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Antonio André Novotny
Jan Sokołowski

Topological Derivatives in Shape Optimization

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Topological Derivatives in Shape Optimization

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This book is dedicated to

Bożena and Vanessinha

Preface

The topological derivative is defined as the first term (correction) of the asymptotic expansion of a given shape functional with respect to a small parameter that measures the size of singular domain perturbations, such as holes, inclusions, defects, source-terms and cracks. Over the last decade, topological asymptotic analysis has become a broad, rich and fascinating research area from both theoretical and numerical standpoints. It has applications in many different fields such as shape and topology optimization, inverse problems, imaging processing and mechanical modeling including synthesis and/or optimal design of microstructures, fracture mechanics sensitivity analysis and damage evolution modeling.

Since there is no monograph on the subject at present, the authors intend to provide here the first detailed account of the theory that combines classical sensitivity analysis in shape optimization with asymptotic analysis by means of compound asymptotic expansions for elliptic boundary value problems. The presented theory of topological derivatives is a natural continuation of the shape sensitivity analysis techniques developed in the monograph *Introduction to shape optimization – shape sensitivity analysis*, Springer-Verlag (1992), by Sokołowski and Zolésio. We show that the velocity method of shape optimization can be combined with the asymptotic analysis in singularly perturbed domains and as a result the new properties of shape functionals are derived for the purposes of optimality conditions and numerical solutions in shape and topology optimization problems. The explicit formulae for the topological derivatives are well suited for the numerical algorithms of shape optimization and are already used in many research papers.

In the book we recall the classical approach to shape optimization problems and extend the analysis to some singular perturbations of the reference domains for elliptic boundary value problems. This means that the topological derivatives are the main subject of our studies. The topological derivative can be considered as the singular limit of the classical shape derivative. It is obtained by the asymptotic analysis of classical solutions to the elliptic boundary value problems in singularly perturbed domains combined with the asymptotic analysis of the shape functionals, all together with respect to the small parameter. In particular, we are interested in the closed form of the topological derivatives for shape and topology optimization problems governed by the elliptic boundary value problems. Therefore, we consider the following aspects of the theory of topological derivatives:

- Descriptions of mathematical theory of shape sensitivity analysis and of domain variations technique in continuum mechanics.
- Asymptotic analysis in singularly perturbed domains by the compound asymptotic expansions.
- Topological derivatives of shape functionals for linear and nonlinear elliptic boundary value problems.
- Mathematical properties of topological derivatives for nonsmooth variational problems.
- Topological derivatives with respect to singular domain perturbations close to the boundary.
- Relationship between shape gradients and topological derivatives.
- Closed formulae for the topological derivatives of the energy-based shape functionals.
- Examples and applications to mathematical physics and structural mechanics.

This book is largely based on lecture notes prepared by the authors for the courses and summer schools held at the Institute Elie Cartan (IECN) in Nancy (France) and at the Laboratório Nacional de Computação Científica (LNCC) in Petrópolis (Brazil). Much of the theory presented here has been developed as a result of scientific collaboration between France, Poland, Russia, and Brazil, as well as on the research work of former PhD students in Nancy and Petrópolis. The joint research on applications of asymptotic analysis to shape optimization were performed in the framework of international scientific projects between IECN in France, Systems Research Institute of the Polish Academy of Sciences and Technical Warsaw University in Poland, Universities in Moscow, St. Petersburg and Lavrentyev Institute of Hydrodynamics, Novosibirsk in Russia, and LNCC in Brazil during the years 1994–2012. We want to point out the research record and joint publications with A. Zochowski (Warsaw, Poland), S.A. Nazarov (St. Petersburg, Russia), T. Lewinski (Warsaw, Poland), A.M. Khludnev (Novosibirsk, Russia), and with the former PhD students Antoine Laurain (Berlin & Graz) and Katarzyna Kedzierska-Szulc (Nancy, Petrópolis & Warsaw). Also, the collaboration with R.A. Feijóo and E. Taroco (Petrópolis, Brazil), C. Padra (Bariloche, Argentina), E.A. de Souza Neto (Swansea, UK), S. Amstutz (Avignon, France) and with the former PhD students Sebastián Miguel Giusti (Córdoba, Agentina) and Jairo Rocha de Faria (João Pessoa, Brazil) has also been fruitful.

We consider the problem of how to derive topological asymptotic expansions of shape functionals associated with elliptic boundary value problems. In particular, we present the calculation of the topological derivative for two-dimensional elliptic problems including scalar (Laplace) and vectorial (Navier) second-order partial differential equations and scalar fourth-order partial differential equations (Kirchhoff). We also consider the topological derivative associated with three-dimensional linear elasticity problems. In addition, we provide the asymptotics for spectral problems. The full mathematical justification for the asymptotic expansion associated with the singular domain perturbations is presented for the semilinear elliptic boundary value problems. Finally, we provide the topological derivatives in linear elasticity contact problem. The results are presented in their closed form, which are useful for numerical methods in shape optimization. We also remark that some exercises are proposed at the end of each chapter.

This book is intended for researchers and graduate students in applied mathematics and computational mechanics interested in any aspect of topological asymptotic analysis. In particular, it can be adopted as a textbook in advanced courses on the subject. Some chapters are self-contained and can be used as lecture notes for mini-courses covering specific classes of problems. The material at the beginning of the book is accessible to a broader audience, while the last chapters may require more mathematical background. Finally, we believe that this book shall be useful for readers interested on the mathematical aspects of topological asymptotic analysis as well as on applications of topological derivatives in computational mechanics.

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Petrópolis, Nancy & Warsaw, June 2012

Laboratório Nacional de Computação Científica — Antonio André Novotny
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Contents

Notation

Geometrical Domains, Sets and Related Objects

$\mathbb{N}$	set of integers; $\mathbb{N}^* := \{0\} \cup \mathbb{N}$.
$\mathbb{R}^d$	Euclidian space of dimension d; $\mathbb{R} \equiv \mathbb{R}^1$ and $\mathbb{R}_+ := (0,\infty)$.
$\mathfrak{D}$	open domain in $\mathbb{R}^d$.
$\overline{\mathfrak{D}}$	closure of $\mathfrak{D}$.
$\partial\mathfrak{D}$	boundary of $\mathfrak{D}$.
$\|\mathfrak{D}\|$	Lebesgue measure of $\mathfrak{D}$.
n	outward unit normal vector to $\partial\mathfrak{D}$.
τ	tangent unit vector on $\partial\mathfrak{D}$, for $d=2$.
Γ	a part of the boundary $\partial\mathfrak{D}$; $\Gamma \subseteq \partial\mathfrak{D}$.
Ω	an open subset of $\mathfrak{D}$; $\overline{\Omega} \Subset \mathfrak{D}$.
ω	an open subset of Ω; $\overline{\omega} \Subset \Omega$.
Υ	a crack; $\overline{\Upsilon} \Subset \Omega \subset \mathbb{R}^d$, with $d=2$.
Υ_l	a crack of length l.
Ω_Υ	domain with a crack; $\Omega_\Upsilon = \Omega \setminus \overline{\Upsilon}$.

Banach and Hilbert Spaces

$C(\Omega)$	Banach space of continuous and bounded functions in Ω.
$C^k(\Omega)$	linear subspace of $C(\Omega)$: functions with derivatives up to order k in $C(\Omega)$, $k \in \mathbb{N} \cup \{\infty\}$.
$C_0^k(\Omega)$	linear subspace of $C^k(\Omega)$: functions vanishing on $\partial\Omega$.
$C_c^\infty(\Omega)$	linear subspace of $C^\infty(\Omega)$: functions with compact supports.
$\mathscr{D}(\Omega)$	space of test functions for distributions.
$\mathscr{D}'(\Omega)$	space of distributions: dual space of $\mathscr{D}(\Omega)$.
$C^{0,1}(\Omega)$	Lipschitz continuous functions in Ω.
$L^p(\Omega)$	p-integrable Lebesgue functions in Ω, with $p \in [0,\infty)$.
$L^p_{\text{loc}}(\Omega)$	locally p-integrable Lebesgue functions in Ω.
$L^\infty(\Omega)$	essentially bounded Lebesgue functions in Ω.
$W^{k,p}(\Omega)$	space of Sobolev functions: generalized derivatives up to the order k are in $L^p(\Omega)$, $k \in \mathbb{N}$ and $p \in [0,\infty]$.

$W^{k,p}_{\mathrm{loc}}(\Omega)$	locally Sobolev functions.
$H^k(\Omega)$	space of Sobolev functions: generalized derivatives up to order k are in $L^2(\Omega)$, $k \in \mathbb{N}$; $W^{k,2}(\Omega) \equiv H^k(\Omega)$ and $L^2(\Omega) \equiv H^0(\Omega)$.
$H^k_{\mathrm{loc}}(\Omega)$	locally Sobolev functions.
$H^k_0(\Omega)$	linear subspace of $H^k(\Omega)$: traces of derivatives vanish on $\partial\Omega$ up to the order $(k-1)$.
$H^{-k}(\Omega)$	dual of $H^k_0(\Omega)$.
$H^{1/2}(\Gamma)$	space of Dirichlet traces on $\Gamma \subseteq \partial\Omega$ for $H^1(\Omega)$.
$H^{-1/2}(\partial\Omega)$	dual of $H^{1/2}(\partial\Omega)$.
$\mathscr{K}(\Omega)$	convex cone of unilateral constraints in Sobolev space.
$\mathscr{S}(\Omega)$	convex cone of *admissible directions* defined for the Hadamard differential of metric projection onto $\mathscr{K}(\Omega)$.

Convergence in Function Spaces

$\to$ in $U(\Omega)$	strong convergence in a Banach space $U(\Omega)$.
$\rightharpoonup$ in $U(\Omega)$	weak convergence in a Banach space $U(\Omega)$.
$\rightharpoondown$ in $L^\infty(\Omega)$	weak star convergence in $L^\infty(\Omega)$.

Norms and Scalar Product in Function Spaces

$\Vert\cdot\Vert_{U(\Omega)}$	norm in a Banach space $U(\Omega)$.
$\vert\cdot\vert_{U(\Omega)}$	seminorm in a Banach space $U(\Omega)$.
$\langle\cdot,\cdot\rangle_{U(\Omega)\times V(\Omega)}$	duality pairing between spaces $U(\Omega)$ and $V(\Omega)$.
$U(\Omega;\mathbb{R}^d)$	cartesian product of $U(\Omega)$ for $d=2,3$; $U(\Omega;\mathbb{R}) \equiv U(\Omega)$.
$U(\Omega;\mathbb{R}^d\times\mathbb{R}^d)$	cartesian product of $U(\Omega;\mathbb{R}^d)$ for $d=2,3$.

Shape Transformations

Ω_t	transformed geometrical domain in $\mathbb{R}^d$ of the form $\Omega_t = \mathfrak{T}_t(\Omega)$, for $t \in \mathbb{R}$; $\Omega := \Omega_t\vert_{t=0}$.
$\partial\Omega_t$	boundary of Ω_t; $\partial\Omega_t = \mathfrak{T}_t(\partial\Omega)$, $\partial\Omega := \partial\Omega_t\vert_{t=0}$.
Γ_t	a part of the boundary $\partial\Omega_t$; $\Gamma_t = \mathfrak{T}_t(\Gamma) \subseteq \partial\Omega_t$, $\Gamma := \Gamma_t\vert_{t=0}$.
n_t	outward unit normal vector to $\partial\Omega_t$; $n := n_t\vert_{t=0}$.
X	material (Lagrangean) coordinate $X \in \Omega$.
x	spatial (Eulerian) coordinate $x \in \Omega_t$.
t	parameter of the domain transformation.
$\mathfrak{T}_t$	mapping $\mathfrak{T}_t : \Omega \to \Omega_t$ ($\mathfrak{T}_t : \mathbb{R}^d \to \mathbb{R}^d$); $x = \mathfrak{T}_t(X)$.
$\mathfrak{T}_t^{-1}$	inverse mapping $\mathfrak{T}_t^{-1} : \Omega_t \to \Omega$ ($\mathfrak{T}_t^{-1} : \mathbb{R}^d \to \mathbb{R}^d$); $X = \mathfrak{T}_t^{-1}(x)$.
$\mathfrak{V}$	shape velocity field $\mathfrak{V} = \mathfrak{V}(X,t)$.
dX	differential element in Ω.
dx	differential element in Ω_t.
∂_X	material gradient operator $\partial_X := \nabla_X$.
∂_x	spatial gradient operator $\partial_x := \nabla_x$.
$\mathfrak{J}$	Jacobian transformation tensor; $\mathfrak{J} = \mathfrak{J}(X,t) := \nabla_X \mathfrak{T}_t(X)$.
div_X	material divergence operator.

div_x	spatial divergence operator.
Δ_X	material Laplacian operator.
Δ_x	spatial Laplacian operator.
φ^t	material description of a spatial field $\varphi(x,t)$; $\varphi^t = \varphi^t(X) = (\varphi \circ \mathfrak{T}_t)(X)$, i.e. $\varphi^t(X) = \varphi(\mathfrak{T}_t(X),t)$.
$D\varphi^t$	Jacobian of a material vector field φ^t, i.e. $D\varphi^t := (\nabla_X \varphi^t)^\top$; $D\mathfrak{T}_t = \mathfrak{J}^\top$.
φ_t	spatial description of a material field $\varphi(X,t)$, $\varphi_t = \varphi_t(x) = (\varphi \circ \mathfrak{T}_t^{-1})(x)$, i.e. $\varphi_t(x) = \varphi(\mathfrak{T}_t^{-1}(x),t)$.
$D\varphi_t$	Jacobian of a spatial vector field φ_t, i.e. $D\varphi_t := (\nabla_x \varphi_t)^\top$.
φ'	shape derivative of the spatial field $\varphi(x,t)$, $\varphi'(x,t) := \partial_t \varphi(x,t)$.
$\dot{\varphi}$	material derivative of the spatial field $\varphi(x,t)$, $\dot{\varphi}(x,t) := \dfrac{d}{dt}\varphi(x,t)$.

Topological Perturbations

$\varepsilon \to 0$	small parameter in $\mathbb{R}_+$ associated to the size of topological perturbations far from the boundary.
$h \to 0$	small parameter in $\mathbb{R}_+$ associated to the size of singular perturbations close to the boundary.
$\omega_\varepsilon(\widehat{x})$	small geometrical perturbation; usually $\omega_\varepsilon(\widehat{x}) = \widehat{x} + \varepsilon\omega$, where $\widehat{x} \in \Omega$ and $\omega \subset \mathbb{R}^d$.
$\Omega_\varepsilon(\widehat{x})$	singularly perturbed geometrical domain in $\mathbb{R}^d$; $\Omega_\varepsilon(\widehat{x}) = \Omega \setminus \overline{\omega_\varepsilon(\widehat{x})}$.
$B_\varepsilon(\widehat{x})$	a ball of radius ε and center at $\widehat{x} \in \Omega$.
$\mathscr{S}_\varepsilon$	set of shape change velocity fields that represents an uniform expansion of $B_\varepsilon(\widehat{x})$.
γ_ε	contrast parameter for material properties; $\gamma_\varepsilon(x) = 1$ for $x \in \Omega \setminus \overline{\omega_\varepsilon}$ and $\gamma_\varepsilon(x) = \gamma$ for $x \in \omega_\varepsilon$, with constant $\gamma \in (0,\infty)$.
χ	characteristic function; $x \mapsto \chi(x)$, $x \in \mathbb{R}^d$, with $\chi(x) = 1$ for $x \in \Omega$ and $\chi(x) = 0$ for $x \in \mathbb{R}^d \setminus \Omega$, or simply $\chi = \mathbb{1}_\Omega$.
$\chi_\varepsilon(\widehat{x})$	function describing the topological perturbation; $x \mapsto \chi_\varepsilon(\widehat{x};x)$, $x \in \mathbb{R}^d$, with $\chi_\varepsilon(\widehat{x}) = \mathbb{1}_\Omega - \mathbb{1}_{\omega_\varepsilon(\widehat{x})}$ for holes or $\chi_\varepsilon(\widehat{x}) = \mathbb{1}_\Omega - (1-\gamma)\mathbb{1}_{\omega_\varepsilon(\widehat{x})}$ for inclusions.
$\psi(\chi)$	unperturbed shape functional.
$\psi(\chi_\varepsilon(\widehat{x}))$	perturbed shape functional.
$f(\varepsilon)$	positive first order correction function depending on the small parameter ε, such that $f(\varepsilon) \to 0$, with $\varepsilon \to 0$.
$O(\varepsilon)$	remainder of order ε; $O(\varepsilon) \to 0$, with $\varepsilon \to 0$; or $\lvert O(\varepsilon)\rvert \leqslant C\varepsilon$, with constant C independent of ε.
$o(\varepsilon)$	remainder of higher order compared to ε; $o(\varepsilon)/\varepsilon \to 0$, with $\varepsilon \to 0$.
$\mathscr{T}(\widehat{x})$	topological derivative function; $\widehat{x} \mapsto \mathscr{T}(\widehat{x})$, with $\widehat{x} \in \Omega$.
$\mathscr{O}$	origin in $\mathbb{R}^d$.

Unperturbed Boundary Value Problems

$\mathscr{U}$	set of admissible functions; $\mathscr{U} \subset U(\Omega)$.
$\mathscr{V}$	space of admissible variations; $\mathscr{V} \subset V(\Omega)$.
u	solution of an elliptic boundary value problem; $u \in \mathscr{U}$.

u' shape derivative of the solution u.
$\dot{u}$ material derivative of the solution u.
q heat flux vector.
K second order conductivity tensor.
σ second order Cauchy stress tensor.
σ_i principal stresses associated to σ, for $i = 1, ..., d$, with $d = 2, 3$.
M second order momentum tensor.
m_i principal moments associated to M, for $i = 1, 2$.
Σ second order Eshelby energy-momentum tensor.
P second order polarization tensor.
$\mathbb{P}$ fourth order polarization tensor.
$\mathbb{C}$ fourth order elasticity or Hooke's tensor.
$\mathscr{J}_\Omega$ shape functional; $\mathscr{J}_\Omega : U(\Omega) \to \mathbb{R}$.

Perturbed Boundary Value Problems

$\mathscr{U}_\varepsilon$ perturbed set of admissible functions; $\mathscr{U}_\varepsilon \subset U(\Omega)$.
$\mathscr{V}_\varepsilon$ perturbed space of admissible variations; $\mathscr{V}_\varepsilon \subset V(\Omega)$.
u_ε solution of a topologically perturbed elliptic boundary value problem.
u'_ε shape derivative of the solution u_ε.
$\dot{u}_\varepsilon$ material derivative of the solution u_ε.
q_ε perturbed heat flux vector; $q_\varepsilon = \gamma_\varepsilon q$ for inclusions.
σ_ε perturbed second order Cauchy stress tensor; $\sigma_\varepsilon = \gamma_\varepsilon \sigma$ for inclusions.
M_ε perturbed second order momentum tensor; $M_\varepsilon = \gamma_\varepsilon M$ for inclusions.
Σ_ε second order Eshelby energy-momentum tensor depending on the small parameter ε.
$\mathscr{J}_{\chi_\varepsilon}$ regularly perturbed shape functional; $\mathscr{J}_{\chi_\varepsilon} : U(\Omega) \to \mathbb{R}$.
$\mathscr{J}_{\Omega_\varepsilon}$ singularly perturbed shape functional; $\mathscr{J}_{\Omega_\varepsilon} : U(\Omega_\varepsilon) \to \mathbb{R}$.
ξ fast variable $\xi = \varepsilon^{-1} x$.
w boundary layer independent of the small parameter ε in asymptotic expansion of u_ε.
w_ε boundary layer dependent on the small parameter ε in asymptotic expansion of u_ε.
$\widetilde{u}_\varepsilon$ remainder in asymptotic expansion of u_ε.

Tensor Calculus

$a \cdot b$ scalar product of two vectors; $a \cdot b = \alpha \in \mathbb{R}$, with $\alpha = a_i b_i := \sum_{i=1}^d a_i b_i$.
$\|a\|$ Euclidian norm of the vector a; $\|a\| = \sqrt{a \cdot a}$.
A, B second order tensors.
Ab application of a second order tensor A to a vector b; the vector $(Ab)_i = A_{ik} b_k := \sum_{k=1}^d A_{ik} b_k$.
AB application of a second order tensor A to a second order tensor B; the second order tensor $(AB)_{ij} = A_{ik} B_{kj} := \sum_{k=1}^d A_{ik} B_{kj}$.
I second order identity tensor; $\mathrm{I}a = a$ and $\mathrm{I}A = A$.

$A \cdot B$	scalar product of two tensors; $A \cdot B = \alpha \in \mathbb{R}$, with $\alpha = A_{ij}B_{ij} := \sum_{i,j=1}^{d} A_{ij}B_{ij}$.
$A^\top$	transpose of the second order tensor A.
$a \otimes b$	tensor product of two vectors; $a \otimes b = A$, for $d = 2,3$, with $A_{ij} = a_i b_j$.
$a \otimes_s b$	symmetric tensor product of two vectors; $a \otimes_s b = \frac{1}{2}(a \otimes b + b \otimes a)$.
$\mathrm{tr}A$	trace of the second order tensor A; $\mathrm{tr}A = \mathrm{I} \cdot A = A_{ii} := \sum_{i=1}^{d} A_{ii}$, $\mathrm{tr}(A^\top B) = A \cdot B$ and $\mathrm{tr}(a \otimes b) = a \cdot b$.
$\det A$	determinant of the second order tensor A.
∇	gradient operator; $\nabla\varphi(x) \in \mathbb{R}^d$ for a scalar field φ and $\nabla\varphi(x) \in \mathbb{R}^d \times \mathbb{R}^d$ for a vector field φ.
$\nabla\varphi^s$	symmetric part of the gradient of a vector field φ; $\nabla\varphi^s = (\nabla\varphi + \nabla\varphi^\top)/2$.
∇_Γ	tangential gradient.
rot	curl operator.
div	divergence operator; $\mathrm{div}\varphi(x) \in \mathbb{R}$ for a vector field φ and $\mathrm{div}\varphi(x) \in \mathbb{R}^d$ for a second order tensor field φ.
div_Γ	tangential divergence.
∂_n	normal derivative.
∂_τ	tangential derivative.
Δ	Laplacian operator.
$\mathbb{A}, \mathbb{B}$	fourth order tensors.
$\mathbb{A}B$	product of a fourth order tensor $\mathbb{A}$ with a second order tensor B; the second order tensor $(\mathbb{A}B)_{ij} = \mathbb{A}_{ijkl}B_{kl}$.
$\mathbb{A}\mathbb{B}$	product of a fourth order tensor $\mathbb{A}$ with a fourth order tensor $\mathbb{B}$; the fourth order tensor $(\mathbb{A}\mathbb{B})_{ijkl} = \mathbb{A}_{ijpq}\mathbb{B}_{pqkl}$.
$\mathbb{I}$	fourth order identity tensor; $\mathbb{I}A = A$ and $\mathbb{I}\mathbb{A} = \mathbb{A}$.
$A \otimes B$	tensor product of two tensors; $A \otimes B = \mathbb{A}$, with $\mathbb{A}_{ijkl} = A_{ij}B_{kl}$.

Miscellaneous

$\varphi_{\vert\Omega}$	restriction of function φ in Ω.
$\varphi_{\vert\partial\Omega}$	trace of function φ on $\partial\Omega$.
$[\![\varphi]\!]$ on $\partial\omega$	jump of φ across $\partial\omega$; $[\![\varphi]\!] = \varphi_{\vert\Omega\setminus\overline{\omega}} - \varphi_{\vert\omega}$ on $\partial\omega$, with $\overline{\omega} \Subset \Omega$.
(r,θ)	polar coordinate system.
(r,θ,ϕ)	spherical coordinate system.
e_i	canonical orthonormal basis of the Euclidian space $\mathbb{R}^d$ for $i = 1,...,d$, with $d = 2,3$.

Chapter 1
Introduction

The topological derivative measures the sensitivity of a given shape functional with respect to an infinitesimal singular domain perturbation, such as the insertion of holes, inclusions, source-terms or even cracks. The topological derivative was rigorously introduced by Sokołowski & Żochowski 1999 [204]. In particular, it can be seen as a mathematical justification for the so-called bubble method [53] (see for instance [136]). Since then, this concept has proved to be extremely useful in the treatment of a wide range of problems, namely topology optimization [5, 16, 19, 21, 38, 40, 77, 78, 115, 133, 185, 186, 187, 207, 217], inverse analysis [18, 42, 59, 84, 94, 96, 101, 102, 142] and image processing [31, 32, 93, 95, 129], and has became a subject of intensive research. See, for instance, applications of the topological derivative in the multi-scale constitutive modeling context [17, 74, 75, 76, 188], fracture mechanics sensitivity analysis [79] and damage evolution modeling [6]. Concerning the theoretical development of the topological asymptotic analysis, the reader may refer to the papers [13, 15, 48, 49, 60, 70, 97, 109, 134, 135, 172, 173, 175, 176, 206, 208], and to the monograph project in progress by Nazarov, Sokołowski & Żochowski.

The topological derivative is obtained by the asymptotic analysis of classical solutions to elliptic boundary value problems in singularly perturbed domains combined with the asymptotic analysis of the shape functionals all together with respect to the small parameter which measures the size of the perturbation. Therefore, the asymptotic analysis of elliptic boundary value problems in singularly perturbed geometrical domains is the main ingredient of the mathematical theory of topological derivatives.

In the seventies and eighties of the last century two asymptotic methods, namely the method of matched [100] and compound [143] expansions, were successfully developed to construct asymptotic expansions of solutions to elliptic boundary value problems in domains with singularly perturbed boundaries as well as of intrinsic functionals calculated for these solutions. In this context the singular perturbation of the boundary means e.g., the creation of a small hole or cavity inside the domain, smoothing a corner, a conical point or an edge on the nonsmooth boundary among others. The functionals considered include e.g., the energy functional associated with elliptic boundary values problems [144, 161, 172, 176], eigenvalues of spectral problems [105, 145, 147, 192, 193] and the *capacity functional* (cf. Note 10.3) which is an example of the energy functional.

The theory of elliptic problems in singularly perturbed domains is covered in [143, 146] for the systems of partial differential equations, elliptic in the Agmon-Douglis-Nirenberg sense. In particular monograph [143] contains the procedures of construction and justification of asymptotics for solutions of equations, the derivation of asymptotically sharp estimates in weighted norms. Asymptotic analysis of elliptic problems in singularly perturbed domains e.g., methods of matched and compound asymptotic expansions, has become the most appropriate and relevant to obtain *almost explicit* formulae for the topological derivatives as it has been demonstrated in [172, 176] and others. We refer the reader to books by V.G. Maz'ya, S.A. Nazarov and B.A. Plamenevsky [148, 170] for the state of art in the asymptotic analysis of elliptic boundary value problems in singularly perturbed geometrical domains. We also mention the books [10] and [158] where the subject is studied, to some extend, from physical and numerical point of view. The formulae for asymptotic expansions obtained for the energy functionals [144] or for the eigenvalues [147] could be used in shape optimization. However, for practical applications of such derivatives in computational shape optimization the results already known are extended to more general shape functionals by introduction of an appropriate adjoint state [204] as well as by using the singular limits of the first order shape derivatives [205]. We note that this monograph concerns the questions which are out of the scope of the books [148, 170] and we believe are related mainly to the numerical methods in shape optimization. There are two main constructions used here. The first one concerns singular domain perturbations associated to nucleation of holes. The second case concerns regular perturbation of the differential operator associated to nucleation of inclusions. Our analysis is performed for the classical solutions of elliptic boundary value problems in order to avoid unnecessary technical difficulties. Most of the results of local nature are valid in Lipschitzian domains. For cracks, a special treatment is necessary as rigorously demonstrated in [172]. In the context of crack detection, for instance, the corresponding inverse problem can be formulated as a shape optimization problem and the associated topological derivative should obviously be evaluated for cracks.

The topological derivative concept is introduced in this chapter and several illustrative examples are provided. In addition, the relationship between classical shape gradients and topological derivatives is presented. In particular, the topological derivative is given by a singular limit of shape derivatives with respect to the size of the parameter which governs the singular domain perturbations. This result leads to a simple and constructive method for the topological derivative evaluation purposes. For the new concept, an example concerning optimal control theory is presented (see, for instance [116, 125]), where the topological derivative is obtained for a tracking type shape functional.

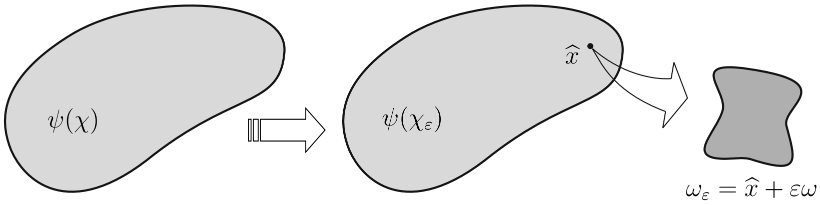


Fig. 1.1 The topological derivative concept

1.1 The Topological Derivative Concept

Let us consider an open and bounded domain $\Omega \subset \mathbb{R}^d$, with $d \geqslant 2$, which is subject to a nonsmooth perturbation confined in a small region $\omega_\varepsilon(\widehat{x}) = \widehat{x} + \varepsilon\omega$ of size ε, with $\overline{\omega_\varepsilon} \Subset \Omega$, as shown in fig. 1.1. Here, $\widehat{x}$ is an arbitrary point of Ω and ω is a fixed domain of $\mathbb{R}^d$. We introduce a *characteristic function* $x \mapsto \chi(x)$, $x \in \mathbb{R}^d$, associated to the unperturbed domain, namely $\chi = \mathbb{1}_\Omega$, such that

$$|\Omega| = \int_{\mathbb{R}^d} \chi \,, \tag{1.1}$$

where $|\Omega|$ is the *Lebesgue measure* of Ω. Then, we define a characteristic function associated to the topologically perturbed domain of the form $x \mapsto \chi_\varepsilon(\widehat{x};x)$, $x \in \mathbb{R}^d$. In the case of a perforation, for instance, $\chi_\varepsilon(\widehat{x}) = \mathbb{1}_\Omega - \mathbb{1}_{\omega_\varepsilon(\widehat{x})}$ and the perforated domain is obtained as $\Omega_\varepsilon = \Omega \setminus \overline{\omega_\varepsilon}$. Then, we assume that a given shape functional $\psi(\chi_\varepsilon(\widehat{x}))$, associated to the topologically perturbed domain, admits the following *topological asymptotic expansion*

$$\psi(\chi_\varepsilon(\widehat{x})) = \psi(\chi) + f(\varepsilon)\mathscr{T}(\widehat{x}) + o(f(\varepsilon)) \,, \tag{1.2}$$

where $\psi(\chi)$ is the shape functional associated to the reference (unperturbed) domain, $f(\varepsilon)$ is a positive *first order correction function* of ψ, and $o(f(\varepsilon))$ is the remainder, namely $o(f(\varepsilon))/f(\varepsilon) \to 0$ with $\varepsilon \to 0$. The function $\widehat{x} \mapsto \mathscr{T}(\widehat{x})$ is called the topological derivative of ψ at $\widehat{x}$. Therefore, this derivative can be seen as a first order correction of $\psi(\chi)$ to approximate $\psi(\chi_\varepsilon(\widehat{x}))$. In fact, after rearranging (1.2) we have

$$\frac{\psi(\chi_\varepsilon(\widehat{x})) - \psi(\chi)}{f(\varepsilon)} = \mathscr{T}(\widehat{x}) + \frac{o(f(\varepsilon))}{f(\varepsilon)} \,. \tag{1.3}$$

The limit passage $\varepsilon \to 0$ in the above expression leads to the general definition for the *topological derivative*

$$\mathscr{T}(\widehat{x}) := \lim_{\varepsilon \to 0} \frac{\psi(\chi_\varepsilon(\widehat{x})) - \psi(\chi)}{f(\varepsilon)} \,. \tag{1.4}$$

If we know that the functional $\psi(\chi_\varepsilon(\widehat{x}))$ admits the asymptotic expansion (1.2), the applicability of this expansion depends on the procedure of evaluation of the unknown function $\widehat{x} \mapsto \mathscr{T}(\widehat{x})$. In particular, we are looking for an explicit form for the topological derivatives. Thus, this evaluation should be performed in such a way that the explicitly given function $\widehat{x} \mapsto \mathscr{T}(\widehat{x})$ can be used in numerical methods of shape optimization. Therefore, we need some properties of the shape functional and of the asymptotic expansion in order to apply a simple method for evaluation of the topological derivative. Actually, we need for these purposes the following framework for the topological sensitivity analysis of a shape functional which accepts (1.2) at a given *reference domain* Ω.

Condition 1.1. Let us suppose that the expansion (1.2) holds true. Then, the following properties have to be fulfilled:

1. For fixed $\varepsilon \in (0, \varepsilon_0]$, with $\varepsilon_0 > 0$, the shape (domain) functional $\omega_\varepsilon \mapsto J(\Omega_\varepsilon) := \psi(\chi_\varepsilon(\widehat{x}))$ is shape differentiable for $\widehat{x} \in \Omega$. The *shape differentiability* means that there is the shape gradient of $\omega_\varepsilon \mapsto J(\Omega_\varepsilon)$ supported on the boundary or interface $\partial \omega_\varepsilon$ for a given $\varepsilon \in (0, \varepsilon_0]$.
2. The shape functional $\varepsilon \mapsto j(\varepsilon) := \psi(\chi_\varepsilon(\widehat{x}))$ is continuous with respect to *topological perturbation* at 0^+, i.e., $\lim_{\varepsilon \to 0^+} f(\varepsilon) = 0$.
3. The function $\varepsilon \mapsto f(\varepsilon)$ is continuously differentiable on $(0, \varepsilon_0]$.
4. The limit passage $\lim_{\varepsilon \to 0^+} o(f(\varepsilon))/f(\varepsilon) = 0$ holds true.

Remark 1.1. According to Condition 1.1, we need the following ingredients for evaluation of topological derivatives:

- Classical *shape sensitivity analysis* [210].
- *Asymptotic analysis* of shape functionals in singularly perturbed domains [131, 160, 172, 177, 178, 179, 180].
- A formula for the *topological derivative* which can be applied in order to determine its explicit form [204, 205].

Since we are dealing with singular perturbations consisting of nucleation of holes, the shape functionals $\psi(\chi_\varepsilon(\widehat{x}))$ and $\psi(\chi)$ are associated with topologically different domains. Therefore, the evaluation of the limit (1.4) is not trivial in general. In particular, we need to perform an asymptotic analysis of the shape functional $\psi(\chi_\varepsilon(\widehat{x}))$ with respect to the small parameter ε. This is, in fact, the main concern of this monograph. However, we will also consider regular perturbations in the form of nucleation of inclusions. The singular case is much more complicated from the mathematical point of view than the regular one. Therefore, in order to emphasize this difference, we will introduce specific notation for each case of topological perturbation in the following chapters. Note, however, that for the shape functional $\psi(\chi_\varepsilon(\widehat{x}))$ we keep the same notation for both cases, i.e. we redefine $\psi(\chi_\varepsilon) := \mathscr{J}_{\Omega_\varepsilon}(u_\varepsilon)$ and $\psi(\chi_\varepsilon) := \mathscr{J}_{\chi_\varepsilon}(u_\varepsilon)$ for singular and regular perturbations, respectively, where u_ε is solution to a perturbed boundary value problem. Despite their lack of rigor, we believe these definitions will make the presentation easier to follow by avoiding a cumbersome notation. In the case of singular perturbations χ_ε is in fact a characteristic function, but this is not true in general. Therefore, function χ_ε shall be defined according to the context under consideration.

In order to fix these ideas, we present three simple examples. The first one concerns singular domain perturbation. The second example is associated to regular perturbation of the integrand coefficients. Finally, the last one shows that the topological derivative obeys the basic rules of differential calculus.

Example 1.1. Let us consider the shape functional

$$\psi(\chi_\varepsilon(\widehat{x})) := \int_{\Omega_\varepsilon} g(x) \,, \tag{1.5}$$

where $\chi_\varepsilon(\widehat{x}) = \mathbb{1}_\Omega - \mathbb{1}_{\omega_\varepsilon(\widehat{x})}$ and $\Omega_\varepsilon = \Omega \setminus \overline{\omega_\varepsilon}$. The function $g : \mathbb{R}^d \to \mathbb{R}$ is *Lipschitz continuous* in $\omega_\varepsilon(\widehat{x})$, i.e. $|g(x) - g(\widehat{x})| \leqslant C\|x - \widehat{x}\|$, $\forall x \in \omega_\varepsilon(\widehat{x})$, where $C \geqslant 0$ is the Lipschitz constant. This is the case of singular domain perturbations. Since $|\omega_\varepsilon| \to 0$ as $\varepsilon \to 0$, we have

$$\psi(\chi) := \int_\Omega g(x) \,. \tag{1.6}$$

We are looking for an asymptotic expansion of the form (1.2), namely

$$\begin{aligned} \psi(\chi_\varepsilon(\widehat{x})) &= \int_{\Omega_\varepsilon} g(x) + \int_{\omega_\varepsilon} g(x) - \int_{\omega_\varepsilon} g(x) \\ &= \int_\Omega g(x) - \int_{\omega_\varepsilon} g(x) \\ &= \psi(\chi) - |\omega_\varepsilon| g(\widehat{x}) + o(|\omega_\varepsilon|) \,. \end{aligned} \tag{1.7}$$

For the simple example, the term $-g(\widehat{x})$ is called the topological derivative of the shape functional ψ, that is, $\mathscr{T}(\widehat{x}) = -g(\widehat{x})$, and we recognize $f(\varepsilon) = |\omega_\varepsilon| \sim \varepsilon^d$.

Example 1.2. Let us now consider a shape functional of the form

$$\psi(\chi_\varepsilon(\widehat{x})) := \int_\Omega g_\varepsilon(x) \,, \tag{1.8}$$

where $\chi_\varepsilon(\widehat{x}) = \mathbb{1}_\Omega - (1-\gamma)\mathbb{1}_{\omega_\varepsilon(\widehat{x})}$ and $g_\varepsilon = \chi_\varepsilon g$ is defined as

$$g_\varepsilon(x) := \begin{cases} g(x) \text{ if } x \in \Omega \setminus \overline{\omega_\varepsilon(\widehat{x})} \\ \gamma g(x) \text{ if } x \in \omega_\varepsilon(\widehat{x}) \end{cases} , \tag{1.9}$$

with a *Lipschitz continuous* function g in ω_ε (see Example 1.1). It means that the set Ω includes the interface $\partial\omega_\varepsilon$. This is the case of shape functionals depending on the characteristic function of small sets. Since $|\omega_\varepsilon| \to 0$ as $\varepsilon \to 0$, we have

$$\psi(\chi) := \int_\Omega g(x) \,. \tag{1.10}$$

We are looking for an asymptotic expansion of the form (1.2), that is

$$\begin{aligned}\psi(\chi_\varepsilon(\widehat{x})) &= \int_{\Omega\setminus\overline{\omega_\varepsilon}} g(x) + \int_{\omega_\varepsilon} \gamma g(x)\\ &= \int_{\Omega\setminus\overline{\omega_\varepsilon}} g(x) + \int_{\omega_\varepsilon} \gamma g(x) + \int_{\omega_\varepsilon} g(x) - \int_{\omega_\varepsilon} g(x)\\ &= \int_{\Omega} g(x) - (1-\gamma)\int_{\omega_\varepsilon} g(x)\\ &= \psi(\chi) - |\omega_\varepsilon|(1-\gamma)g(\widehat{x}) + o(|\omega_\varepsilon|)\,. \end{aligned} \tag{1.11}$$

For the simple example, the term $-(1-\gamma)g(\widehat{x})$ is called the topological derivative of the shape functional ψ, that is, $\mathscr{T}(\widehat{x}) = -(1-\gamma)g(\widehat{x})$, and we recognize $f(\varepsilon) = |\omega_\varepsilon| \sim \varepsilon^d$. In addition, we note that for the limit case $\gamma \to 0$, we have $\mathscr{T}(\widehat{x}) = -g(\widehat{x})$. It means that the first example can be seen as the singular limit of this last one.

Example 1.3. Let us consider two *Lipschitz continuous* functions g and h in ω_ε (see Example 1.1). We are interested again in the case of singular domain perturbation of the form $\Omega_\varepsilon(\widehat{x}) = \Omega \setminus \overline{\omega_\varepsilon(\widehat{x})}$. Then, according to Example 1.1, we have the following results, for instance:

$$\psi(\chi) := \left(\int_\Omega g(x)\right)^\alpha \Rightarrow \mathscr{T}(\widehat{x}) = -\alpha g(\widehat{x})\left(\int_\Omega g(x)\right)^{\alpha-1}, \tag{1.12}$$

with $\alpha \in \mathbb{Z}$,

$$\psi(\chi) := \int_\Omega g(x)\int_\Omega h(x) \Rightarrow \mathscr{T}(\widehat{x}) = -g(\widehat{x})\int_\Omega h(x) - h(\widehat{x})\int_\Omega g(x) \tag{1.13}$$

and

$$\psi(\chi) := \frac{1}{|\Omega|}\int_\Omega g(x) \Rightarrow \mathscr{T}(\widehat{x}) = -\frac{1}{|\Omega|^2}\left(g(\widehat{x})|\Omega| - \int_\Omega g(x)\right). \tag{1.14}$$

Before proceed, we consider two examples for the second and the fourth order ordinary differential equations, respectively. Thus, the examples concern the topological derivatives in the simple case of one dimensional boundary value problems.

Example 1.4. Let us consider the second order ordinary differential equation

$$u_\varepsilon''(x) = 0\,, \qquad 0 < x < 1\,, \tag{1.15}$$

with the boundary condition

$$u_\varepsilon(0) = 0 \qquad \text{and} \qquad u_\varepsilon'(1) = 1\,, \tag{1.16}$$

and the transmission conditions over the interface

$$u_\varepsilon(\varepsilon^+) = u_\varepsilon(\varepsilon^-) \qquad \text{and} \qquad u_\varepsilon'(\varepsilon^+) = \gamma u_\varepsilon'(\varepsilon^-)\,. \tag{1.17}$$

where $\gamma \in \mathbb{R}^+$ is the contrast. The above boundary value problem has an explicit solution, namely

$$\begin{cases} u_\varepsilon(x) = \frac{x}{\gamma}\,, & 0 < x \leqslant \varepsilon\,, \\ u_\varepsilon(x) = x + \varepsilon\frac{1-\gamma}{\gamma}\,, & \varepsilon < x < 1\,. \end{cases} \tag{1.18}$$

Let us consider the shape functional

$$\psi(\chi_\varepsilon(\hat{x})) := \int_0^1 \gamma_\varepsilon (u_\varepsilon')^2\,, \tag{1.19}$$

where $\Omega = (0,1)$, $\chi_\varepsilon(\hat{x}) = \mathbb{1}_\Omega - (1-\gamma)\mathbb{1}_{\omega_\varepsilon(\hat{x})}$, and $\gamma_\varepsilon := \chi_\varepsilon$. It means that $\gamma_\varepsilon(x) = \gamma$ for $0 < x \leqslant \varepsilon$, and $\gamma_\varepsilon(x) = 1$ for $\varepsilon < x < 1$. In addition we have

$$\psi(\chi) := \int_0^1 (u')^2\,, \tag{1.20}$$

where u is solution to the above boundary value problem for $\varepsilon = 0$, namely

$$u(x) = x\,. \tag{1.21}$$

We are looking for an asymptotic expansion of the form (1.2). Therefore, we have

$$\psi(\chi_\varepsilon(\hat{x})) = \int_0^\varepsilon \gamma(u_\varepsilon')^2 + \int_\varepsilon^1 (u_\varepsilon')^2 = 1 + \varepsilon\frac{1-\gamma}{\gamma} = \psi(\chi) + |\omega_\varepsilon|\,\frac{1-\gamma}{\gamma}\,. \tag{1.22}$$

For the simple example, the topological derivative is given by

$$\mathscr{T}(\hat{x}) = \frac{1-\gamma}{\gamma}\,, \tag{1.23}$$

with $f(\varepsilon) = |\omega_\varepsilon| = \varepsilon$. In addition, we note that for the limit case $\gamma \to \infty$, $\mathscr{T}(\hat{x}) = -1$, and for $\gamma \to 0$ the topological derivative doesn't exist. This is an intrinsic property of one dimensional boundary value problems.

Example 1.5. Let us now consider a fourth order ordinary differential equation of the form

$$u_\varepsilon''''(x) = 0\,, \qquad 0 < x < 1\,, \tag{1.24}$$

with boundary condition given by

$$u_\varepsilon(0) = u_\varepsilon'(0) = u_\varepsilon'''(1) = 0 \quad \text{and} \quad u_\varepsilon''(1) = 1\,, \tag{1.25}$$

and transmission conditions of the form

$$\begin{aligned} &u_\varepsilon(\varepsilon^+) = u_\varepsilon(\varepsilon^-)\,, \quad u_\varepsilon'(\varepsilon^+) = u_\varepsilon'(\varepsilon^-)\,, \\ &u_\varepsilon''(\varepsilon^+) = \gamma u_\varepsilon''(\varepsilon^-)\,, \, u_\varepsilon'''(\varepsilon^+) = \gamma u_\varepsilon'''(\varepsilon^-)\,, \end{aligned} \tag{1.26}$$

where $\gamma \in \mathbb{R}^+$ is the contrast. The above boundary value problem has explicit solution, namely

$$\begin{cases} u_\varepsilon(x) = \frac{x^2}{2\gamma}\,, & 0 < x \leqslant \varepsilon\,, \\ u_\varepsilon(x) = \frac{x^2}{2} + \varepsilon\frac{1-\gamma}{2\gamma}(2x - \varepsilon)\,, & \varepsilon < x < 1\,. \end{cases} \tag{1.27}$$

Let us consider a shape functional of the form

$$\psi(\chi_\varepsilon(\widehat{x})) := \int_0^1 \gamma_\varepsilon (u_\varepsilon'')^2 ,$$

where $\Omega = (0,1)$, $\chi_\varepsilon(\widehat{x}) = \mathbb{1}_\Omega - (1-\gamma)\mathbb{1}_{\omega_\varepsilon(\widehat{x})}$ and $\gamma_\varepsilon := \chi_\varepsilon$. It means that $\gamma_\varepsilon(x) = \gamma$ for $0 < x \leqslant \varepsilon$, and $\gamma_\varepsilon(x) = 1$, for $\varepsilon < x < 1$. In addition we have

$$\psi(\chi) := \int_0^1 (u'')^2 , \tag{1.28}$$

where u is solution to the above boundary value problem for $\varepsilon = 0$, namely

$$u(x) = \frac{x^2}{2} . \tag{1.29}$$

We are looking for an asymptotic expansion of the form (1.2). Therefore, we have

$$\psi(\chi_\varepsilon(\widehat{x})) = \int_0^\varepsilon \gamma(u_\varepsilon'')^2 + \int_\varepsilon^1 (u_\varepsilon'')^2 = 1 + \varepsilon\frac{1-\gamma}{\gamma} = \psi(\chi) + |\omega_\varepsilon|\,\frac{1-\gamma}{\gamma} . \tag{1.30}$$

For the simple example, the topological derivative is given by

$$\mathcal{T}(\widehat{x}) = \frac{1-\gamma}{\gamma} , \tag{1.31}$$

with $f(\varepsilon) = |\omega_\varepsilon| = \varepsilon$. In addition, we note that for the limit case $\gamma \to \infty$, $\mathcal{T}(\widehat{x}) = -1$, and for $\gamma \to 0$ the singular limit is not defined.

Finally, in order to explain the significance of the topological derivative in shape optimization we present an example whose global minimizer $\Omega^\star$ is known.

Example 1.6. Let $B_R = \{\|x\| < R\} \subset \mathbb{R}^2$, with $1 < R < \infty$, be a fixed hold all domain, and consider the multiply connected admissible domains $\Omega \subset B_R$ with the volume constraints $|\Omega| \geqslant \pi(1-\rho^2)$, where $0 < \rho < 1$ is fixed. The shape functional is of the tracking type

$$\psi(\chi) = \int_\Omega (u - z_d)^2 dx, \tag{1.32}$$

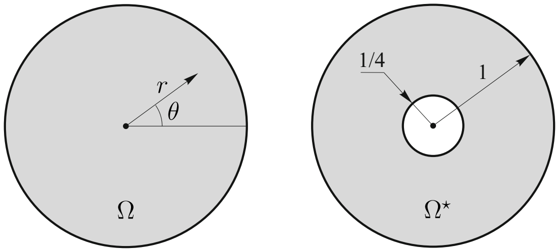
where z_d, defined in polar coordinate system (r,θ) centered at the origin, is a given function of r, namely

$$z_d(r) := \begin{cases} 0 & \text{for } 0 < r \leqslant \rho , \\ g(r) & \text{for } \rho < r < 1 , \\ 0 & \text{for } 1 \leqslant r < R , \end{cases} \tag{1.33}$$

where

$$g(r) := -(1-r)^2(1+2r-24r^2) . \tag{1.34}$$

Fig. 1.2 Example with global optimizer: geometrical domains



(a) initial guess Ω (b) optimal domain $\Omega^\star$

The scalar field u is a solution to the following boundary value problem:

$$\begin{cases} \text{Find } u, \text{ such that} \\ -\Delta u = b \text{ in } \Omega \ , \\ \quad u = 0 \text{ on } \partial\Omega \ . \end{cases} \tag{1.35}$$

Here the source b is defined in polar coordinates as follows

$$b(r) := -\frac{1}{r}(rg'(r))' \ . \tag{1.36}$$

From the above elements, we can find:

- if the initial guess is the unit ball $B = \{\|x\| < 1\}$, the shape gradient of $\psi(\chi)$ is null;
- by computing the topological derivative of $\psi(\chi)$ at B and taking the condenser type domain, the optimal domain is obtained from an analysis of the sign of the topological derivative;
- optimal cost is null, therefore the optimal domain is the global minimizer.

Now, we give more details. Let us consider an optimal domain $\Omega^\star \subset \mathbb{R}^2$. It is given by a ring of the form $\Omega^\star = B \setminus \overline{B_\rho}$, where B_ρ is a ball centered at the origin with radius $\rho < 1$. See fig. 1.2. We have constructed the source b in such way that the solution u can be obtained explicitly as a function of r, namely

$$u(r) = g(r) \quad \text{for} \quad 0 < r < 1 \ . \tag{1.37}$$

The graph of $u(r)$ is plotted in fig. 1.3(a). The function z_d is defined for $\rho = 1/4$ as follows

$$z_d(r) := \begin{cases} 0 & \text{for } 0 < r \leqslant \rho \ , \\ u(r) & \text{for } \rho < r < 1 \ . \end{cases} \tag{1.38}$$

The graph of $z_d(r)$ is shown in fig. 1.3(b), where the grey scale is used to denote the region where the target functions is non-null. Therefore, the tracking type shape functional is zero over the optimal domain $\Omega^\star$. In fact the optimal solution $u^\star = u_{|\Omega^\star} = z_d$. The shape derivative of $\psi(\chi)$ is given by [210]

$$d\psi(\chi; \mathfrak{V}) = -\int_{\partial B} (\partial_n u \, \partial_n v) \, n \cdot \mathfrak{V} \ . \tag{1.39}$$

In the above formula, $\mathfrak{V}$ is the shape change velocity field [210] and v is solution to the adjoint problem, namely

$$\begin{cases} \text{Find } v, \text{ such that} \\ -\Delta v = -(u - z_d) \ \text{ in } \ \Omega = B \,, \\ \quad v = 0 \qquad\qquad \text{on } \partial B \,. \end{cases} \tag{1.40}$$

The solution to the above boundary value problem can also be obtained by hand as a function of r. The graph of $v(r)$ is shown in fig. 1.3(c). Thus, the shape derivative of $\psi(\chi)$ can be calculated explicitly, which is given by $d\psi(\chi;\mathfrak{V}) = 0$, since in this particular case $\partial_n u_{|\partial B} = u'(1) = 0$. It means that the shape functional cannot be improved by using the information provided by the shape derivative. On the other hand, let us now compute the topological derivative, which is given by the following formula for homogeneous Dirichlet boundary condition on the hole (see Section 4.1)

$$\mathscr{T}(\widehat{x}) = u(\widehat{x})\, v(\widehat{x}) \qquad \forall\, \widehat{x} \in \Omega = B \,. \tag{1.41}$$

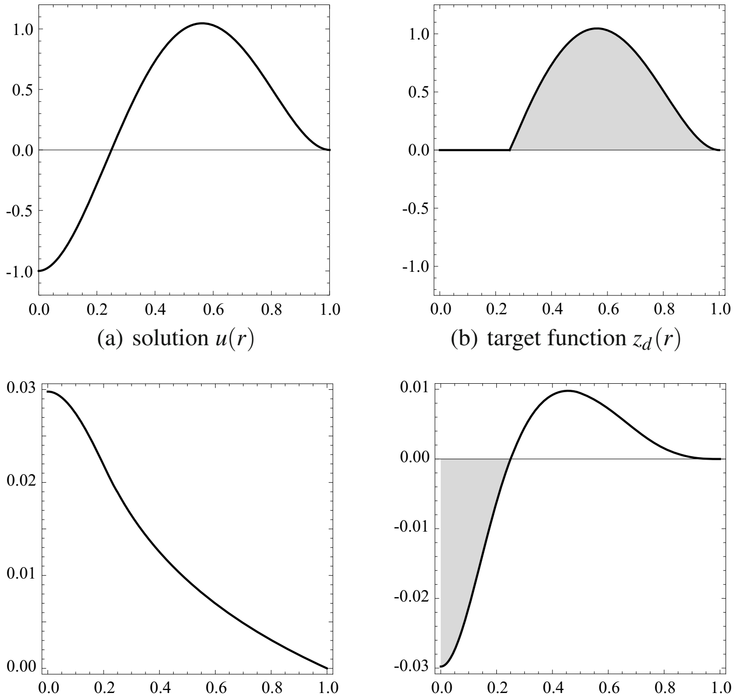
In this example, the topological derivative is a function of r given by $\mathscr{T}(r) = u(r)\,v(r)$, for $0 < r < 1$. The topological derivative is plotted in fig. 1.3(d), where the grey scale is used to denote the region where $\mathscr{T}(r)$ is negative. It means that in order to improve the shape functional, the hole must be nucleated at the center of the disk. In addition, the threshold of the topological derivative, namely for $r < \rho$, gives information on the optimal size of the hole. In fact, once a hole of size ρ is introduced, $u^\star = u_{|\Omega^\star} = z_d$ by construction, and the corresponding adjoint state $v^\star$ satisfies

$$\begin{cases} \text{Find } v^\star, \text{ such that} \\ -\Delta v^\star = 0 \ \text{ in } \ \Omega^\star = B \setminus \overline{B_\rho} \,, \\ \quad v^\star = 0 \text{ on } \partial B \,, \\ \quad v^\star = 0 \text{ on } \partial B_\rho \,, \end{cases} \tag{1.42}$$

which has a unique trivial solution $v^\star = 0$. Therefore, the optimal domain $\Omega^\star$ is the global minimizer of the shape functional $\psi(\chi)$, since the optimality conditions $d\psi(\chi^\star;\mathfrak{V}) = 0$ and $\mathscr{T}(\widehat{x}) \geqslant 0 \; \forall \widehat{x} \in \Omega^\star$ are fulfilled, provided that $v^\star = 0$, where $\chi^\star$ is the characteristic function associated to $\Omega^\star$, that is, $\chi^\star = \mathbb{1}_B - \mathbb{1}_{B_\rho}$. In this example, the global optimum was obtained in one step by using subsequently the shape and the topological derivatives. This result is impossible to achieve by taking into account only the shape derivative.

1.2 Relationship between Shape and Topological Derivatives

The topological derivative of a functional can be considered as the singular limit of its shape derivative, so it is a generalization of the classical tool in shape optimization. In order to fix this idea, let us present an example concerning the relation between shape and topological derivatives.



(a) solution $u(r)$ (b) target function $z_d(r)$

(c) solution $v(r)$ (d) topological derivative $\mathscr{T}(r)$

Fig. 1.3 Example with global optimizer: direct and adjoint solutions, target function and topological derivative

Example 1.7. Let as consider a bar under torsion effects. The cross section of the shaft is represented by an open bounded domain $\Omega \subset \mathbb{R}^2$, as shown in fig. 1.4. Following the Prandtl's approach, we consider the complementary dissipation energy shape functional of the form

$$\psi(\chi) = \frac{1}{2}\int_\Omega \|\nabla u\|^2 - \int_\Omega bu \,, \tag{1.43}$$

where the scalar field u is solution to the following boundary value problem

$$\begin{cases} \text{Find } u, \text{ such that} \\ -\Delta u = b \ \text{ in } \ \Omega \,, \\ \quad u = 0 \text{ on } \partial\Omega \,, \end{cases} \tag{1.44}$$

with the constant b used to denote a rigid twist of the cross-section of the shaft. The shape derivative of $\psi(\chi)$ is given by [210]

$$d\psi(\chi;\mathfrak{V}) = \frac{1}{2}\int_{\partial\Omega} (\partial_n u)^2 \, n\cdot\mathfrak{V} \,, \tag{1.45}$$

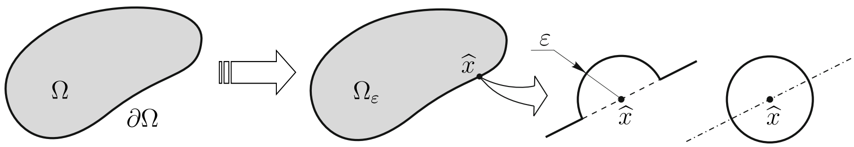


Fig. 1.4 Cross section of a shaft under torsion effects: original and singulary perturbed domains

where $\mathfrak{V}$ is the shape change velocity field [210]. The topological asymptotic expansion for the above problem is known [185] and given by (see analogous results in Section 4.1)

$$\psi(\chi_\varepsilon(\widehat{x})) = \psi(\chi) + \pi\varepsilon^2\|\nabla u(\widehat{x})\|^2 + o(\varepsilon^2) \qquad \forall\,\widehat{x} \in \Omega\ , \tag{1.46}$$

where we recognize the topological derivative as $\mathscr{T}(\widehat{x}) = \|\nabla u(\widehat{x})\|^2$. This last result can be extended to the boundary by using the odd extension of the problem, as shown in fig. 1.4. In addition, since $u = 0$ on $\partial\Omega$, then its tangential derivative vanishes on the boundary, namely $\partial_\tau u = 0$ on $\partial\Omega$. Therefore, the topological asymptotic expansion on the boundary leads to

$$\psi(\chi_\varepsilon(\widehat{x})) = \psi(\chi) + \frac{1}{2}\pi\varepsilon^2(\partial_n u(\widehat{x}))^2 + o(\varepsilon^2) \qquad \forall\,\widehat{x} \in \partial\Omega\ . \tag{1.47}$$

It means that in this simple example, the topological derivative $\mathscr{T}(\widehat{x}) = \frac{1}{2}(\partial_n u(\widehat{x}))^2$ coincides with the density of the shape derivative at the point $\widehat{x} \in \partial\Omega$. This fact motivates us to state the main result of this monograph.

1.2.1 The Topological-Shape Sensitivity Method

Now, the method of evaluation of topological derivatives is introduced. Such a method should be sufficiently simple and robust. We restrict ourselves to the elliptic boundary value problems which are well understood from the point of view of the asymptotic analysis in singularly perturbed domains. The proposed method should be applicable to the cavities as well as to the inclusions, since both cases are important for applications, in particular in solid and fluid mechanics. Among the evaluation methods of topological derivatives for elliptic boundary value problems currently available in the literature on numerical methods of shape optimization (see, for instance, [11, 130, 213]), we adopt the methodology developed in [184], which uses the following properties of the shape functional under considerations.

Proposition 1.1. *Let $\psi(\chi_\varepsilon(\widehat{x}))$ be the shape functional associated to the topologically perturbed domain, which admits, for ε small enough, the topological asymptotic expansion of the form*

$$\psi(\chi_\varepsilon(\widehat{x})) = \psi(\chi) + f(\varepsilon)\mathcal{T}(\widehat{x}) + \mathcal{R}(f(\varepsilon)) , \tag{1.48}$$

where $\psi(\chi)$ is the shape functional associated to the original (unperturbed) domain, the positive function $f(\varepsilon)$ is such that $f(\varepsilon) \to 0$, with $\varepsilon \to 0$, and the function $\mathcal{T}(\widehat{x})$ is the topological derivative of the shape functional ψ. We assume that the remainder $\mathcal{R}(f(\varepsilon)) = o(f(\varepsilon))$ has the following additional property $\mathcal{R}'(f(\varepsilon)) \to 0$, when $\varepsilon \to 0$. Then, the topological derivative *can be written as*

$$\mathcal{T}(\widehat{x}) = \lim_{\varepsilon \to 0} \frac{1}{f'(\varepsilon)} \frac{d}{d\varepsilon} \psi(\chi_\varepsilon(\widehat{x})) , \tag{1.49}$$

where $\frac{d}{d\varepsilon}\psi(\chi_\varepsilon(\widehat{x}))$ is the (shape) derivative of $\psi(\chi_\varepsilon(\widehat{x}))$ with respect to the small positive parameter ε.

Proof. Let us calculate the total derivative of the expansion (1.48) with respect to the real parameter ε, that is

$$\frac{d}{d\varepsilon}\psi(\chi_\varepsilon(\widehat{x})) = f'(\varepsilon)\mathcal{T}(\widehat{x}) + \mathcal{R}'(f(\varepsilon))f'(\varepsilon) . \tag{1.50}$$

After division by $f'(\varepsilon)$ we have

$$\mathcal{T}(\widehat{x}) = \frac{1}{f'(\varepsilon)} \frac{d}{d\varepsilon} \psi(\chi_\varepsilon(\widehat{x})) - \mathcal{R}'(f(\varepsilon)) . \tag{1.51}$$

Finally, by taking the limit $\varepsilon \to 0$ in the above expression, the result holds provided that $\mathcal{R}'(f(\varepsilon)) \to 0$, when $\varepsilon \to 0$. □

Remark 1.2. We propose here a simple method for evaluation of topological derivatives, which can be used for elliptic boundary value problems. The method relies on the properties of the compound asymptotic expansions obtained for the solutions of elliptic boundary value problems in singularly perturbed domains. In order to apply the method, the required convergence of the remainders

$$\mathcal{R}'(f(\varepsilon)) \to 0, \quad \text{for} \quad \varepsilon \to 0 \tag{1.52}$$

should be verified in each specific case of a shape functional considered for the boundary value problems defined in singularly perturbed geometrical domains. Actually, the convergence follows by the property of the asymptotic expansions of solutions which can be *differentiated term by term* under the appropriate decrease order rule for the remainders of the expansions. It means that the procedure presented in the above proposition for the evaluation of the topological derivative can be performed for the boundary value problems which enjoy such a property. We point out that this property is positively confirmed for a class of second order elliptic boundary value problems considered in [172]. However, we also refer to [172] for some counterexamples on the lack of topological differentiability. In particular, it seems that such a property cannot be confirmed for hyperbolic boundary value problems

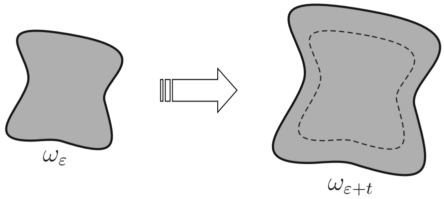


Fig. 1.5 Uniform expansion of the perturbation ω_ε

which makes the evaluation of topological derivatives much more involved, when it is possible.

The derivative of $\psi(\chi_\varepsilon(\widehat{x}))$ with respect to ε can be seen as the sensitivity of $\psi(\chi_\varepsilon(\widehat{x}))$, in the classical sense [50, 210], to the domain variation produced by an uniform expansion of the perturbation ω_ε, as shown in fig. 1.5. In fact, we have

$$\frac{d}{d\varepsilon}\psi(\chi_\varepsilon(\widehat{x})) = \lim_{t\to 0}\frac{\psi(\chi_{\varepsilon+t}(\widehat{x})) - \psi(\chi_\varepsilon(\widehat{x}))}{t}\,, \tag{1.53}$$

where $\varepsilon > 0$ and $\psi(\chi_{\varepsilon+t}(\widehat{x}))$ is the shape functional associated to the perturbed domain, whose perturbation is given by $\omega_{\varepsilon+t}$. Therefore, since $\psi(\chi_{\varepsilon+t}(\widehat{x}))$ and $\psi(\chi_\varepsilon(\widehat{x}))$ are now associated to topologically identical domains, we can use the concept of shape sensitivity analysis as an intermediate step in the topological derivative calculation. We will see later that this procedure enormously simplifies the analysis.

1.2.2 An Example of Topological Derivative Evaluation

Before conclude this chapter, let us present a last example concerning the simplest case of topological perturbation. It is given by a perturbation on the right hand side of a boundary value problem, which can be seen as a simple variant of the singulary perturbed domain. In particular we will compute the topological derivative by using the result stated through Proposition 1.1.

Example 1.8. Let us consider again the tracking type shape functional, which is useful in many practical applications such as optimal control and image processing. It is given by a functional of the form

$$\psi(\chi) = \frac{1}{2}\int_\Omega (u - z_d)^2\,, \tag{1.54}$$

where $\Omega \subset \mathbb{R}^2$, z_d is the target function, and the scalar field u is a solution to the following variational problem

$$\begin{cases} \text{Find } u \in H_0^1(\Omega), \text{ such that} \\ \displaystyle\int_\Omega \nabla u\cdot\nabla\eta = \int_\Omega b\eta \quad \forall \eta \in H_0^1(\Omega)\,. \end{cases} \tag{1.55}$$

Now, we introduce a topological perturbation on the source term of the form $b_\varepsilon = \chi_\varepsilon b$, with $\chi_\varepsilon(\widehat{x}) = \mathbb{1}_\Omega - (1-\gamma)\mathbb{1}_{B_\varepsilon(\widehat{x})}$. Therefore the perturbed source term b_ε reads

$$b_\varepsilon(x) := \begin{cases} b(x) \text{ if } x \in \Omega \setminus \overline{B_\varepsilon(\widehat{x})} \,, \\ \gamma b(x) \text{ if } x \in B_\varepsilon(\widehat{x}) \,, \end{cases} \tag{1.56}$$

with γ used to denote the contrast on the source term. In order to simplify the presentation of this simple example, we have assumed that the source term $b(x)$ is constant in the neighborhood of the point $\widehat{x}$. Therefore, the shape functional associated to the perturbed problem is defined as

$$\psi(\chi_\varepsilon) = \frac{1}{2}\int_\Omega (u_\varepsilon - z_d)^2 \,, \tag{1.57}$$

where u_ε is solution to the following variational problem

$$\begin{cases} \text{Find } u_\varepsilon \in H_0^1(\Omega), \text{ such that} \\ \displaystyle\int_\Omega \nabla u_\varepsilon \cdot \nabla\eta = \int_\Omega b_\varepsilon \eta \quad \forall \eta \in H_0^1(\Omega) \,. \end{cases} \tag{1.58}$$

Lemma 1.1. *Let the remainder be $\widetilde{u}_\varepsilon = u_\varepsilon - u$, where u and u_ε are solutions to (1.55) and (1.58), respectively. Then, we have the following estimate for $\widetilde{u}_\varepsilon$*

$$\|\widetilde{u}_\varepsilon\|_{H^1(\Omega)} \leqslant C\varepsilon \,, \tag{1.59}$$

with constant C independent of the small parameter ε.

Proof. We start by recalling that $b_\varepsilon = b$ in $\Omega \setminus \overline{B_\varepsilon}$ and $b_\varepsilon = \gamma b$ in B_ε. Thus, the right hand side of (1.58) can be written as

$$\begin{aligned} \int_\Omega b_\varepsilon \eta &= \int_{\Omega\setminus\overline{B_\varepsilon}} b\eta + \gamma\int_{B_\varepsilon} b\eta \pm \int_{B_\varepsilon} b\eta \\ &= \int_\Omega b\eta - (1-\gamma)\int_{B_\varepsilon} b\eta \,. \end{aligned} \tag{1.60}$$

After subtracting the variational problems (1.58) and (1.55), we obtain

$$\widetilde{u}_\varepsilon \in H_0^1(\Omega) : \int_\Omega \nabla\widetilde{u}_\varepsilon \cdot \nabla\eta = -(1-\gamma)\int_{B_\varepsilon} b\eta \quad \forall \eta \in H_0^1(\Omega) \,, \tag{1.61}$$

with $\widetilde{u}_\varepsilon = u_\varepsilon - u$. Now, by taking $\eta = \widetilde{u}_\varepsilon$ in the above equation we have

$$\int_\Omega \|\nabla\widetilde{u}_\varepsilon\|^2 = -(1-\gamma)\int_{B_\varepsilon} b\widetilde{u}_\varepsilon \,. \tag{1.62}$$

From the *Cauchy-Schwarz inequality*, we obtain

$$\begin{aligned}\int_\Omega \|\nabla\widetilde{u}_\varepsilon\|^2 &\leqslant C_1\|b\|_{L^2(B_\varepsilon)}\|\widetilde{u}_\varepsilon\|_{L^2(B_\varepsilon)}\\ &\leqslant C_2\varepsilon\|\widetilde{u}_\varepsilon\|_{L^2(B_\varepsilon)}\\ &\leqslant C_3\varepsilon\|\widetilde{u}_\varepsilon\|_{H^1(\Omega)}\,,\end{aligned} \tag{1.63}$$

where we have used the continuity of the function b at the point $\widehat{x}\in\Omega$. Finally, from the *coercivity* of the bilinear form on the left hand side of (1.61), namely,

$$c\|\widetilde{u}_\varepsilon\|^2_{H^1(\Omega)} \leqslant \int_\Omega \|\nabla\widetilde{u}_\varepsilon\|^2\,, \tag{1.64}$$

we have

$$c\|\widetilde{u}_\varepsilon\|_{H^1(\Omega)} \leqslant C_3\varepsilon\,, \tag{1.65}$$

which leads to the result, with $C = C_3/c$. □

Remark 1.3. The previous result can be slightly improved by using the *Hölder inequality* together with the *Sobolev embedding theorem*. In fact, we can find an estimate for the remainder $\widetilde{u}_\varepsilon$ of the form $\|\widetilde{u}_\varepsilon\|_{H^1(\Omega)} \leqslant C\varepsilon^{1+\delta}$, with $\delta > 0$ small. In particular, for $1/p+1/q = 1$, we have

$$\begin{aligned}\|\widetilde{u}_\varepsilon\|_{L^2(B_\varepsilon)} &\leqslant \left[\left(\int_{B_\varepsilon}(|\widetilde{u}_\varepsilon|^2)^p\right)^{\frac{1}{p}}\left(\int_{B_\varepsilon}1^q\right)^{\frac{1}{q}}\right]^{\frac{1}{2}}\\ &= \pi^{1/2q}\varepsilon^{1/q}\left(\int_{B_\varepsilon}|\widetilde{u}_\varepsilon|^{2p}\right)^{\frac{1}{2p}}\\ &= \pi^{1/2q}\varepsilon^{1/q}\|\widetilde{u}_\varepsilon\|_{L^{2p}(B_\varepsilon)}\\ &= \pi^{1/2q}\varepsilon^{1/q}\|\widetilde{u}_\varepsilon\|_{L^{2q/(q-1)}(B_\varepsilon)}\\ &\leqslant C\varepsilon^\delta\|\widetilde{u}_\varepsilon\|_{H^1(\Omega)}\,,\end{aligned} \tag{1.66}$$

where $p = q/(q-1)$, with $q > 1$, and $\delta = 1/q$.

Before proceed, we introduce the adjoint state v_ε for further simplification. It is solution to the following variational problem

$$\begin{cases}\text{Find } v_\varepsilon \in H^1_0(\Omega), \text{ such that}\\ \displaystyle\int_\Omega \nabla v_\varepsilon\cdot\nabla\eta = -\int_\Omega (u_\varepsilon - z_d)\eta \quad \forall\eta\in H^1_0(\Omega)\,.\end{cases} \tag{1.67}$$

In addition, the adjoint state associated to the unperturbed problem is given by taking $\varepsilon = 0$ in the previous equation. Namely, v is the solution to the adjoint equation of the form

$$\begin{cases}\text{Find } v \in H^1_0(\Omega), \text{ such that}\\ \displaystyle\int_\Omega \nabla v\cdot\nabla\eta = -\int_\Omega (u - z_d)\eta \quad \forall\eta\in H^1_0(\Omega)\,.\end{cases} \tag{1.68}$$

Lemma 1.2. *Let be $\widetilde{v}_\varepsilon = v_\varepsilon - v$, where v and v_ε are solutions to (1.68) and (1.67), respectively. Then, we have the following estimate for $\widetilde{v}_\varepsilon$*

$$\|\widetilde{v}_\varepsilon\|_{H^1(\Omega)} \leqslant C\varepsilon \,, \tag{1.69}$$

with constant C independent of the small parameter ε.

Proof. Let us subtract the variational problems (1.67) and (1.68), which leads to

$$\widetilde{v}_\varepsilon \in H_0^1(\Omega) : \int_\Omega \nabla\widetilde{v}_\varepsilon \cdot \nabla\eta = -\int_\Omega \widetilde{u}_\varepsilon \eta \quad \forall \eta \in H_0^1(\Omega) \,, \tag{1.70}$$

with $\widetilde{v}_\varepsilon = v_\varepsilon - v$ and $\widetilde{u}_\varepsilon = u_\varepsilon - u$. By taking $\eta = \widetilde{v}_\varepsilon$ in the above equation we have

$$\int_\Omega \|\nabla\widetilde{v}_\varepsilon\|^2 = -\int_\Omega \widetilde{u}_\varepsilon \widetilde{v}_\varepsilon \,. \tag{1.71}$$

From the *Cauchy-Schwarz inequality*, we obtain

$$\begin{aligned} \int_\Omega \|\nabla\widetilde{v}_\varepsilon\|^2 &\leqslant \|\widetilde{u}_\varepsilon\|_{L^2(\Omega)} \|\widetilde{v}_\varepsilon\|_{L^2(\Omega)} \\ &\leqslant \|\widetilde{u}_\varepsilon\|_{H^1(\Omega)} \|\widetilde{v}_\varepsilon\|_{H^1(\Omega)} \\ &\leqslant C_1\varepsilon \|\widetilde{v}_\varepsilon\|_{H^1(\Omega)} \,, \end{aligned} \tag{1.72}$$

where we have used the result (1.59). Finally, from the *coercivity* of the bilinear form on the left hand side of (1.70), namely,

$$c\|\widetilde{v}_\varepsilon\|^2_{H^1(\Omega)} \leqslant \int_\Omega \|\nabla\widetilde{v}_\varepsilon\|^2 \,, \tag{1.73}$$

we have

$$c\|\widetilde{v}_\varepsilon\|_{H^1(\Omega)} \leqslant C_1\varepsilon \,, \tag{1.74}$$

which leads to the result, with $C = C_1/c$. □

In this particular case, the geometrical domain remains fixed and the application of the result given by Proposition 1.1 is straightforward. In fact, let us calculate the derivative of the shape functional with respect to the small parameter ε, leading to

$$\dot{\psi}(\chi_\varepsilon) = \int_\Omega (u_\varepsilon - z_d)\dot{u}_\varepsilon \,, \tag{1.75}$$

where the overhead dot is used to denote the total derivative with respect to ε. Since the above equation involves $\dot{u}_\varepsilon$, we need to calculate the derivative of the state equation (1.58) with respect to ε.

Note 1.1. In this case of *regular perturbations of the domain*, it is easy to see that the shape functional $\varepsilon \mapsto \psi(\chi_\varepsilon)$ is differentiable for $\varepsilon > 0$, ε small enough.

Indeed, assuming that $B_\varepsilon = \{\|x\| < \varepsilon\}$, by the passage to polar coordinates and differentiation of the resulting parametric integral with respect to ε, the real function of one variable

$$\varepsilon \mapsto \int_{B_\varepsilon} g \tag{1.76}$$

is differentiable on $(0, \varepsilon_0]$ for $\varepsilon_0 > 0$, ε_0 small enough, and the derivative is continuous and given by the boundary integral over $\partial B_\varepsilon = \{\|x\| = \varepsilon\}$. Hence we have the first order Taylor's expansion

$$\int_{B_{\varepsilon+t}} g = \int_{B_\varepsilon} g + t \int_{\partial B_\varepsilon} g + o(t) \,. \tag{1.77}$$

Thus, the weak solution to (1.58) is also differentiable in $H_0^1(\Omega)$ with respect to ε by an application of the implicit function theorem. In fact, by recalling that $b_\varepsilon = b$ in $\Omega \setminus \overline{B_\varepsilon}$ and $b_\varepsilon = \gamma b$ in B_ε, we can rewrite the right hand side of (1.58) as follows

$$\int_\Omega b_\varepsilon \eta = \int_\Omega b\eta - (1-\gamma) \int_{B_\varepsilon} b\eta \,. \tag{1.78}$$

Whence the function $\varepsilon \mapsto u_\varepsilon$ admits the derivative $\dot{u}_\varepsilon \in H_0^1(\Omega)$ with respect to $\varepsilon \in (0, \varepsilon_0]$ of the form

$$u_{\varepsilon+t}(x) = u_\varepsilon(x) + t\dot{u}_\varepsilon(x) + o(t) \quad x \in \Omega \,, \tag{1.79}$$

where $\dot{u}_\varepsilon$ is given by the solution of the *equation in variations*

$$\begin{cases} \text{Find } \dot{u}_\varepsilon \in H_0^1(\Omega), \text{ such that} \\ \displaystyle\int_\Omega \nabla \dot{u}_\varepsilon \cdot \nabla \eta = (\gamma - 1) \int_{\partial B_\varepsilon} b\eta \quad \forall \eta \in H_0^1(\Omega) \,. \end{cases} \tag{1.80}$$

We can now turn back to the shape functional and obtain its expansion in ε with help of an appropriate *adjoint state*. Since $\dot{u}_\varepsilon \in H_0^1(\Omega)$, we can take $\eta = \dot{u}_\varepsilon$ as test function in the adjoint equation (1.67) and $\eta = v_\varepsilon$ as test function in (1.80), which leads to

$$\int_\Omega \nabla \dot{u}_\varepsilon \cdot \nabla v_\varepsilon = -(1-\gamma) \int_{\partial B_\varepsilon} b v_\varepsilon \tag{1.81}$$

and

$$\int_\Omega \nabla v_\varepsilon \cdot \nabla \dot{u}_\varepsilon = -\int_\Omega (u_\varepsilon - z_d)\dot{u}_\varepsilon \,. \tag{1.82}$$

By comparing both equations, we obtain the following important result

$$\int_\Omega (u_\varepsilon - z_d)\dot{u}_\varepsilon = (1-\gamma) \int_{\partial B_\varepsilon} b v_\varepsilon \,. \tag{1.83}$$

Therefore, the derivative of the shape functional is given by

$$\dot{\psi}(\chi_\varepsilon) = (1-\gamma)\int_{\partial B_\varepsilon} b v_\varepsilon = (1-\gamma)\int_{\partial B_\varepsilon} b v + (1-\gamma)\int_{\partial B_\varepsilon} b \widetilde{v}_\varepsilon \ , \tag{1.84}$$

where $\widetilde{v}_\varepsilon = v_\varepsilon - v$. For the first integral on the right hand side in the above equation, the following expansion in power of ε holds

$$(1-\gamma)\int_{\partial B_\varepsilon} b v = 2\pi\varepsilon(1-\gamma)b(\widehat{x})v(\widehat{x}) + o(\varepsilon) \ , \tag{1.85}$$

where we have used the continuity of the function b at the point $\widehat{x} \in \Omega$ and the interior *elliptic regularity* of the solution v. Finally, from the result (1.69), the second integral is

$$(1-\gamma)\int_{\partial B_\varepsilon} b \widetilde{v}_\varepsilon = o(\varepsilon) \ . \tag{1.86}$$

Therefore, the following expansion in power of ε for the derivative of the shape functional holds

$$\dot{\psi}(\chi_\varepsilon) = 2\pi\varepsilon(1-\gamma)b(\widehat{x})v(\widehat{x}) + o(\varepsilon) \ . \tag{1.87}$$

The above result together with the relation between shape and topological derivative given by (1.49) yields

$$\mathscr{T}(\widehat{x}) = \lim_{\varepsilon\to 0} \frac{1}{f'(\varepsilon)} \left(2\pi\varepsilon(1-\gamma)b(\widehat{x})v(\widehat{x}) + o(\varepsilon)\right) \ . \tag{1.88}$$

Now, in order to identify the leading term of the above expansion, we choose $f(\varepsilon) = \pi\varepsilon^2$, which leads to the final formula for the topological derivative, namely

$$\mathscr{T}(\widehat{x}) = (1-\gamma)b(\widehat{x})v(\widehat{x}) \ . \tag{1.89}$$

We note that the expansion (1.87) holds the hypothesis of Proposition 1.1, namely $\mathscr{R}'(f(\varepsilon)) = o(\varepsilon)/\varepsilon \to 0$, when $\varepsilon \to 0$.

Remark 1.4. This kind of topological perturbation, namely on the right hand side of a boundary value problem, can be handle by using very simple arguments. In particular, we have used only the well-posedness properties of the boundary value problems. Therefore, in this framework, we can consider even some classes of nonlinear problems. However, this monograph is dedicated mainly to the case of singular domain perturbation, such as the one produced by nucleation of holes. The mathematical treatment to this kind of topological perturbation is much more involved and will be deeper discussed in what follows.

1.3 Monograph Organization

The *topological derivative* is introduced in Section 1.2 as the singular limit of shape derivatives with respect to a small parameter. The proposed method of evaluation is constructive for elliptic boundary value problems and it seems to be the simplest way to derive one term asymptotics for shape functionals [205]. The small parameter of asymptotic analysis measures the size of singular (topological) or configurational (regular) domain perturbations. This means that in the associated numerical optimization procedure the changes of the material properties or of the geometrical domain by creation of small inclusions or voids are allowed in order to improve the shape design for a given shape functional to be minimized. In our framework of the *topological-shape sensitivity analysis* there are combined the well known methods of mathematics and continuum mechanics:

- The material and shape derivatives in variable geometrical domains are developed in the setting of continuum mechanics (Chapter 2). The Eshelby energy-momentum tensor concept naturally appears in the shape sensitivity analysis derivation.
- The shape sensitivity analysis of classical calculus of variations is recalled in great detail (Chapter 3) and then used (Chapter 11). There are defined the important concepts of the material and shape derivatives for weak and strong solutions (in the scale of Sobolev or Kondratiev spaces) to partial differential equations of elliptic type and of the shape gradients for the associated integral functionals.
- The asymptotic analysis of boundary value problems in singularly perturbed geometrical domains (Chapters 9 and 10) coming from the theory of partial differential equations of elliptic type is applied. The compound asymptotics method in the weighted Kondratiev spaces is used for approximation of singularly perturbed solutions to the elliptic boundary value problems. As a result, the rigorous derivation of the asymptotics for shape functionals is provided.
- The evaluation of the closed form of the topological derivatives is performed for shape functionals associated with linear elliptic boundary value problems (Chapters 4–8). The obtained formulae are easy to implement and turn out to be useful for numerical solution of the applied shape and topology optimization problems. The method of evaluation is extended, with full proofs, to some nonlinear boundary value problems important for applications, namely, semilinear (Chapter 10) and nonsmooth (Chapter 11) problems.

Shape sensitivity analysis is introduced in Chapter 2 from the continuum mechanics point of view. The framework for such an analysis includes the Reynolds' transport theorem combined with the material derivatives of spacial fields in mechanics. The Eshelby energy-momentum tensor is derived in the context of analysis of defects in three-dimensional elastic bodies.

The shape derivatives which describe the dependence of solutions to elliptic boundary value problems with respect to the boundary variations of the geometrical domains are investigated in Chapter 3. The variational solutions of boundary value problems are considered in the scale of Sobolev spaces. The shape and material derivatives are obtained for weak and strong solutions of the elliptic boundary value problems. The elliptic regularity results apply to the regularity of shape and material derivatives which obviously depends on the regularity of the data, including the domain, sources and boundary conditions.

The topological-shape sensitivity analysis of the energy shape functionals with respect to singular and regular domain perturbations is performed in Chapter 4, for the perturbations in the form of small holes, and in Chapter 5, for the perturbations in the form of inclusions with appropriated transmission conditions. The closed form of topological derivatives is obtained for the Poisson, Navier and Kirchhoff elliptic problems.

In Chapter 6 the topological derivatives are obtained for a general class of shape functionals. For the shape functionals not being of energy type, the adjoint method is required in order to simplify the formulae for the shape gradients and the topological derivatives. A generalization of the Eshelby-energy momentum tensor depending on the direct and adjoint states is introduced for the problem under consideration.

In Chapter 7 the energy asymptotics for orthotropic materials with respect to the small parameter governing the nucleation of an inclusion is constructed in order to evaluate the topological derivative. The obtained result contains as a particular case the isotropic material.

The results presented in Chapter 8 are important for applications in structural mechanics. Namely, the analysis of singular energy perturbation in the form of small spherical cavities in three spatial dimensions is performed in this chapter. The closed forms of the topological derivatives for the energy functional are obtained for two constitutive models. The first one concerns the classical linear elasticity. The second model is introduced in Section 8.6, it is a multi-scale constitutive model. The topological sensitivity analysis of the energy functional for the multi-scale constitutive model leads to the topological derivative of the homogenized elasticity tensor, which is useful for the purpose of synthesis and optimal design of microstructures.

In Chapter 9, the asymptotics of simple and multiple eigenvalues of elliptic spectral problems are introduced. The cases of voids close and far from the boundary are analyzed in all details, and the full proofs of the results presented are provided in the framework of the compound asymptotic method. The asymptotics of multiple eigenvalues are investigated using Lemma A.1 of Appendix A on *almost eigenvalues and eigenvectors*. The case of simple eigenvalues turns out to be easy and it is considered in Section 9.2 for a scalar spectral problem in three spatial dimensions and the cavities located far from the boundary. The cavities located close to the boundary are considered in Section 9.3 for a scalar spectral problem and in Section 9.4 for the elasticity spectral problem. The asymptotics for the scalar and elasticity spectral problems are presented in Appendices B and C, respectively. The polarization tensor and its properties are derived in Appendix D in the context of three-dimensional elasticity.

The topological derivatives for semilinear elliptic boundary value problems are obtained in Chapter 10 by the compound asymptotic method in singularly perturbed geometrical domains. Since there are very few results on topological derivatives for nonlinear problems available in the literature, the full proofs of the derived results are presented in Appendix E.

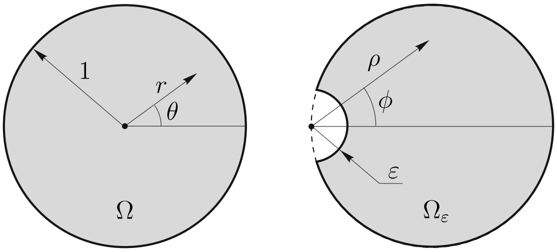
The topological derivatives for variational inequalities including the Signorini problem and the frictionless contact problems in elasticity are derived in Chapter 11. This is also a solution to a challenging problem in topological and shape sensitivity analysis, since the standard approach of asymptotic analysis requires in this particular case the hypothesis of *strict complementarity* to be fulfilled. The proposed method which avoids such a restrictive hypothesis combines the domain decomposition method with the Hadamard differentiability of solutions to the unilateral problems with respect to the data. The abstract result of this sort is presented in Appendix F.

Some useful basic results of tensor calculus are included in Appendix G for the reader convenience. In particular, inner, vector and tensor products are defined. In addition, gradient, divergence and curl formulae, together with some integral theorems, are presented. Finally, some useful decompositions in curvilinear, polar and spherical coordinate systems are provided.

The main idea of the monograph is the presentation of topological derivatives for a wide class of elliptic problems with the applications in numerical methods of shape and topology optimization, accessible for both communities of applied mathematics and computational mechanics.

1.4 Exercises

1. Show that the remainder of the topological asymptotic expansion in Example 1.1 behaves like $o(\varepsilon^d)$.
2. Let us consider one more term in the topological asymptotic expansion of the form
$$\psi(\chi_\varepsilon(\widehat{x})) = \psi(\chi) + f(\varepsilon)\mathcal{T}(\widehat{x}) + f_2(\varepsilon)\mathcal{T}^2(\widehat{x}) + o(f_2(\varepsilon)) ,$$
where $f_2(\varepsilon)$ is such that
$$\lim_{\varepsilon\to 0}\frac{f_2(\varepsilon)}{f(\varepsilon)} = 0 .$$
Then, $\mathcal{T}(\widehat{x})$ and $\mathcal{T}^2(\widehat{x})$ are the first and second order topological derivatives of ψ, respectively. Suppose that the function $g(x)$ in Example 1.2 is of class $C^2(\Omega)$, with its second order gradient *Lipschitz continuous* in ω_ε ($\exists\, C \geqslant 0 : \|\nabla\nabla g(x) - \nabla\nabla g(\widehat{x})\| \leqslant C\|x-\widehat{x}\|,\ \forall x \in \omega_\varepsilon$). Consider the particular case associated to the nucleation of a circular inclusion of the form $\omega_\varepsilon(\widehat{x}) = B_\varepsilon(\widehat{x})$, with $B_\varepsilon(\widehat{x})$ used to denote a ball of radius ε and center at $\widehat{x}\in\Omega$, with $\Omega\subset\mathbb{R}^2$. Then, show that the topological asymptotic expansion of the functional $\psi(\chi_\varepsilon(\widehat{x}))$ is given by
$$\psi(\chi_\varepsilon(\widehat{x})) = \psi(\chi) - (1-\gamma)\pi\varepsilon^2 g(\widehat{x}) - \frac{1-\gamma}{8}\pi\varepsilon^4\Delta g(\widehat{x}) + o(\varepsilon^4) .$$
3. Using the definition for the topological derivative given by (1.2), show the results presented in Example 1.3.
4. Repeat Example 1.4 with the following conditions: $-u''(x) = 1$ for $0 < x < 1$ and $u(0) = u'(1) = 0$.
5. Repeat Example 1.5 with the following conditions: $-u''''(x) = 0$ for $0 < x < 1$, $u(0) = u'(0) = u''(1) = 0$ and $u'''(1) = 1$.
6. Find the functions $b(r)$, $v(r)$ and $\mathcal{T}(r)$ in Example 1.6.
7. Let us consider Example 1.7 for the particular case of a shaft with circular cross section, with $\Omega = B_1$, where B_1 is a ball of radius 1 and center at the origin (see fig. 1.6(a)). Consider a singulary perturbed domain of the form $\Omega_\varepsilon = \Omega\setminus\overline{B_\varepsilon}$, where B_ε is a ball of radius ε and center on $\partial\Omega$ (see fig. 1.6(b)). Show that the topological asymptotic expansion of the complementary dissipation energy is given by
$$\psi(\chi_\varepsilon) = -\pi\frac{b^2}{16} + \pi\varepsilon^2\frac{b^2}{8} + o(\varepsilon^2) .$$
Compare the above expansion with the general result given by (1.47). Hint: use the polar coordinate systems as shown in fig. 1.6. The closed solutions to both original and perturbed problems are respectively given by
$$u(r) = \frac{b}{4}(1-r^2) \quad \text{and} \quad u_\varepsilon(\rho,\phi) = -\frac{b}{4}(\rho^2-\varepsilon^2)\left(1-\frac{2}{\rho}\cos\phi\right) .$$



(a) unperturbed domain (b) perturbed domain

Fig. 1.6 Shaft with circular cross section under torsion effects: original and singulary perturbed domains

8. By taking into account Example 1.8:

   a. Show that the expansions (1.85) and (1.86) hold.

   b. Replace the tracking type shape functional by the total potential energy, namely

$$\psi(\chi) = \frac{1}{2}\int_{\Omega} \|\nabla u\|^2 - \int_{\Omega} bu\ ,$$

   and repeat the same steps to obtain the associated topological derivative. Repeat the derivation by using directly the definition (1.2) for the topological asymptotic expansion.

   c. Take the total potential energy defined in a disk B_1 of unity radius and center at the origin, submitted to a constant source-term b. As topological perturbation, consider the particular case given by

$$b_\varepsilon(x) := \begin{cases} b & \text{if } x \in B_1 \setminus \overline{B_\varepsilon}\ , \\ \gamma b & \text{if } x \in B_\varepsilon\ , \end{cases}$$

   where B_ε is a disk of radius ε and center at the origin. Then, develop $\psi(\chi_\varepsilon)$ in power of ε around the origin and compare with the previous obtained result.

Chapter 2
Domain Derivation in Continuum Mechanics

In this chapter the formal shape sensitivity analysis is performed in the setting of continuum mechanics. The word *formal* is used in the sense that all objects are assumed to be sufficiently smooth. It means that we do not state smoothness hypotheses, since standard differentiability assumptions sufficient to make an argument rigorous are generally obvious to mathematicians and of little interest to engineers and physicists. In addition, we do not employ any function spaces setting for all the developments. The case of elliptic boundary value problems is considered separately in Chapter 3 in the framework of the variational solutions in functional spaces. Therefore the required results on the shape and material derivatives are proved e.g. in [210] by an application of the so-called speed method. The demand on shape sensitivity analysis for our purposes of the topological differentiability is not involved, since we restrict ourselves to the shape gradients of the energy type shape functionals for the elliptic boundary value problems with the absence of singularities. We refer to Chapter 3 for a presentation of the complete arguments on shape differentiability for the solutions of the Poisson, Kirchhoff plate, linear elasticity. These results are of independent interest and the proofs are borrowed from the monograph [210]. The results on boundary value problems of fluid mechanics are formally obtained by the method proposed in [196].

The shape functional, the constraints and the state equations are written in general as domain and/or boundary integrals, whose integrands may depend on scalar and/or vector fields and their gradients of first or second orders, etc. The shape sensitivity analysis concerns the study of the behavior of these functionals with respect to shape perturbations in the geometrical domain of the problem definition. In order to obtain the sensitivity (derivative) of the shape functional under consideration with respect to shape perturbations, it is sufficient to adequately parameterize the moving boundaries and apply the concept of Gâteaux and Fréchet derivatives together with material derivatives of spatial fields and the Reynold's transport theorem. In this chapter, therefore, we present the basic tools to perform the shape sensitivity analysis from the continuum mechanics point of view, leading to a systematic and general methodology applicable to a wide range of problems.

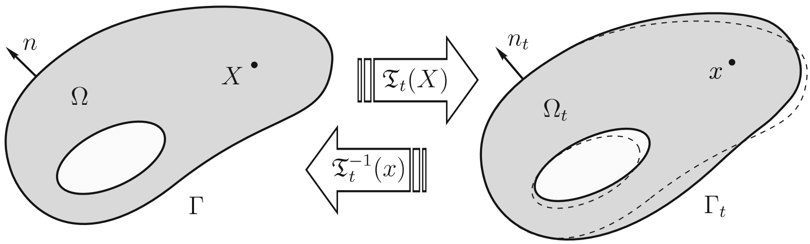


Fig. 2.1 Mapping $\mathfrak{T}_t$ between the original (material) Ω and the perturbed (spacial) Ω_t domains

From historical point of view, a remarkable development of this field was observed during the conference *Optimization of Distributed Parameters Structures*, held in 1981 [89], mainly due to the works by Céa [43] and Zolésio [219]. These papers describe the mathematical foundation of the shape sensitivity analysis in the Sobolev spaces by a smooth boundary variation technique (see also Haslinger & Neittaanmäki 1988 [88], Sokołowski & Zolésio 1992 [210], Delfour & Zolésio 2001 [50] and Henrot & Pierre 2005 [91]). Furthermore, it is possible to establish a closed relation between shape sensitivity analysis and modern continuum mechanics theory (see, for instance, [214]), which is discussed at the end of this chapter through an example on the analysis of defects in three-dimensional elastic bodies.

2.1 Material and Spatial Descriptions

Let us consider an open and bounded domain $\Omega \subset \mathbb{R}^d$, with $d \geqslant 2$, whose boundary, denoted by $\Gamma := \partial\Omega$, is smooth enough, i.e., class C^2 or Lipschitz boundaries shall be sufficient for our purposes. We assume that the domain Ω is subject to a smooth perturbation (its topology is preserved) represented by a smooth and invertible mapping denoted by $\mathfrak{T}_t(X)$, where $X \in \Omega$ and $t \in [0,\delta)$, with $\delta \in \mathbb{R}_+$. Then, for each t, we have

$$\mathfrak{T}_t : \Omega \to \Omega_t \qquad \text{with} \qquad \mathfrak{T}_t^{-1} : \Omega_t \to \Omega \ . \tag{2.1}$$

Thus, the perturbed domain Ω_t, bounded by $\Gamma_t := \partial\Omega_t$, parameterized through t, can be written as (see fig. 2.1)

$$\Omega_t := \left\{ x \in \mathbb{R}^d : x = \mathfrak{T}_t(X), X \in \Omega \text{ and } t \in [0,\delta) \right\} \ . \tag{2.2}$$

Therefore, $x_{|_{t=0}} = \mathfrak{T}_t(X)_{|_{t=0}} = X$ and $\Omega_{t|_{t=0}} = \Omega$.

By using the classical notation from the continuum mechanics (Gurtin 1981 [82]), Ω and Ω_t represent the *material and spatial configurations*, respectively. In addition, $X \in \Omega$ and $x \in \Omega_t$ are also referred as the Lagrangian and Eulerian coordinates, respectively. Therefore, we consider the reference domain Ω with the *Lagrangian coordinate system*, and the variable domain Ω_t equipped with the

Eulerian coordinate system. The domain Ω_t is constructed in the form of the flow of a given velocity field.

The spatial differential element dx (defined in Ω_t) is associated to the material differential element dX (defined in Ω) as

$$x = \mathfrak{T}_t(X) \quad \Rightarrow \quad dx = \partial_X \mathfrak{T}_t(X) dX \, , \tag{2.3}$$

which can be written in a compact form as

$$\mathfrak{J}(X,t) := \partial_X \mathfrak{T}_t(X) \quad \Rightarrow \quad dx = \mathfrak{J} dX \, , \tag{2.4}$$

where $\mathfrak{J}$ can be interpreted as the Jacobian transformation tensor of Ω to Ω_t. We can differentiate the mapping $\mathfrak{T}_t(X)$ with respect to t, to obtain

$$x = \mathfrak{T}_t(X) \quad \Rightarrow \quad \dot{x} := \partial_t \mathfrak{T}_t(X) = \mathfrak{V}(X,t) \, , \tag{2.5}$$

where, by an analogy with the continuum mechanics, $\mathfrak{V}(X,t)$ can be seen as the *material description of the velocity field* characterizing the shape change of the body.

Remark 2.1. In Chapter 3 the *Jacobian domain transformation tensor* $\mathfrak{J}(X,t)$ is specified for the mapping $\mathfrak{T}_t$ and represented by the matrix function $D\mathfrak{T}_t$. Its determinant is denoted by $\mathfrak{g}(t) = \det(D\mathfrak{T}_t)$. We have also an appropriate notation for the boundary Jacobian in the case of the transformation $\mathfrak{T}_t$.

Remark 2.2. In Chapter 3 we use the notation $\mathfrak{V}(x,t) := \mathfrak{V}_t(x)$ for the velocity field written in the Eulerian coordinates. The associated homeomorphism $\mathfrak{T}_t : \mathbb{R}^d \mapsto \mathbb{R}^d$ is always written in the Lagrangian coordinates. The mapping $\mathfrak{T}_t$ actually depends on the velocity vector field $\mathfrak{V}$ and the real variable t, and it defines $\Omega_t = \mathfrak{T}_t(\Omega)$. For the evaluation of the topological derivatives of the energy functionals in perturbed domains with the smooth inclusions, voids or cavities, in our framework the normal component of the field $\mathfrak{V}$ on the moving boundary or interface is usually given by the negative outward normal vector $-n$. But it is the only simplification in our procedure, since the shape gradient of the energy functional should be determined in its full generality for our purposes.

The complete dependence of the material $X \in \Omega$ and spatial $x \in \Omega_t$ points with respect to the parameter t is respectively given by

$$\mathfrak{T}_t^{-1}(\mathfrak{T}_t(X)) = X \qquad \text{and} \qquad \mathfrak{T}_t(\mathfrak{T}_t^{-1}(x)) = x \, . \tag{2.6}$$

Therefore, given two functions $g(X,t)$ and $h(x,t)$, we respectively denote their spatial and material descriptions as follows

$$g_t(x) := g(\mathfrak{T}_t^{-1}(x),t) \qquad \text{and} \qquad h^t(X) := h(\mathfrak{T}_t(X),t) \, . \tag{2.7}$$

Let us introduce φ^t and φ_t to denote the material and spatial descriptions of a (scalar, vector or tensor) field φ, respectively. Then, the *spatial description of the material field* φ^t is defined as

$$[\varphi^t]_t(x) := \varphi^t(\mathfrak{T}_t^{-1}(x)) \,. \tag{2.8}$$

In the same way, the *material description of the spatial field* φ_t is written as

$$[\varphi_t]^t(X) := \varphi_t(\mathfrak{T}_t(X)) \,. \tag{2.9}$$

By combining (2.8) and (2.9), we obtain

$$\varphi^t(X) = [\varphi_t(x)]^t = \varphi_t(x)|_{x=\mathfrak{T}_t(X)} \,, \tag{2.10}$$

$$\varphi_t(x) = [\varphi^t(X)]_t = \varphi^t(X)|_{X=\mathfrak{T}_t^{-1}(x)} \,, \tag{2.11}$$

leading to

$$\varphi^t = [\varphi_t]^t = \left[[\varphi^t]_t\right]^t \qquad \text{and} \qquad \varphi_t = [\varphi^t]_t = \left[[\varphi_t]^t\right]_t \,. \tag{2.12}$$

The following notation for composed functions is often used

$$\varphi^t(X) = (\varphi_t \circ \mathfrak{T}_t)(X) \qquad \text{and} \qquad \varphi_t(x) = (\varphi^t \circ \mathfrak{T}_t^{-1})(x) \,, \tag{2.13}$$

which can be found in many references on the subject (see, for instance, the books by Sokołowski & Zolésio 1992 [210] and Delfour & Zolésio 2001 [50]).

2.1.1 Gradient of Scalar Fields

Let φ^t and φ_t be the material and spatial descriptions of a scalar field φ, respectively. Then, we can calculate the total differential of φ^t and φ_t, namely

$$d\varphi^t = \partial_X \varphi^t \cdot dX = \nabla_X \varphi^t \cdot dX \quad \text{and} \quad d\varphi_t = \partial_x \varphi_t \cdot dx = \nabla_x \varphi_t \cdot dx \,, \tag{2.14}$$

where $\nabla_X := \partial_X$ and $\nabla_x := \partial_x$ are gradients with respect to Lagrangian and Eulerian coordinates, respectively. Thus, since $d\varphi^t = [d\varphi_t]^t$, the relation between $\nabla_X \varphi^t$ and $\nabla_x \varphi_t$ can be obtained as follows

$$\begin{aligned} [d\varphi_t]^t &= [\nabla_x \varphi_t \cdot dx]^t = [\nabla_x \varphi_t]^t \cdot \mathfrak{J} dX \\ &= \mathfrak{J}^\top [\nabla_x \varphi_t]^t \cdot dX \Rightarrow \nabla_X \varphi^t = \mathfrak{J}^\top [\nabla_x \varphi_t]^t \,. \end{aligned} \tag{2.15}$$

2.1.2 Gradient of Vector Fields

Let φ^t and φ_t be the material and spatial descriptions of a vector field φ, respectively. Then, we can calculate the total differential of φ^t and φ_t, that is

$$d\varphi^t = (\partial_X \varphi^t)dX = (\nabla_X \varphi^t)dX \quad \text{and} \quad d\varphi_t = (\partial_x \varphi_t)dx = (\nabla_x \varphi_t)dx \,, \tag{2.16}$$

where $\nabla_X := \partial_X$ and $\nabla_x := \partial_x$. Thus, since $d\varphi^t = [d\varphi_t]^t$, the relation between $\nabla_X \varphi^t$ and $\nabla_x \varphi_t$ is given by

$$[d\varphi_t]^t = [(\nabla_x \varphi_t)dx]^t = [\nabla_x \varphi_t]^t \mathfrak{J} dX \Rightarrow \nabla_X \varphi^t = [\nabla_x \varphi_t]^t \mathfrak{J} \,. \tag{2.17}$$

2.1.3 Spatial Description of Velocity Fields

The material description of the velocity field is obtained by differentiation of the mapping $X \mapsto \mathfrak{T}_t(X)$ with respect to the parameter t (cf. equation (2.5)). On the other hand, to obtain the *spatial description of the velocity field*, we need to transport its material description $\mathfrak{V}(X,t)$ to the spatial configuration Ω_t. Thus, the spatial description of the velocity field is defined as

$$\mathfrak{V}_t(x) := \mathfrak{V}(\mathfrak{T}_t^{-1}(x), t) = \partial_t \mathfrak{T}_t(X)_{|_{X=\mathfrak{T}_t^{-1}(x)}} \,. \tag{2.18}$$

Therefore, the material and spatial descriptions of a velocity field are respectively given by (2.5) and (2.18). In addition, at $t = 0$, we observe that

$$\mathfrak{V}_t(x)_{|_{t=0}} = \mathfrak{V}(X,0) \,. \tag{2.19}$$

Taking into account (2.17) for the particular case in which the vector field φ is the shape change velocity $\mathfrak{V}$, we have

$$\nabla_X \mathfrak{V} = [\nabla_x \mathfrak{V}_t]^t \mathfrak{J} \,, \tag{2.20}$$

which can be written in a compact form by introducing the following notation

$$L := \nabla_X \mathfrak{V} \qquad \text{and} \qquad L_t := \nabla_x \mathfrak{V}_t \,, \tag{2.21}$$

leading to

$$L = [L_t]^t \mathfrak{J} \,. \tag{2.22}$$

In addition

$$\operatorname{tr}(L) = \mathrm{I} \cdot \nabla_X \mathfrak{V} = \operatorname{div}_X \mathfrak{V} \quad \text{and} \quad \operatorname{tr}(L_t) = \mathrm{I} \cdot \nabla_x \mathfrak{V}_t = \operatorname{div}_x \mathfrak{V}_t \,. \tag{2.23}$$

Remark 2.3. In the matrix notation of Chapter 3 the gradient with respect to the Lagrangian coordinates of a function depending on the Eulerian coordinates is written in the following way

$$D(\varphi \circ \mathfrak{T}_t) = D\mathfrak{T}_t (D\varphi \circ \mathfrak{T}_t) \,. \tag{2.24}$$

Such a transformation is used for the transport of the gradient from the domain Ω_t to the reference domain Ω, for example. The material derivatives of solutions to the boundary value problems in variational form can be evaluated in the reference domain Ω.

2.2 Material Derivatives of Spatial Fields

As already mentioned, the shape functional, the constraints and the state equations are in general written as domain and/or boundary integrals, whose integrands may depend on scalar and/or vector fields and their gradients of first or second orders, etc. Thus, for a given scalar or vector field, we determine its total derivative with respect to the control parameter t as well as the associated material and spatial descriptions.

Let φ be a given field, whose material and spatial descriptions are respectively denoted by φ^t and φ_t. Then, the material (total) derivative of the material description φ^t of a field φ is trivially defined as

$$\dot{\varphi}^t(X) := \partial_t \varphi^t(X) \,. \tag{2.25}$$

On the other hand, the spatial description of the material (total) derivative of the field φ written spatially φ_t is defined by

$$\dot{\varphi}_t(x) := \left(\partial_t \varphi_t(\mathfrak{T}_t(X))\right)_{|_{X=\mathfrak{T}_t^{-1}(x)}} \,. \tag{2.26}$$

That is, in order to obtain the spatial description of the material derivative of a field φ written spatially φ_t, we first need to transport the field φ_t to the material configuration Ω, then calculate its derivative with respect to the parameter t and, finally, come back to the spatial configuration Ω_t. Therefore, from the notation introduced by (2.12), we have

$$\dot{\varphi}_t(x) = [\dot{\varphi}^t(X)]_t \qquad \text{and} \qquad \dot{\varphi}^t(X) = [\dot{\varphi}_t(x)]^t \,. \tag{2.27}$$

Finally, the *relation between material and spatial derivatives* is given by the following important result:

Theorem 2.1. *Let φ_t be the spatial description of a smooth enough scalar or vector field φ, then*

$$\dot{\varphi}_t = \varphi_t' + \langle \nabla_x \varphi_t, \mathfrak{V}_t \rangle \,, \qquad \textit{with} \qquad \varphi_t'(x) := \partial_t \varphi_t(x) \,. \tag{2.28}$$

Proof. From the chain rule and taking into account the definition of the spatial description of the velocity field given by (2.18), we have

$$\begin{aligned} \dot{\varphi}_t(x) &= \left(\partial_t \varphi_t(\mathfrak{T}_t(X))\right)_{|_{X=\mathfrak{T}_t^{-1}(x)}} \\ &= \langle \nabla_x \varphi_t(x), \partial_t \mathfrak{T}_t(X)_{|_{X=\mathfrak{T}_t^{-1}(x)}} \rangle + \partial_t \varphi_t(x) \\ &= \langle \nabla_x \varphi_t(x), \mathfrak{V}_t(x) \rangle + \varphi_t'(x) \,, \end{aligned} \tag{2.29}$$

leading to the result. □

Corollary 2.1. *Taking into account Theorem 2.1 together with (2.19), we have the following relation between the material and spatial derivatives:*

- *For a scalar field* φ_t
$$\dot{\varphi}_t = \varphi_t' + \nabla_x \varphi_t \cdot \mathfrak{V}_t \,. \tag{2.30}$$
- *For a vector field* φ_t
$$\dot{\varphi}_t = \varphi_t' + (\nabla_x \varphi_t)\mathfrak{V}_t \,. \tag{2.31}$$

Remark 2.4. For the purposes of the shape differentiability of the solutions to elliptic boundary value problems developed in Chapter 3 the matrix notation is used which is briefly explained in that chapter. The notation is traditionally employed in the shape sensitivity analysis [210], and therefore is included in our presentation for the convenience of the reader. We point out that in the framework of the boundary variations technique we are able to determine the shape gradient of the functional, e.g., the energy functional. If the shape gradient is given by a function, it provides the normal component of the velocity field at the moving boundary for the descent method of the gradient type in shape optimization. We also use the shape gradient on the moving boundary of a domain singular perturbation in order to determine the topological derivatives of the energy functionals. Therefore, we are in fact interested only in mappings which are defined by the specific normal component of the velocity field on the moving boundary. That is why, the special notation of the shape sensitivity analysis borrowed from [210] is required for our purposes, even if we do not perform any shape optimization using the shape gradients. In fact, we evaluate the singular limits of the shape gradients in order to identify the topological derivatives.

2.2.1 Derivative of the Gradient of a Scalar Field

In order to obtain the spatial description of the material derivative of the gradient of a scalar field φ spatially written φ_t, we need to differentiate both sides of (2.15) with respect to t, which leads to

$$\begin{aligned} \partial_t(\nabla_X \varphi^t) &= \partial_t(\mathfrak{J}^\top [\nabla_x \varphi_t]^t) \\ &= \partial_t \mathfrak{J}^\top [\nabla_x \varphi_t]^t + \mathfrak{J}^\top \partial_t([\nabla_x \varphi_t]^t) \,. \end{aligned} \tag{2.32}$$

Let us multiply from the left both sides of (2.32) by $\mathfrak{J}^{-\top}$. Then, after some rearrangements we obtain

$$\partial_t([\nabla_x \varphi_t]^t) = \mathfrak{J}^{-\top} \partial_t(\nabla_X \varphi^t) - \mathfrak{J}^{-\top} \partial_t \mathfrak{J}^\top [\nabla_x \varphi_t]^t \,. \tag{2.33}$$

However,

$$\partial_t(\nabla_X \varphi^t) = \nabla_X(\partial_t \varphi^t) = \nabla_X \dot{\varphi}^t = \nabla_X [\dot{\varphi}_t]^t = \mathfrak{J}^\top [\nabla_x \dot{\varphi}_t]^t \,, \tag{2.34}$$

and, from the definition to the Jacobian tensor $\mathfrak{J}$ given by (2.4) and taking into account (2.22), we have

$$\begin{aligned} \partial_t \mathfrak{J} &= \partial_t (\nabla_X \mathfrak{T}_t) = \nabla_X \partial_t \mathfrak{T}_t = \nabla_X \mathfrak{V} = [\nabla_x \mathfrak{V}_t]^t \mathfrak{J} \\ &\Rightarrow \partial_t \mathfrak{J} = [L_t]^t \mathfrak{J} \qquad \text{and} \qquad \partial_t \mathfrak{J}^\top = \mathfrak{J}^\top ([L_t]^t)^\top . \end{aligned} \tag{2.35}$$

By considering the equations (2.33), (2.34) and (2.35), we obtain

$$\partial_t ([\nabla_x \varphi_t]^t) = [\nabla_x \dot{\varphi}_t]^t - ([L_t]^t)^\top [\nabla_x \varphi_t]^t . \tag{2.36}$$

After taking the spatial description of the above relation, we have

$$\left[\partial_t ([\nabla_x \varphi_t]^t)\right]_t = \left[[\nabla_x \dot{\varphi}_t]^t\right]_t - \left[([L_t]^t)^\top [\nabla_x \varphi_t]^t\right]_t , \tag{2.37}$$

which finally results in

$$(\nabla_x \varphi_t)^\cdot = \nabla_x \dot{\varphi}_t - L_t^\top (\nabla_x \varphi_t) . \tag{2.38}$$

2.2.2 Derivative of the Gradient of a Vector Field

In the same way, the spatial description of the material derivative of the gradient of a vector field φ spatially written φ_t can be obtained by differentiating both sides of (2.17) with respect to t, that is

$$\begin{aligned} \partial_t (\nabla_X \varphi^t) &= \partial_t ([\nabla_x \varphi_t]^t \mathfrak{J}) \\ &= \partial_t ([\nabla_x \varphi_t]^t) \mathfrak{J} + [\nabla_x \varphi_t]^t \partial_t \mathfrak{J} . \end{aligned} \tag{2.39}$$

Let us multiply from the right both sides of (2.39) by $\mathfrak{J}^{-1}$. Then, after some rearrangements we obtain

$$\partial_t ([\nabla_x \varphi_t]^t) = \partial_t (\nabla_X \varphi^t) \mathfrak{J}^{-1} - [\nabla_x \varphi_t]^t (\partial_t \mathfrak{J}) \mathfrak{J}^{-1} . \tag{2.40}$$

Furthermore,

$$\partial_t (\nabla_X \varphi^t) = \nabla_X (\partial_t \varphi^t) = \nabla_X \dot{\varphi}^t = \nabla_X [\dot{\varphi}_t]^t = [\nabla_x \dot{\varphi}_t]^t \mathfrak{J} , \tag{2.41}$$

and, from equations (2.40), (2.41) and (2.35), we obtain

$$\partial_t ([\nabla_x \varphi_t]^t) = [\nabla_x \dot{\varphi}_t]^t - [\nabla_x \varphi_t]^t [L_t]^t . \tag{2.42}$$

After taking the spatial description of the above relation, we have

$$\left[\partial_t ([\nabla_x \varphi_t]^t)\right]_t = \left[[\nabla_x \dot{\varphi}_t]^t\right]_t - \left[[\nabla_x \varphi_t]^t [L_t]^t\right]_t , \tag{2.43}$$

which finally leads to

$$(\nabla_x \varphi_t)^\cdot = \nabla_x \dot{\varphi}_t - (\nabla_x \varphi_t) L_t . \tag{2.44}$$

2.3 Material Derivatives of Integral Expressions

As mentioned in the beginning of this chapter, the shape functional, constraints and the state equations are given in general by functionals defined through domain and/or boundary integrals, whose integrands depend on scalar and/or vector fields as well as their gradients of first or second orders, etc. In the previous sections we have shown how to differentiate the gradients of scalar and vector fields with respect to the shape. Now, we will show how to differentiate a class of functionals defined over a domain which is submitted to smooth changes on its shape.

2.3.1 Domain Integral

In order to obtain the spatial description of the material derivative of a functional given by integrals defined in the spatial configuration Ω_t, that is,

$$\frac{d}{dt}\int_{\Omega_t} \varphi_t \, d\Omega_t \ , \tag{2.45}$$

we first need to transport the domain of integration and the integrand φ_t, representing the spatial description of a scalar field φ, to the material configuration Ω. This procedure allows us to introduce the total derivative operator inside the integral. Finally, we can calculate the derivative with respect to the control parameter t by using standard calculus rules and come back to the spatial configuration Ω_t.

Taking into account, therefore, the differential elements dx, dy and dz defined in Ω_t, then the relation between $d\Omega_t$ and $d\Omega$ can be obtained from (2.4) as following

$$\begin{aligned} d\Omega_t &= dx \times dy \cdot dz \\ &= \mathfrak{J}dX \times \mathfrak{J}dY \cdot \mathfrak{J}dZ \\ &= \frac{\mathfrak{J}dX \times \mathfrak{J}dY \cdot \mathfrak{J}dZ}{dX \times dY \cdot dZ} d\Omega \\ &\Rightarrow d\Omega_t = (\det\mathfrak{J}) d\Omega \ , \end{aligned} \tag{2.46}$$

where dX, dY and dZ are the differential elements defined in Ω.

Now, in order to obtain all necessary elements to derive the main result in this section, which is given by the Reynolds' transport theorem, we only have to calculate the derivative of $\det\mathfrak{J}$, namely

$$(\det\mathfrak{J}(X,t))^{\cdot} = \left\langle \partial_{\mathfrak{J}}(\det\mathfrak{J}(X,t)), \dot{\mathfrak{J}}(X,t) \right\rangle , \tag{2.47}$$

where we employ the following first order expansion

$$\det(\mathfrak{J} + \dot{\mathfrak{J}}) = \det(\mathfrak{J}) + \left\langle \partial_{\mathfrak{J}}(\det\mathfrak{J}), \dot{\mathfrak{J}} \right\rangle + o(\|\dot{\mathfrak{J}}\|) \ . \tag{2.48}$$

The term $\partial_{\mathfrak{J}}(\det\mathfrak{J})$ is identified below, and the remainder $o(\|\dot{\mathfrak{J}}\|)$ is of higher order with respect to the matrix norm $\|\dot{\mathfrak{J}}\|$.

On the other hand, given a second order tensor T, $\det(T - s\mathrm{I})$ admits the following representation (Gurtin 1981 [82])

$$\det(T - s\mathrm{I}) = -s^3 + I_1(T)s^2 - I_2(T)s + I_3(T) \quad \forall s \in \mathbb{R} , \tag{2.49}$$

where $I_1(T)$, $I_2(T)$ and $I_3(T)$ are the invariants of the tensor T respectively defined as

$$I_1(T) = \mathrm{tr}(T) , \tag{2.50}$$

$$I_2(T) = \frac{1}{2}[\mathrm{tr}(T)^2 - \mathrm{tr}(T^2)] , \tag{2.51}$$

$$I_3(T) = \det T . \tag{2.52}$$

By setting $s = -1$ in (2.49), we have

$$\det(T + \mathrm{I}) = 1 + \mathrm{tr}(T) + o(\|T\|) . \tag{2.53}$$

In addition, we note that

$$\det(\mathfrak{J} + \dot{\mathfrak{J}}) = \det[(\mathrm{I} + \dot{\mathfrak{J}}\mathfrak{J}^{-1})\mathfrak{J}] = \det(\dot{\mathfrak{J}}\mathfrak{J}^{-1} + \mathrm{I})\det\mathfrak{J} . \tag{2.54}$$

Thus, by setting $T = \dot{\mathfrak{J}}\mathfrak{J}^{-1}$ in (2.53) and considering (2.54), we have

$$\begin{aligned} \det(\mathfrak{J} + \dot{\mathfrak{J}}) &= [1 + \mathrm{tr}(\dot{\mathfrak{J}}\mathfrak{J}^{-1}) + o(\|\dot{\mathfrak{J}}\|)]\det\mathfrak{J} \\ &= \det\mathfrak{J} + \mathrm{tr}(\dot{\mathfrak{J}}\mathfrak{J}^{-1})\det\mathfrak{J} + o(\|\dot{\mathfrak{J}}\|) \end{aligned} \tag{2.55}$$

and, by comparing (2.48) with (2.55) and using (2.35), we obtain

$$\begin{aligned} \left\langle \partial_{\mathfrak{J}}(\det\mathfrak{J}), \dot{\mathfrak{J}} \right\rangle &= \mathrm{tr}(\dot{\mathfrak{J}}\mathfrak{J}^{-1})\det\mathfrak{J} = \mathrm{tr}([L_t]^t\mathfrak{J}\mathfrak{J}^{-1})\det\mathfrak{J} \\ &= \mathrm{tr}([\nabla_x\mathfrak{V}_t]^t)\det\mathfrak{J} = [\mathrm{div}_x\mathfrak{V}_t]^t\det\mathfrak{J} , \end{aligned} \tag{2.56}$$

leading to

$$(\det\mathfrak{J})^{\cdot} = [\mathrm{div}_x\mathfrak{V}_t]^t\det\mathfrak{J} . \tag{2.57}$$

Finally, by using the above results, we are ready to prove the *domain integral version of the Reynolds' transport theorem* (Gurtin 1981 [82]):

Theorem 2.2. *Let us consider a functional defined through an integral in Ω_t, whose integrand is given by the spatial description φ_t of a smooth enough scalar field φ. Then,*

$$\frac{d}{dt}\int_{\Omega_t} \varphi_t \, d\Omega_t = \int_{\Omega_t} (\dot{\varphi}_t + \varphi_t \mathrm{div}_x\mathfrak{V}_t) d\Omega_t \tag{2.58}$$

$$= \int_{\Omega_t} \varphi_t' d\Omega_t + \int_{\partial\Omega_t} \varphi_t(\mathfrak{V}_t \cdot n_t) d\Gamma_t , \tag{2.59}$$

where n_t is the outward unit normal vector on $\partial\Omega_t$.

Proof. From formulae (2.46) and (2.57), it follows that

$$\begin{aligned}\frac{d}{dt}\int_{\Omega_t}\varphi_t\,d\Omega_t &= \partial_t\int_{\Omega}\varphi^t(\det\mathfrak{J})d\Omega\\ &= \int_{\Omega}\partial_t(\varphi^t\det\mathfrak{J})d\Omega\\ &= \int_{\Omega}(\dot{\varphi}^t\det\mathfrak{J}+\varphi^t(\det\mathfrak{J})^{\cdot})d\Omega\\ &= \int_{\Omega}(\dot{\varphi}^t+\varphi^t[\mathrm{div}_x\mathfrak{V}_t]^t)(\det\mathfrak{J})d\Omega\\ &= \int_{\Omega_t}(\dot{\varphi}_t+\varphi_t\mathrm{div}_x\mathfrak{V}_t)d\Omega_t\ .\end{aligned} \tag{2.60}$$

On the other hand, from the result of Theorem 2.1 given by (2.28) and after applying the divergence theorem (G.35), (2.60) can be rewritten as

$$\begin{aligned}\frac{d}{dt}\int_{\Omega_t}\varphi_t\,d\Omega_t &= \int_{\Omega_t}(\varphi_t'+\nabla_x\varphi_t\cdot\mathfrak{V}_t+\varphi_t\mathrm{div}_x\mathfrak{V}_t)d\Omega_t\\ &= \int_{\Omega_t}\varphi_t'd\Omega_t+\int_{\Omega_t}\mathrm{div}_x(\varphi_t\mathfrak{V}_t)d\Omega_t\\ &= \int_{\Omega_t}\varphi_t'd\Omega_t+\int_{\partial\Omega_t}\varphi_t(\mathfrak{V}_t\cdot n_t)d\Gamma_t\ .\end{aligned} \tag{2.61}$$

Thus, from equations (2.60) and (2.61) we have the result. □

2.3.2 Boundary Integral

In this section we show how to obtain the spatial description of the material derivative of a functional given by boundary integrals, that is

$$\frac{d}{dt}\int_{\partial\Omega_t}\varphi_t\,d\Gamma_t\ , \tag{2.62}$$

where the integrand φ_t represents the spatial description of a scalar field φ and $\Gamma_t=\partial\Omega_t$ is used to denote the boundary of the spatial configuration Ω_t.

Let n and n_t respectively be the normal unit vector fields to the boundaries $\Gamma=\partial\Omega$ and $\Gamma_t=\partial\Omega_t$, such that $(d\Gamma_t)n_t=dx\times dy$ and $(d\Gamma)n=dX\times dY$. Then, taking into account that dz and dZ are the differential elements in the directions n_t and n, we have (see fig. 2.2)

$$d\Gamma_t(n_t\cdot dz)=d\Omega_t \qquad \text{and} \qquad d\Gamma(n\cdot dZ)=d\Omega\ . \tag{2.63}$$

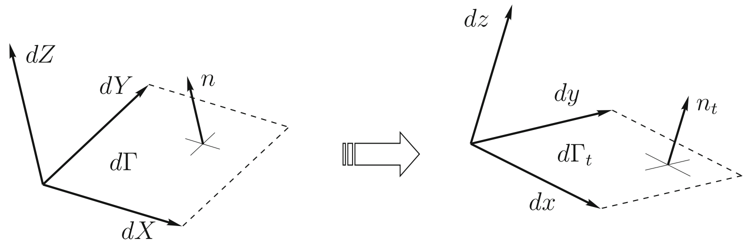


Fig. 2.2 Surface differential elements $d\Gamma$ and $d\Gamma_t$ defined on the material and spatial configurations, respectively

Thus, from (2.46), we obtain

$$\begin{aligned} d\Gamma_t(n_t \cdot dz) &= (\det\mathfrak{J}) d\Gamma (n \cdot dZ) \\ &= (\det\mathfrak{J}) d\Gamma (n \cdot \mathfrak{J}^{-1} dz) \\ &= (\det\mathfrak{J}) d\Gamma (\mathfrak{J}^{-\top} n) \cdot dz \\ &\Rightarrow (d\Gamma_t) n_t = (\det\mathfrak{J}) d\Gamma (\mathfrak{J}^{-\top} n) \; . \end{aligned} \tag{2.64}$$

Therefore, the relation between $d\Gamma_t$ and $d\Gamma$ is given by

$$d\Gamma_t = \|(d\Gamma_t) n_t\| = \|\det\mathfrak{J}(\mathfrak{J}^{-\top} n)\| d\Gamma = \|\mathfrak{J}^{-\top} n\| (\det\mathfrak{J}) d\Gamma \; . \tag{2.65}$$

The derivative of $\det\mathfrak{J}$ is given by (2.57). However, we still need to calculate the derivative of $\|\mathfrak{J}^{-\top} n\|$. For that, firstly we obtain the material description of the normal n_t in the following way

$$n_t = \frac{n_t d\Gamma_t}{d\Gamma_t} \quad \Rightarrow \quad \frac{\mathfrak{J}^{-\top} n (\det\mathfrak{J}) d\Gamma}{\|\mathfrak{J}^{-\top} n\| (\det\mathfrak{J}) d\Gamma} = \frac{\mathfrak{J}^{-\top} n}{\|\mathfrak{J}^{-\top} n\|} = [n_t]^t \; . \tag{2.66}$$

By defining

$$m := \mathfrak{J}^{-\top} n \; , \tag{2.67}$$

we have

$$[n_t]^t = \frac{m}{\|m\|} \; . \tag{2.68}$$

After differentiating both sides of the equation below

$$\mathfrak{J}^{-1}\mathfrak{J} = \mathrm{I} \; , \tag{2.69}$$

we note that

$$(\mathfrak{J}^{-1}\mathfrak{J})^{\cdot} = (\mathfrak{J}^{-1})^{\cdot}\mathfrak{J} + \mathfrak{J}^{-1}\dot{\mathfrak{J}} = 0 \; . \tag{2.70}$$

Let us multiply from the right the above expression by $\mathfrak{J}^{-1}$. Then, after some rearrangements, we can obtain the derivative of the inverse Jacobian tensor, namely

$$(\mathfrak{J}^{-1})^{\cdot} = -\mathfrak{J}^{-1}\dot{\mathfrak{J}}\mathfrak{J}^{-1} = -\mathfrak{J}^{-1}[L_t]^t \mathfrak{J}\mathfrak{J}^{-1} = -\mathfrak{J}^{-1}[L_t]^t \; , \tag{2.71}$$

where we have used the result (2.35). Thus,

$$(\mathfrak{J}^{-\top})^{\cdot} = -[L_t^{\top}]^t \mathfrak{J}^{-\top} . \tag{2.72}$$

In addition, from (2.67), we have

$$\|m\| = \|\mathfrak{J}^{-\top} n\| \tag{2.73}$$

and its derivative takes the form

$$\|m\|^{\cdot} = \partial_t (m \cdot m)^{\frac{1}{2}} = \frac{1}{2}(m \cdot m)^{-\frac{1}{2}} 2(m \cdot \dot{m}) = \frac{1}{\|m\|} m \cdot \dot{m} . \tag{2.74}$$

From equations (2.72) and (2.68) we note that

$$\begin{aligned} \dot{m} &= (\mathfrak{J}^{-\top} n)^{\cdot} \\ &= -[L_t^{\top}]^t \mathfrak{J}^{-\top} n = -[L_t^{\top}]^t m \\ &= -[L_t^{\top}]^t [n_t]^t \|m\| = -[L_t^{\top} n_t]^t \|m\| . \end{aligned} \tag{2.75}$$

By substituting (2.75) in (2.74) and taking into account (2.68), we have

$$\begin{aligned} \|m\|^{\cdot} &= -\frac{1}{\|m\|} m \cdot [L_t^{\top} n_t]^t \|m\| \\ &= -m \cdot [L_t^{\top} n_t]^t = -[n_t]^t \cdot [L_t^{\top} n_t]^t \|m\| \\ &= -[n_t \cdot L_t^{\top} n_t]^t \|m\| = -[L_t n_t \cdot n_t]^t \|m\| . \end{aligned} \tag{2.76}$$

By using the formulae (2.57) and (2.76), and since that $m = \mathfrak{J}^{-\top} n$, we can calculate the derivative of $\|\mathfrak{J}^{-\top} n\| \det \mathfrak{J}$, namely

$$\begin{aligned} (\|\mathfrak{J}^{-\top} n\| \det \mathfrak{J})^{\cdot} &= \|\mathfrak{J}^{-\top} n\| [\operatorname{div}_x \mathfrak{V}_t]^t \det \mathfrak{J} - [n_t \cdot L_t n_t]^t \|\mathfrak{J}^{-\top} n\| \det \mathfrak{J} \\ &= [\operatorname{div}_x \mathfrak{V}_t - n_t \cdot L_t n_t]^t \|\mathfrak{J}^{-\top} n\| \det \mathfrak{J} \\ &= [\operatorname{div}_{\Gamma_t} \mathfrak{V}_t]^t \|\mathfrak{J}^{-\top} n\| \det \mathfrak{J} , \end{aligned} \tag{2.77}$$

where $\operatorname{div}_{\Gamma_t} \mathfrak{V}_t$ is the tangential divergence of the velocity field defined as

$$\operatorname{div}_{\Gamma_t} \mathfrak{V}_t = \operatorname{div}_x \mathfrak{V}_t - n_t \cdot L_t n_t = \mathrm{I} \cdot L_t - (n_t \otimes n_t) \cdot L_t = (\mathrm{I} - n_t \otimes n_t) \cdot L_t . \tag{2.78}$$

Finally, by using the previous results, we can prove the *boundary integrals version of the Reynolds's transport theorem*:

Theorem 2.3. *Let us consider a functional defined through an integral on $\partial\Omega_t$, whose integrand is given by the spatial description φ_t of a smooth enough scalar field φ. Then,*

$$\frac{d}{dt} \int_{\partial\Omega_t} \varphi_t \, d\Gamma_t = \int_{\partial\Omega_t} (\dot{\varphi}_t + \varphi_t \operatorname{div}_{\Gamma_t} \mathfrak{V}_t) d\Gamma_t , \tag{2.79}$$

where $\operatorname{div}_{\Gamma_t} \mathfrak{V}_t$ is the tangential divergence of the velocity field given by (2.78).

Proof. Taking into account the results (2.65) and (2.77), we have

$$\begin{aligned}\frac{d}{dt}\int_{\partial\Omega_t}\varphi_t\,d\Gamma_t &= \partial_t\int_{\partial\Omega}\varphi^t\|\mathfrak{J}^{-\top}n\|\det\mathfrak{J}\,d\Gamma\\ &= \int_{\partial\Omega}\partial_t(\varphi^t\|\mathfrak{J}^{-\top}n\|\det\mathfrak{J})d\Gamma\\ &= \int_{\partial\Omega}(\dot{\varphi}^t\|\mathfrak{J}^{-\top}n\|\det\mathfrak{J}+\varphi^t(\|\mathfrak{J}^{-\top}n\|\det\mathfrak{J})^{\cdot})d\Gamma\\ &= \int_{\partial\Omega}(\dot{\varphi}^t+\varphi^t[\mathrm{div}_{\Gamma_t}\mathfrak{V}_t]^t)\|\mathfrak{J}^{-\top}n\|\det\mathfrak{J}\,d\Gamma\\ &= \int_{\partial\Omega_t}(\dot{\varphi}_t+\varphi_t\mathrm{div}_{\Gamma_t}\mathfrak{V}_t)d\Gamma_t\,,\end{aligned} \tag{2.80}$$

leading to the result. □

2.4 Summary of the Derived Formulae

Let us summarize the results presented in this chapter. We consider the material (total) derivatives evaluated at $t = 0$. Since at $t = 0$ we have $\Omega_{t\,|_{t=0}} = \Omega$, then the subscript X can be suppressed, namely, $\nabla := \nabla_X$ and $\mathrm{div} := \mathrm{div}_X$. In addition, for the sake of simplicity we denote $x \in \Omega$, instead of X. Therefore, for a given (scalar, vector or tensor) field φ, the *relation between its material and spatial derivatives* is given by

$$\dot{\varphi} = \varphi' + \langle\nabla\varphi, \mathfrak{V}\rangle\ . \tag{2.81}$$

In particular, we have:

- In the case of a *scalar field* φ

$$\dot{\varphi} = \varphi' + \nabla\varphi\cdot\mathfrak{V}\,. \tag{2.82}$$

- For a *vector field* φ

$$\dot{\varphi} = \varphi' + (\nabla\varphi)\mathfrak{V}\,. \tag{2.83}$$

The material and shape derivatives forms of the *Reynolds' transport theorem* are given by

$$\left(\int_\Omega\varphi\right)^{\cdot} = \int_\Omega(\dot{\varphi}+\varphi\,\mathrm{div}\mathfrak{V}) \tag{2.84}$$

$$= \int_\Omega\varphi' + \int_{\partial\Omega}\varphi(\mathfrak{V}\cdot n)\,, \tag{2.85}$$

for *domain integral*, respectively, and by

$$\left(\int_{\partial\Omega}\varphi\right)^{\cdot} = \int_{\partial\Omega}(\dot{\varphi}+\varphi\,\mathrm{div}_\Gamma\mathfrak{V})\,, \tag{2.86}$$

for *boundary integral*, where the *tangential divergence of the velocity* is defined as

$$\mathrm{div}_\Gamma \mathfrak{V} := (\mathrm{I} - n \otimes n) \cdot \nabla \mathfrak{V}\,, \tag{2.87}$$

with n standing for the outward unit normal vector on $\partial\Omega$.

Remark 2.5. Let us consider a subset $\omega \subset \Omega$. If the scalar function φ is *discontinuous* on the boundary $\partial\omega$, then, in this case the Reynolds' transport theorem reads

$$\begin{aligned}
\left(\int_\Omega \varphi\right)^{\cdot} &= \left(\int_{\Omega\setminus\overline{\omega}} \varphi + \int_\omega \varphi\right)^{\cdot} \\
&= \int_{\Omega\setminus\overline{\omega}} (\dot{\varphi} + \varphi \mathrm{div}\mathfrak{V}) + \int_\omega (\dot{\varphi} + \varphi \mathrm{div}\mathfrak{V}) \\
&= \int_{\Omega\setminus\overline{\omega}} (\varphi' + \nabla\varphi \cdot \mathfrak{V} + \varphi \mathrm{div}\mathfrak{V}) + \int_\omega (\varphi' + \nabla\varphi \cdot \mathfrak{V} + \varphi \mathrm{div}\mathfrak{V}) \\
&= \int_\Omega \varphi' + \int_{\Omega\setminus\overline{\omega}} \mathrm{div}(\varphi\mathfrak{V}) + \int_\omega \mathrm{div}(\varphi\mathfrak{V}) \\
&= \int_\Omega \varphi' + \int_{\partial\Omega} \varphi(\mathfrak{V}\cdot n) + \int_{\partial\omega} \varphi_e(\mathfrak{V}\cdot n) - \int_{\partial\omega} \varphi_i(\mathfrak{V}\cdot n) \\
&= \int_\Omega \varphi' + \int_{\partial\Omega} \varphi(\mathfrak{V}\cdot n) + \int_{\partial\omega} [\![\varphi]\!](\mathfrak{V}\cdot n)\,,
\end{aligned} \tag{2.88}$$

where n is the outward unit normal vector to $\Omega\setminus\overline{\omega}$ and $[\![\varphi]\!]$ is used to denote the jump of φ across to the boundary $\partial\omega$, namely $[\![\varphi]\!] = \varphi_e - \varphi_i$ on $\partial\omega$, with $\varphi_e = \varphi_{|_{\Omega\setminus\overline{\omega}}}$ and $\varphi_i = \varphi_{|_\omega}$.

In addition, for a *scalar field* φ we have

$$(\nabla\varphi)^{\cdot} = \nabla\dot{\varphi} - (\nabla\mathfrak{V})^\top \nabla\varphi\,. \tag{2.89}$$

In the case of a *vector field* φ, there is

$$(\nabla\varphi)^{\cdot} = \nabla\dot{\varphi} - \nabla\varphi\nabla\mathfrak{V}\,. \tag{2.90}$$

The *symmetric gradient of a vector field* is defined as

$$\nabla\varphi^s := \frac{1}{2}(\nabla\varphi + \nabla\varphi^\top) \tag{2.91}$$

and its material derivative can be obtained by applying formula (2.90), namely

$$\begin{aligned}
(\nabla\varphi^s)^{\cdot} &= \frac{1}{2}(\nabla\varphi + \nabla\varphi^\top)^{\cdot} \\
&= \frac{1}{2}((\nabla\varphi)^{\cdot} + (\nabla\varphi^\top)^{\cdot}) \\
&= \frac{1}{2}[(\nabla\varphi)^{\cdot} + ((\nabla\varphi)^{\cdot})^\top] \\
&= [(\nabla\varphi)^{\cdot}]^s = \nabla\dot{\varphi}^s - (\nabla\varphi\nabla\mathfrak{V})^s\,.
\end{aligned} \tag{2.92}$$

The *divergence of a vector field* is defined as

$$\mathrm{div}\varphi := \mathrm{tr}(\nabla\varphi) \tag{2.93}$$

and its material derivative is easily obtained from (2.90), that is

$$(\mathrm{div}\varphi)^{\cdot} = [\mathrm{tr}(\nabla\varphi)]^{\cdot} = \mathrm{tr}(\nabla\varphi)^{\cdot} = \mathrm{tr}(\nabla\dot{\varphi}) - \mathrm{tr}(\nabla\varphi\nabla\mathfrak{V}) = \mathrm{div}\dot{\varphi} - \nabla\varphi^{\top}\cdot\nabla\mathfrak{V}\,. \tag{2.94}$$

The *Laplacian of a scalar field* is defined as

$$\Delta\varphi := \mathrm{div}(\nabla\varphi)\,. \tag{2.95}$$

Then, by taking into account (2.94) and (2.89), we have

$$\begin{aligned}(\Delta\varphi)^{\cdot} &= [\mathrm{div}(\nabla\varphi)]^{\cdot}\\ &= \mathrm{div}(\nabla\varphi)^{\cdot} - (\nabla\nabla\varphi)^{\top}\cdot\nabla\mathfrak{V}\\ &= \mathrm{div}[\nabla\dot{\varphi} - \nabla\mathfrak{V}^{\top}\nabla\varphi] - \nabla\nabla\varphi\cdot\nabla\mathfrak{V}\\ &= \Delta\dot{\varphi} - \mathrm{div}(\nabla\mathfrak{V}^{\top}\nabla\varphi) - \nabla\nabla\varphi\cdot\nabla\mathfrak{V}\,.\end{aligned} \tag{2.96}$$

On the other hand, it is interesting to note that the Laplacian of a scalar field can also be written as

$$\Delta\varphi = \mathrm{tr}(\nabla\nabla\varphi)\,, \tag{2.97}$$

where $\nabla\nabla\varphi = (\nabla\nabla\varphi)^{\top}$. Thus, by applying (2.90) and (2.89), we have the material derivative of the *second order gradient of a scalar field*

$$\begin{aligned}(\nabla\nabla\varphi)^{\cdot} &= \nabla(\nabla\varphi)^{\cdot} - (\nabla\nabla\varphi)\nabla\mathfrak{V}\\ &= \nabla(\nabla\dot{\varphi} - \nabla\mathfrak{V}^{\top}\nabla\varphi) - (\nabla\nabla\varphi)\nabla\mathfrak{V}\\ &= \nabla\nabla\dot{\varphi} - \nabla(\nabla\mathfrak{V}^{\top}\nabla\varphi) - (\nabla\nabla\varphi)\nabla\mathfrak{V}\,.\end{aligned} \tag{2.98}$$

After taking the trace in both sides of (2.98), we obtain the same result as (2.96).

2.5 The Eshelby Energy-Momentum Tensor

In this section, we discuss the relation between shape sensitivity analysis and modern continuum mechanics theory, which is based on the Eshelby energy-momentum tensor concept introduced in the fundamental work by *Eshelby* 1975 [57]. This notion is due to Taroco and Feijóo 2006 [214] derived in the context of torsion problem of elastic shafts. Let us present this idea through an example concerning the analysis of defects in three-dimensional elastic bodies.

Example 2.1 (Eshelby energy-momentum tensor). Let $\Omega \subset \mathbb{R}^3$ be an open and bounded domain with smooth boundary $\partial\Omega$, and $\omega \subset \mathbb{R}^3$ be an open domain embedded in Ω, such that $\overline{\omega} \Subset \Omega$, with smooth boundary $\partial\omega$. We assume that

$\Omega_\omega = \Omega \setminus \overline{\omega}$ represents an elastic body with a small cavity ω inside. The total potential strain energy is given by the following functional:

$$\mathscr{J}_\omega(u) = \frac{1}{2}\int_{\Omega_\omega} \sigma(u)\cdot\nabla u^s - \int_{\Omega_\omega} b\cdot u\,, \tag{2.99}$$

where the vector function u is the solution to the variational problem:

$$\begin{cases} \text{Find } u \in H_0^1(\Omega_\omega;\mathbb{R}^3), \text{ such that} \\ \displaystyle\int_{\Omega_\omega} \sigma(u)\cdot\nabla\eta^s = \int_{\Omega_\omega} b\cdot\eta \quad \forall\eta\in H_0^1(\Omega_\omega;\mathbb{R}^3)\,, \\ \text{with} \quad \sigma(u) = \mathbb{C}\nabla u^s\,. \end{cases} \tag{2.100}$$

In the above equation, b is a constant body force distributed in the domain Ω and $\mathbb{C}$ is the constitutive tensor given by

$$\mathbb{C} = 2\mu\mathbb{I} + \lambda \mathrm{I}\otimes\mathrm{I}\,, \tag{2.101}$$

where I and $\mathbb{I}$ are the second and fourth order identity tensors, respectively, μ and λ are the Lamé's coefficients, both considered constants everywhere. Suppose that the cavity ω represents a defect embedded in Ω and that we want to know the sensitivity of the total potential strain energy with respect to the shape of the defect ω. Let us suppose that the cavity ω is submitted to a smooth perturbation of its shape. The *distributed shape gradient* of $\mathscr{J}_\omega(u)$ with respect to the shape of the cavity ω is given by

$$\dot{\mathscr{J}}_\omega(u) = \int_{\Omega_\omega} \Sigma\cdot\nabla\mathfrak{V}\,, \tag{2.102}$$

where $\mathfrak{V}$ is the shape change velocity field over Ω_ω, such that $\mathfrak{V}_{|\partial\Omega} = 0$, since $\partial\Omega$ remains fixed, and Σ is a divergence-free tensor field given by

$$\Sigma = \frac{1}{2}(\sigma(u)\cdot\nabla u^s - 2b\cdot u)\mathrm{I} - \nabla u^\top\sigma(u)\,. \tag{2.103}$$

Therefore, the distributed shape gradient (2.102) can be replaced by the *boundary shape gradient*

$$\dot{\mathscr{J}}_\omega(u) = \int_{\partial\omega} \Sigma n\cdot\mathfrak{V}\,, \tag{2.104}$$

where n is the normal unit vector field pointing toward the interior of the cavity ω. Finally, since $\sigma(u)n = 0$ on the boundary of the cavity $\partial\omega$, we have a further simplification of this formula. In particular, for the boundary shape gradient, the corresponding tensor Σ reduces itself to a hydrostatic tensor proportional to the specific strain energy. In fact,

$$\dot{\mathscr{J}}_\omega(u) = \int_{\partial\omega} \phi(u)\, n\cdot\mathfrak{V}\,, \tag{2.105}$$

where $\phi(u)$ is the strain energy density concentrated on $\partial\omega$, that is

$$\phi(u) = \frac{1}{2}\sigma(u)\cdot\nabla u^s - b\cdot u\,. \tag{2.106}$$

The above results have been derived using formulae summarized in the previous section together with Appendix G. The derivation of these results we leave as an exercise.

Let us now analyze the results obtained in the example. We can recognize Σ as the energy-momentum tensor introduced by *Eshelby* 1975 [57]. This tensor appears in the analysis of defects in three-dimensional elasticity and it plays a central role in the continuum mechanics theory involving inhomogeneities (inclusions, pores, cracks, etc.) in solids. Since the distributed shape gradient of the total potential energy is given by the product of Σ and $\nabla\mathfrak{V}$, it follows that Σ can be interpreted in terms of the *configurational forces* [83] acting in the elastic body with a small defect inside. Thus, $\mathrm{div}\Sigma = g$ in Ω, with $g = 0$ in this particular case, can be referred to the balance of configurational forces or simply *configurational balance* in *configurational mechanics* theory [83]. Finally, the shape gradient of the functional $\mathscr{J}_\omega(u)$ takes the form of a boundary integral concentrated on the moving boundary $\partial\omega$ and depending on the normal component of the velocity field $\mathfrak{V}$. This latter result fits into the so-called *Hadarmard's structure theorem* of shape optimization, proved in [210], for instance.

2.6 Exercises

1. Let u be a smooth enough scalar or vector field defined over an open bounded domain $\Omega \in \mathbb{R}^d$, $d \geqslant 2$. Compute the material derivative of the function $\phi(u)$ for the following cases:

    a. Thermal energy density associated to a steady-state heat conduction problem, that is
    $$\phi(u) := -\frac{1}{2} q(u) \cdot \nabla u \,,$$
    where $q(u) := -K\nabla u$, with K used to denote a second order symmetric tensor ($K^\top = K$) which doesn't depend on the shape of the body Ω. Then,
    $$\dot{\phi}(u) = -q(u) \cdot \nabla \dot{u} + (\nabla u \otimes q(u)) \cdot \nabla \mathfrak{V} \,.$$

    b. Strain energy density associated to a linear elasticity system, namely
    $$\phi(u) := \frac{1}{2} \sigma(u) \cdot \nabla u^s \,,$$
    where $\sigma(u) := \mathbb{C}\nabla u^s$, with $\mathbb{C}$ used to denote a fourth order symmetric tensor ($\mathbb{C}^\top = \mathbb{C}$) that doesn't depend on the shape of the body Ω. Then,
    $$\dot{\phi}(u) = \sigma(u) \cdot \nabla \dot{u}^s - \nabla u^\top \sigma(u) \cdot \nabla \mathfrak{V} \,.$$

    c. Energy density associated to a Kirchhoff plate bending problem, that is
    $$\phi(u) := -\frac{1}{2} M(u) \cdot \nabla\nabla u \,,$$
    where $M(u) = -\mathbb{C}\nabla\nabla u$, with $\mathbb{C}$ used to denote a fourth order symmetric tensor ($\mathbb{C}^\top = \mathbb{C}$) independent of the shape of the body Ω. Thus,
    $$\begin{aligned} \dot{\phi}(u) = & -M(u) \cdot \nabla\nabla \dot{u} + (\nabla\nabla u) M(u) \cdot \nabla \mathfrak{V} \\ & - (\nabla u \otimes \operatorname{div} M(u)) \cdot \nabla \mathfrak{V} + \operatorname{div}\left(M(u) \nabla \mathfrak{V}^\top \nabla u \right) \,. \end{aligned}$$

    d. Complementary energy density associated to a steady-state creep Prandtl shaft problem under torsion effects, which is given by
    $$\phi(u) := -\frac{1}{p} q(u) \cdot \nabla u \,,$$
    where $q(u) := -k\|\nabla u\|^{p-2}\nabla u$, with the material parameters k and p independent of the shape of the body Ω. Then,
    $$\dot{\phi}(u) = -q(u) \cdot \nabla \dot{u} + (\nabla u \otimes q(u)) \cdot \nabla \mathfrak{V} \,.$$

e. Quadratic form of the difference between the von Mises stress field $\sigma_{eq}(u)$ and an admissible equivalent stress $\overline{\sigma}$, that is

$$\phi(u) := (\sigma_{eq}(u) - \overline{\sigma})^2 ,$$

where $\overline{\sigma}$ is a given constant and

$$\sigma_{eq}(u) := \sqrt{\frac{1}{2}\mathbb{B}\sigma(u) \cdot \sigma(u)} \qquad \text{with} \qquad \mathbb{B} = 3\mathbb{I} - \mathrm{I} \otimes \mathrm{I} .$$

In the above equation, $\mathbb{I}$ and I are the fourth and second order identity tensors, respectively, and $\sigma(u) := \mathbb{C}\nabla u^s$, with $\mathbb{C}$ used to denote a fourth order symmetric tensor ($\mathbb{C}^\top = \mathbb{C}$) that doesn't depend on the shape of the body Ω. Therefore,

$$\dot{\phi}(u) = \left(1 - \frac{\overline{\sigma}}{\sigma_{eq}(u)}\right)\left(\mathbb{C}\mathbb{B}\sigma(u) \cdot \nabla \dot{u}^s - \nabla u^\top \mathbb{C}\mathbb{B}\sigma(u) \cdot \nabla \mathfrak{V}\right) .$$

Hint: use the formulas in the Appendix G.

2. Let us consider the p-Poisson problem given by the following nonlinear boundary value problem:

$$\begin{cases} \text{Find } u, \text{ such that} \\ -\mathrm{div}(\|\nabla u\|^{p-2}\nabla u) = 1 \ \text{ in } \ \Omega , \\ \qquad\qquad\qquad u = 0 \text{ on } \partial\Omega , \end{cases}$$

where $p \geqslant 2$. By taking into account the shape functional of the form

$$\mathscr{J}_\Omega(u) = \frac{1}{p}\int_\Omega \|\nabla u\|^p - \int_\Omega u ,$$

which represents the complementary dissipation energy associated to a steady-state creep Prandtl shaft problem under torsion effects, derive the weak formulation to the above problem, namely:

$$\begin{cases} \text{Find } u \in W_0^{1,p}(\Omega), \text{ such that} \\ \int_\Omega \|\nabla u\|^{p-2}\nabla u \cdot \nabla \eta = \int_\Omega \eta \quad \forall \eta \in W_0^{1,p}(\Omega) . \end{cases}$$

Now, from the Reynolds' transport theorem and by using the material derivatives of spatial fields concept, show that the shape derivative of the functional $\mathscr{J}_\Omega(u)$ leads to

$$\dot{\mathscr{J}}_\Omega(u) = \int_\Omega \Sigma \cdot \nabla \mathfrak{V} ,$$

where Σ can be seen as a generalization of the Eshelby energy momentum tensor, which is given by

$$\Sigma = \left(\frac{1}{p}\|\nabla u\|^p - u\right)\mathrm{I} - \|\nabla u\|^{p-2}(\nabla u \otimes \nabla u) \ .$$

Show that Σ is a divergence-free tensor field, namely $\mathrm{div}\Sigma = 0$, and derive the shape sensitivity of the functional $\mathscr{J}_\Omega(u)$ as a boundary integral of the form

$$\dot{\mathscr{J}}_\Omega(u) = \int_{\partial\Omega} \Sigma n \cdot \mathfrak{V} \ ,$$

where n is the outward unit normal vector to $\partial\Omega$. Hint: compute the divergence of the tensor Σ and rearrange the obtained expression in the form

$$\int_\Omega \mathrm{div}\Sigma \cdot \mathfrak{V} = -\int_\Omega (\mathrm{div}(\|\nabla u\|^{p-2}\nabla u) + 1)\nabla u \cdot \mathfrak{V} \qquad \forall \mathfrak{V} \ .$$

Since u is solution to the boundary value problem, we have $\mathrm{div}\Sigma = 0$ a.e. in Ω. Show that this last result can also be obtained by using purely variational arguments.

3. It is well known that only the normal component of the velocity field $\mathfrak{V}$ is relevant in the shape sensitivity analysis. This result is known as the *Hadamard's structure theorem* [210]. Thus, show that for the previous result the structure theorem holds.
4. Repeat Example 2.1 by considering the inclusion with appropriated transmission conditions instead of a cavity.

Chapter 3
Material and Shape Derivatives for Boundary Value Problems

In this chapter the mathematical background of shape sensitivity analysis is established, in contrast to Chapter 2 where the formal shape differentiability of functions and functionals is presented. Chapters 2 and 3 furnish the complete description of the differentiation technique with respect to the boundary variations of geometric domains.

The shape sensitivity analysis is extended to the singular boundary perturbations in the framework of the asymptotic analysis in singularly perturbed domains in Chapters 4–11. The new technique furnishes the closed formulae for the topological derivatives of shape functionals. In view of this additional information on sensitivity of shape functionals, we are able in numerical methods of shape and topology optimization to propose the appropriate changes of topology by creation of the new voids or inclusions in the reference domain, which improve the shape design and diminish the value of the cost. In particular, smooth boundary perturbations are performed here within the boundary variation technique. Non smooth perturbations should be analyzed by the asymptotic analysis in the singularly perturbed geometrical domains, and in fact lead directly to the asymptotic expansions of the shape functionals. The method of compound asymptotic expansions is introduced in the monograph in a restricted fashion only, in order to simplify the presentation. Therefore, the weighted spaces of Kondratiev or Hölder types are not considered in full range, we refer the reader to the references [144, 161, 163, 166, 170, 171, 172, 174, 176] for such developments.

We briefly describe the contents of this chapter. The weak solutions of elliptic boundary value problems are considered in Sobolev spaces. The shape differentiability of solutions is shown for the Poisson, Kirchhoff plate, linear elasticity and boundary value problems of fluid mechanics. In all cases, the weak and strong material derivatives of solutions to the boundary problems are obtained in the standard way by an application of the implicit function theorem. Then, the shape derivatives of solutions are specified as weak solutions of elliptic boundary value problems. The importance of shape derivatives is twofold, by the structure theorem of the shape gradients of shape functionals the knowledge of the shape derivatives of solutions is sufficient to obtain the shape gradients of functionals. It is also evident, that the shape derivatives can be easily obtained by a formal differentiation of the equation and the boundary conditions. However, sometimes the formal differentiation cannot be justified, we refer the reader to [196] for such an example in the case of the drag functional.

Preliminaries are presented in Section 3.1. In Sections 3.2 and 3.3 the velocity method for boundary variations in all its generality is used in order to obtain the boundary value problems for the material and shape derivatives of the solutions to the second order elliptic equations. The presentation follows that of [210], however it is restricted to the Laplacian for the sake of simplicity. Simple examples of shape derivatives can be also found e.g., in [87]. The shape derivative of the solution to the system of equations of linear elasticity is determined in Section 3.4. In Section 3.5 the shape derivative of the solution to the Kirchhoff plate problem is derived. In Section 3.6 the new method of shape differentiability, particularly well adapted to the nonlinear boundary value problems of fluid dynamics [197, 196], is presented. The particularity of this method is that it is reduced to the stability analysis of the solutions to the boundary value problem in the reference domain with respect to the coefficients of the differential operator. In this stability analysis the coefficients of the operator depend exclusively on the adjugate matrix function of the domain transformation. In particular, the adjugate matrix fully characterized the shape dependence of the boundary value problem posed in the reference domain with respect to the boundary perturbations. Thus, it is sufficient to show that the solutions of the boundary value problem in the reference domain are stable with respect to the coefficients of the operator to obtain the shape differentiability with respect to the domain variations reflected by the adjugate matrix. The elementary proofs of properties of the adjugate matrix with respect to the shape parameter are given. An example of application of this method to the boundary value problems of fluid mechanics is presented.

3.1 Preliminaries

We assume that there is given a solution $x \mapsto u(\Omega;x)$ of the boundary value problem posed in the reference domain Ω. We introduce a family of perturbed domains Ω_t defined by the change of variables $x \mapsto y = y(x)$ of the specific form $\mathfrak{T}_t$, where t is the shape parameter.

We denote by $y \mapsto u_t(\Omega_t;y)$ the solutions of the perturbed boundary value problem i.e., of the boundary value problem defined in the perturbed domain $\Omega_t := \mathfrak{T}_t(\Omega)$. The inverse relation $x = x(y)$, which takes the form $\Omega = \mathfrak{T}_t^{-1}(\Omega_t)$, allows us to introduce an auxiliary family of functions $x \mapsto u^t(\Omega;x)$ defined in the fixed reference domain, however the functions defined have no physical meaning for the model under considerations.

Finally, we consider a shape functional $J(\Omega)$ depending on $u(\Omega)$, which is minimized with respect to Ω. The shape differentiability is defined for the solutions

$t \mapsto u_t(\Omega_t; y) = u^t(\Omega; x)$, with $y = y(x)$, of the boundary value problems, and for the associated shape functional $t \mapsto J(\Omega_t)$ with respect to the shape parameter $t \to 0$.

We are interested in three basic concepts of the *shape differentiability* used in the framework of *shape sensitivity analysis* [210] (see also [50, 196]) as well as in the numerical methods of *shape optimization*, which are:

- The *material derivatives* are obtained by the differentiation of the mapping

$$t \mapsto u^t(x), \quad x \in \Omega.$$

- The *shape derivatives* are defined by derivatives of the mapping

$$t \mapsto u_t(y), \quad y \in \Omega_t.$$

- The *shape gradient* is given by the derivative of the shape functional

$$t \mapsto J(\Omega_t).$$

3.1.1 Sobolev-Slobodetskii Spaces

We use the *elliptic regularity* of solutions to the elliptic boundary value problems both for the weak and the classical solutions. We present a general result of this sort for the scalar equation of order m posed in a smooth, bounded domain. In our case $m = 1, 2$ for the Laplacian and the Kirchhoff plate, respectively.

First we recall some basic facts from the theory of *Sobolev-Slobodetskii spaces* which can be found in [2] and [215], for instance. Let Ω be an open subset of $\mathbb{R}^d$. For every multi-index $\alpha = (\alpha_1, \dots, \alpha_d)$ with nonnegative integers α_i and $f \in L^1_{\text{loc}}(\Omega)$, a function $g \in L^1_{\text{loc}}(\Omega)$ is the α-th *generalized* (or *distributional*) *derivative* of f (denoted $g = \partial^\alpha f$) if

$$\int_\Omega g\varphi\, dx = (-1)^{\alpha_1 + \dots + \alpha_d} \int_\Omega f \partial^\alpha \varphi\, dx$$

for all $\varphi \in C_0^\infty(\Omega)$. The number $|\alpha| = \alpha_1 + \dots + \alpha_d$ is the *order* of the derivative g.

For an integer $l \geqslant 1$ and for an exponent $r \in [1, \infty)$, we denote by $W^{l,r}(\Omega)$ the *Sobolev space* of functions having all generalized derivatives up to order l in $L^r(\Omega)$. Endowed with the norm

$$\|u\|_{W^{l,r}(\Omega)} = \sup_{|\alpha| \leqslant l} \|\partial^\alpha u\|_{L^r(\Omega)},$$

it becomes a Banach space. In the scale of Sobolev spaces, by convention we have $W^{0,r}(\Omega) \equiv L^r(\Omega)$ for $l = 0$. For the negative indices $-l < 0$, the *negative Sobolev spaces* are defined by duality [2, 196].

Remark 3.1. Since $L^2(\Omega)$ is a Hilbert space, thus for $r = 2$ the Sobolev spaces $H^l(\Omega) := W^{l,2}(\Omega)$ are Hilbert spaces with the appropriate scalar products and norms.

For real $0 < s < 1 < r < \infty$, the *fractional Sobolev space* $W^{s,r}(\Omega)$ is obtained by the real interpolation method [215] between $L^r(\Omega)$ and $W^{1,r}(\Omega)$, i.e., $W^{s,r}(\Omega) = [L^r(\Omega), W^{1,r}(\Omega)]_{s,r}$, and consists of all measurable functions with the finite norm

$$\|u\|_{W^{s,r}(\Omega)} = \|u\|_{L^r(\Omega)} + |u|_{s,r,\Omega},$$

where

$$|u|^r_{s,r,\Omega} = \int_{\Omega\times\Omega} \|x-y\|^{-d-rs} |u(x)-u(y)|^r \, dx dy. \tag{3.1}$$

In particular, if Ω is a bounded domain of class C^1, then $C^\infty(\Omega)$ is dense in $W^{s,r}(\Omega)$.

In general, the Sobolev space $W^{l+s,r}(\Omega)$, $0 < s < 1 < r < \infty$, $l \geqslant 0$ an integer, is defined as the space of measurable functions with the finite norm

$$\|u\|_{W^{l+s,r}(\Omega)} = \|u\|_{W^{l,r}(\Omega)} + \sup_{|\alpha|=l} \|\partial^\alpha u\|_{W^{s,r}(\Omega)}.$$

Furthermore, the notation $W_0^{s,r}(\Omega)$, $0 \leqslant s \leqslant 1$, stands for the closed subspace of $W^{s,r}(\mathbb{R}^d)$ which consists of all $u \in W^{s,r}(\mathbb{R}^d)$ vanishing outside of Ω. We identify functions of $W_0^{s,r}(\Omega)$ with their restrictions to Ω. We have $W^{s,r}(\Omega) = W_0^{s,r}(\Omega)$ for $sr < 1$.

3.1.2 Elliptic Regularity

Let Ω be a bounded domain in $\mathbb{R}^d$ with C^∞ boundary. Denote by α a vector with nonnegative integer components

$$\alpha = (\alpha_1, \dots, \alpha_d), \quad \alpha_i \in \mathbb{N}^* := \mathbb{N} \cup \{0\}, \quad |\alpha| = \alpha_1 + \cdots + \alpha_d,$$

and set

$$\xi^\alpha = \xi_1^{\alpha_1} \dots \xi_d^{\alpha_d} \quad \text{for } \xi \in \mathbb{R}^d, \quad \partial^\alpha = \partial_{x_1}^{\alpha_1} \cdots \partial_{x_d}^{\alpha_d}.$$

Assume that functions $b_{\alpha\beta} \in C^\infty(\overline{\Omega})$, $|\alpha| = |\beta| = m$, satisfy the *ellipticity condition*

$$c_b^{-1} \|\xi\|^{2m} \leqslant b_{\alpha\beta} \xi^\alpha \xi^\beta \leqslant c_b \|\xi\|^{2m} \quad \text{for all } \xi \in \mathbb{R}^d, \quad c_b > 0.$$

Let us consider the boundary value problem

$$\sum_{|\alpha|=|\beta|=m} \partial^\beta (b_{\alpha\beta} \partial^\alpha v) = f \quad \text{in } \Omega, \quad \partial^\kappa v = 0 \quad \text{on } \partial\Omega, \quad 0 \leqslant |\kappa| \leqslant m-1. \tag{3.2}$$

The following theorem (see [3] or [138]) is a particular case of the general theory of boundary value problems for elliptic equations.

Theorem 3.1. *Let $s \geqslant -m$ be an integer. Then for any $f \in W^{s,2}(\Omega)$ problem* (3.2) *has a unique solution*

$$v \in W^{2m+s,2}(\Omega), \quad \text{with} \quad v \in W_0^{m,2}(\Omega),$$

which satisfies the estimate

$$\|v\|_{W^{2m+s,2}(\Omega)} \leqslant c\,\|f\|_{W^{s,2}(\Omega)}.$$

Here, the constant c depends only on $b_{\alpha\beta}$, s and Ω.

Remark 3.2. For $s \in [-m,0]$ equation (3.2) is understood in the sense of distributions, which means that we have the integral identity

$$(-1)^{|\beta|} \int_\Omega b_{\alpha\beta} \partial^\alpha v \partial^\beta \varphi \, dx = \langle f, \varphi \rangle \quad \text{for all } \varphi \in C_0^\infty(\Omega).$$

3.1.3 Elliptic Problems in Nonsmooth Domains

In this monograph we avoid, when it is unnecessary, to consider the boundary value problems posed in nonsmooth domains. However, the theory of elliptic problems is well developed in such domains in the scale of Kondratiev spaces. In particular, we refer the reader to [62] for the shape sensitivity analysis in nonsmooth domains.

There are some exceptions concerning the cracks in solids. In Example 9.1 of Chapter 9 the polarization matrix is given for a crack. It means that the results on topological derivatives of eigenvalues in elliptic spectral problems can be extended to the shape-topological perturbations in the form of small cracks.

The cracks on the boundaries of rigid inclusions are considered in Section 11.4 of the chapter on unilateral problems. However, the shape-topological perturbations allowed in this section is located far from the crack.

In general, the local regularity of solutions to elliptic problems [170] is sufficient for the derivation of topological derivatives [206]. In fact, the topological derivatives can be evaluated far from the singular points of the boundary.

The singularities can be also caused by the change of the type of the boundary conditions e.g., from Dirichlet to Neumann. We can assume that this cannot happen or that shape-topological perturbation occurs far from such an interface of the bundary conditions change.

In general, the topological derivatives can be evaluated in nonsmooth domains for the elliptic boundary value problems far from the singularities.

3.1.4 Shape Derivatives

The differentiability of families of functions $u_t = u(\Omega_t)$, with $\Omega_t \subset \mathbb{R}^d$, $d = 2,3$, with respect to the shape parameter $t \geqslant 0$, at $t = 0^+$, is considered in this chapter. The space dimension $d = 2$ is usually fixed, most of the results are valid in three spatial dimensions. Usually a family of functions is defined by solutions to elliptic boundary value problems defined in variable domain of integration. The family of domains Ω_t is defined by the transformation of the speed method with $\Omega_t = \mathfrak{T}_t(\mathfrak{V})(\Omega)$, for a fixed velocity field $\mathfrak{V} \in C([0,\delta);C^2(\mathbb{R}^d;\mathbb{R}^d))$. For a velocity field $\mathfrak{V} \in C([0,\delta);C^2(\mathbb{R}^d;\mathbb{R}^d))$ we need some additional assumptions which are required in order to assure that for a given reference domain Ω the family of variable domains $\Omega_t = \mathfrak{T}_t(\mathfrak{V})(\Omega)$ for $t \in [0,\delta)$ belongs to the hold-all domain $B := \mathfrak{D}$.

Condition 3.1. The vector field $(t,x) \mapsto \mathfrak{V}(t,x)$ is compactly supported in the hold-all domain B, i.e., $\mathfrak{V} \in C([0,\delta);C_0^2(B;\mathbb{R}^d))$.

In Section 3.6 a new approach to the speed method [196, 197] well suited for the fluid dynamics is employed, depending on the adjugate matrix function. All the properties of the domain transformation required in the stability analysis of boundary value problems which leads to the material derivatives of solutions are shown by elementary arguments in Section 3.6.1 for the new method. The change of variables by this method is performed for the boundary value problems of fluid mechanics. We refer the reader to [196] for the general results obtained for shape sensitivity analysis of the compressible Navier-Stokes equations.

The differentiability properties can also be considered for a family of functions $z_t = z(\Gamma_t)$ defined on the surfaces $\Gamma_t := \partial\Omega_t$. We consider also the evolution of an *interface* $\Gamma_t \subset \Omega$ in the interior of the reference domain, by an interface we understand the boundary of an inclusion for the elasticity boundary value problems. We need the properties (cf. Note 3.3) for the shape sensitivity analysis with respect to the perturbations of an interface or of an inclusion for the elasticity boundary value problems. Therefore, we introduce the material and the shape derivatives for the families of functions defined on the moving domains and on the moving surfaces. The shape derivatives for the families u_t and of z_t are defined in a slightly different manner, since for the restriction $g_t := g_{|\Omega_t}$ to Ω_t of a given function g defined in all space $\mathbb{R}^d$, the domain shape derivative $g'(\Omega;\mathfrak{V})$ is null, but for the restriction to $\Gamma_t = \partial\Omega_t$ of the same function, its boundary shape derivative $g'(\Gamma;\mathfrak{V})$ depending on the *Neumann trace* or on the normal derivative of the function on Γ in general is non-null.

There are material derivatives, domain shape derivatives and boundary shape derivatives which are associated to a given family of functions defined by boundary variations of a given domain, its boundary or an interface in the interior of the domain. The domain dependence of $\Omega \mapsto u(\Omega)$ usually reflects the dependence of a solution to the boundary value problem on its domain of definition or on an interface inside of the domain of definition. All the derivatives are listed below for a scalar function u.

- The *material derivative* $\dot{u}_\Omega = \dot{u}(\Omega;\mathfrak{V})$ of the function $u_\Omega = u(\Omega)$ in the direction of the vector field $\mathfrak{V}$ is simply the derivative of the composed function $t \mapsto u(\Omega_t) \circ \mathfrak{T}_t$ defined in a fixed domain Ω. Since the composed function is defined in the fixed domain Ω, we say that the function $u(\Omega_t)$, defined in the variable domain Ω_t, is transported to the fixed domain Ω using the change of variables defined by the transformation $\mathfrak{T}_t(\mathfrak{V})$. The material derivative can be evaluated with respect to the weak or strong convergence in the associated function space over Ω.
- The *shape derivative* $u'_\Omega = u'(\Omega;\mathfrak{V})$ of the function $u_\Omega = u(\Omega)$ in the direction of the vector field $\mathfrak{V}$ is related to the material derivative as follows

$$u'(\Omega;\mathfrak{V}) = \dot{u}(\Omega;\mathfrak{V}) - \nabla u(\Omega) \cdot \mathfrak{V} \tag{3.3}$$

and leads to the formulae for the shape derivatives of domain functionals.
- The *shape derivative* at $t = 0$ of the shape functional

$$\mathscr{J}_{\Omega_t}(u(\Omega_t)) = \int_{\Omega_t} u(\Omega_t)\, d\Omega_t \ , \tag{3.4}$$

takes the forms

$$\begin{aligned}
\dot{\mathscr{J}}_\Omega(u(\Omega)) &= \frac{d}{dt} \int_{\Omega_t} u(\Omega_t)\, d\Omega_t \bigg|_{t=0} \\
&= \int_\Omega u'(\Omega;\mathfrak{V})\, d\Omega + \int_\Gamma u(\Omega)(\mathfrak{V}\cdot n)\, d\Gamma \\
&= \int_\Omega u'(\Omega;\mathfrak{V}) + \operatorname{div}(u(\Omega)\mathfrak{V})\, d\Omega \\
&= \frac{d}{dt} \int_\Omega (u(\Omega_t) \circ \mathfrak{T}_t)(x) \mathfrak{g}(t)\, d\Omega \bigg|_{t=0} \\
&= \int_\Omega \dot{u}(\Omega;\mathfrak{V}) + u(\Omega) \operatorname{div}\mathfrak{V}\, d\Omega \ ,
\end{aligned} \tag{3.5}$$

where $\mathfrak{g}(t)$ is the Jacobian of the domain transformation and $\dot{\mathscr{J}}_\Omega(u(\Omega))$ is the derivative of the shape functional $\mathscr{J}_\Omega(u(\Omega))$ in the direction of the vector field $\mathfrak{V}$, namely $\mathfrak{g}(t) = \det(D\mathfrak{T}_t)$ and $\dot{\mathscr{J}}_\Omega(u(\Omega)) = D\mathscr{J}_\Omega(u(\Omega);\mathfrak{V})$, respectively.
- The *boundary shape derivative* or the displacement derivative denoted by

$$u'(\Gamma;\mathfrak{V}) = \dot{u}(\Omega;\mathfrak{V}) - \nabla_\Gamma u(\Omega) \cdot \mathfrak{V} \tag{3.6}$$

is a shape derivative of a family of functions defined e.g., on the surfaces which are domains boundaries. Here, $\nabla_\Gamma \varphi$ is the tangential gradient of a scalar function φ on the boundary Γ, that is

$$\nabla_\Gamma \varphi = \nabla \varphi - \partial_n \varphi\, n \quad \text{on} \quad \Gamma \ . \tag{3.7}$$

The formula of shape derivative of boundary integrals makes possible to define the boundary shape derivatives of functions, such definition is conform with the so-called displacement derivative in mechanics [119]. The boundary shape derivative z'_Γ of a function $z_\Gamma = z(\Gamma)$ given on the boundary (or on the interface) Γ is defined from the relation

$$z'(\Gamma;\mathfrak{V}) = \dot{z}(\Gamma;\mathfrak{V}) - \nabla_\Gamma z(\Gamma)\cdot\mathfrak{V}\,. \tag{3.8}$$

If z_Γ is the restriction or the trace on Γ of a function u_Ω, the above definition leads to the relation between the shape derivatives, i.e., between the domain shape derivative $u'(\Omega;\mathfrak{V})$ and the boundary shape derivative $z'(\Gamma;\mathfrak{V})$,

$$z'(\Gamma;\mathfrak{V}) = u'(\Omega;\mathfrak{V}) + \partial_n u(\Omega)\, n\cdot\mathfrak{V}\,. \tag{3.9}$$

The boundary shape derivatives or equivalently the displacement derivatives can be employed for the shape sensitivity analysis of boundary value problems for the shells or for the boundary control problems in the framework of shape sensitivity analysis.

We point out in Section 3.2.1, that the transport of distributions from the variable domain Ω_t to the fixed domain Ω is defined by *transposition*, and that the differentiability of the *transported distribution* might be obtained only for a *weak convergence* in negative Sobolev spaces.

The material derivatives for elliptic boundary value problems can be defined for the strong, weak and very weak variational formulations. It means that for the Poisson's equation we can consider the solution $u(\Omega)$ in the scale of the Sobolev spaces: a very weak solution in $L^2(\Omega)$, a weak solution in $H^1_0(\Omega)$ and a strong solution in $H^1_0(\Omega)\cap H^2(\Omega)$, and we obtain the weak or the strong material derivatives $\dot{u}(\Omega;\mathfrak{V})$ in all the spaces listed above, under the appropriate assumptions on the data of the problem and on the velocity vector field of the speed method. The specific differentiability result required for the solutions of boundary value problems depends on the nature of the shape functionals considered.

The mathematical analysis for material and shape derivatives can be performed independently. The existence of the material derivative is usually shown by an application of the Implicit Function Theorem for the boundary value problem transformed to the fixed or reference domain, i.e. the domain Ω independent of the shape parameter t. The existence of the material derivative in the Sobolev space $H^{k+1}(\Omega)$ for sufficiently smooth velocity vector field $\mathfrak{V}$ implies the existence of the shape derivative in $H^k(\Omega)$ in view of the relation (3.3), provided that $\nabla u(\Omega)\cdot\mathfrak{V}\in H^k(\Omega)$. Once the existence of the shape derivative is assured, it remains to identify the boundary value problem whose solution is the shape derivative itself.

3.2 Material Derivatives for Second Order Elliptic Equations

We derive the form of material derivatives of solutions to elliptic boundary value problems under some regularity assumptions on the date of the problems. Depending on the regularity of solutions, we obtain the weak material derivatives for the very weak solutions in $L^2(\Omega)$, and the strong material derivatives of the strong solutions in the Sobolev spaces $H^k(\Omega)$, $k = 1,2$, for the second order elliptic boundary value problem. In analysis of the weak and very weak solutions, it turns out that the transported distributions in the negative Sobolev spaces are only weakly differentiable with respect to the shape parameter $t \to 0$, the related result is given by Lemma 3.1.

3.2.1 Weak Material Derivatives for the Dirichlet Problem

Let the velocity field $\mathfrak{V}$ which defines the deformed domain Ω_t be given. Let us consider the homogeneous Dirichlet problem for the Poisson's equation

$$\begin{cases} -\Delta u(\Omega_t) = b \text{ in } H^{-1}(\Omega_t) \,, \\ u(\Omega_t) = 0 \text{ on } \Gamma_t \,, \end{cases} \tag{3.10}$$

with the right hand side $b \in L^2(\Omega_t)$. We determine the weak material derivative $\dot{u}(\Omega;\mathfrak{V})$ of the solution $u(\Omega)$ at $t = 0$.

First, the Poisson's equation with the Dirichlet boundary conditions is transformed to the fixed domain Ω using the change of variables defined by the transformation $\mathfrak{T}_t(\mathfrak{V})$. In other words, the form of boundary value problems for elements $u^t := u^t(\Omega) \equiv u(\Omega_t) \circ \mathfrak{T}_t$, $t \in [0,\delta)$, is derived.

The right hand side of the Laplace equation is transformed to the fixed domain Ω. Hence one has to consider two distributions in negative Sobolev spaces:

$$b_{|\Omega_t} \in H^{-1}(\Omega_t) \tag{3.11}$$

and

$$(b_{|\Omega_t}) * \mathfrak{T}_t \in H^{-1}(\Omega) \,, \tag{3.12}$$

where $H^{-1}(\Omega_t)$ stands for the dual space of $H_0^1(\Omega_t)$ for $t \in [0,\delta)$. We shall derive sufficient conditions for the mapping

$$t \mapsto (h_{\Omega_t}) * \mathfrak{T}_t \tag{3.13}$$

to be weakly differentiable in the Sobolev space $H^{-1}(\mathfrak{D})$, where $\mathfrak{D}$ is used to denote the hold-all domain such that the domains Ω and Ω_t, for t small enough, are included in $\mathfrak{D}$.

Let $b \in H^{-1}(\mathfrak{D})$ be a given element, the transformed distribution $b * \mathfrak{T}_t \in H^{-1}(\mathfrak{D})$ is defined by transposition,

$$\langle b * \mathfrak{T}_t, \phi \rangle_{H^{-1}(\mathfrak{D}) \times H_0^1(\mathfrak{D})} = \langle b, (\mathfrak{g}(t)^{-1}\phi) \circ \mathfrak{T}_t^{-1} \rangle_{H^{-1}(\mathfrak{D}) \times H_0^1(\mathfrak{D})} \quad \forall \phi \in H_0^1(\mathfrak{D}) . \tag{3.14}$$

The restriction

$$b_{|\Omega} \in \mathscr{D}'(\Omega) \tag{3.15}$$

of the distribution $b \in H^{-1}(\mathfrak{D})$ is given by

$$\langle b_{|\Omega}, \phi \rangle_{\mathscr{D}'(\mathfrak{D}) \times \mathscr{D}(\mathfrak{D})} = \langle b, \phi^0 \rangle_{\mathscr{D}'(\mathfrak{D}) \times \mathscr{D}(\mathfrak{D})} \quad \forall \phi \in \mathscr{D}(\Omega) , \tag{3.16}$$

where ϕ^0 denotes the extension of $\phi \in \mathscr{D}(\Omega)$ to $\overline{\mathfrak{D}}$, $\phi^0(x) = 0$ on $\overline{\mathfrak{D}} \setminus \Omega$. In addition, $\mathscr{D}(\mathfrak{D})$ is the space of test functions and $\mathscr{D}'(\mathfrak{D})$ is the space of distributions, dual of $\mathscr{D}(\mathfrak{D})$. Since $b_{|\Omega} \in H^{-1}(\Omega)$, then

$$\|b_{|\Omega}\|_{H^{-1}(\Omega)} = \sup_{\|\phi\|_{H_0^1(\Omega)} \leqslant 1} |\langle b, \phi \rangle| \leqslant \sup_{\|\phi\|_{H_0^1(\mathfrak{D})} \leqslant 1} |\langle b, \phi \rangle| = \|b\|_{H^{-1}(\mathfrak{D})} . \tag{3.17}$$

Let $\Omega_t = \mathfrak{T}_t(\mathfrak{V})(\Omega)$ and

$$b_{|\Omega_t} = \chi_{\Omega_t} b \in H^{-1}(\Omega_t) . \tag{3.18}$$

The transformed distribution is defined by

$$(b_{|\Omega_t}) * \mathfrak{T}_t = (\chi_{\Omega_t} b) * \mathfrak{T}_t \in H^{-1}(\Omega) . \tag{3.19}$$

Proposition 3.1. *Let* $\Omega_t = \mathfrak{T}_t(\mathfrak{V})(\Omega)$ *then*

$$(b_{|\Omega_t}) * \mathfrak{T}_t = (b * \mathfrak{T}_t)_{|\Omega} . \tag{3.20}$$

Proof. For any $\phi \in H_0^1(\Omega)$ we have

$$\langle b_{|\Omega_t} * \mathfrak{T}_t, \phi \rangle_{H^{-1}(\Omega) \times H_0^1(\Omega)} = \langle b_{|\Omega_t}, (\mathfrak{g}(t)^{-1}\phi) \circ \mathfrak{T}_t^{-1} \rangle_{H^{-1}(\Omega_t) \times H_0^1(\Omega_t)} . \tag{3.21}$$

With the extension ϕ^0 of ϕ the right hand side of the above equation becomes

$$\langle b, (\mathfrak{g}(t)^{-1}\phi^0) \circ \mathfrak{T}_t^{-1} \rangle_{H^{-1}(\mathfrak{D}) \times H_0^1(\mathfrak{D})} = \langle b * \mathfrak{T}_t, \phi^0 \rangle_{H^{-1}(\mathfrak{D}) \times H_0^1(\mathfrak{D})} \tag{3.22}$$

and since $\phi^0 = 0$ on $\overline{\mathfrak{D}} \setminus \Omega$

$$\langle b_{|\Omega_t} * \mathfrak{T}_t, \phi \rangle_{H^{-1}(\Omega) \times H_0^1(\Omega)} = \langle (b * \mathfrak{T}_t)_{|\Omega}, \phi \rangle_{H^{-1}(\Omega) \times H_0^1(\Omega)} . \tag{3.23}$$

For $u(\Omega_t) = u_t \in H_0^1(\Omega_t)$ the following integral identity holds:

$$\int_{\Omega_t} \nabla u_t \cdot \nabla \phi \, d\Omega_t = \langle b, \phi^0 \rangle_{H^{-1}(\mathfrak{D}) \times H_0^1(\mathfrak{D})} \quad \forall \phi \in H_0^1(\Omega_t) , \tag{3.24}$$

or equivalently

$$\langle -\mathrm{div}(\chi_{\Omega_t}\nabla u_t), \phi\rangle_{H^{-1}(\Omega_t)\times H_0^1(\Omega_t)} = \langle b_{|\Omega_t}, \phi\rangle_{H^{-1}(\Omega_t)\times H_0^1(\Omega_t)} . \tag{3.25}$$

Applying the change of variables $\mathfrak{T}_t(\mathfrak{V})$ to the left hand side of this equality, we have

$$\int_\Omega A(t)\nabla(u_t\circ\mathfrak{T}_t)\cdot\nabla(\phi\circ\mathfrak{T}_t)d\Omega = \langle b_{|\Omega_t}, \phi\rangle , \tag{3.26}$$

where $A(t) = \mathfrak{g}(t)D\mathfrak{T}_t^{-1}D\mathfrak{T}_t^{-\top}$. Thus

$$\langle -\mathrm{div}(\chi_\Omega A(t)\nabla(u_t\circ\mathfrak{T}_t)), \varphi\rangle_{H^{-1}(\Omega)\times H_0^1(\Omega)} = \langle b_{|\Omega_t}, \varphi\circ\mathfrak{T}_t\rangle_{H^{-1}(\Omega_t)\times H_0^1(\Omega_t)} \quad \forall\varphi = \phi\circ\mathfrak{T}_t^{-1}\in H_0^1(\Omega) . \tag{3.27}$$

Let us observe that for any element $\Lambda\in\mathscr{D}'(\mathfrak{D})$, the element $\Lambda * \mathfrak{T}_t^{-1}$ is defined as follows:

$$\langle\Lambda * \mathfrak{T}_t^{-1}, \varphi\rangle = \langle\Lambda, (\mathfrak{g}(t)\varphi)\circ\mathfrak{T}_t\rangle \quad \forall\varphi\in\mathscr{D}(\mathfrak{D}) . \tag{3.28}$$

Therefore

$$\langle -\mathfrak{g}(t)^{-1}\mathrm{div}(\chi_\Omega A(t)\nabla(u_t\circ\mathfrak{T}_t)), \mathfrak{g}(t)\varphi\rangle_{H^{-1}(\Omega)\times H_0^1(\Omega)} = \langle b_{|\Omega_t}, (\mathfrak{g}(t)\varphi)\circ\mathfrak{T}_t\rangle_{H^{-1}(\Omega_t)\times H_0^1(\Omega_t)} . \tag{3.29}$$

Whence it follows that

$$[-\mathfrak{g}(t)^{-1}\mathrm{div}(\chi_\Omega A(t)\nabla(u_t\circ\mathfrak{T}_t))] * \mathfrak{T}_t^{-1} = b_{|\Omega_t} \tag{3.30}$$

or

$$-\mathfrak{g}(t)^{-1}\mathrm{div}(\chi_\Omega A(t)\nabla(u_t\circ\mathfrak{T}_t)) = (b_{|\Omega_t}) * \mathfrak{T}_t = (b * \mathfrak{T}_t)_{|\Omega} , \tag{3.31}$$

which concludes the proof. □

Let $u^t = u(\Omega_t)\circ\mathfrak{T}_t\in H_0^1(\Omega)$ be a solution to the following problem

$$\int_\Omega A(t)\nabla u^t\cdot\nabla\phi\rangle\, d\Omega = \langle\mathfrak{g}(t)(b * \mathfrak{T}_t)_{|\Omega}, \phi\rangle_{H^{-1}(\Omega)\times H_0^1(\Omega)} \quad \forall\phi\in H_0^1(\Omega) . \tag{3.32}$$

It has been already shown that the mapping $t\mapsto b * \mathfrak{T}_t$ is weakly differentiable in the space $H^{-2}(\mathfrak{D})$, however the mapping $t\mapsto (b * \mathfrak{T}_t)_{|\Omega}$ fails to have this property in the space $H^{-1}(\mathfrak{D})$. In order to obtain the required differentiability of the mapping $t\mapsto u^t$, it is necessary to introduce additional assumptions on the distribution b, the domain Ω and the speed field $\mathfrak{V}$.

For $b\in H^{-1}(\mathfrak{D})$ there are $g\in L^2(\mathfrak{D})$ and $h\in L^2(\mathfrak{D};\mathbb{R}^d)$ such that $b = g - \mathrm{div}h$. It is assumed that the support of the singular part $\mathrm{div}h$ of b is included in Ω and in Ω_t for $t>0$, t small enough. Therefore we assume that there exists a compact set $\overline{\mathfrak{C}}$, such that $\overline{\mathfrak{C}}\subset\Omega\cup\Omega^c$,

$$h(x) = 0 \quad \text{for} \quad x\in\overline{\mathfrak{D}}\setminus\overline{\mathfrak{C}} \quad \text{a.e.} \tag{3.33}$$

Lemma 3.1. *Let* (3.33) *be satisfied, then the mapping* $t \mapsto (b * \mathfrak{T}_t)_{|\Omega}$ *is weakly differentiable in* $(H_0^1(\Omega) \cap H^2(\Omega))'$, *the dual of* $H_0^1(\Omega) \cap H^2(\Omega)$.

Proof. Let $\phi \in H_0^1(\Omega) \cap H^2(\Omega)$ be a given element, then on the set $\overline{\Omega} \setminus \overline{\mathfrak{C}}$ the element ϕ can be modified, i.e. there exists an element $\widetilde{\phi} \in H^2(\Omega)$ such that

$$\phi - \widetilde{\phi} \in H^2(\mathfrak{D} \setminus \overline{\mathfrak{C}}) . \tag{3.34}$$

From (3.33) it follows that

$$\langle \mathrm{div} h, \phi \rangle_{H^{-1}(\mathfrak{D}) \times H_0^1(\mathfrak{D})} = \langle \mathrm{div} h, \widetilde{\phi} \rangle_{H^{-1}(\mathfrak{D}) \times H_0^1(\mathfrak{D})} , \tag{3.35}$$

thus

$$\langle (b * \mathfrak{T}_t)_{|\Omega}, \phi \rangle = \langle (b * \mathfrak{T}_t)_{|\Omega}, \widetilde{\phi}^0 \rangle_{H^{-2}(\mathfrak{D}) \times H_0^2(\mathfrak{D})} , \tag{3.36}$$

and the proof is completed. □

Proposition 3.2. *Let* $\mathfrak{V}$ *satisfy Condition 3.1 and* $b = g + \mathrm{div} h$ *with* $g \in L^2(\mathfrak{D})$ *and* $h \in L^2(\mathfrak{D}; \mathbb{R}^d)$. *Moreover, let* h *satisfy* (3.33) *for a compact* $\overline{\mathfrak{C}}$, *such that* $\overline{\mathfrak{C}} \subset \Omega \cup \Omega^c$. *Then the mapping* $t \mapsto u^t = u(\Omega_t) \circ \mathfrak{T}_t \in H^1(\Omega)$ *is weakly differentiable in* $L^2(\Omega)$, *its derivative is given by the linear form on* $L^2(\Omega)$,

$$L^2(\Omega) \ni \varphi \mapsto \int_\Omega \dot{u}(\Omega; \mathfrak{V}) \varphi \, d\Omega := \int_\Omega \mathrm{div}(g\mathfrak{V})((-\Delta)^{-1}\varphi) \, d\Omega - \tag{3.37}$$
$$\int_\Omega (\mathrm{div}\mathfrak{V}\mathrm{I} - 2\nabla\mathfrak{V}^s)\nabla u(\Omega) \cdot \nabla((-\Delta)^{-1}\varphi) \, d\Omega + \int_\Omega \nabla(\nabla((-\Delta)^{-1}\varphi)\mathfrak{V}) \cdot h \, d\Omega \in \mathbb{R} ,$$

where

$$\nabla\mathfrak{V}^s = \frac{1}{2}(\nabla\mathfrak{V} + \nabla\mathfrak{V}^\top) . \tag{3.38}$$

Proof. For a given element $\phi \in H_0^1(\Omega) \cap H^2(\Omega)$ we have

$$\int_\Omega A(t)\nabla\phi \cdot \nabla u^t \, d\Omega = \int_\Omega (g \circ \mathfrak{T}_t)\mathfrak{g}(t)\phi \, d\Omega - \int_{\mathfrak{D}} \nabla(\widetilde{\phi}^0 \circ \mathfrak{T}_t) \cdot h \, d\Omega , \tag{3.39}$$

where $\widetilde{\phi} \in H_0^2(\Omega)$ is an element such that $\widetilde{\phi} = \phi$ in an open neighborhood in $\mathbb{R}^d$ of the compact set $\overline{\mathfrak{C}}$. Let $\widetilde{\phi}^0$ be an extension of $\widetilde{\phi}$ to $\overline{\mathfrak{D}}$. Green's formula leads to

$$-\int_\Omega u^t \Delta\phi \, d\Omega = \int_\Omega u^t \mathrm{div}((A(t) - \mathrm{I})\nabla\phi) d\Omega - \int_{\mathfrak{D}} \nabla(\widetilde{\phi}^0 \circ \mathfrak{T}_t) \cdot h \, d\Omega . \tag{3.40}$$

Since the inverse $(-\Delta)^{-1}$ of the Laplace operator with homogeneous Dirichlet boundary condition (*Dirichlet Laplacian*) is an isomorphism from $L^2(\Omega)$ onto $H^2(\Omega) \cap H_0^1(\Omega)$, the right hand side of (3.40) is differentiable with respect to t at $t = 0$

$$\frac{d}{dt}\left[\int_\Omega u^t \operatorname{div}((A(t)-\mathrm{I})\nabla\phi)d\Omega - \int_{\mathfrak{D}} \nabla(\widetilde{\phi}^0 \circ \mathfrak{T}_t)\cdot h\, d\Omega\right]_{t=0} =$$
$$\int_\Omega u \operatorname{div}(A'(0)\nabla\phi)d\Omega + \int_{\mathfrak{D}} \nabla(\nabla\widetilde{\phi}^0 \cdot \mathfrak{V})\cdot h\, d\Omega\,. \quad (3.41)$$

On the other hand

$$\nabla(\nabla\widetilde{\phi}^0 \cdot \mathfrak{V}) = \nabla(\nabla\phi\cdot\mathfrak{V}) \quad \text{on} \quad \overline{\mathfrak{C}}\,, \quad (3.42)$$

and $h \equiv 0$ on $\Omega\setminus\overline{\mathfrak{C}}$. For $h \neq 0$ on $\overline{\mathfrak{C}}$ and $\phi \in H^2(\Omega)\cap H_0^1(\Omega)$, the integral on $\mathfrak{D}$ is rewritten,

$$\int_{\mathfrak{D}} \nabla(\nabla\widetilde{\phi}^0 \cdot \mathfrak{V})\cdot h\, d\Omega = \int_\Omega \nabla(\nabla\phi\cdot\mathfrak{V})\cdot h\, d\Omega\,. \quad (3.43)$$

For ϕ, φ related by equations $-\Delta\phi = \varphi$, or equivalently $\phi = (-\Delta)^{-1}\varphi$, with $\phi \in H^2(\Omega)\cap H_0^1(\Omega)$ and $\varphi \in L^2(\Omega)$ we have

$$\int_\Omega \dot{u}(\Omega;\mathfrak{V})\varphi\, d\Omega = \int_\Omega u \operatorname{div}(A'(0)\nabla\phi)d\Omega + \int_\Omega \operatorname{div}(g\mathfrak{V})\phi\, d\Omega$$
$$+ \int_\Omega \nabla(\nabla\phi\cdot\mathfrak{V})\cdot h\, d\Omega\,. \quad (3.44)$$

Applying Green's formula we obtain

$$\int_\Omega \dot{u}(\Omega;\mathfrak{V})\varphi\, d\Omega = -\int_\Omega A'(0)\nabla u\cdot\nabla\phi\, d\Omega$$
$$+ \int_\Omega \operatorname{div}(g\mathfrak{V})\phi\, d\Omega + \int_\Omega \nabla(\nabla\phi\cdot\mathfrak{V})\cdot h\, d\Omega\,, \quad (3.45)$$

which completes the proof. □

For the particular case of the Poisson's equation with homogeneous Dirichlet boundary conditions and with the right hand side $b \in L^2(\Omega)$, the weak differentiability is established.

Corollary 3.1. *Let $u(\Omega_t) \in H_0^1(\Omega_t)$ be the solution to the problem:*

$$\begin{cases} -\Delta u(\Omega_t) = b \ \ in \ \ \Omega_t\,, \\ \quad u(\Omega_t) = 0 \ on \ \Gamma_t\,, \end{cases} \quad (3.46)$$

where $b \in L^2(\mathfrak{D})$ and $\mathfrak{V}$ verify Condition 3.1. Then the weak L^2-material derivative of the mapping $t \mapsto u(\Omega_t)\circ\mathfrak{T}_t$ is given by the linear form

$$L^2(\Omega) \ni \varphi \mapsto \int_\Omega \dot{u}(\Omega;\mathfrak{V})\varphi\, d\Omega := \int_\Omega \operatorname{div}(g\mathfrak{V}((-\Delta)^{-1}\varphi)\, d\Omega -$$
$$\int_\Omega (\operatorname{div}\mathfrak{V}\mathrm{I} - 2\nabla\mathfrak{V}^s)\nabla u(\Omega)\cdot\nabla((-\Delta)^{-1}\varphi)\, d\Omega \in \mathbb{R}\,. \quad (3.47)$$

Remark 3.3. The linear form

$$H^{-1}(\Omega) \ni \varphi \mapsto \int_\Omega \operatorname{div}(g\mathfrak{V}((-\Delta)^{-1}\varphi)\,d\Omega - \int_\Omega (\operatorname{div}\mathfrak{V}\mathrm{I} - 2\nabla\mathfrak{V}^s)\nabla u(\Omega)\cdot\nabla((-\Delta)^{-1}\varphi)\,d\Omega \in \mathbb{R} \quad (3.48)$$

is continuous because the inverse operator $(-\Delta)^{-1}$ is an isomorphism from $H^{-1}(\Omega)$ onto $H_0^1(\Omega)$. Thus the material derivative $\dot{u}(\Omega;\mathfrak{V})$ is well defined in $H_0^1(\Omega)$ for any vector field $\mathfrak{V}$ given by Condition 3.1. For $b \in H^1(\mathfrak{D})$ it is easy to show that the strong material derivative exists.

3.2.2 *Strong Material Derivatives for the Dirichlet Problem*

We assume that $b \in H^1(\mathfrak{D})$, $\Omega \subset \mathfrak{D}$ is of class C^k, $k \geqslant 1$, and $\mathfrak{V}$ satisfies Condition 3.1. The transformed domain is denoted by $\Omega_t = \mathfrak{T}_t(\mathfrak{V})(\Omega)$.

Let $u(\Omega_t) \in H_0^1(\Omega_t)$ be a weak solution to the Poisson's equation with homogeneous Dirichlet boundary conditions in Ω_t,

$$\begin{cases} -\Delta u(\Omega_t) = b \text{ in } \Omega_t \,, \\ \quad u(\Omega_t) = 0 \text{ on } \Gamma_t = \partial\Omega_t \,. \end{cases} \quad (3.49)$$

The weak solution denoted $u_t := u(\Omega_t)$ satisfies

$$\int_{\Omega_t} \nabla u_t \cdot \nabla\phi_t \, d\Omega_t = \int_{\Omega_t} b\phi_t d\Omega_t \quad \forall\phi_t \in H_0^1(\Omega_t)\,. \quad (3.50)$$

The transformed function to the reference domain

$$u^t = u(\Omega_t)\circ\mathfrak{T}_t \in H_0^1(\Omega)\,, \quad (3.51)$$

satisfies

$$\int_\Omega A(t)\nabla u_t \cdot \nabla\varphi\, d\Omega = \int_\Omega \mathfrak{g}(t)(b\circ\mathfrak{T}_t)\varphi\, d\Omega \quad \forall\varphi = \phi_t\circ\mathfrak{T}_t \in H_0^1(\Omega)\,. \quad (3.52)$$

In order to determine the material derivative we denote

$$z^t = \frac{1}{t}(u^t - u) \in H_0^1(\Omega)\,, \quad (3.53)$$

and find the linear equation for z^t

$$\int_\Omega \nabla z^t\cdot\nabla\varphi\, d\Omega = -\frac{1}{t}\int_\Omega (A(t)-\mathrm{I})\nabla u^t\cdot\nabla\varphi\, d\Omega + \frac{1}{t}\int_\Omega (\mathfrak{g}(t)b\circ\mathfrak{T}_t - b)\varphi\, d\Omega\,. \quad (3.54)$$

From (3.52) it follows that

$$\|u^t\|_{H_0^1(\Omega)} \leqslant C\,. \tag{3.55}$$

Moreover, using (3.54) we can show that u^t converges strongly to $u(\Omega)$ in $H_0^1(\mathfrak{D})$ as $t \to 0$. Applying this convergence result to the right hand side of (3.54) we have

$$\frac{1}{t}(A(t) - \mathrm{I}) \to A'(0) \quad \text{strongly in } L^\infty(\mathfrak{D};\mathbb{R}^d) \tag{3.56}$$

and

$$\frac{1}{t}(\mathfrak{g}(t)b \circ \mathfrak{T}_t - b) \to \operatorname{div}(b\mathfrak{V}) \quad \text{strongly in } L^2(\mathfrak{D})\,, \tag{3.57}$$

here, it is assumed here that $k \geqslant 1$. From the foregoing it can be inferred that z^t is bounded, i.e.

$$\|z^t\|_{H_0^1(\Omega)} \leqslant C\,. \tag{3.58}$$

We can suppose that for a subsequence $z^k = z^{t_k} \rightharpoonup z$ weakly in $H_0^1(\Omega)$ (for a sequence $\{t_k\}$, $t_k \to 0$ as $k \to \infty$); for a weak limit z the following integral identity holds

$$\begin{aligned}\int_\Omega \nabla z \cdot \nabla\phi\, d\Omega = &- \int_\Omega A'(0)\nabla u \cdot \nabla\phi\, d\Omega \\ &+ \int_\Omega \operatorname{div}(b\mathfrak{V})\phi\, d\Omega \qquad \forall \phi \in H_0^1(\Omega)\,.\end{aligned} \tag{3.59}$$

Let us assume that in (3.54) ϕ is taken as $z^k = z^{t_k}$. It is known that the sequence $\{\nabla u^{t_k}\}$ converges strongly to ∇u in $L^2(\Omega;\mathbb{R}^d)$ as $k \to +\infty$. Furthermore

$$\frac{1}{t_k}(A(t_k) - \mathrm{I})\nabla u^{t_k} \to A'(0)\nabla u \quad \text{strongly in } L^2(\Omega;\mathbb{R}^d)\,, \tag{3.60}$$

$$\nabla z^k \rightharpoonup \nabla z \quad \text{weakly in } L^2(\Omega;\mathbb{R}^d)\,. \tag{3.61}$$

We can pass to the limit in (3.54) and obtain

$$\|z^k\|^2_{H_0^1(\Omega)} \to \|z\|^2_{H_0^1(\Omega)} \quad \text{as} \quad k \to +\infty\,. \tag{3.62}$$

As it has been already shown, the convergence of z^k to z in $H_0^1(\Omega)$ assures the strong convergence; the element z is uniquely determined, hence z^t converges to z strongly in $H_0^1(\mathfrak{D})$.

Proposition 3.3. *Let $\Omega \subset \mathfrak{D}$ be of class C^k, $k \geqslant 1$, $\mathfrak{V}$ satisfy Condition 3.1 and $b \in H^1(\mathfrak{D})$. Then the solution $u(\Omega_t)$ of the Poisson's equation with homogeneous Dirichlet boundary conditions* (3.47) *admits the unique strong H^1-material derivative z in the direction $\mathfrak{V}$*

$$\frac{1}{t}(u(\Omega_t) \circ \mathfrak{T}_t(\mathfrak{V}) - u(\Omega)) \to z \quad \textit{strongly in } H_0^1(\Omega) \tag{3.63}$$

as $t \to 0$.

We now turn to the case $k \geqslant 2$. In order to apply the classical implicit function theorem let us consider the mapping

$$\Phi : [0,\delta) \times (H^2(\Omega) \cap H_0^1(\Omega)) \to L^2(\Omega) , \tag{3.64}$$

which is given by

$$\Phi(t,u) = -\mathrm{div}(A(t)\nabla u) - \mathfrak{g}(t) b \circ \mathfrak{T}_t . \tag{3.65}$$

By standard regularity results applied to the elliptic problem defined in the domain Ω with the boundary Γ of class C^k (see e.g. [181]), it follows that for any t, $0 \leqslant t < \delta$, $u \mapsto \Phi(t,u)$ is an isomorphism from $H^2(\Omega) \cap H_0^1(\Omega)$ onto $L^2(\Omega)$.

On the other hand, for $b \in H^1(\mathfrak{D})$ the mapping $t \mapsto \Phi(t,u)$ is strongly differentiable in $L^2(\Omega)$. By the standard implicit function theorem it follows that the mapping $t \mapsto u^t$, where u^t is a unique solution to (3.49) and satisfies $\Phi(t,u^t) = 0$, is strongly differentiable in $H^2(\Omega) \cap H_0^1(\Omega)$. The derivative at $t = 0$ is of the form

$$z = -D_u \Phi(0,u)^{-1} \partial_t \Phi(0,u) . \tag{3.66}$$

Thus, we have the result.

Proposition 3.4. *Let $\Omega \subset \mathfrak{D}$ be of class C^k, $k \geqslant 2$, $\mathfrak{V}$ satisfy Condition 3.1 and $b \in H^2(\mathfrak{D})$. Then the solution $u(\Omega_t)$ to the Poisson's equation with homogeneous Dirichlet boundary conditions* (3.47) *has the unique strong H^2-material derivative z in the direction $\mathfrak{V}$,*

$$\frac{1}{t}(u(\Omega_t) \circ \mathfrak{T}_t(\mathfrak{V}) - u(\Omega)) \to z \quad \textit{strongly in } H^2(\Omega) \cap H_0^1(\Omega) \tag{3.67}$$

as $t \to 0$.

3.2.3 Material Derivatives for the Neumann Problem

Let Ω be a domain in $\mathfrak{D}$ with the boundary Γ of class C^k, $k \geqslant 1$, let $\mathfrak{V}$ satisfy Condition 3.1 and $b \in L^2(\mathfrak{D})$ be given.

We denote by $u(\Omega_t) \in H^1(\Omega)/\mathbb{R}$ a weak solution of the Neumann boundary value problem *(Neumann Laplacian)*

$$\begin{cases} -\Delta u(\Omega_t) = b - \bar{b} \ \text{ in } \ \Omega_t , \\ \partial_n u(\Omega_t) = 0 \qquad \text{on } \Gamma_t = \partial\Omega_t , \end{cases} \tag{3.68}$$

where $|\Omega|$ is the Lebesgue measure of Ω and

$$\bar{b} = \frac{1}{|\Omega_t|} \int_{\Omega_t} b \, d\Omega_t . \tag{3.69}$$

The weak solution u_t satisfies

$$\int_{\Omega_t} \nabla u_t \cdot \nabla \phi_t \, d\Omega_t = \int_{\Omega_t} (b - \bar{b}) \phi_t \, d\Omega \tag{3.70}$$

for all test functions ϕ_t in $H^1(\Omega_t)/\mathbb{R}$.

By the change of variables defined by the transformation $\mathfrak{T}_t(\mathfrak{V})$ the above integral identity in variable domain Ω_t is transformed to the reference domain

$$\int_{\Omega} A(t) \nabla u^t \cdot \nabla \phi \, d\Omega = \int_{\Omega} F(t) \phi \, d\Omega \, . \tag{3.71}$$

The mean value of

$$F(t) = \mathfrak{g}(t) \left(b \circ \mathfrak{T}_t - \frac{1}{|\Omega_t|} \int_{\Omega_t} b \, d\Omega_t \right) \tag{3.72}$$

is null

$$\int_{\Omega} F(t) \, d\Omega = \int_{\Omega_t} b \, d\Omega_t - \frac{1}{|\Omega_t|} \int_{\Omega_t} b \, d\Omega_t \int_{\Omega} \mathfrak{g}(t) d\Omega = 0 \, . \tag{3.73}$$

To check this property it is enough to recall that

$$\int_{\Omega} \mathfrak{g}(t) b \circ \mathfrak{T}_t \, d\Omega = \int_{\Omega_t} b \, d\Omega \quad \text{and} \quad \int_{\Omega} \mathfrak{g}(t) \, d\Omega = \int_{\Omega_t} d\Omega_t = |\Omega_t| \, . \tag{3.74}$$

We replace ϕ by u^t in (3.71), hence

$$\|u^t\|_{H^1(\Omega)/\mathbb{R}} \leqslant C \, , \tag{3.75}$$

for $k \geqslant 1$ and

$$\|A(t)\|_{W^{1,\infty}(\mathfrak{D};\mathbb{R}^2 \times \mathbb{R}^2)} \leqslant C \quad \text{for} \quad t \in [0, \delta) \, . \tag{3.76}$$

For $b \in L^2(\mathfrak{D})$ we have that $F(t) \to F(0)$ strongly in $L^2(\mathfrak{D})$ as $t \to 0$, where

$$F(0) = b - \frac{1}{|\Omega|} \int_{\Omega} b \, d\Omega \, . \tag{3.77}$$

From (3.71) it follows that $u^t \to u$ strongly in $H^1(\Omega)/\mathbb{R}$. First assuming that $\phi = u^t$ in (3.71) we get

$$\|u^t\|^2_{H^1(\Omega)/\mathbb{R}} \leqslant C \, . \tag{3.78}$$

Let us consider a subsequence

$$u^k = u^{t_k} \, , \quad t_k \to 0 \text{ as } k \to \infty \, , \tag{3.79}$$

then

$$u^k \rightharpoonup u = u(\Omega) \quad \text{weakly in } H^1(\Omega)/\mathbb{R} \, , \tag{3.80}$$

as $t \to 0$. Hence $u^t \rightharpoonup u(\Omega)$ weakly in $H^1(\Omega)/\mathbb{R}$ as $t \to 0$. For $z^t = (u^t - u)/t$ one obtains

$$\int_\Omega \nabla z^t \cdot \nabla \phi \, d\Omega = -\int_\Omega \frac{1}{t}(A(t) - \mathrm{I})\nabla u^t \cdot \nabla \phi \, d\Omega \\ + \int_\Omega \frac{1}{t}(F(t) - F(0))\phi \, d\Omega \quad \forall \phi \in H^1(\Omega)/\mathbb{R} . \tag{3.81}$$

Furthermore

$$\frac{1}{t}(A(t) - \mathrm{I})\nabla u^t \rightharpoonup A'(0)\nabla u \quad \text{weakly in } L^2(\Omega; \mathbb{R}^d) . \tag{3.82}$$

For $b \in H^1(\mathfrak{D})$ we have

$$\frac{1}{t}(F(t) - F(0)) \to F'(0) \quad \text{strongly in } L^2(\Omega) , \tag{3.83}$$

as $t \to 0$, where $F'(0) \in L^2(\Omega)$ is given by

$$F'(0) = \operatorname{div}(b\mathfrak{V}) + \int_\Gamma \mathfrak{V} \cdot n \, d\Gamma \frac{1}{|\Omega|^2} \int_\Omega b \, d\Omega \\ - \frac{1}{|\Omega|} \int_\Gamma b\mathfrak{V} \cdot n \, d\Gamma - \operatorname{div}\mathfrak{V} \frac{1}{|\Omega|} \int_\Omega b \, d\Omega . \tag{3.84}$$

Thus

$$\int_\Omega F'(0) \, d\Omega = \int_\Gamma b \, \mathfrak{V} \cdot n \, d\Gamma + \frac{1}{|\Omega|} \int_\Omega b \, d\Omega \int_\Gamma \mathfrak{V} \cdot n \, d\Gamma \\ - \int_\Gamma b \, \mathfrak{V} \cdot n \, d\Gamma - \frac{1}{|\Omega|} \int_\Omega b \, d\Omega \int_\Gamma \mathfrak{V} \cdot n \, d\Gamma = 0 . \tag{3.85}$$

3.3 Shape Derivatives for Second Order Elliptic Equations

In this section the form of the shape derivatives for the second order linear elliptic boundary value problems is derived. Our goal is to obtain the complete information for the shape derivatives, including the boundary value problems and the explicit form of nonhomogeneous boundary conditions. The form of the shape derivative for the second order elliptic boundary value problem with nonhomogeneous Dirichlet boundary conditions is determined in Section 3.3.1. In Section 3.3.2 the same equation but with nonhomogeneous Neumann boundary conditions is considered.

3.3.1 Shape Derivatives for the Dirichlet Problem

Let $\mathfrak{D}$ be a given domain in $\mathbb{R}^d$. It is assumed that for any domain Ω of class C^k in $\mathfrak{D}$ there are given three elements $b(\Omega)$, $z(\Gamma)$, $u(\Omega)$ such that $b(\Omega) \in L^2(\Omega)$,

$z(\Gamma) \in H^{1/2}(\Gamma)$, and $u(\Omega) \in H^1(\Omega)$. In this section, $u(\Omega)$ denotes a solution to the Poisson's equation with the Dirichlet boundary conditions

$$\begin{cases} -\Delta u(\Omega) = b(\Omega) \text{ in } L^2(\Omega)\,, \\ \quad u(\Omega) = z(\Gamma) \text{ in } H^{1/2}(\Gamma)\,. \end{cases} \tag{3.86}$$

Let $\mathfrak{V}$ satisfy Condition 3.1 and the elements $b(\Omega)$, $z(\Gamma)$, $u(\Omega)$ admit the shape derivatives $b'(\Omega)$, $z'(\Gamma)$, $u'(\Omega)$ in $L^2(\Omega)$, $H^{1/2}(\Gamma)$, $H^1(\Omega)$, respectively. We have established that

$$\frac{1}{t}(u(\Omega_t) \circ \mathfrak{T}_t(\mathfrak{V}) - u(\Omega)) \rightharpoonup \dot{u}(\Omega;\mathfrak{V}) \quad \text{weakly in } H^1(\Omega)\,, \tag{3.87}$$

as $t \to 0$, and in addition

$$\nabla u(\Omega) \cdot \mathfrak{V} \in H^1(\Omega)\,. \tag{3.88}$$

In order to determine the shape derivative let us consider the weak form of (3.86) obtained by transposition

$$\int_\Omega u(\Omega)\Delta\phi\, d\Omega = \int_\Gamma z(\Gamma)\partial_n\phi\, d\Gamma - \int_\Omega b(\Omega)\phi\, d\Omega \quad \forall\phi \in H^2(\Omega)\cap H_0^1(\Omega)\,. \tag{3.89}$$

In order to determine the boundary conditions for the shape derivative we consider the boundary condition in (3.86) written as the integral identity

$$\int_{\Gamma_t} u(\Omega_t)\phi\, d\Gamma_t = \int_{\Gamma_t} z(\Gamma_t)\phi\, d\Gamma_t\,, \tag{3.90}$$

with the test function $\phi \in \mathscr{D}(\mathbb{R}^d)$.

Taking the derivative with respect to t at $t = 0$ of both sides of this identity, we obtain

$$\int_\Gamma u'(\Omega;\mathfrak{V})_{|\Gamma}\phi\, d\Gamma + \int_\Gamma (\partial_n(u(\Omega)\phi) + \kappa u(\Omega)\phi)\mathfrak{V}\cdot n\, d\Gamma = \int_\Gamma (z(\Gamma)\phi)'(\Gamma;\mathfrak{V})\, d\Gamma + \int_\Gamma \kappa z(\Gamma)\phi\,\mathfrak{V}\cdot n\, d\Gamma\,, \tag{3.91}$$

where κ is the mean curvature of Γ. For a given element $\phi \in \mathscr{D}(\mathbb{R}^d)$ we have the expression for the boundary shape derivative of its restriction to Γ

$$\phi'(\Gamma;\mathfrak{V}) = \partial_n\phi(\Gamma)\,\mathfrak{V}\cdot n\,. \tag{3.92}$$

Since we need test functions in a dense subset of the Sobolev space $H^1(\Omega)$, without loss of generality we can take the boundary shape derivative of the test function null, i.e., $\partial_n\phi = 0$ on Γ, then

$$\int_\Gamma u'(\Omega;\mathfrak{V})_{|\Gamma}\phi\,d\Gamma + \int_\Gamma (\partial_n u(\Omega)+\kappa u(\Omega))\phi\,\mathfrak{V}\cdot n\,d\Gamma = \int_\Gamma z'(\Gamma;\mathfrak{V})\phi\,d\Gamma + \int_\Gamma \kappa z(\Gamma)\phi\,\mathfrak{V}\cdot n\,d\Gamma\,. \quad (3.93)$$

From the boundary condition in (3.86) it follows that

$$u'(\Omega;\mathfrak{V})_{|\Gamma} = -\partial_n u(\Omega)\mathfrak{V}\cdot n + z'(\Gamma;\mathfrak{V}) \quad \text{on} \quad \Gamma\,. \quad (3.94)$$

On the other hand, for a test function $\phi\in\mathscr{D}(\Omega)$ we have the property that $\phi\in\mathscr{D}(\Omega_t)$ for $t>0$, t small enough. Therefore,

$$\int_{\Omega_t}\nabla u(\Omega_t)\cdot\nabla\phi\,d\Omega = \int_{\Omega_t} b(\Omega_t)\phi\,d\Omega\,. \quad (3.95)$$

Taking the derivative with respect to t at $t=0$ of both sides of this identity we have

$$\int_\Omega \nabla u'(\Omega;\mathfrak{V})\cdot\nabla\phi\,d\Omega = \int_\Omega b'(\Omega;\mathfrak{V})\phi\,d\Omega\,, \quad (3.96)$$

that is

$$-\Delta u'(\Omega;\mathfrak{V}) = b'(\Omega;\mathfrak{V}) \quad \text{in} \quad \mathscr{D}'(\Omega)\,. \quad (3.97)$$

Proposition 3.5. *Let* $(b(\Omega),z(\Gamma))\in L^2(\Omega)\times H^{1/2}(\Gamma)$ *be given elements such that there exist the shape derivatives* $(b'(\Omega),z'(\Gamma))$ *in* $L^2(\Omega)\times H^{1/2}(\Gamma)$. *Then the solution* $u(\Omega)$ *to the Poisson's equation with the Dirichlet boundary conditions* (3.86) *has the shape derivative* $u'(\Omega;\mathfrak{V})$ *in* $H^1(\Omega)$ *determined as the unique solution to the Poisson's equation* (3.97) *with the Dirichlet boundary conditions* (3.94).

3.3.2 Shape Derivatives for the Neumann Problem

Let $\mathfrak{D}$ be a given domain in $\mathbb{R}^d$. It is assumed that for any domain Ω of class C^k in $\mathfrak{D}$ there are given three elements $b(\Omega)$, $z(\Gamma)$ and $u(\Omega)$ such that $b(\Omega)\in L^2(\Omega)$, $z(\Gamma)\in H^{1/2}(\Omega)/\mathbb{R}$, and

$$\int_\Omega b(\Omega)\,d\Omega + \int_\Gamma z(\Gamma)\,d\Gamma = 0\,. \quad (3.98)$$

In this section $u(\Omega)$ denotes a solution to the Neumann boundary value problem

$$\begin{cases} -\Delta u(\Omega) = b(\Omega) \text{ in } L^2(\Omega)\,, \\ \partial_n u(\Omega) = z(\Gamma) \text{ in } H^{1/2}(\Gamma)\,. \end{cases} \quad (3.99)$$

Let us consider the following integral identity

$$\int_{\Omega_t}\nabla u(\Omega_t)\cdot\nabla\phi\,d\Omega = \int_{\Omega_t} b(\Omega_t)\phi\,d\Omega + \int_{\Gamma_t} z(\Gamma)\phi\,d\Gamma\,, \quad (3.100)$$

where $\phi \in \mathscr{D}(\mathbb{R}^d)$ is a given element and $u(\Omega_t) \in H^1(\Omega_t)/\mathbb{R}$. Taking the derivative of (3.100) with respect to t at $t = 0$ we obtain

$$\int_\Omega \nabla u'(\Omega;\mathfrak{V}) \cdot \nabla\phi \, d\Omega + \int_\Gamma \nabla u \cdot \nabla\phi \, \mathfrak{V}\cdot n \, d\Gamma = \int_\Omega b'(\Omega;\mathfrak{V})\phi \, d\Omega + \int_\Gamma b(\Omega)\phi \, \mathfrak{V}\cdot n \, d\Gamma + \int_\Gamma [z'(\Gamma;\mathfrak{V})\phi + (z(\Gamma)\partial_n\phi + \kappa z(\Gamma)\phi) \, \mathfrak{V}\cdot n] \, d\Gamma \,. \quad (3.101)$$

Assuming that ϕ is in $\mathscr{D}(\Omega)$ we get

$$-\Delta u'(\Omega;\mathfrak{V}) = b'(\Omega;\mathfrak{V}) \quad \text{in} \quad \Omega \,. \quad (3.102)$$

If the test function ϕ is such that its displacement derivative is null on the boundary i.e., $\partial_n\phi = 0$ on Γ, then Green's formula yields

$$\int_\Gamma \partial_n u'(\Omega;\mathfrak{V}) \, \phi \, d\Gamma - \int_\Gamma \mathrm{div}_\Gamma(\mathfrak{V}\cdot n \nabla_\Gamma u)\phi \, d\Gamma = \int_\Gamma (b(\Omega) \, \mathfrak{V}\cdot n + z'(\Gamma;\mathfrak{V}) + \kappa z(\Gamma) \, \mathfrak{V}\cdot n)\phi \, d\Gamma \,, \quad (3.103)$$

where $\mathrm{div}_\Gamma \varphi$ is the tangential divergence of a vector function φ on the boundary Γ, that is

$$\mathrm{div}_\Gamma \varphi = (\mathrm{I} - n \otimes n) \cdot \nabla\varphi \quad \text{on} \quad \Gamma \,. \quad (3.104)$$

If $v_n = \mathfrak{V}\cdot n$ on Γ, then the following Neumann boundary conditions can be set out for $u'(\Omega;\mathfrak{V})$

$$\partial_n u'(\Omega;\mathfrak{V}) = \mathrm{div}_\Gamma(v_n \nabla_\Gamma u(\Omega)) + (b(\Omega) + \kappa z(\Gamma))v_n + z'(\Gamma;\mathfrak{V}) \text{ on } \Gamma \,. \quad (3.105)$$

We shall show that the compatibility condition (3.98) is satisfied in an appropriate way for the problem (3.102) and (3.105).

Proposition 3.6. *For the terms on the right hand side of formulae* (3.102) *and* (3.105) *the compatibility condition* (3.98) *holds, i.e.*

$$\int_\Omega b'(\Omega;\mathfrak{V}) d\Omega + \int_\Gamma \mathrm{div}_\Gamma(v_n \nabla_\Gamma u(\Omega)) d\Gamma + \int_\Gamma (b(\Omega) + \kappa z(\Gamma)) v_n \, d\Gamma + \int_\Gamma z'(\Gamma;\mathfrak{V}) d\Gamma = 0 \,, \quad (3.106)$$

hence there exists the unique solution $u'(\Omega;\mathfrak{V}) \in H^1(\Omega)/\mathbb{R}$ *to the problem* (3.102) *and* (3.105).

Proof. From (3.98) it follows that in (3.100) ϕ can be replaced with $\phi + c$, where c is any constant. Differentiation with respect to t does not change this property. Therefore ϕ can be replaced by $\phi + c$ in the integral identity obtained after differentiation of (3.106) with respect to t. This yields

$$\int_{\Omega} b'\, d\Omega + \int_{\Gamma} b v_n \, d\Gamma + \int_{\Gamma} z' \, d\Gamma + \int_{\Gamma} \kappa z v_n \, d\Gamma = 0\,. \tag{3.107}$$

On the other hand we have

$$\int_{\Gamma} \mathrm{div}_{\Gamma}(v_n \nabla_{\Gamma} u)\, d\Gamma = -\int_{\Gamma} v_n \nabla_{\Gamma} u \cdot \nabla_{\Gamma} 1 \, d\Gamma = 0\,, \tag{3.108}$$

as it was to be shown. □

Proposition 3.7. *Let* $(b(\Omega), z(\Gamma)) \in L^2(\Omega) \times H^{1/2}(\Gamma)$ *be given elements such that there exist the shape derivatives* $(b'(\Omega;\mathfrak{V}), z'(\Gamma;\mathfrak{V}))$ *in* $L^2(\Omega) \times H^{1/2}(\Gamma)$*. Then the solution* $u(\Omega)$ *to the Neumann boundary value problem has the shape derivative* $u'(\Omega;\mathfrak{V})$ *in* $H^1(\Omega)/\mathbb{R}$*. This derivative is given by the unique solution to the Neumann boundary value problem* (3.102) *and* (3.105).

3.4 Material and Shape Derivatives for Elasticity Problems

In this section the form of the material derivatives and the shape derivatives for the second order linear elliptic system is derived. In particular the shape sensitivity analysis is performed for anisotropic elasticity boundary value problems with the full range of boundary conditions. The existence of the strong or weak H^k-material derivatives, $k = 0, 1, 2$, can be shown by the exactly same arguments as it is in the case of the Poisson's equation by an application of the implicit function theorem. Then, from the relation between the material and the shape derivatives it follows the existence of the associated H^{k-1}-shape derivatives.

3.4.1 Problem Formulation

The elliptic boundary value problems in elasticity are formulated in this section.

Let $\eta \in H^1(\Gamma)$ be the trace on a smooth manifold $\Gamma = \partial\Omega$ of a vector function $\phi \in H^2(\Omega;\mathbb{R}^3)$, then

$$\nabla_{\Gamma} \eta = (\mathrm{I} - n \otimes n)\nabla\phi \quad \text{on} \quad \Gamma\,, \tag{3.109}$$

which implies

$$\mathrm{div}_{\Gamma} \eta = \mathrm{tr}(\nabla_{\Gamma} \eta) = (\mathrm{I} - n \otimes n) \cdot \nabla\phi \quad \text{on} \quad \Gamma\,. \tag{3.110}$$

We point out that η is defined only on Γ, hence $\nabla\eta$ is not defined.

For any vector function $\phi \in H^1(\mathbb{R}^3;\mathbb{R}^3)$ the following notation is used

$$(\nabla\phi)_{ij} = \phi_{i,j} \quad \text{and} \quad (\nabla\phi^{\top})_{ij} = \phi_{j,i}\,, \quad i,j = 1,2,3\,. \tag{3.111}$$

The linearized strain tensor $\varepsilon(\phi)$ is of the form

$$\varepsilon(\phi) = \frac{1}{2}(\nabla\phi + \nabla\phi^\top) . \tag{3.112}$$

Let us consider the fourth order tensor field $\mathbb{C} = \{c_{ijkl}\}$, $i,j,k,l = 1,2,3$, such that the following symmetry conditions are satisfied

$$c_{ijkl}(x) = c_{jikl}(x) = c_{klij}(x) \quad x \in \mathbb{R}^3, \qquad i,j,k,l = 1,2,3 . \tag{3.113}$$

Furthermore $c_{ijkl}(\cdot) \in L^\infty_{loc}(\mathbb{R}^3)$, $i,j,k,l = 1,2,3$, and there exists $\alpha_0 > 0$ such that

$$\mathbb{C}(x)\xi \cdot \xi = c_{ijkl}(x)\xi_{ij}\xi_{kl} \geqslant \alpha_0 \xi_{ij}\xi_{kl} = \alpha_0 \xi \cdot \xi \tag{3.114}$$

for all $x \in \mathbb{R}^3$ and for all second order symmetric tensors ξ, where the summation convention over repeated indices $i,j,k,l = 1,2,3$ is used.

The stress tensor $\sigma = \sigma(\phi)$ is defined by

$$\sigma(\phi) = \mathbb{C}\varepsilon(\phi) \quad \text{i.e.} \quad \sigma_{ij} = c_{ijkl}\varepsilon_{kl} = c_{ijkl}\phi_{k,l} \quad i,j,k,l = 1,2,3 . \tag{3.115}$$

For $\phi \in H^2(\mathbb{R}^3;\mathbb{R}^3)$ there are well defined

- the normal component σ_{nn} of the stress tensor on the boundary Γ,

$$\sigma_{nn} = n \cdot \sigma n = \sigma_{ij} n_i n_j , \tag{3.116}$$

- the tangential component σ_τ,

$$\sigma_\tau = \sigma n - \sigma_{nn} n . \tag{3.117}$$

We introduce for the elasticity boundary value problems

- the bilinear form

$$a(\varphi,\phi) = \int_\Omega \mathbb{C}\varepsilon(\varphi) \cdot \varepsilon(\phi)\, d\Omega \quad \forall \varphi,\phi \in H^1(\Omega;\mathbb{R}^3) , \tag{3.118}$$

- and the linear form

$$l(\phi) = \int_\Omega b \cdot \phi \, d\Omega + \int_{\Gamma_1} z \cdot \phi \, d\Gamma . \tag{3.119}$$

Here $\Omega \subset \mathbb{R}^3$ is a given domain with the smooth boundary $\Gamma = \overline{\Gamma}_0 \cup \overline{\Gamma}_1 \cup \overline{\Gamma}_2$, $\overline{\Gamma}_i \cap \overline{\Gamma}_j = \varnothing$, $i \neq j$, $|\Gamma_0| > 0$; $b \in L^2(\Omega;\mathbb{R}^3)$ and $z \in H^1(\Gamma_2;\mathbb{R}^3)$ are given elements.

Remark 3.4. The above constraints on Γ_0, Γ_1 and Γ_2 require explanation. If

- $\partial\Gamma_i \cap \partial\Gamma_j \neq \varnothing$, $i \neq j$, then the singularities of weak solutions on $\partial\Gamma_i \cap \partial\Gamma_j$ should be taken into account in evaluations of material and shape derivatives.
- $|\Gamma_0| = 0$ then the compability conditions generated by rigid body motions are required for the solvability of boundary value problems.

Proposition 3.8. *Under the above assumptions there exists a weak solution to the variational equation*

$$u \in \mathscr{V} : a(u,\phi) = l(\phi) \quad \forall \phi \in \mathscr{V} , \tag{3.120}$$

where

$$\mathscr{V} = \{\phi \in H^1(\Omega;\mathbb{R}^3) : \phi = 0 \text{ on } \Gamma_0,\ \phi_n = \phi \cdot n = 0 \text{ on } \Gamma_2\} . \tag{3.121}$$

It can be shown [61] that for the weak solution u, the following system of equations is satisfied

$$\begin{cases} -\mathrm{div}\sigma = b \text{ in } \Omega , \\ u = 0 \text{ on } \Gamma_0 , \\ \sigma n = z \text{ on } \Gamma_1 , \\ u \cdot n = 0 \text{ on } \Gamma_2 , \\ \sigma_\tau = 0 \text{ on } \Gamma_2 , \end{cases} \tag{3.122}$$

in the weak sense. It is well known that for $|\Gamma_0| > 0$ the bilinear form $a(\cdot,\cdot)$ is coercive [61], i.e. there exists a constant $\alpha > 0$ such that

$$\int_\Omega \mathbb{C}\varepsilon(\phi) \cdot \varepsilon(\phi)\, d\Omega \geqslant \alpha \|\phi\|^2_{H^1(\Omega;\mathbb{R}^3)} \quad \forall \phi \in \mathscr{V} . \tag{3.123}$$

This implies the existence and uniqueness of the weak solution to (3.122) defined by (3.120). The equivalent form of (3.122) expressed in terms of the displacement u is as follows

$$\begin{cases} -\mathrm{div}\sigma(u) = b & \text{in } \Omega , \\ \sigma(u) = \mathbb{C}\varepsilon(u) , & \\ u = 0 & \text{on } \Gamma_0 , \\ \sigma(u)n = z & \text{on } \Gamma_1 , \\ u \cdot n = 0 & \text{on } \Gamma_2 , \\ \sigma_\tau(u) = 0 & \text{on } \Gamma_2 . \end{cases} \tag{3.124}$$

Let us examine the linear model (3.122). The principal aim of our consideration is the shape sensitivity analysis of the system (3.122), therefore it is assumed that data are smooth enough, e.g.

$$z, b \in C^1(\mathbb{R}^3;\mathbb{R}^3) , \tag{3.125}$$

$$c_{ijkl} \in C^1(\mathbb{R}^3) \quad i,j,k,l = 1,2,3 . \tag{3.126}$$

The system (3.122) is to be defined in the domain $\Omega_t \in \mathbb{R}^3$, with the boundary $\Gamma_t = \overline{\Gamma}{}^t_0 \cup \overline{\Gamma}{}^t_1 \cup \overline{\Gamma}{}^t_2$ for $t \in [0,\delta)$. For this purpose the following notation is introduced

$$a_t(\varphi,\phi) = \int_{\Omega_t} \mathbb{C}\varepsilon(\varphi) \cdot \varepsilon(\phi)\, d\Omega_t \quad \forall \varphi, \phi \in \mathscr{V}_t , \tag{3.127}$$

$$l_t(\phi) = \int_{\Omega_t} b \cdot \phi\, d\Omega_t + \int_{\Gamma_1^t} z \cdot \phi\, d\Gamma_t \quad \forall \phi \in \mathscr{V}_t , \tag{3.128}$$

where

$$\mathscr{V}_t = \{\phi \in H^1(\Omega_t;\mathbb{R}^3) : \phi = 0 \text{ on } \Gamma_0^t,\ \phi \cdot n_t = 0 \text{ on } \Gamma_2^t\} \,. \tag{3.129}$$

The following variational equation holds

$$u_t \in \mathscr{V}_t : a_t(u_t,\phi) = l_t(\phi) \quad \forall \phi \in \mathscr{V}_t \tag{3.130}$$

for a weak solution to (3.122).

Note 3.1. The *frictionless contact* problems and the *contact problems with given friction* for linear elastic solids take the form of *variational inequalities*.

Note 3.2. For the contact problems, the *nonpenetration condition* $u_t \cdot n_t \geqslant 0$ on Γ_c^t is not preserved for the function $u^t := u_t \circ \mathfrak{T}_t$ on the boundary Γ_c in view of

$$n^t(x) := (n_t \circ \mathfrak{T}_t)(x) = (\|(D\mathfrak{T}_t)^{-\top} n\|_{\mathbb{R}^3}^{-1} (D\mathfrak{T}_t)^{-\top} n)(x)$$

for $x \in \Gamma_c \subset \partial\Omega$, where n is the unit normal vector on $\partial\Omega$. It is convenient to replace the unknown vector function $u_t \circ \mathfrak{T}_t$ by

$$\mathfrak{z}^t = D\mathfrak{T}_t(u_t \circ \mathfrak{T}_t) \,, \tag{3.131}$$

since

$$\mathfrak{z}^t \cdot n^t = (u_t \circ \mathfrak{T}_t)(D\mathfrak{T}_t)^\top (n_t \circ \mathfrak{T}_t) = \|(D\mathfrak{T}_t)^{-\top} n\|_{\mathbb{R}^3} u^t \cdot n \,. \tag{3.132}$$

Thus the unilateral condition on the moving boundary Γ_c^t

$$u_t \cdot n_t \geqslant 0 \tag{3.133}$$

is transformed to the fixed domain, but for the function $\mathfrak{z}^t = D\mathfrak{T}_t \cdot u^t$,

$$\mathfrak{z}^t \cdot n \geqslant 0 \,. \tag{3.134}$$

3.4.2 Material Derivatives for Elasticity

The elasticity boundary value problem defined in variable domain is transformed to the reference domain. To this end we introduce the notation

- the bilinear form transformed to the reference domain

$$\begin{aligned} a^t(\varphi,\phi) &= a_t(\varphi \circ \mathfrak{T}_t^{-1}, \phi \circ \mathfrak{T}_t^{-1}) \\ &= \int_\Omega \mathfrak{g}(t)\mathbb{C}^t \varepsilon^t(\varphi) \cdot \varepsilon^t(\phi)\, d\Omega \quad \forall \varphi,\phi \in \mathscr{V} \,, \end{aligned} \tag{3.135}$$

- the linear form transformed to the reference domain

$$\begin{aligned} l^t(\phi) &= l_t(\phi \circ \mathfrak{T}_t^{-1}) \\ &= \int_\Omega b^t \cdot \phi \, d\Omega + \int_{\Gamma_1} z^t \cdot \phi d\Gamma \quad \forall \phi \in \mathscr{V} , \end{aligned} \tag{3.136}$$

where

$$\varepsilon^t(\phi) = \frac{1}{2}(D\phi (D\mathfrak{T}_t)^{-1} + (D\mathfrak{T}_t)^{-\top} D\phi^\top) , \tag{3.137}$$

$$b^t = \mathfrak{g}(t) b \circ \mathfrak{T}_t , \tag{3.138}$$

$$z^t = \|D\mathfrak{T}_t^{-\top} n\| \mathfrak{g}(t) \, z \circ \mathfrak{T}_t . \tag{3.139}$$

Proposition 3.9. *The solution transformed to the reference domain*

$$u^t = u_t \circ \mathfrak{T}_t \tag{3.140}$$

satisfies

$$u^t \in \mathscr{V} : a^t(u^t, \phi) = l^t(\phi) \quad \forall \phi \in \mathscr{V} . \tag{3.141}$$

The solution of (3.141) is differentiated with respect to t. First, the bilinear and the linear forms are differentiated. We denote

- derivative of mapping $t \mapsto \varepsilon^t(\phi)$

$$\varepsilon'(\phi) = -\frac{1}{2}(\nabla \phi \nabla \mathfrak{V} + \nabla \mathfrak{V}^\top \nabla \phi^\top) , \tag{3.142}$$

- derivative of mapping $t \mapsto \mathbb{C}^t := \mathbb{C} \circ \mathfrak{T}_t$

$$\mathbb{C}' = \{c'_{ijkl}\}, \quad c'_{ijkl} = c_{ijkl} \mathrm{div} \mathfrak{V} + \nabla(c_{ijkl}) \cdot \mathfrak{V} , \tag{3.143}$$

- tangential component of the velocity field

$$\mathfrak{V}_\tau = \mathfrak{V} - (\mathfrak{V} \cdot n) \, n . \tag{3.144}$$

Proposition 3.10. *The derivatives $a'(\cdot,\cdot)$, $l'(\cdot)$ of the bilinear form $a^t(\cdot,\cdot)$ and the linear form $l^t(\cdot)$ with respect to t at $t = 0$ are given by*

$$a'(\varphi, \phi) = \int_\Omega (\varepsilon'(\varphi) \cdot \sigma(\phi) + \sigma(\varphi) \cdot \varepsilon'(\phi) + \mathbb{C}' \varepsilon(\varphi) \cdot \varepsilon(\phi)) \, d\Omega \qquad \forall \varphi, \phi \in \mathscr{V} , \tag{3.145}$$

and

$$\begin{aligned} l'(\phi) &= \int_\Omega (b \, \mathrm{div} \mathfrak{V} + (\nabla b) \mathfrak{V}) \cdot \phi \, d\Omega \\ &+ \int_{\Gamma_1} (z \, \mathrm{div}_\Gamma \mathfrak{V} + (\nabla_\Gamma z) \mathfrak{V}_\tau) \cdot \phi \, d\Gamma \quad \forall \phi \in \mathscr{V} . \end{aligned} \tag{3.146}$$

Theorem 3.2. *The following variational equation*

$$\dot{u} \in H^1(\Omega;\mathbb{R}^3) : a(\dot{u},\phi) = l'(\phi) - a'(u,\phi) \quad \forall \phi \in \mathscr{V} \tag{3.147}$$

with the additional conditions

$$\dot{u} = 0 \quad on \quad \Gamma_0, \quad \dot{u}\cdot n = n\cdot(\nabla\mathfrak{V})u_\tau \quad on \quad \Gamma_2\,, \tag{3.148}$$

holds for the strong material derivative $\dot{u} \in H^1(\Omega;\mathbb{R}^3)$ *of the solution* $u(\Omega)$ *to* (3.122) *in the direction of a vector field* $\mathfrak{V}$.

Proof. From our assumptions it follows that the mappings

$$[0,\delta) \ni t \mapsto b\circ\mathfrak{T}_t \in L^2(\Omega;\mathbb{R}^3)\,, \tag{3.149}$$

$$[0,\delta) \ni t \mapsto z\circ\mathfrak{T}_t \in L^2(\Gamma_1;\mathbb{R}^3)\,, \tag{3.150}$$

are strongly differentiable. Therefore we can differentiate the integral identity (3.141) with respect to t at $t = 0$. This yields the integral identity (3.148). Since $u^t = 0$ on Γ_0, then $\dot{u} = 0$ on Γ_0. On the other hand, $u_t \cdot n_t = 0$ on Γ_2^t, thus

$$u^t \cdot n^t = 0 \quad \text{on} \quad \Gamma_2\,, \tag{3.151}$$

where

$$n^t = n_t \circ \mathfrak{T}_t = \|(D\mathfrak{T}_t)^{-\top}n\|^{-1}(D\mathfrak{T}_t)^{-\top}n\,. \tag{3.152}$$

Hence

$$\frac{d}{dt}(u^t\cdot n^t)_{|t=0} = 0 \quad \text{on} \quad \Gamma_2\,, \tag{3.153}$$

or equivalently

$$\dot{u}\cdot n - u\cdot(\nabla\mathfrak{V})^\top n = 0 \quad \text{on} \quad \Gamma_2\,. \tag{3.154}$$

Taking into account that $u \cdot n = 0$ on Γ_2, one can show that (3.147) holds. □

3.4.3 Shape Derivatives for Elasticity

In this section the form of the shape derivative $u' = u'(\Omega;\mathfrak{V})$ of the solution $u(\Omega)$ to (3.122) is derived.

Proposition 3.11. *Let us assume*

$$(\nabla u)\mathfrak{V} \in H^1(\Omega;\mathbb{R}^3)\,, \tag{3.155}$$

then the shape derivative

$$u' = \dot{u} - (\nabla u)\mathfrak{V} \in H^1(\Omega;\mathbb{R}^3) \tag{3.156}$$

satisfies for all test functions $\phi \in \mathscr{V}$ *the relation*

$$a(u',\phi) = l'(\phi) - a'(u,\phi) - a((\nabla u)\mathfrak{V},\phi)\,. \tag{3.157}$$

Now we establish the boundary value problem for the shape derivative.

Condition 3.2. We assume that the sets $\overline{\Gamma}_0 \cap \overline{\Gamma}_1$, $\overline{\Gamma}_1 \cap \overline{\Gamma}_2$, $\overline{\Gamma}_0 \cap \overline{\Gamma}_2$ are empty.

Lemma 3.2. *Shape derivative of the stress tensor satisfies*

$$\int_\Omega \sigma' \cdot \varepsilon(\phi)\, d\Omega = \int_\Gamma v_n b_\tau \cdot \phi_\tau\, d\Gamma + \int_{\Gamma_1} (v_n b + v_n \kappa z - \mathrm{div}_\Gamma(v_n \sigma_\tau)) \cdot \phi\, d\Gamma \,. \tag{3.158}$$

Proof. Let us suppose that $\mathfrak{V} \cdot n = 0$ on Γ, then $\Omega = \Omega_t$. Thus $u' = 0$ and

$$l'(\phi) - a'(u, \phi) - a((\nabla u)\mathfrak{V}, \phi) = 0 \,. \tag{3.159}$$

Let us recall, that for $u_t \in H^1(\Omega_t; \mathbb{R}^3)$ the following integral identity holds

$$\int_{\Omega_t} \sigma_t \cdot \varepsilon(\phi)\, d\Omega_t = \int_{\Omega_t} b \cdot \phi\, d\Omega_t + \int_{\Gamma_1^t} z \cdot \phi d\Gamma_t \,. \tag{3.160}$$

Differentiation of (3.160) with respect to t at $t = 0$ yields

$$\int_\Omega \sigma' \cdot \varepsilon(\phi)\, d\Omega + \int_\Gamma v_n \sigma \cdot \varepsilon(\phi)\, d\Gamma = \int_\Gamma v_n b \cdot \phi\, d\Gamma + \int_{\Gamma_1} v_n \kappa z \cdot \phi\, d\Gamma \tag{3.161}$$

for all $\phi \in H^2(\Omega; \mathbb{R}^3)$. Let us assume that $\partial_n \phi = 0$ on Γ, and let $\phi_\tau = \phi - (\phi \cdot n)n$, then

$$\begin{aligned}\int_\Gamma v_n \sigma \cdot \varepsilon(\phi)\, d\Gamma &= \int_\Gamma v_n \sigma \cdot \nabla \phi\, d\Gamma = \int_\Gamma v_n \sigma \cdot \nabla_\Gamma \phi\, d\Gamma \\ &= \int_\Gamma (-\mathrm{div}_\Gamma(v_n \sigma) + v_n \kappa \sigma n) \cdot \phi\, d\Gamma \,,\end{aligned} \tag{3.162}$$

or equivalently

$$\begin{aligned}\int_\Gamma v_n \sigma \cdot \varepsilon(\phi)\, d\Gamma = -\int_\Gamma (&\phi_n \mathrm{div}_\Gamma(v_n \sigma) \cdot n + \\ &\phi_\tau \cdot \mathrm{div}_\Gamma(v_n \sigma) - v_n \kappa \sigma n \cdot \phi)\, d\Gamma \,.\end{aligned} \tag{3.163}$$

Hence

$$\begin{aligned}\int_\Omega \sigma' \cdot \varepsilon(\phi)\, d\Omega &= -\int_\Omega \mathrm{div} \sigma' \cdot \phi\, d\Omega + \int_\Gamma \sigma' n \cdot \phi\, d\Gamma \\ &= -\int_\Gamma (\mathrm{div}_\Gamma(v_n \sigma) - v_n \kappa \sigma n - v_n b - v_n \kappa z) \cdot \phi\, d\Gamma \,.\end{aligned} \tag{3.164}$$

In this equation we have used the conditions: $\phi = 0$ on Γ_0 and $\phi \cdot n = 0$ on Γ_2. Hence $\phi = \phi_\tau$ on Γ_2, $\sigma n = z$ on Γ_1 and $\sigma n = \sigma_{nn} n$ on Γ_2 because of $\sigma_\tau = 0$ on Γ_2. Thus, we obtain (3.158). □

Now we are in position to establish the boundary value problem for the shape derivative.

Theorem 3.3. *If*

- *Condition 3.2 holds,*
- *otherwise, the vector field* $\mathfrak{V}$ *satisfies*

$$\mathfrak{V} = 0 \quad on \quad \overline{\Gamma}_0 \cap \overline{\Gamma}_1, \quad \overline{\Gamma}_1 \cap \overline{\Gamma}_2, \quad \overline{\Gamma}_0 \cap \overline{\Gamma}_2 \,. \tag{3.165}$$

Then the shape derivative $u' = u'(\Omega;\mathfrak{V}) \in H^1(\Omega;\mathbb{R}^3)$ *of the solution* $u(\Omega)$ *to* (3.122) *satisfies the boundary value problem*

$$\begin{cases} -\mathrm{div}\sigma' = 0 & in\ \Omega\,, \\ u' = -v_n\,\partial_n u & on\ \Gamma_0\,, \\ \sigma' n = v_n b + v_n \kappa z - \mathrm{div}_\Gamma(v_n \sigma_\tau) & on\ \Gamma_1\,, \\ u'\cdot n = (\nabla\mathfrak{V})u_\tau \cdot n & on\ \Gamma_2\,, \\ \sigma'_\tau = v_n b_\tau & on\ \Gamma_2\,. \end{cases} \tag{3.166}$$

Proof. The equation (3.166) follows from

$$\begin{aligned} \int_\Omega \sigma'\cdot\varepsilon(\phi)\,d\Omega &= \int_\Gamma \sigma' n\cdot\phi d\Gamma - \int_\Omega \mathrm{div}\sigma'\cdot\phi\,d\Omega \\ &= \int_\Gamma (v_n\kappa\sigma n + v_n b + v_n\kappa z - \mathrm{div}_\Gamma(v_n\sigma))\cdot\phi\,d\Gamma \\ &= \int_\Gamma v_n\phi_\tau\cdot b_\tau\,d\Gamma \\ &\quad + \int_{\Gamma_1}(v_n b + v_n\kappa z - \mathrm{div}_\Gamma(v_n\sigma_\tau))\cdot\phi\,d\Gamma \end{aligned} \tag{3.167}$$

for the test functions $\phi \in \mathscr{D}(\Omega;\mathbb{R}^3)$. We derive the boundary conditions in (3.166). We have

$$u' = \dot{u} - (\nabla u)\mathfrak{V} = -v_n\,\partial_n u - (\nabla_\Gamma u)\mathfrak{V}_\tau = -v_n\,\partial_n u \quad \text{on} \quad \Gamma_0\,. \tag{3.168}$$

Hence the condition on Γ_0 is obtained. The condition on Γ_1 follows from (3.167). In order to derive the first condition on Γ_2, the following equation

$$u_t\cdot n_t = 0 \quad \text{on} \quad \Gamma_2^t = \mathfrak{T}_t(\Gamma_2) \tag{3.169}$$

is to be used. From (3.169) it follows that

$$u'\cdot n = -u\cdot n' \quad \text{on} \quad \Gamma_2\,. \tag{3.170}$$

On the other hand

$$n' = \dot{n} - (\nabla_\Gamma n)\mathfrak{V}_\tau = -(\nabla\mathfrak{V})^\top n\,. \tag{3.171}$$

Since $\mathfrak{V}_\tau = 0$, then

$$u'\cdot n = (\nabla\mathfrak{V})u\cdot n\,. \tag{3.172}$$

Taking into account that (3.169) holds on Γ_2 we get the first condition on Γ_2. Finally the second condition on Γ_2 follows from (3.167), which concludes the proof. □

3.4.4 Shape Derivatives for Interfaces

Given the domain Ω with the boundary denoted by $\partial\Omega$, and $\overline{\Omega}^{\alpha} \Subset \Omega$ with the boundary $\Gamma := \partial\Omega^{\alpha}$, we split the domain Ω into two subdomains and an interface: $\Omega := \Omega^{\alpha} \cup \Gamma \cup \Omega^{\beta}$. The Hook's tensor $\mathbb{C}(x) = \alpha\,\mathbb{C}$ in Ω^{α} and $\mathbb{C}(x) = \beta\,\mathbb{C}$ in Ω^{β}, where $\mathbb{C}$ is a constant tensor. The solution in displacements $u(x)$ we also split into $u_{\alpha}(x)$ and $u_{\beta}(x)$. From the variational formulation of the transmission problem

$$\int_{\Omega} \sigma(u) \cdot \varepsilon(\varphi)\, d\Omega = \int_{\Omega} b \cdot \varphi\, d\Omega\,, \tag{3.173}$$

where $\sigma(u(x)) = \mathbb{C}(x)\varepsilon(u(x))$ is the Cauchy stress tensor and $\varepsilon(u(x))$ is the linearized Green strain tensor, and with the smooth vector test function $\varphi \in C_0^{\infty}(\Omega)$ we obtain

$$\int_{\Omega^{\alpha}} \sigma_{\alpha}(u_{\alpha}) \cdot \varepsilon(\varphi_{\alpha})\, d\Omega + \int_{\Omega^{\beta}} \sigma_{\beta}(u_{\beta}) \cdot \varepsilon(\varphi_{\beta})\, d\Omega = \int_{\Omega^{\alpha}} b_{\alpha} \cdot \varphi_{\alpha}\, d\Omega + \int_{\Omega^{\beta}} b_{\beta} \cdot \varphi_{\beta}\, d\Omega\,, \tag{3.174}$$

where $\sigma_{\alpha}(u_{\alpha}(x)) = \alpha\mathbb{C}\varepsilon(u_{\alpha}(x))$ and $\sigma_{\beta}(u_{\beta}(x)) = \beta\mathbb{C}\varepsilon(u_{\beta}(x))$. The transmission conditions on the interface come out from the continuity of the solution and of the tractions over the interface

$$u_{\alpha} = u_{\beta} \quad \text{and} \quad \sigma_{\alpha}(u_{\alpha})n = \sigma_{\beta}(u_{\beta})n\,, \tag{3.175}$$

where n is the exterior normal to Ω^{α}. Note that we have also considered a jump on the body force b of the form $b(x) = b_{\alpha}$ in Ω^{α} and $b(x) = b_{\beta}$ in Ω^{β}.

We determine the shape derivative of the variational problem with respect to the boundary variations of the interface. Analogously to the previous section, we have to write the above problem in the variable domain Ω_t. Then, by simple differentiation of this formulation with respect to t at $t = 0$, we obtain

$$\int_{\Omega^{\alpha}} \sigma_{\alpha}(u'_{\alpha}) \cdot \varepsilon(\varphi_{\alpha})\, d\Omega + \int_{\Omega^{\beta}} \sigma_{\beta}(u'_{\beta}) \cdot \varepsilon(\varphi_{\beta})\, d\Omega + \int_{\Gamma} \sigma_{\alpha}(u_{\alpha}) \cdot \varepsilon(\varphi_{\alpha})(\mathfrak{V} \cdot n)\, d\Gamma - \int_{\Gamma} \sigma_{\beta}(u_{\beta}) \cdot \varepsilon(\varphi_{\beta})(\mathfrak{V} \cdot n)\, d\Gamma = \int_{\Gamma} b_{\alpha}\varphi_{\alpha}(\mathfrak{V} \cdot n)\, d\Gamma - \int_{\Gamma} b_{\beta}\varphi_{\beta}(\mathfrak{V} \cdot n)\, d\Gamma\,, \tag{3.176}$$

where we have assumed that the boundary shape derivative of the test function on the interface for $t = 0$ is null. The above derivation requires the following additional explanation:

Note 3.3. We recall that, for a vector function $u(\Omega_t)(x) = u_t(x) = U(t,x)$ defined on the variable domain Ω_t, the domain shape derivative associated with the derivatives of volume integrals equals $u'(\Omega;\mathfrak{V})(x) = u'(x) := \partial_t U(0,x)$ in the reference domain Ω, in contrast with the boundary shape derivative of the same function written as $z(\Gamma_t)(x) = z_t(x) = U(t,x)$. For such a function depending on the surface $\Gamma_t = \partial\Omega_t$ the appropriate notion associated with the derivatives of surface integrals is called the displacement derivative given by $z'(\Gamma;\mathfrak{V})(x) = z'(x) := \partial_t U(0,x) + \partial_n U(0,x)(\mathfrak{V}\cdot n)$. From the definitions we get the relations with the material derivatives

$$\dot{u}(\Omega;\mathfrak{V}) = u'(\Omega;\mathfrak{V}) + (\nabla u)\mathfrak{V}, \tag{3.177}$$

$$\dot{z}(\Gamma;\mathfrak{V}) = z'(\Gamma;\mathfrak{V}) + (\nabla_\Gamma z)\mathfrak{V}. \tag{3.178}$$

Therefore, by taking into account that for the test function φ the displacement derivative $\varphi'(\Gamma;\mathfrak{V}) = \partial_n\varphi(\mathfrak{V}\cdot n)$ is null on Γ by our assumption, we get after integrations by parts, the transmission conditions on Γ for the shape derivative u'. Indeed, for a test function supported in Ω^α it follows that $\operatorname{div}\sigma_\alpha(u'_\alpha) = 0$ in Ω^α, and for a test function supported in Ω^β it follows that $\operatorname{div}\sigma_\beta(u'_\beta) = 0$ in Ω^β. Then the solution u' lives in $H^1(\Omega)$, which requires the continuity of displacements

$$u' := u'_\alpha = u'_\beta \quad \text{on} \quad \Gamma\,, \tag{3.179}$$

and from the variational formulation we obtain the nonhomogeneous transmission conditions for the tractions

$$\sigma_\alpha(u'_\alpha)n - \sigma_\beta(u'_\beta)n = (\alpha-\beta)\operatorname{div}_\Gamma\left((\mathfrak{V}\cdot n)\sigma_\Gamma(u)\right) + (b_\alpha - b_\beta)(\mathfrak{V}\cdot n)\,, \tag{3.180}$$

with $\sigma_\Gamma(u) := \mathbb{C}(\nabla_\Gamma u)^s$. Finally, given the shape derivative, we can find the shape gradient of the energy shape functional, which we leave as an exercise.

3.5 Material and Shape Derivatives for Kirchhoff Plates

In this section the material and shape derivatives for the fourth order linear elliptic equation are obtained. The derivation is performed in the same framework as in the case of the elasticity boundary value problems. In particular, the linear model of thin, solid elastic Kirchhoff plate is considered.

3.5.1 Problem Formulation

The static response of the plate $u = u(\Omega)$, with $\Omega \subset \mathbb{R}^2$, can be determined from the Kirchhoff plate model, namely

$$\begin{cases} -\mathrm{div}(\mathrm{div}M) = b \ \text{in} \ \Omega \ , \\ u = \partial_n u = 0 \ \text{on} \ \Gamma_0 \ , \\ u = M_{nn} = 0 \ \text{on} \ \Gamma_1 \ , \\ M_{nn} = Q = 0 \ \text{on} \ \Gamma_2 \ , \end{cases} \tag{3.181}$$

i.e. the plate is clamped, simply supported and free on the portions Γ_0, Γ_1 and Γ_2 of the boundary $\partial\Omega$, respectively. The following condition is assumed for simplicity

Condition 3.3. The sets $\overline{\Gamma}_i \cap \overline{\Gamma}_j = \emptyset$ for $i \neq j$, $i, j = 0, 1, 2$.

In (3.181), $M_{nn} = n \cdot Mn$ denotes the normal component of the moment and Q is the effective shear force given by

$$Q = -\partial_\tau M_{\tau n} - \mathrm{div}M \cdot n \ , \quad \text{with} \quad M_{\tau n} = \tau \cdot Mn \ . \tag{3.182}$$

In addition, we consider the following constitutive relation

$$M(u) = \mathbb{C}\nabla\nabla u \ . \tag{3.183}$$

For the fourth order tensor field $\mathbb{C} = \{c_{ijkl}\}$, with $c_{ijkl} \in C^2(\mathbb{R}^2)$, $i, j, k, l = 1, 2$, the usual symmetry conditions hold

$$c_{ijkl}(x) = c_{jikl}(x) = c_{klij}(x) \quad x \in \mathbb{R}^2, \quad i, j, k, l = 1, 2 \ . \tag{3.184}$$

Let us assume that there exists a constant $\alpha_0 > 0$ such that

$$\mathbb{C}\xi \cdot \xi = c_{ijkl}(x)\xi_{ij}\xi_{kl} \geqslant \alpha_0 \xi_{ij}\xi_{kl} = \alpha_0 \xi \cdot \xi \tag{3.185}$$

for all $x \in \mathbb{R}^2$ and for all second order symmetric tensors ξ. The problem (3.181) can be formulated in terms of the transversal displacement u as follows

$$\begin{cases} -\mathrm{div}(\mathrm{div}M(u)) = b & \text{in} \ \Omega \ , \\ M(u) = \mathbb{C}\nabla\nabla u \ , & \\ u = \partial_n u = 0 & \text{on} \ \Gamma_0 \ , \\ u = M_{nn}(u) = 0 & \text{on} \ \Gamma_1 \ , \\ M_{nn}(u) = Q(u) = 0 & \text{on} \ \Gamma_2 \ . \end{cases} \tag{3.186}$$

For a weak solution $u \in H^2(\Omega)$ to (3.181) the following integral identity is satisfied

$$u \in \mathscr{V} : a(u, \phi) = l(\phi) \quad \forall \phi \in \mathscr{V} \ , \tag{3.187}$$

where

$$\mathscr{V} = \{\phi \in H^2(\Omega) : \phi = 0 \ \text{on} \ \Gamma_0 \cup \Gamma_1, \ \partial_n u = 0 \ \text{on} \ \Gamma_0\} \ , \tag{3.188}$$

and

$$a(\varphi,\phi) = \int_{\Omega} \mathbb{C}\nabla\nabla\varphi \cdot \nabla\nabla\phi \, d\Omega \quad \forall \varphi,\phi \in H^2(\Omega)\,, \tag{3.189}$$

$$l(\phi) = \int_{\Omega} b\phi \, d\Omega\,. \tag{3.190}$$

The following Green's formula holds for $\varphi \in H^4(\Omega)$ and $\phi \in H^2(\Omega)$:

$$a(\varphi,\phi) = \int_{\Omega} \mathrm{div}(\mathrm{div} M(\varphi))\phi \, d\Omega + \int_{\Gamma} (Q(\varphi)\phi + M_{nn}(\varphi)\partial_n\phi) \, d\Gamma\,. \tag{3.191}$$

Using (3.191) the weak form of (3.181) can be defined, along with the nonhomogeneous boundary conditions prescribed on the portions Γ_0, Γ_1 and Γ_2 of the boundary. However, for the sake of simplicity we restrict our considerations to (3.181) with homogeneous boundary conditions.

3.5.2 Material Derivatives for the Kirchhoff Plate

Let $u_t \in \mathscr{V}_t$ denote a solution to (3.181) now defined in the variable domain $\Omega_t \subset \mathbb{R}^2$, with $\Omega_t = \mathfrak{T}_t(\mathfrak{V})(\Omega)$, for $t \in [0,\delta)$,

$$u_t \in \mathscr{V}_t : a_t(u_t,\phi) = l_t(\phi) \quad \forall \phi \in \mathscr{V}_t\,, \tag{3.192}$$

where

$$\mathscr{V}_t = \{\phi \in H^2(\Omega_t) : \phi = 0 \text{ on } \Gamma_0^t \cup \Gamma_1^t,\ \partial_{n_t}\phi = 0 \text{ on } \Gamma_0^t\}\,, \tag{3.193}$$

and

$$a_t(\varphi,\phi) = \int_{\Omega_t} \mathbb{C}\nabla\nabla\varphi \cdot \nabla\nabla\phi \, d\Omega_t \quad \forall \varphi,\phi \in \mathscr{V}_t\,, \tag{3.194}$$

$$l_t(\phi) = \int_{\Omega_t} b\phi \, d\Omega_t \quad \forall \phi \in \mathscr{V}_t\,. \tag{3.195}$$

First, the form of the material derivative is derived

$$\dot{u} = \lim_{t\to 0} \frac{1}{t}(u_t \circ \mathfrak{T}_t - u)\,. \tag{3.196}$$

From (3.192) it follows that $u^t = u_t \circ \mathfrak{T}_t \in H^2(\Omega)$ satisfies

$$u^t \in \mathscr{V} : a^t(u^t,\phi) = l^t(\phi) \quad \forall \phi \in \mathscr{V}\,, \tag{3.197}$$

where

$$a^t(\varphi,\phi) = \int_\Omega \mathbb{C}^t \xi^t(\varphi)\cdot\xi^t(\phi)\,d\Omega \quad \forall\varphi,\phi\in\mathscr{V}\,, \tag{3.198}$$

$$l^t(\phi) = \int_\Omega b^t\phi\,d\Omega \quad \forall\phi\in\mathscr{V}\,, \tag{3.199}$$

with

$$\xi^t(\varphi) = D((D\mathfrak{T}_t)^{-\top}D\varphi)(D\mathfrak{T}_t)^{-1}\,, \tag{3.200}$$

$$\mathbb{C}^t = \{c^t_{ijkl}\}, \quad c_{ijkl} = \mathfrak{g}(t)(c_{ijkl}\circ\mathfrak{T}_t)\,, \tag{3.201}$$

$$b^t = \mathfrak{g}(t)(b\circ\mathfrak{T}_t)\,. \tag{3.202}$$

Note 3.4. Since by Proposition 2.41 in [210] the mapping

$$[0,\delta)\ni t\mapsto b\circ\mathfrak{T}_t\in(\mathscr{V})' \tag{3.203}$$

is strongly differentiable, then the following result is a consequence of Theorem 4.30 of Chapter 4 in [210].

Theorem 3.4. *The strong material derivative for the Kirhchoff model is given by*

$$\dot{u}\in\mathscr{V}: a(\dot{u},\phi) = l'(\phi) - a'(u,\phi) \quad \forall\phi\in\mathscr{V}\,, \tag{3.204}$$

where

$$a'(\varphi,\phi) = \int_\Omega(\mathbb{C}\xi'(\varphi)\cdot\xi(\phi) + \mathbb{C}'\xi(\varphi)\cdot\xi(\phi) + \mathbb{C}\xi(\varphi)\cdot\xi'(\phi))\,d\Omega \qquad \forall\varphi,\phi\in\mathscr{V}\,, \tag{3.205}$$

and

$$l'(\phi) = \int_\Omega b'\xi(\phi)\,d\Omega \quad \forall\phi\in\mathscr{V}\,, \tag{3.206}$$

with

$$\xi'(\varphi) = -D((D\mathfrak{V})^\top D\varphi) - D(D\varphi)D\mathfrak{V}\,, \tag{3.207}$$

$$\mathbb{C}' = \{c'_{ijkl}\}, \quad c'_{ijkl} = \operatorname{div}(c_{ijkl}\mathfrak{V})\,, \tag{3.208}$$

$$\xi(\phi) = D(D\phi)\,, \tag{3.209}$$

$$b' = \operatorname{div}(b\mathfrak{V})\,. \tag{3.210}$$

Proof. The proof is left as an exercise. □

3.5.3 Shape Derivatives for the Kirchhoff Plate

Finally the form of the shape derivative u' is to be determined

$$u' = \dot{u} - \nabla u\cdot\mathfrak{V}\,. \tag{3.211}$$

It is supposed that

$$\nabla u \cdot \mathfrak{V} \in H^2(\Omega) , \tag{3.212}$$

then $u' \in H^2(\Omega)$.

Differentiating (3.192) with respect to t at $t = 0$, for the test functions $\phi \in H^2(\Omega_t)$ given by restrictions to Ω_t of $\phi \in H^2(\mathbb{R}^2)$, we have

$$\int_\Omega M' \cdot \nabla\nabla\phi \, d\Omega + \int_\Gamma v_n M \cdot \nabla\nabla\phi \, d\Gamma = \int_\Gamma v_n b\phi \, d\Gamma . \tag{3.213}$$

Here it is assumed that the trace of the source term b is well defined, that is $b \in L^2(\Gamma)$. Integration by parts of the first integral on the left hand side of (3.213), yields

$$\int_\Omega M' \cdot \nabla\nabla\phi \, d\Omega = \int_\Omega \mathrm{div}(\mathrm{div} M')\phi \, d\Omega + \int_\Gamma (M'n \cdot \nabla\phi - \mathrm{div} M' \cdot n\phi) \, d\Gamma . \tag{3.214}$$

It should be remarked that on $\Gamma = \partial\Omega$ we have

$$\nabla\phi = \nabla_\Gamma \phi + \partial_n \phi \, n . \tag{3.215}$$

Therefore, from integrating by parts on Γ we get

$$\begin{aligned}\int_\Gamma M'n \cdot \nabla\phi \, d\Gamma &= \int_\Gamma M'_{nn} \partial_n \phi \, d\Gamma + \int_\Gamma M'n \cdot \nabla_\Gamma \phi \, d\Gamma \\ &= \int_\Gamma (M'_{nn} \partial_n \phi - \mathrm{div}_\Gamma (M'n)\phi) \, d\Gamma \\ &= \int_\Gamma (M'_{nn} \partial_n \phi - \partial_\tau (M'_{\tau n})\phi) \, d\Gamma ,\end{aligned} \tag{3.216}$$

where $M'_{nn} = n \cdot M'n$ and $M'_{\tau n} = \tau \cdot M'n$. Let us consider an appropriate extension $\widetilde{n}$ of the normal vector field n on Γ with $\partial\widetilde{n}/\partial n = 0$, and ϕ such that $\partial^2\phi/\partial n^2 = 0$ on Γ. Then, integration by parts on Γ accomplished for the second term on the left hand side of (3.213) leads to

$$\int_\Gamma v_n M \cdot \nabla\nabla\phi \, d\Gamma = -\int_\Gamma (2\partial_\tau (v_n M_{\tau n}) \partial_n \phi - \partial_\tau (\partial_\tau (v_n M_{\tau\tau}))\phi) \, d\Gamma . \tag{3.217}$$

By considering the above results in (3.213) it follows that

$$\begin{aligned}&\int_\Omega \mathrm{div}(\mathrm{div} M')\phi \, d\Omega + \int_\Gamma (M'_{nn} - 2\partial_\tau (v_n M_{\tau n}))\partial_n \phi \, d\Gamma - \\ &\qquad \int_\Gamma (\partial_\tau (M'_{\tau n}) + \mathrm{div} M' \cdot n - \partial_\tau (\partial_\tau (v_n M_{\tau\tau})))\phi \, d\Gamma = \int_\Gamma v_n b\phi \, d\Gamma .\end{aligned} \tag{3.218}$$

Hence the *shape derivative* u' is a solution to the following boundary value problem

$$\begin{cases} -\mathrm{div}(\mathrm{div} M') = 0 & \text{in } \Omega\,, \\ u' = -v_n \partial_n u,\ \partial_n u' = -v_n \partial_n(\partial_n u) & \text{on } \Gamma_0\,, \\ u' = -v_n \partial_n u,\ M'_{nn} = 2\partial_\tau(v_n M_{\tau n}) & \text{on } \Gamma_1\,, \\ M'_{nn} = 2\partial_\tau(v_n M_{\tau n}),\ Q' = v_n b - \partial_\tau(\partial_\tau(v_n M_{\tau\tau})) & \text{on } \Gamma_2\,, \end{cases} \tag{3.219}$$

with $Q' = -\partial_\tau(M'_{\tau n}) - \mathrm{div} M' \cdot n$. The boundary conditions for u' and $\partial_n u'$ in (3.219) are derived from (3.211).

3.6 Material and Shape Derivatives in Fluid Mechanics

The velocity method of shape optimization is used in this chapter. We have no results on mathematical properties of the method, we refer the reader to [210] for the proofs. It turns out, that the properties of the method can be investigated in an elementary fashion by using the particular form of the change of variables defined by the adjugate matrix. Such a formalism is recently introduced and employed in fluid mechanics [196, 197]. It is important to mention, that within this formalism the evaluation of material derivatives can be performed for local solutions of the nonlinear problems including compressible Navier-Stokes equations [197]. The new method of shape sensitivity analysis proposed in [197] includes three steps. First the existence of material derivatives is proved by using the change of variables combined with the stability result of solutions with respect to the coefficients of differential operators. Then the shape derivatives are obtained by the singular limit passage in the formulae for the material derivatives. In the limit passage, the support of the shape velocity field is reduced to the moving boundary. We refer the reader to [196] for the mathematical analysis of the method for the drag minimization in the framework of the local, strong solutions for the nonhomogeneous, stationary, compressible flow problem. In particular, all results on shape sensitivity analysis are given with the complete proofs in Chapter 11 of the monograph [196].

Below the formal evaluations only of the material and shape derivatives of solutions to the homogeneous, stationary, compressible flow problem are presented. The *topological differentiability of the drag functional* in the case of such a flow governed by a *nonlinear elliptic & hyperbolic boundary value problem* can be analyzed. However, this is a new topic which is out of scope of the monograph, therefore, it is left to the motivated reader.

3.6.1 The Adjugate Matrix Concept

Now, we describe the proposed method in details in three spacial dimensions. As usually, the family of mappings $\mathfrak{T}_t : \Omega \to \Omega_t$ is introduced, parameterized by t. The mappings $\mathfrak{T}_t$ can be defined in many ways. First, we recall here the classic velocity method. Let $y = y(x,t)$ denote the solution to the system of ordinary differential equations

$$\begin{cases} \frac{d}{dt}y(x,t) = \mathfrak{V}(y(x,t),t) , \\ y(x,0) = x . \end{cases} \tag{3.220}$$

Then the mapping associated with the shape velocity field $\mathfrak{V}$ takes the form

$$\mathfrak{T}_t(x) := y(x,t) . \tag{3.221}$$

In the method employed in this section, we define the mapping

$$\mathfrak{T}_t(x) := x + t\mathfrak{T}(x) . \tag{3.222}$$

Therefore, the associated velocity field with the above mapping $\mathfrak{T}_t$ is uniquely determined

$$\mathfrak{V}(y,t) := \mathfrak{T}((1+t\mathfrak{T})^{-1}(y)) , \tag{3.223}$$

and we find that

$$\mathfrak{V}(x,0) := \mathfrak{T}(x) . \tag{3.224}$$

We introduce the *adjugate matrix* $N(x)$ for the Jacobian matrix $(\mathrm{I} + tD\mathfrak{T})(x)$

$$N(x) := \det((\mathrm{I} + tD\mathfrak{T})(x))((\mathrm{I} + tD\mathfrak{T})(x))^{-1}. \tag{3.225}$$

Remark 3.5. In Chapter 2 the velocity field is defined in the Lagrangian (material) coordinates. Here, the velocity field $\mathfrak{V}$ is written in the Eulerian (spatial) coordinates and uniquely determined by the mapping $\mathfrak{T}_t$.

3.6.1.1 Dependence of Adjugate Matrix N on Shape Parameter $t \to 0$

We are interested in the dependence of the adjugate matrix N of the Jacobian matrix $\mathrm{I} + tD\mathfrak{T}$ with respect to the small parameter $t \to 0$. To this end let us consider

$$\mathfrak{g}(x) = \sqrt{\det N} = \det(\mathrm{I} + tD\mathfrak{T}(x)) . \tag{3.226}$$

The characteristic equation (or secular equation) for a square matrix T is the equation in one variable s

$$\det(T - s\mathrm{I}) = \det T - I_2(T)s + \mathrm{tr}(T)s^2 - s^3 , \tag{3.227}$$

where $I_2(T)$ is the sum of the principal minors of the matrix T. Thus, it follows that

$$\mathfrak{g}(x) = \det(D\mathfrak{T}(x))t^3 + I_2(D\mathfrak{T}(x))t^2 + \mathrm{tr}(D\mathfrak{T}(x))t + 1 . \tag{3.228}$$

Therefore,

$$\mathfrak{g}(x) = 1 + \mathrm{tr}(D\mathfrak{T}(x))t + o(t) . \tag{3.229}$$

On the other hand, the elementary equality

$$\frac{1}{1-s} = 1 + s + s^2 + \cdots + s^k + \frac{s^{k+1}}{1-s} \tag{3.230}$$

leads to the Neumann series for the Jacobian matrix function

$$\begin{aligned}(\mathrm{I} + tD\mathfrak{T}(x))^{-1} &= \mathrm{I} - tD\mathfrak{T}(x) + t^2(D\mathfrak{T}(x))^2 + \\ &\cdots + (-1)^k(t)^k(D\mathfrak{T}(x))^k + (t)^{k+1}(D\mathfrak{T}(x))^{k+1}(\mathrm{I} + tD\mathfrak{T}(x))^{-1}\,. \end{aligned} \tag{3.231}$$

Proposition 3.12. *We have the following first order expansion of the adjugate matrix function N,*

$$N(x) = \mathrm{I} + tQ(x) + t^2\widetilde{Q}(x,t)\,, \tag{3.232}$$

where we denote

$$Q(x) := \mathrm{tr}(D\mathfrak{T}(x))\mathrm{I} - D\mathfrak{T}(x)\,, \tag{3.233}$$

and the remainder $o(t) := t^2\widetilde{Q}(x,t)$ *in* (3.232) *is obtained from* (3.229). *In addition, the derivatives with respect to* t *at* $t = 0$ *take the form*

$$\dot{N} := \frac{dN}{dt} = Q(x) \qquad \text{and} \qquad \dot{\mathfrak{g}} := \frac{d\mathfrak{g}}{dt} = \mathrm{div}\mathfrak{T}(x)\,. \tag{3.234}$$

3.6.1.2 Change of Variables in Stationary, Homogeneous, Compressible Navier-Stokes Problem

In this paragraph a stationary model of compressible gas is considered.

Let $(\overline{u}_t, \overline{\rho}_t)$ denote a solution to the following boundary value problem posed in variable domain Ω_t.

$$\begin{cases} \Delta u + \nabla \mathrm{div} u = \nabla p(\rho) + \rho b & \text{in } \Omega_t\,, \\ \mathrm{div}(\rho u) = 0 & \text{in } \Omega_t\,, \\ u = 0 & \text{on } \partial\Omega_t\,, \\ \dfrac{1}{|\Omega_t|}\displaystyle\int_{\Omega_t} \rho(y)\,dy = \mathfrak{m}\,. \end{cases} \tag{3.235}$$

In the model, u stands for the fluid velocity field, ρ is the density, $\mathfrak{m}|\Omega_t|$ is the mass of gas contained in Ω_t, and $\rho \mapsto p(\rho)$ is the pressure under constant temperature. We refer the reader to [194, 195] for the mathematical analysis of the boundary value problem (3.235), and to [196] for physical modeling of compressible gases.

We want to determine the equations for the couple (u_t, ρ_t) defined by

$$u_t(x) = N\overline{u}_t(x + t\mathfrak{T}(x)) \quad \text{and} \quad \rho_t(x) = \overline{\rho}_t(x + t\mathfrak{T}(x))\,, \tag{3.236}$$

in the unperturbed domain Ω, starting from the system (3.235). The procedure is divided into two steps. First, the equations for the couple

$$(\widetilde{u}(x),\widetilde{\rho}(x)) := (\overline{u}_t(y(x)),\overline{\rho}_t(y(x))) \tag{3.237}$$

are derived by a simple change of variables $y(x) := x+t\mathfrak{T}(x)$ in (3.235). Here the dependence of the couple $(\widetilde{u}(x),\widetilde{\rho}(x))$ on the shape parameter t is omitted. Then, in the second step of our procedure, by the replacement

$$(\widetilde{u}(x),\widetilde{\rho}(x)) := (N^{-1}u_t(x),\rho_t(x)) \; , \tag{3.238}$$

the equations for the unknown couple $(u_t(x),\rho_t(x))$ defined in the unperturbed domain Ω are identified. For the couple $(u_t(x),\rho_t(x))$ the differentiability with respect to the shape parameter t can be established, but it is out of the scope of the book. The reader interested on these mathematical aspects may refer to [197] for the general case of shape sensitivity analysis in compressible gas dynamics. Here, we present the change of variables technique for an example which is a representative model for fluid dynamics.

Lemma 3.3. *By the change of variables, the following boundary value problem is obtained for the couple* (u_t,ρ_t),

$$\begin{cases} \Delta u_t + \nabla(\mathfrak{g}^{-1}\mathrm{div} u_t - p(\rho_t)) = \mathscr{A}(\rho_t,u_t) & in\ \Omega\ , \\ \mathrm{div}(\rho_t u_t) = 0 & in\ \Omega\ , \\ u_t = 0 & on\ \partial\Omega\ , \\ \displaystyle\int_\Omega \rho_t(x)\mathfrak{g}(x)\,dx = \mathfrak{m}\int_\Omega \mathfrak{g}(x)\,dx\ . \end{cases} \tag{3.239}$$

Here, the linear operator $\mathscr{A}$ *is defined in terms of the adjugate matrix* N,

$$\mathscr{A}(\rho,u) = \rho\widetilde{b} + \Delta u - N^{-\top}\mathrm{div}(\mathfrak{g}^{-1}NN^{\top}\nabla(N^{-1}u)) \; . \tag{3.240}$$

Proof. For a function $\varphi(y)$, $y\in\Omega_t$, the composed function $\widetilde{\varphi}(x) := \varphi(y(x))$, $x\in\Omega$, with the transformation $\Omega \ni x \mapsto y(x) \in \Omega_t$ given by

$$y(x) = x+t\mathfrak{T}(x), \quad x\in\Omega, \quad y\in\Omega_t \; , \tag{3.241}$$

is defined in the unperturbed domain Ω. Since the transformation (3.241) explicitly depends on the shape parameter t, even if φ is defined by the restriction to Ω_t of a function defined over all space $\mathbb{R}^3$, the composed function $\widetilde{\varphi}(x)$ depends on the shape parameter, and its material derivative with respect to t is non-null, in general. Therefore, we multiply the equations (3.235) by smooth vector $\varphi(y)$ and scalar $\phi(y)$ test functions, with $y\in\Omega_t$, and integrate over Ω_t,

$$\int_{\Omega_t} (\Delta u + \nabla\mathrm{div} u - \nabla p(\rho))(y)\cdot\varphi(y)\,dy = \int_{\Omega_t} \rho(y)b(y)\cdot\varphi(y)\,dy\ , \tag{3.242}$$

$$\int_{\Omega_t} \mathrm{div}(\rho u)(y)\phi(y)\,dy = 0\ . \tag{3.243}$$

By the change of variables (3.241) we obtain the integral identities in Ω,

$$\int_\Omega (\rho b)(y(x)) \cdot \varphi(y(x)) \det M \, dx = \int_\Omega (\Delta u + \nabla \mathrm{div} u - \nabla p(\rho))(y(x)) \cdot \varphi(y(x)) \det M \, dx \,, \tag{3.244}$$

and

$$\int_\Omega \mathrm{div}(\rho u)(y(x)) \phi(y(x)) \det M \, dx = 0 \,. \tag{3.245}$$

The change of variables in the first integral of (3.244) is straightforward,

$$\int_\Omega \widetilde{\rho}(x) \widetilde{b}(x) \cdot \widetilde{\varphi}(x) \det M \, dx := \int_\Omega (\rho b)(y(x)) \cdot \varphi(y(x)) \det M \, dx \,. \tag{3.246}$$

Therefore, we make the change of variables in the remaining integrals. Now we transport the partial differential operators to the unperturbed domain. To this end the solutions of (3.235) are denoted by $u(y)$ and $\rho(y)$, $y \in \Omega_t$, and we have the following notation for the change of variables, its Jacobian, and the composed functions

$$y = x + t\mathfrak{T}(x),\ M(x) = \mathrm{I} + tD\mathfrak{T}(x),\ \widetilde{u}(x) = u(y(x)),\ \widetilde{\rho}(x) = \rho(y(x)), \tag{3.247}$$

and, we set

$$u_t(x) := N\widetilde{u}(x) \quad \text{and} \quad \rho_t(x) := \widetilde{\rho}(x) \,. \tag{3.248}$$

The Jacobian matrix M is given in terms of the matrix N by the relations

$$\det M = \sqrt{\det N} \equiv \mathfrak{g} \quad \text{and} \quad M = \mathfrak{g} N^{-1} \,. \tag{3.249}$$

For any function $\phi \in C^1(\Omega_t)$ we have $\nabla_y \phi = M^{-\top} \nabla_x \widetilde{\phi}$, where $\widetilde{\phi}(x) = \phi(y(x))$. It follows that the identities

$$\begin{aligned}
\int_\Omega (\mathrm{div}_y u)(y(x))\, \widetilde{\phi}(x) \det M \, dx &= \int_{\Omega_t} (\mathrm{div}_y u)(y) \phi(y) \, dy = -\int_{\Omega_t} u \cdot \nabla_y \phi \, dy \\
&= -\int_\Omega \widetilde{u} \cdot M^{-\top} \nabla_x \widetilde{\phi}(x) \det M \, dx \\
&= \int_\Omega \mathrm{div}_x((\det M) M^{-1} \widetilde{u})\, \widetilde{\phi}(x) \, dx
\end{aligned} \tag{3.250}$$

hold true for all $\phi \in C_0^\infty(\Omega_t)$. On the other hand, by (3.249) we have $(\det M) M^{-1} \widetilde{u} = u_t(x,t)$. This leads to the equalities

$$(\mathrm{div}_y u)(y(x)) = \mathfrak{g}^{-1} \mathrm{div}_x(N\widetilde{u}(x)) \equiv \mathfrak{g}^{-1} \mathrm{div}_x u_t(x) \,, \tag{3.251}$$

$$\mathrm{div}_y(\rho u)(y(x)) = \mathfrak{g}^{-1} \mathrm{div}_x(\rho_t u_t)(x) \,, \tag{3.252}$$

which imply the modified mass balance in equation (3.239). From the identity $M^{-\top} = \mathfrak{g}^{-1} N^{\top}$ we obtain

$$\nabla(\mathrm{div} u - p(\rho)) = \mathfrak{g}^{-1} N^{\top} \nabla(\mathfrak{g}^{-1} \mathrm{div} u_t - p(\rho_t)) \,. \tag{3.253}$$

In view of the identity $\Delta = \mathrm{div}\nabla$ we obtain

$$\begin{aligned} \Delta u(y) &= \mathfrak{g}^{-1} \mathrm{div}(N M^{-\top} \nabla \widetilde{u}) \\ &= \mathfrak{g}^{-1} \mathrm{div}(\mathfrak{g}^{-1} N N^{\top} \nabla(N^{-1} u_t)) \\ &= \mathfrak{g}^{-1} N^{\top} (\Delta u_t - \mathscr{A}(\rho_t, u_t)) \,, \end{aligned} \tag{3.254}$$

which concludes the proof. □

3.6.2 Shape Derivatives for the Stationary, Homogeneous Navier-Stokes Problem

The shape derivatives (u', ρ') are simply obtained from (3.235) by differentiation with respect to the shape parameter t at $t = 0$. In this differentiation the attention should be payed to the boundary conditions, here we have only homogeneous Dirichlet condition to be taken into account. Therefore, the *shape derivatives* (u', ρ') for the boundary value problem (3.235) are given by the system

$$\begin{cases} \Delta u' + \nabla \mathrm{div} u' = \nabla(p'(\rho)\rho') + \rho' b + \rho b' & \text{in } \Omega \,, \\ \mathrm{div}(\rho' u + \rho u') = 0 & \text{in } \Omega \,, \\ u' = -\partial_n u (\mathfrak{T} \cdot n) & \text{on } \partial\Omega \,, \\ \displaystyle\int_\Omega \rho'(x)\, dx = \int_{\partial\Omega} (\mathfrak{m} - \rho(x))(\mathfrak{T} \cdot n)\, ds(x) \,. \end{cases} \tag{3.255}$$

3.6.3 Material Derivatives for the Stationary, Homogeneous Navier-Stokes Problem

Since we have the relation

$$\overline{u}_t = N^{-1} u_t \,, \tag{3.256}$$

then the *material derivative* $\dot{u}$ is defined by the relation

$$\dot{u} := \frac{d\overline{u}_t}{dt} = -Qu + u_{,t} \,, \tag{3.257}$$

where $u_{,t}$ stands for the derivative

$$u_{,t} := \frac{du_t}{dt} \,. \tag{3.258}$$

The derivatives $(u_{,t}, \dot{\rho})$ are obtained from the boundary value problem (3.239) by simple differentiation with respect to the shape parameter t, at $t = 0$.

$$\begin{cases} \Delta u_{,t} + \nabla(-\mathrm{div}\mathfrak{T}\,\mathrm{div}u + \mathrm{div}u_{,t} - p'(\rho)\dot{\rho}) = \dot{\mathscr{A}}(\rho, \dot{\rho}, u) & \text{in } \Omega\,, \\ \mathrm{div}(\dot{\rho}u + \rho u_{,t}) = 0 & \text{in } \Omega\,, \\ u_{,t} = 0 & \text{on } \partial\Omega\,, \\ \int_\Omega \dot{\rho}(x)\,dx = \int_\Omega (\mathfrak{m} - \rho)\mathrm{div}\mathfrak{T}(x)\,dx\,. \end{cases} \tag{3.259}$$

Here, the linear operator $\dot{\mathscr{A}}$ is defined in terms of $\dot{N} = Q$,

$$\dot{\mathscr{A}}(\rho, \dot{\rho}, u) = \dot{\rho}b + \rho\dot{b} + Q\Delta u - \mathrm{div}[(-(\mathrm{div}\mathfrak{T})\mathrm{I} + Q + Q^\top)\nabla u] + \Delta(Qu)\,. \tag{3.260}$$

3.7 Exercises

Please derive using the adjugate matrix formalism the material derivatives for the following boundary value problems:

- Dirichlet Poisson equation.
- Neumann Poisson equation.
- Elasticity system.
- Kirchhoff plate problem.

Chapter 4
Singular Perturbations of Energy Functionals

The closed formulae for the topological derivatives are identified and a method for its evaluation is presented in this chapter. To this end the shape sensitivity analysis is combined with the asymptotic expansions of solutions to singularly perturbed elliptic boundary value problems.

The full proofs of the method for the specific boundary value problems necessarily include the compound asymptotic expansions of solutions in singularly perturbed geometrical domains. The proofs are relegated to Chapters 9 and 10 as well as to Appendices B, C and E for some selected problems.

In this chapter the topological derivatives for the energy shape functionals associated to a representative class of linear elliptic boundary value problems are obtained. Namely, scalar (Laplace) and vectorial (Navier) second-order partial differential equations and scalar fourth-order partial differential equation (Kirchhoff) are considered in a smooth, bounded domain Ω.

The domain is topologically perturbed by the nucleation of a small circular hole, as shown in fig. 4.1. Since $\Omega \subset \mathbb{R}^2$ is the original (unperturbed) domain, therefore, $\Omega_\varepsilon(\widehat{x}) = \Omega \setminus \overline{B_\varepsilon(\widehat{x})}$ is the topologically perturbed domain, where $B_\varepsilon(\widehat{x})$, with $\overline{B_\varepsilon} \Subset \Omega$, is a ball of radius ε and center at $\widehat{x} \in \Omega$ representing a circular hole.

In the particular case of circular holes, for a given $\widehat{x} \in \Omega$ and $0 < \varepsilon < \ell$, with $\ell := \operatorname{dist}(\widehat{x}, \partial\Omega)$, we can construct a shape change velocity field $\mathfrak{V}$ that represents an uniform expansion of $B_\varepsilon(\widehat{x})$. In fact, it is sufficient to define $\mathfrak{V}$ on the boundaries $\partial\Omega$ and ∂B_ε and consider the family of admissible fields for given centre $\widehat{x}$ and size ε of the singular perturbation $B_\varepsilon(\widehat{x})$

$$\mathscr{S}(\varepsilon,\widehat{x}) = \{\mathfrak{V} \in C_0^2(\Omega;\mathbb{R}^2) : \mathfrak{V}_{|\partial B_\varepsilon(\widehat{x})} = -n\} \,, \tag{4.1}$$

where $n = -(x - \widehat{x})/\varepsilon$, with $x \in \partial B_\varepsilon$, is the normal unit vector field pointing toward the center of the circular hole B_ε, as it can be seen in fig. 4.1. It means that for a given centre of the singular domain perturbation, the shape change velocity fields $\mathfrak{V}$ always belongs to the family of fields denoted, for the sake of simplicity, by

$$\mathscr{S}_\varepsilon := \bigcup_{\widehat{x}\in\Omega} \bigcup_{0<\varepsilon<\ell} \mathscr{S}(\varepsilon,\widehat{x}) \,. \tag{4.2}$$

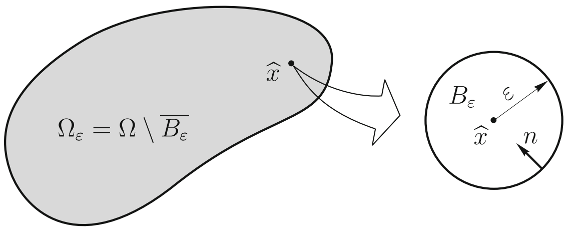


Fig. 4.1 Topologically perturbed domain by the nucleation of a small circular hole

By this construction of velocity fields $\mathfrak{V} \in \mathscr{S}_\varepsilon$ combined with Proposition 1.1, we can use the concept of shape derivatives as an intermediate step in the topological asymptotic analysis, leading to a simple and constructive method for evaluation of the topological derivatives through formula (1.49).

4.1 Second Order Elliptic Equation: The Poisson Problem

In this section we evaluate the topological derivative of the total potential energy associated to steady-state heat conduction problem, considering homogeneous Neumann and Dirichlet conditions on the boundary of the hole ∂B_ε.

4.1.1 *Problem Formulation*

The shape functional in the unperturbed domain Ω is given by

$$\psi(\chi) := \mathscr{J}_\Omega(u) = \frac{1}{2}\int_\Omega \|\nabla u\|^2 - \int_\Omega bu + \int_{\Gamma_N} \overline{q}u \, , \tag{4.3}$$

where the scalar function u is the solution to the variational problem:

$$\begin{cases} \text{Find } u \in \mathscr{U}, \text{ such that} \\ \displaystyle\int_\Omega \nabla u \cdot \nabla \eta = \int_\Omega b\eta - \int_{\Gamma_N} \overline{q}\eta \quad \forall \eta \in \mathscr{V} \, . \end{cases} \tag{4.4}$$

In the above equation, b is a source-term assumed to be constant everywhere. The set $\mathscr{U}$ and the space $\mathscr{V}$ are respectively defined as

$$\mathscr{U} := \{\varphi \in H^1(\Omega) : \varphi_{|_{\Gamma_D}} = \overline{u}\} \, , \tag{4.5}$$

$$\mathscr{V} := \{\varphi \in H^1(\Omega) : \varphi_{|_{\Gamma_D}} = 0\} \, . \tag{4.6}$$

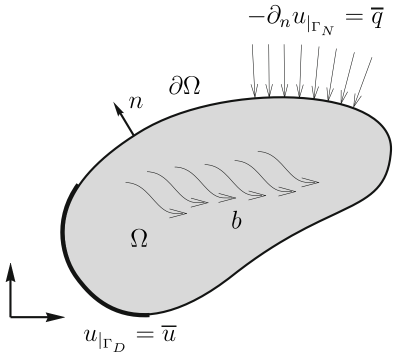


Fig. 4.2 The Poisson problem defined in the unperturbed domain Ω

In addition, $\partial\Omega = \overline{\Gamma}_D \cup \overline{\Gamma}_N$ with $\Gamma_D \cap \Gamma_N = \varnothing$, where Γ_D and Γ_N are Dirichlet and Neumann boundaries, respectively. Thus $\overline{u}$ is a Dirichlet data on Γ_D and $\overline{q}$ is a Neumann data on Γ_N, both functions are assumed to be smooth enough. See the details in fig. 4.2. The strong formulation associated to the variational problem (4.4) leads to the so-called Poisson equation, namely:

$$\begin{cases} \text{Find } u, \text{ such that} \\ \quad -\Delta u = b \ \text{ in } \ \Omega \ , \\ \qquad u = \overline{u} \text{ on } \Gamma_D \ , \\ -\partial_n u = \overline{q} \text{ on } \Gamma_N \ . \end{cases} \tag{4.7}$$

Now, let us state the same problem in the perturbed domain Ω_ε. In this case, the total potential energy reads

$$\psi(\chi_\varepsilon) := \mathscr{J}_{\Omega_\varepsilon}(u_\varepsilon) = \frac{1}{2}\int_{\Omega_\varepsilon} \|\nabla u_\varepsilon\|^2 - \int_{\Omega_\varepsilon} b u_\varepsilon + \int_{\Gamma_N} \overline{q} u_\varepsilon \ , \tag{4.8}$$

where the scalar function u_ε solves the variational problem:

$$\begin{cases} \text{Find } u_\varepsilon \in \mathscr{U}_\varepsilon, \text{ such that} \\ \displaystyle\int_{\Omega_\varepsilon} \nabla u_\varepsilon \cdot \nabla \eta = \int_{\Omega_\varepsilon} b\eta - \int_{\Gamma_N} \overline{q}\eta \quad \forall \eta \in \mathscr{V}_\varepsilon \ . \end{cases} \tag{4.9}$$

The set $\mathscr{U}_\varepsilon$ and the space $\mathscr{V}_\varepsilon$ must be defined according to the boundary condition on ∂B_ε. In particular, we have

$$\mathscr{U}_\varepsilon := \{\varphi \in H^1(\Omega_\varepsilon) : \varphi_{|_{\Gamma_D}} = \overline{u},\ \beta\varphi_{|_{\partial B_\varepsilon}} = 0\} \ , \tag{4.10}$$

$$\mathscr{V}_\varepsilon := \{\varphi \in H^1(\Omega_\varepsilon) : \varphi_{|_{\Gamma_D}} = 0,\ \beta\varphi_{|_{\partial B_\varepsilon}} = 0\} \ , \tag{4.11}$$

with $\beta \in \{0,1\}$. This notation have to be understood as follows:

- When $\beta = 1$, we have homogeneous Dirichlet boundary condition on ∂B_ε, since $u_\varepsilon = 0$ and $\eta = 0$ on ∂B_ε.

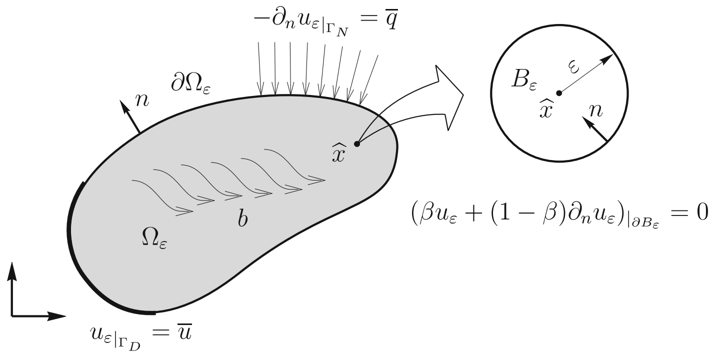


Fig. 4.3 The Poisson problem defined in the perturbed domain Ω_ε

- When $\beta = 0$, u_ε and η are free on the boundary of the hole ∂B_ε, then we have homogeneous Neumann boundary condition on ∂B_ε.

The *strong formulation* associated to the variational problem (4.9) reads (see the details in fig. 4.3):

$$\begin{cases} \text{Find } u_\varepsilon, \text{ such that} \\ \qquad -\Delta u_\varepsilon = b \text{ in } \Omega_\varepsilon \,, \\ \qquad u_\varepsilon = \overline{u} \text{ on } \Gamma_D \,, \\ \qquad -\partial_n u_\varepsilon = \overline{q} \text{ on } \Gamma_N \,, \\ \beta u_\varepsilon + (1-\beta)\partial_n u_\varepsilon = 0 \text{ on } \partial B_\varepsilon \,. \end{cases} \tag{4.12}$$

4.1.2 Shape Sensitivity Analysis

In order to apply the result presented in Proposition 1.1, we need to evaluate the shape derivative of functional $\mathscr{J}_{\Omega_\varepsilon}(u_\varepsilon)$ with respect to an uniform expansion of the hole B_ε. Before starting, let us introduce the *Eshelby energy-momentum tensor* [57] of the form

$$\Sigma_\varepsilon = \frac{1}{2}(\|\nabla u_\varepsilon\|^2 - 2bu_\varepsilon)\mathrm{I} - \nabla u_\varepsilon \otimes \nabla u_\varepsilon \,. \tag{4.13}$$

Therefore, we can state the following result:

Proposition 4.1. *Let $\mathscr{J}_{\Omega_\varepsilon}(u_\varepsilon)$ be the shape functional defined by (4.8). Then, the derivative of this functional with respect to the small parameter ε is given by*

$$\dot{\mathscr{J}}_{\Omega_\varepsilon}(u_\varepsilon) = \int_{\Omega_\varepsilon} \Sigma_\varepsilon \cdot \nabla \mathfrak{V} \,, \tag{4.14}$$

where $\mathfrak{V}$ is the shape change velocity field defined through (4.2) and Σ_ε is the Eshelby energy-momentum tensor given by (4.13).

Proof. We want to differentiate the function $(0,\varepsilon_0] \ni \varepsilon \mapsto \mathscr{J}_{\Omega_\varepsilon}(u_\varepsilon) \in \mathbb{R}$ at $\varepsilon > 0$. Thus, by making use of the Reynolds' transport theorem through formula (2.84), the shape derivative (the material or total derivative with respect to the parameter ε) of the functional (4.8) is given by

$$\dot{\mathscr{J}}_{\Omega_\varepsilon}(u_\varepsilon) = \frac{1}{2}\int_{\Omega_\varepsilon} ((\|\nabla u_\varepsilon\|^2)^{\cdot} + \|\nabla u_\varepsilon\|^2 \mathrm{div}\mathfrak{V}) - \int_{\Omega_\varepsilon} b(\dot{u}_\varepsilon + u_\varepsilon \mathrm{div}\mathfrak{V}) + \int_{\Gamma_N} \overline{q}\dot{u}_\varepsilon \,, \tag{4.15}$$

since Γ_N remains fixed according to (4.2). Next, by using the concept of material derivative of spatial fields through formula (2.89), we find that the first term of the above right hand side integral can be written as

$$\begin{aligned}(\|\nabla u_\varepsilon\|^2)^{\cdot} &= (\nabla u_\varepsilon \cdot \nabla u_\varepsilon)^{\cdot} \\ &= 2\nabla u_\varepsilon \cdot \nabla \dot{u}_\varepsilon - 2\nabla\mathfrak{V}^\top \nabla u_\varepsilon \cdot \nabla u_\varepsilon \\ &= 2\nabla u_\varepsilon \cdot \nabla \dot{u}_\varepsilon - 2(\nabla u_\varepsilon \otimes \nabla u_\varepsilon)\cdot \nabla\mathfrak{V} \,. \end{aligned} \tag{4.16}$$

From these last results we obtain

$$\dot{\mathscr{J}}_{\Omega_\varepsilon}(u_\varepsilon) = \frac{1}{2}\int_{\Omega_\varepsilon} ((\|\nabla u_\varepsilon\|^2 - 2bu_\varepsilon)\mathrm{I} - 2\nabla u_\varepsilon \otimes \nabla u_\varepsilon)\cdot \nabla\mathfrak{V} + \int_{\Omega_\varepsilon} \nabla u_\varepsilon \cdot \nabla \dot{u}_\varepsilon - \int_{\Omega_\varepsilon} b\dot{u}_\varepsilon + \int_{\Gamma_N} \overline{q}\dot{u}_\varepsilon \,, \tag{4.17}$$

where we have made use of the identity $\mathrm{div}\mathfrak{V} = \mathrm{I}\cdot\nabla\mathfrak{V}$. Since $\dot{u}_\varepsilon$ is a variation of u_ε in the direction of the velocity field $\mathfrak{V}$, then $\dot{u}_\varepsilon \in \mathscr{V}_\varepsilon$ [210]. Finally, by taking $\dot{u}_\varepsilon$ as test function in the variational problem (4.9), we have that the last three terms of the above equation vanish. □

Now, we can prove that the shape derivative of the functional $\mathscr{J}_{\Omega_\varepsilon}(u_\varepsilon)$ can be written in terms of quantities concentrated on the boundary $\partial\Omega_\varepsilon$. In fact, the following result holds:

Proposition 4.2. *Let $\mathscr{J}_{\Omega_\varepsilon}(u_\varepsilon)$ be the shape functional defined by (4.8). Then, the derivative of this functional with respect to the small parameter ε is given by*

$$\dot{\mathscr{J}}_{\Omega_\varepsilon}(u_\varepsilon) = \int_{\partial\Omega_\varepsilon} \Sigma_\varepsilon n \cdot \mathfrak{V} \,, \tag{4.18}$$

where $\mathfrak{V}$ is the shape change velocity field defined through (4.2) and tensor Σ_ε is given by (4.13).

Proof. From the tensor relation (G.23) and by applying the divergence theorem (G.32) in (4.14), we have

$$\dot{\mathscr{J}}_{\Omega_\varepsilon}(u_\varepsilon) = \int_{\partial\Omega_\varepsilon} \Sigma_\varepsilon n \cdot \mathfrak{V} - \int_{\Omega_\varepsilon} \mathrm{div}\Sigma_\varepsilon \cdot \mathfrak{V} \,. \tag{4.19}$$

Let us evaluate the divergence of the Eshelby tensor (4.13). Then, from (G.20), (G.22) and (G.24), we obtain

$$\begin{aligned}\operatorname{div}\Sigma_\varepsilon &= \frac{1}{2}\nabla(\nabla u_\varepsilon\cdot\nabla u_\varepsilon - 2bu_\varepsilon) - \operatorname{div}(\nabla u_\varepsilon\otimes\nabla u_\varepsilon)\\ &= (\nabla\nabla u_\varepsilon)^\top\nabla u_\varepsilon - b\nabla u_\varepsilon - \nabla u_\varepsilon\operatorname{div}\nabla u_\varepsilon - (\nabla\nabla u_\varepsilon)\nabla u_\varepsilon\\ &= (\nabla\nabla u_\varepsilon)^\top\nabla u_\varepsilon - (\nabla\nabla u_\varepsilon)\nabla u_\varepsilon - (\Delta u_\varepsilon + b)\nabla u_\varepsilon\,. \end{aligned}\tag{4.20}$$

Thus, since $\nabla\nabla u_\varepsilon = (\nabla\nabla u_\varepsilon)^\top$ and taking into account that u_ε is the solution to the state equation (4.12), namely, $-\Delta u_\varepsilon = b$, we observe that

$$\int_{\Omega_\varepsilon}\operatorname{div}\Sigma_\varepsilon\cdot\mathfrak{V} = 0 \qquad \forall\mathfrak{V}\,, \tag{4.21}$$

which leads to the result. □

Remark 4.1. The proof of Proposition 4.2 requires more regularity of solution u_ε than in its variational form (4.9), namely we need $u_\varepsilon\in H^2(\Omega_\varepsilon)$ instead of $u_\varepsilon\in H^1(\Omega_\varepsilon)$. On the other hand, this requirement can be weakened by proving (4.21) from variational arguments. This task we leave as an exercise.

Corollary 4.1. *According to the obtained result in Proposition 4.2, we have*

$$\dot{\mathscr{J}}_{\Omega_\varepsilon}(u_\varepsilon) = \int_{\partial\Omega_\varepsilon}\Sigma_\varepsilon n\cdot\mathfrak{V} = \int_{\partial B_\varepsilon}\Sigma_\varepsilon n\cdot\mathfrak{V} + \int_{\partial\Omega}\Sigma_\varepsilon n\cdot\mathfrak{V}\,. \tag{4.22}$$

Since we are dealing with an uniform expansion of the circular hole, then by taking into account the associated velocity field defined through (4.2), namely, $\mathfrak{V} = -n$ on ∂B_ε and $\mathfrak{V} = 0$ on $\partial\Omega$, we finally obtain for $\varepsilon > 0$ small enough

$$\frac{d}{d\varepsilon}\psi(\chi_\varepsilon) = \dot{\mathscr{J}}_{\Omega_\varepsilon}(u_\varepsilon) = -\int_{\partial B_\varepsilon}\Sigma_\varepsilon n\cdot n\,. \tag{4.23}$$

From the above corollary, we observe that the *distributed* shape gradient originally defined in the whole domain Ω_ε leads to the *boundary* shape gradient given by an integral defined only on the boundary of the hole ∂B_ε. In particular, the shape derivative of functional $\mathscr{J}_{\Omega_\varepsilon}(u_\varepsilon)$, given by the final formula (4.23), is written in terms of quantities concentrated on ∂B_ε. It means that we need to know the asymptotic behavior of the solution u_ε with respect to ε in the neighborhood of the hole B_ε. We will see later that this result simplifies enormously the next steps of the topological derivative calculation.

Remark 4.2. The final formula (4.23) is conform to the *Hadamard's structure theorem* [210]. This obtained expression for the boundary shape gradient is in general only a distribution, however, under appropriate regularity assumptions the boundary shape gradient for elliptic problems becomes a function, as well. More precisely, here we have assumed that $\Sigma_\varepsilon\in L^2(\Omega_\varepsilon;\mathbb{R}^2\times\mathbb{R}^2)$. Since $\mathfrak{V}$ is a smooth vector field, the shape gradient can be given by a distribution and, (4.23) is written in the form of a duality paring on ∂B_ε. Then the order of the distribution is one. On the other hand, by the *elliptic regularity* we can always require the regularity of the boundary as well as the data $b, \overline{u}$ and $\overline{q}$, which makes the gradient ∇u_ε on ∂B_ε to be a function, and Σ_ε is a function.

4.1.3 Asymptotic Analysis of the Solution

The shape derivative of functional $\mathscr{J}_{\Omega_\varepsilon}(u_\varepsilon)$ is given exclusively in terms of an integral over the boundary of the hole ∂B_ε (4.23). Therefore, in order to apply the result of Proposition 1.1, we need to know the behavior of the function u_ε with respect to ε in the neighborhood of the hole B_ε. In particular, once we know this behavior explicitly, we can identify function $f(\varepsilon)$ and perform the limit passage $\varepsilon \to 0$ in (1.49) to obtain the final formula for the topological derivative $\mathscr{T}$ of the shape functional ψ. However, in general it is not an easy task. In fact, we need to perform the asymptotic analysis of u_ε with respect to ε. In this section we present the formal calculation of the expansions of the solution u_ε associated to both Neumann and Dirichlet boundary conditions on ∂B_ε. For a rigorous justification of the asymptotic expansions of u_ε, the reader may refer to the book by Kozlov et al. 1999 [120], for instance. For the general theory on asymptotic analysis of solutions in singularly perturbed domains we refer the reader to the book by Mazja, Nasarow and Plamenewski, 1991 [148].

4.1.3.1 Neumann Condition on the Boundary of the Hole

For the case $\beta = 0$ in (4.12), let us propose an *ansätz* for the expansion of u_ε in the form [120, 148]

$$\begin{aligned} u_\varepsilon(x) &= u(x) + \varepsilon w(\varepsilon^{-1}x) + \widetilde{u}_\varepsilon(x) \\ &= u(\widehat{x}) + \nabla u(\widehat{x}) \cdot (x - \widehat{x}) + \frac{1}{2} \nabla\nabla u(y)(x - \widehat{x}) \cdot (x - \widehat{x}) \\ &+ \varepsilon w(\varepsilon^{-1}x) + \widetilde{u}_\varepsilon(x) \ , \end{aligned} \tag{4.24}$$

where y is an intermediate point between x and $\widehat{x}$. On the boundary of the hole ∂B_ε we have $\partial_n u_\varepsilon|_{\partial B_\varepsilon} = 0$. Thus, the normal derivative of the above expansion, evaluated on ∂B_ε, leads to

$$\nabla u(\widehat{x}) \cdot n - \varepsilon \nabla\nabla u(y) n \cdot n + \varepsilon \partial_n w(\varepsilon^{-1}x) + \partial_n \widetilde{u}_\varepsilon(x) = 0 \ . \tag{4.25}$$

Thus, we can choose w such that

$$\varepsilon \partial_n w(\varepsilon^{-1}x) = -\nabla u(\widehat{x}) \cdot n \quad \text{on} \quad \partial B_\varepsilon \ . \tag{4.26}$$

In the new variable $\xi = \varepsilon^{-1}x$, which implies $\nabla_\xi w(\xi) = \varepsilon \nabla w(\varepsilon^{-1}x)$, the following exterior problem is considered, and formally obtained as $\varepsilon \to 0$:

$$\begin{cases} \text{Find } w, \text{ such that} \\ \quad \Delta_\xi w = 0 \qquad\qquad \text{in } \mathbb{R}^2 \setminus \overline{B_1}\ , \\ \qquad w \to 0 \qquad\qquad \text{at } \infty\ , \\ \nabla_\xi w \cdot n = -\nabla u(\widehat{x}) \cdot n \text{ on } \partial B_1\ . \end{cases} \tag{4.27}$$

The above boundary value problem admits an explicit solution, namely

$$w(\varepsilon^{-1}x) = \frac{\varepsilon}{\|x - \widehat{x}\|^2} \nabla u(\widehat{x}) \cdot (x - \widehat{x})\ . \tag{4.28}$$

Now we can construct $\widetilde{u}_\varepsilon$ in such a way that it compensates the discrepancies introduced by the higher-order terms in ε as well as by the boundary-layer w on the exterior boundary $\partial\Omega$. It means that the remainder $\widetilde{u}_\varepsilon$ must be solution to the following boundary value problem:

$$\begin{cases} \text{Find } \widetilde{u}_\varepsilon, \text{ such that} \\ \Delta \widetilde{u}_\varepsilon = 0 \qquad\qquad \text{in } \Omega_\varepsilon\ , \\ \quad \widetilde{u}_\varepsilon = -\varepsilon w \qquad \text{on } \Gamma_D\ , \\ \partial_n \widetilde{u}_\varepsilon = -\varepsilon \partial_n w \qquad \text{on } \Gamma_N\ , \\ \partial_n \widetilde{u}_\varepsilon = \varepsilon \nabla\nabla u(y) n \cdot n \text{ on } \partial B_\varepsilon\ , \end{cases} \tag{4.29}$$

where, under appropriate regularity assumption [148], clearly $\widetilde{u}_\varepsilon = O(\varepsilon)$. However, this estimate can be improved [120, 148], namely $\widetilde{u}_\varepsilon = O(\varepsilon^2)$, and the *expansion* for u_ε reads

$$u_\varepsilon(x) = u(x) + \frac{\varepsilon^2}{\|x - \widehat{x}\|^2} \nabla u(\widehat{x}) \cdot (x - \widehat{x}) + O(\varepsilon^2)\ . \tag{4.30}$$

4.1.3.2 Dirichlet Condition on the Boundary of the Hole

For the case $\beta = 1$ in (4.12), initially we consider the following *ansätz* for the expansion of u_ε [120, 148]

$$\begin{aligned} u_\varepsilon(x) &= u(x) + v_\varepsilon(x) + \varepsilon w(\varepsilon^{-1}x) + \widetilde{u}_\varepsilon(x) \\ &= u(\widehat{x}) + \nabla u(\widehat{x}) \cdot (x - \widehat{x}) + \frac{1}{2} \nabla\nabla u(y)(x - \widehat{x}) \cdot (x - \widehat{x}) \\ &+ v_\varepsilon(x) + \varepsilon w(\varepsilon^{-1}x) + \widetilde{u}_\varepsilon(x)\ , \end{aligned} \tag{4.31}$$

where y is an intermediate point between x and $\widehat{x}$. In addition, the function v_ε is defined as

$$v_\varepsilon(x) = \alpha(\varepsilon) u(\widehat{x}) G(x)\ . \tag{4.32}$$

The function G is the solution to the following boundary value problem:

$$\begin{cases} \text{Find } G \text{, such that} \\ -\Delta G = \delta(x-\widehat{x}) & \text{in } \Omega\,, \\ G = 0 & \text{on } \Gamma_D\,, \\ \partial_n G = 0 & \text{on } \Gamma_N\,, \end{cases} \tag{4.33}$$

which, by means of the *fundamental solution* for the Laplacian, admits a representation in the neighborhood of the point $\widehat{x} \in \Omega$ of the form

$$G(x) = -\left(\frac{1}{2\pi}\log\|x-\widehat{x}\| + g(x)\right), \quad \text{with} \quad \|x-\widehat{x}\| > 0\,, \tag{4.34}$$

where g is harmonic in $\overline{\Omega}$ and must compensate the discrepancy on $\partial\Omega$ introduced by the above representation, that is, g is the solution of the auxiliary boundary value problem:

$$\begin{cases} \text{Find } g \text{, such that} \\ \Delta g = 0 & \text{in } \Omega\,, \\ g = -(2\pi)^{-1}\log\|x-\widehat{x}\| & \text{on } \Gamma_D\,, \\ \partial_n g = -(2\pi)^{-1}\dfrac{x-\widehat{x}}{\|x-\widehat{x}\|^2}\cdot n & \text{on } \Gamma_N\,. \end{cases} \tag{4.35}$$

On the boundary of the hole ∂B_ε we have $u_{\varepsilon|_{\partial B_\varepsilon}} = 0$. Thus, the expansion for u_ε, evaluated on ∂B_ε, leads to

$$\begin{aligned} &u(\widehat{x}) - \varepsilon\nabla u(\widehat{x})\cdot n + \varepsilon^2\nabla\nabla u(y)n\cdot n - \\ &\qquad \alpha(\varepsilon)u(\widehat{x})\left(\frac{1}{2\pi}\log\varepsilon + g(\widehat{x}) - \varepsilon\nabla g(\widehat{x})\cdot n + \varepsilon^2\nabla\nabla g(z)n\cdot n\right) + \\ &\qquad\qquad \varepsilon w\left(\varepsilon^{-1}x\right) + \widetilde{u}_\varepsilon(x) = 0\,, \end{aligned} \tag{4.36}$$

where z is an intermediate point between x and $\widehat{x}$. In addition, we have used the regularity of function g around $\widehat{x}$. Now we can construct $\widetilde{u}_\varepsilon$ in such a way that it compensates the discrepancy introduced by the higher-order terms in ε, namely

$$\widetilde{u}_\varepsilon(x) = \varepsilon^2(\alpha(\varepsilon)u(\widehat{x})\nabla\nabla g(z)n - \nabla\nabla u(y)n)\cdot n \quad \text{on} \quad \partial B_\varepsilon\,. \tag{4.37}$$

Furthermore, in the new variable $\xi = \varepsilon^{-1}x$ function w is solution of the exterior problem:

$$\begin{cases} \text{Find } w \text{, such that} \\ \Delta_\xi w = 0 & \text{in } \mathbb{R}^2 \setminus \overline{B_1} \\ w \to 0 & \text{at } \infty \\ w = (\nabla u(\widehat{x}) - \alpha(\varepsilon)u(\widehat{x})\nabla g(\widehat{x}))\cdot n & \text{on } \partial B_1 \end{cases} \tag{4.38}$$

which has a closed solution, given by

$$w(\varepsilon^{-1}x) = -\frac{\varepsilon}{\|x-\widehat{x}\|^2}(\nabla u(\widehat{x}) - \alpha(\varepsilon)u(\widehat{x})\nabla g(\widehat{x}))\cdot(x-\widehat{x})\,. \tag{4.39}$$

Thus, the previous expansion (4.36) reduces itself to

$$u(\widehat{x}) - \alpha(\varepsilon)u(\widehat{x})\left(\frac{1}{2\pi}\log\varepsilon + g(\widehat{x})\right) = 0 \quad \text{on} \quad \partial B_\varepsilon\ , \tag{4.40}$$

which can be solved in terms of $\alpha(\varepsilon)$, leading to

$$\alpha(\varepsilon) = \frac{2\pi}{\log\varepsilon + 2\pi g(\widehat{x})}\ . \tag{4.41}$$

Finally, function $\widetilde{u}_\varepsilon$ is constructed in such a way that it compensates the discrepancy introduced by the previous terms of the expansion for u_ε, thus $\widetilde{u}_\varepsilon$ solves:

$$\begin{cases} \text{Find } \widetilde{u}_\varepsilon, \text{ such that} \\ \Delta\widetilde{u}_\varepsilon = 0 & \text{in } \Omega_\varepsilon\ , \\ \widetilde{u}_\varepsilon = -\varepsilon w & \text{on } \Gamma_D\ , \\ \partial_n\widetilde{u}_\varepsilon = -\varepsilon\partial_n w & \text{on } \Gamma_N\ , \\ \widetilde{u}_\varepsilon = \varepsilon^2(\alpha(\varepsilon)u(\widehat{x})\nabla\nabla g(z)n - \nabla\nabla u(y)n)\cdot n & \text{on } \partial B_\varepsilon\ , \end{cases} \tag{4.42}$$

where y and z are intermediate points between x and $\widehat{x}$. Under appropriate regularity assumption [148], clearly $\widetilde{u}_\varepsilon = O(\varepsilon^2)$, since $w = O(\varepsilon)$ on the exterior boundary $\partial\Omega$. Therefore, the *expansion* for u_ε reads

$$\begin{aligned} u_\varepsilon(x) &= u(x) - \alpha(\varepsilon)u(\widehat{x})\left(\frac{1}{2\pi}\log\|x-\widehat{x}\| + g(x)\right) \\ &\quad - \frac{\varepsilon^2}{\|x-\widehat{x}\|^2}\left(\nabla u(\widehat{x}) - \alpha(\varepsilon)u(\widehat{x})\nabla g(\widehat{x})\right)\cdot(x-\widehat{x}) + O(\varepsilon^2)\ , \end{aligned} \tag{4.43}$$

with $\alpha(\varepsilon)$ given by (4.41).

4.1.4 Topological Derivative Evaluation

From an orthonormal curvilinear coordinate system n and τ on the boundary ∂B_ε (see fig. 4.4), the gradient ∇u_ε can be decomposed into its normal and tangential components, that is

$$\nabla u_{\varepsilon|_{\partial B_\varepsilon}} = (\partial_n u_\varepsilon)n + (\partial_\tau u_\varepsilon)\tau\ . \tag{4.44}$$

Therefore, on the boundary of the hole ∂B_ε we observe that

$$\begin{aligned} \Sigma_\varepsilon n\cdot n_{|_{\partial B_\varepsilon}} &= \frac{1}{2}(\|\nabla u_\varepsilon\|^2 - 2bu_\varepsilon)\mathrm{I}n\cdot n - (\nabla u_\varepsilon\otimes\nabla u_\varepsilon)n\cdot n \\ &= \frac{1}{2}(\|\nabla u_\varepsilon\|^2 - 2bu_\varepsilon) - (\nabla u_\varepsilon\cdot n)^2 \\ &= \frac{1}{2}((\partial_n u_\varepsilon)^2 + (\partial_\tau u_\varepsilon)^2 - 2bu_\varepsilon) - (\partial_n u_\varepsilon)^2 \\ &= \frac{1}{2}((\partial_\tau u_\varepsilon)^2 - (\partial_n u_\varepsilon)^2 - 2bu_\varepsilon)\ . \end{aligned} \tag{4.45}$$

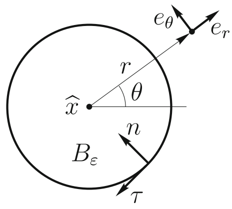


Fig. 4.4 Polar coordinate system (r,θ) centered at the point $\widehat{x} \in \Omega$

Now, we shall analyze the behavior of the total potential energy with respect to the parameter ε by taking into account each type of boundary condition on ∂B_ε, namely, Neumann ($\beta = 0$) and Dirichlet ($\beta = 1$).

4.1.4.1 Neumann Condition on the Boundary of the Hole

By taking $\beta = 0$ in (4.12), we have homogeneous Neumann boundary condition on ∂B_ε, namely $\partial_n u_\varepsilon|_{\partial B_\varepsilon} = 0$. Therefore, the shape derivative of the cost functional (4.23) reads

$$\frac{d}{d\varepsilon}\psi(\chi_\varepsilon) = \dot{\mathscr{J}}_{\Omega_\varepsilon}(u_\varepsilon) = -\frac{1}{2}\int_{\partial B_\varepsilon}((\partial_\tau u_\varepsilon)^2 - 2bu_\varepsilon)\,, \tag{4.46}$$

where we have used the result (4.45). In addition, we have that the following expansion for u_ε holds in the neighborhood of the hole (4.30)

$$\begin{aligned} u_\varepsilon(x) &= u(x) + \frac{\varepsilon^2}{\|x-\widehat{x}\|^2}\nabla u(\widehat{x})\cdot(x-\widehat{x}) + o(\varepsilon) \\ &= u(\widehat{x}) + \nabla u(\widehat{x})\cdot(x-\widehat{x}) + \frac{\varepsilon^2}{\|x-\widehat{x}\|^2}\nabla u(\widehat{x})\cdot(x-\widehat{x}) + o(\varepsilon)\,, \end{aligned} \tag{4.47}$$

which can be written in a polar coordinate system (r,θ) centered at the point $\widehat{x}$ (see fig. 4.4), namely

$$u_\varepsilon(r,\theta) = \varphi_0 + \frac{r^2+\varepsilon^2}{r}(\varphi_1\cos\theta + \varphi_2\sin\theta) + o(\varepsilon)\,, \tag{4.48}$$

where we have introduced the notation $u(\widehat{x}) = \varphi_0$ and $\nabla u(\widehat{x}) = (\varphi_1, \varphi_2)^\top$. The tangential derivative of u_ε is obtained in the following way

$$\begin{aligned} \partial_\tau u_\varepsilon(x) &= -\frac{1}{r}\partial_\theta u_\varepsilon(r,\theta) \\ &= \frac{r^2+\varepsilon^2}{r^2}(\varphi_1\sin\theta - \varphi_2\cos\theta) + o(\varepsilon)\,, \\ \partial_\tau u_\varepsilon(x)|_{\partial B_\varepsilon} &= 2(\varphi_1\sin\theta - \varphi_2\cos\theta) + o(\varepsilon)\,, \end{aligned} \tag{4.49}$$

where the last expression was obtained by taking $r = \varepsilon$ in the previous one. In addition, considering the above expansion in (4.46) and after explicitly evaluating the integral on the boundary of the hole ∂B_ε, we obtain

$$\begin{aligned} \frac{d}{d\varepsilon}\psi(\chi_\varepsilon) &= -\frac{1}{2}\int_0^{2\pi}(4(\varphi_1 \sin\theta - \varphi_2\cos\theta)^2 - 2b\varphi_0)\varepsilon d\theta + o(\varepsilon^2) \\ &= -2\pi\varepsilon((\varphi_1^2+\varphi_2^2) - b\varphi_0) + o(\varepsilon^2)\,. \end{aligned} \tag{4.50}$$

Therefore, the above result together with the relation between shape and topological derivatives given by (1.49) leads to

$$\mathscr{T} = -\lim_{\varepsilon\to 0}\frac{1}{f'(\varepsilon)}\left(2\pi\varepsilon((\varphi_1^2+\varphi_2^2) - b\varphi_0) + o(\varepsilon^2)\right)\,. \tag{4.51}$$

Now, in order to identify the leading term of the above expansion, we choose

$$f(\varepsilon) = \pi\varepsilon^2\,, \tag{4.52}$$

which leads to

$$\mathscr{T} = -(\varphi_1^2+\varphi_2^2) + b\varphi_0\,. \tag{4.53}$$

Recalling that $u(\widehat{x}) = \varphi_0$ and $\nabla u(\widehat{x}) = (\varphi_1,\varphi_2)^\top$, the final formula for the *topological derivative* becomes [185, 204]

$$\mathscr{T}(\widehat{x}) = -\|\nabla u(\widehat{x})\|^2 + bu(\widehat{x})\,. \tag{4.54}$$

This leads to the topological asymptotic expansion of the energy shape functional, namely

$$\psi(\chi_\varepsilon(\widehat{x})) = \psi(\chi) - \pi\varepsilon^2(\|\nabla u(\widehat{x})\|^2 - bu(\widehat{x})) + o(\varepsilon^2)\,. \tag{4.55}$$

The full mathematical justification for the above expansion will be given in details in Chapter 10.

4.1.4.2 Dirichlet Condition on the Boundary of the Hole

By taking $\beta = 1$ in (4.12), we have homogeneous Dirichlet boundary condition on ∂B_ε, namely $u_{\varepsilon|_{\partial B_\varepsilon}} = 0 \Rightarrow \partial_\tau u_{\varepsilon|_{\partial B_\varepsilon}} = 0$. Therefore, the shape derivative of the cost functional (4.23) reads

$$\frac{d}{d\varepsilon}\psi(\chi_\varepsilon) = \dot{\mathscr{J}}_{\Omega_\varepsilon}(u_\varepsilon) = \frac{1}{2}\int_{\partial B_\varepsilon}(\partial_n u_\varepsilon)^2\,. \tag{4.56}$$

In addition, we have that the following expansion for ∇u_ε holds in the neighborhood of the hole (4.43)

$$
\begin{aligned}
\nabla u_\varepsilon(x) &= \nabla u(\widehat{x}) + \nabla\nabla u(y)(x-\widehat{x}) \\
&- \alpha(\varepsilon)u(\widehat{x})\left(\frac{1}{2\pi}\frac{x-\widehat{x}}{\|x-\widehat{x}\|^2} + \nabla g(\widehat{x}) + \nabla\nabla g(z)(x-\widehat{x})\right) \\
&- \frac{\varepsilon^2}{\|x-\widehat{x}\|^2}\left(\mathrm{I} - 2\frac{x-\widehat{x}}{\|x-\widehat{x}\|^2}\otimes(x-\widehat{x})\right)(\nabla u(\widehat{x}) - \alpha(\varepsilon)u(\widehat{x})\nabla g(\widehat{x})) + o(\varepsilon)\,,
\end{aligned}
\tag{4.57}
$$

where y and z are intermediate points between x and $\widehat{x}$. Recalling that g is the solution to (4.35) or, equivalently, solution to the following auxiliary variational problem:

$$
\begin{cases}
\text{Find } g \in \mathscr{V}_g, \text{ such that} \\
\int_\Omega \nabla g\cdot\nabla\eta = \int_{\Gamma_N} g^N\eta \quad \forall\eta\in\mathscr{V}_0\,,
\end{cases}
\tag{4.58}
$$

where the solution g lives in the set $\mathscr{V}_g$, and the test functions belong to the linear space $\mathscr{V}_0$, which are defined, respectively, as

$$
\mathscr{V}_g = \{\varphi\in H^1(\Omega) : \varphi_{|_{\Gamma_D}} = g^D\} \quad\text{and}\quad \mathscr{V}_0 = \{\varphi\in H^1(\Omega) : \varphi_{|_{\Gamma_D}} = 0\}\,, \tag{4.59}
$$

and functions g^D and g^N are respectively given by

$$
g^D(x) = -\frac{1}{2\pi}\log\|x-\widehat{x}\| \quad\text{and}\quad g^N(x) = -\frac{1}{2\pi}\frac{x-\widehat{x}}{\|x-\widehat{x}\|^2}\cdot n\,. \tag{4.60}
$$

Since $\partial_n u_{\varepsilon|_{\partial B_\varepsilon}} = \nabla u_\varepsilon\cdot n_{|_{\partial B_\varepsilon}}$ and $x-\widehat{x} = -\varepsilon n$ on the boundary of the hole ∂B_ε, we have

$$
\begin{aligned}
\partial_n u_{\varepsilon|_{\partial B_\varepsilon}} &= \nabla u(\widehat{x})\cdot n - \varepsilon\nabla\nabla u(y)n\cdot n \\
&- \alpha(\varepsilon)u(\widehat{x})\left(-\frac{1}{2\pi\varepsilon} + \nabla g(\widehat{x})\cdot n - \varepsilon\nabla\nabla g(z)n\cdot n\right) \\
&- (\mathrm{I} - 2n\otimes n)(\nabla u(\widehat{x}) - \alpha(\varepsilon)u(\widehat{x})\nabla g(\widehat{x}))\cdot n + o(\varepsilon) \\
&= \nabla u(\widehat{x})\cdot n - \alpha(\varepsilon)u(\widehat{x})\left(-\frac{1}{2\pi\varepsilon} + \nabla g(\widehat{x})\cdot n\right) \\
&+ (\nabla u(\widehat{x}) - \alpha(\varepsilon)u(\widehat{x})\nabla g(\widehat{x}))\cdot n + O(\varepsilon) \\
&= \frac{\alpha(\varepsilon)}{2\pi\varepsilon}u(\widehat{x}) + 2\nabla u(\widehat{x})\cdot n - 2\alpha(\varepsilon)u(\widehat{x})\nabla g(\widehat{x})\cdot n + O(\varepsilon)\,.
\end{aligned}
\tag{4.61}
$$

Considering the above expansion in (4.56) and after explicitly evaluating the integral on the boundary of the hole ∂B_ε, we obtain

$$
\int_{\partial B_\varepsilon}\left(\frac{\alpha(\varepsilon)}{2\pi\varepsilon}u(\widehat{x})\right)^2 = \frac{\alpha(\varepsilon)^2}{2\pi\varepsilon}u(\widehat{x})^2 = \frac{2\pi}{\varepsilon(\log\varepsilon + 2\pi g(\widehat{x}))^2}u(\widehat{x})^2\,, \tag{4.62}
$$

$$\int_{\partial B_\varepsilon} (\nabla u(\widehat{x}) \cdot n)^2 = (\nabla u(\widehat{x}) \otimes \nabla u(\widehat{x})) \cdot \int_{\partial B_\varepsilon} n \otimes n$$
$$= \pi\varepsilon(\nabla u(\widehat{x}) \otimes \nabla u(\widehat{x})) \cdot \mathrm{I} = \pi\varepsilon \|\nabla u(\widehat{x})\|^2 \,, \tag{4.63}$$

$$\alpha(\varepsilon) u(\widehat{x}) \int_{\partial B_\varepsilon} (\nabla g(\widehat{x}) \cdot n)(\nabla u(\widehat{x}) \cdot n) = O(\varepsilon\alpha(\varepsilon)) = o(\varepsilon) \,, \tag{4.64}$$
$$\alpha(\varepsilon)^2 \int_{\partial B_\varepsilon} (\nabla g(\widehat{x}) \cdot n)^2 = O(\varepsilon\alpha(\varepsilon)^2) = o(\varepsilon) \,, \tag{4.65}$$

where the first term in (4.61) is orthogonal to the following two terms. Therefore we have

$$\frac{d}{d\varepsilon}\psi(\chi_\varepsilon(\widehat{x})) = \frac{\pi}{\varepsilon(\log\varepsilon + 2\pi g(\widehat{x}))^2} u(\widehat{x})^2 + 2\pi\varepsilon\|\nabla u(\widehat{x})\|^2 + o(\varepsilon) \,. \tag{4.66}$$

The above result, together with the relation between shape and topological derivatives given by (1.49), leads to

$$\mathscr{T}(\widehat{x}) = \lim_{\varepsilon \to 0} \frac{1}{f'(\varepsilon)} \left(\frac{\pi}{\varepsilon(\log\varepsilon + 2\pi g(\widehat{x}))^2} u(\widehat{x})^2 + O(\varepsilon) \right) \,. \tag{4.67}$$

Now, in order to identify the leading term of the above expansion, we choose

$$f(\varepsilon) = -\frac{\pi}{\log\varepsilon + 2\pi g(\widehat{x})} \,, \tag{4.68}$$

which leads to the final formula for the *topological derivative*, namely [44, 185]

$$\mathscr{T}(\widehat{x}) = u(\widehat{x})^2 \,. \tag{4.69}$$

Finally, the topological asymptotic expansion of the energy shape functional takes the form

$$\psi(\chi_\varepsilon(\widehat{x})) = \psi(\chi) - \frac{\pi}{\log\varepsilon + 2\pi g(\widehat{x})} u(\widehat{x})^2 + O(\varepsilon) \,. \tag{4.70}$$

The full mathematical justification for the above expansion is given in Chapter 10.

Remark 4.3. It is important to observe that the *domain truncation technique* widely used in the literature introduces an artificial parameter R in the topological asymptotic expansion, which cannot be explicitly evaluated. Thus, the simplification $f(\varepsilon) \approx -\pi/\log\varepsilon$ is often adopted, leading to the following expansion (see, for instance, [80])

$$\psi(\chi_\varepsilon(\widehat{x})) = \psi(\chi) - \frac{\pi}{\log\varepsilon} u(\widehat{x})^2 + o(\frac{-1}{\log\varepsilon}) \,, \tag{4.71}$$

which introduces a discrepancy in the topological asymptotic expansion.

In addition, we can go further in the expansion. In fact, let us consider one more term is the topological asymptotic expansion of the form

$$\psi(\chi_\varepsilon(\widehat{x})) = \psi(\chi) + f(\varepsilon)\mathcal{T}(\widehat{x}) + f_2(\varepsilon)\mathcal{T}^2(\widehat{x}) + \mathcal{R}(f_2(\varepsilon)) \, , \tag{4.72}$$

where $\mathcal{T}$ and $\mathcal{T}^2$ are the first and the *second order topological derivatives* of ψ, respectively. Some terms in the above expansion require explanation. In particular, we make the following assumptions in order to evaluate $\mathcal{T}^2$:

Condition 4.1. Let us consider that expansion (4.72) holds true. Then, the properties bellow have to be fulfilled:

- The term $f_2(\varepsilon)$ is a positive *second order correction function* that decreases monotonically such that $f_2(\varepsilon) \to 0$ with $\varepsilon \to 0$. Furthermore,

$$\lim_{\varepsilon\to 0} \frac{f_2(\varepsilon)}{f(\varepsilon)} = 0 \, . \tag{4.73}$$

- For the remainder we have

$$\lim_{\varepsilon\to 0} \frac{\mathcal{R}(f_2(\varepsilon))}{f_2(\varepsilon)} = 0 \, , \tag{4.74}$$

  and for its derivative

$$\mathcal{R}'(f_2(\varepsilon)) \to 0 \, , \quad \text{for} \quad \varepsilon \to 0 \, . \tag{4.75}$$

Now, if we divide (4.72) by $f_2(\varepsilon)$ and perform the limit passage $\varepsilon \to 0$, then, in view of (4.74), we recognize the second order topological derivative

$$\mathcal{T}^2(\widehat{x}) := \lim_{\varepsilon\to 0} \frac{\psi(\chi_\varepsilon(\widehat{x})) - \psi(\chi) - f(\varepsilon)\mathcal{T}(\widehat{x})}{f_2(\varepsilon)} \, . \tag{4.76}$$

Proposition 4.3. *Let the assumptions of Condition 4.1 be satisfied. Then the second order topological derivative $\mathcal{T}^2$ can be obtained as*

$$\mathcal{T}^2(\widehat{x}) = \lim_{\varepsilon\to 0} \frac{1}{f_2'(\varepsilon)} \left(\frac{d}{d\varepsilon} \psi(\chi_\varepsilon(\widehat{x})) - f'(\varepsilon)\mathcal{T}(\widehat{x}) \right) \, . \tag{4.77}$$

Proof. We differentiate (4.72) with respect to ε, then

$$\frac{d}{d\varepsilon} \psi(\chi_\varepsilon(\widehat{x})) - f'(\varepsilon)\mathcal{T}(\widehat{x}) = f_2'(\varepsilon)\mathcal{T}^2(\widehat{x}) + \mathcal{R}'(f_2(\varepsilon)) f_2'(\varepsilon) \, . \tag{4.78}$$

After division by $f_2'(\varepsilon)$ we have

$$\mathcal{T}^2(\widehat{x}) = \frac{1}{f_2'(\varepsilon)} \left(\frac{d}{d\varepsilon} \psi(\chi_\varepsilon(\widehat{x})) - f'(\varepsilon)\mathcal{T}(\widehat{x}) \right) - \mathcal{R}'(f_2(\varepsilon)) \, . \tag{4.79}$$

In view of (4.75), the limit passage $\varepsilon \to 0$ leads to the result. □

Remark 4.4. The topological derivatives of arbitrary order are derived for the simple eigenvalues in Section 9.2.

Now, we can evaluate the second order topological derivative of the energy shape functional from the obtained relation. More precisely, in view of (4.66) combined with (4.68) and (4.69) we have

$$\frac{d}{d\varepsilon}\psi(\chi_\varepsilon(\widehat{x})) - f'(\varepsilon)\mathscr{T}(\widehat{x}) = 2\pi\varepsilon\|\nabla u(\widehat{x})\|^2 + o(\varepsilon)\,. \tag{4.80}$$

Therefore, the relation between shape derivative and the second order topological derivative given by (4.77) provides

$$\mathscr{T}^2(\widehat{x}) = \lim_{\varepsilon\to 0}\frac{1}{f_2'(\varepsilon)}\left(2\pi\varepsilon\|\nabla u(\widehat{x})\|^2 + o(\varepsilon)\right)\,. \tag{4.81}$$

Now, in order to identify the leading term of the above expansion, we choose

$$f_2(\varepsilon) = \pi\varepsilon^2\,, \tag{4.82}$$

which leads to the final formula for the second order topological derivative [48]

$$\mathscr{T}^2(\widehat{x}) = \|\nabla u(\widehat{x})\|^2\,. \tag{4.83}$$

Finally, the topological asymptotic expansion of the energy shape functional takes the form

$$\psi(\chi_\varepsilon(\widehat{x})) = \psi(\chi) - \frac{\pi}{\log\varepsilon + 2\pi g(\widehat{x})}u(\widehat{x})^2 + \pi\varepsilon^2\|\nabla u(\widehat{x})\|^2 + o(\varepsilon^2)\,. \tag{4.84}$$

Remark 4.5. The mathematical justification for the above expansion follows the same steps as it is presented in Chapter 10.

4.1.5 Examples with Explicit Form of Topological Derivatives

Now, we shall verify, through some examples, the accuracy of the obtained topological asymptotic expansions. For that, we compute an approximation for the shape functional by taking into account the obtained expansions (4.55), (4.70) and also (4.84). Thus, let us consider the Laplace problem defined in the domain $\Omega_\varepsilon = \Omega \setminus \overline{B_\varepsilon}$, where, for $\varepsilon < \rho$, we have

$$\Omega = \left\{x \in \mathbb{R}^2 : \|x\| < \rho\right\} \quad \text{and} \quad B_\varepsilon = \left\{x \in \mathbb{R}^2 : \|x\| < \varepsilon\right\}\,. \tag{4.85}$$

4.1.5.1 Example A: The Neumann's Case

By taking $b = 0$ and $\overline{q} = -\cos\theta$, the problem formulation associated to the perturbed domain Ω_ε reads:

$$\begin{cases} \text{Find } u_\varepsilon, \text{ such that} \\ \Delta u_\varepsilon = 0 \quad \text{in } \Omega_\varepsilon \ , \\ \partial_n u_\varepsilon = \cos\theta \text{ on } \partial\Omega \ , \\ \partial_n u_\varepsilon = 0 \quad \text{on } \partial B_\varepsilon \ . \end{cases} \tag{4.86}$$

The analytical solution is given, up to an arbitrary additive constant, by

$$u_\varepsilon(r,\theta) = \frac{\rho^2}{r}\left(\frac{r^2+\varepsilon^2}{\rho^2-\varepsilon^2}\right)\cos\theta \ . \tag{4.87}$$

Thus, the shape functional can be written as

$$\psi(\chi_\varepsilon) = -\frac{\pi\rho^2}{2}\left(\frac{\rho^2+\varepsilon^2}{\rho^2-\varepsilon^2}\right) \ , \tag{4.88}$$

which can be expanded in powers of ε, namely

$$\psi(\chi_\varepsilon) = -\frac{1}{2}\pi\rho^2 - \pi\varepsilon^2 + O(\varepsilon^4) \ . \tag{4.89}$$

On the other hand, according to (4.55), the topological asymptotic expansion reads

$$\begin{aligned} \psi(\chi_\varepsilon) &= \psi(\chi) - \pi\varepsilon^2\|\nabla u\|^2 + o(\varepsilon^2) \\ &= -\frac{1}{2}\pi\rho^2 - \pi\varepsilon^2 + o(\varepsilon^2) \ , \end{aligned} \tag{4.90}$$

that coincides with the above expansion in powers of ε, since $\|\nabla u\|^2 = 1$. In particular, by taking $\rho = 1$, the topological asymptotic expansion is given by

$$\psi(\chi_\varepsilon) \approx -\frac{\pi}{2} - \pi\varepsilon^2 \ . \tag{4.91}$$

These results are compared in the graphic of fig. 4.5, where we observe that the approximation (4.91) is fairly exact for small values of ε, with the exact values given by (4.88).

4.1.5.2 Example B: The Dirichlet's Case

Now, let us consider $b = 0$ and $\overline{u} = a + \cos\theta$. Then, the problem formulation associated to the perturbed domain Ω_ε reads:

$$\begin{cases} \text{Find } u_\varepsilon, \text{ such that} \\ \Delta u_\varepsilon = 0 \quad \text{in } \Omega_\varepsilon \ , \\ u_\varepsilon = a + \cos\theta \text{ on } \partial\Omega \ , \\ u_\varepsilon = 0 \quad \text{on } \partial B_\varepsilon \ , \end{cases} \tag{4.92}$$

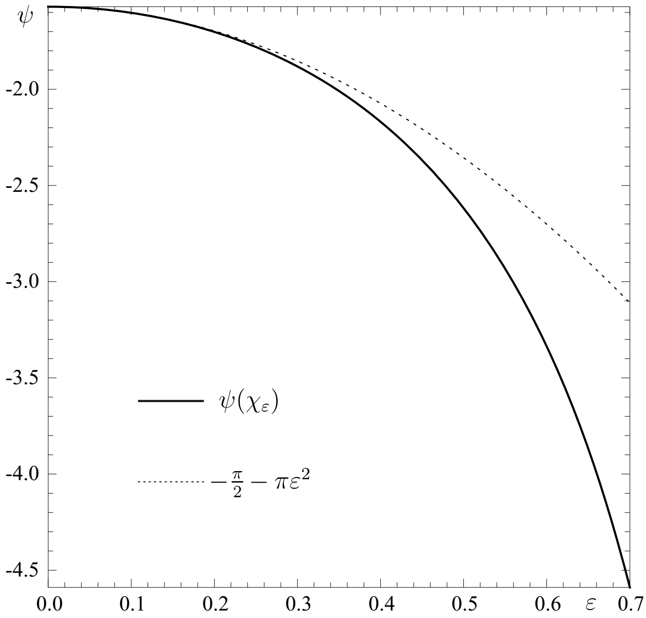


Fig. 4.5 Topological asymptotic expansions explicitly evaluated in the ring: the Neumann's case

whose analytical solution is given by

$$u_\varepsilon(r,\theta) = a\frac{\log(r/\varepsilon)}{\log(\rho/\varepsilon)} + \frac{\rho}{r}\left(\frac{r^2-\varepsilon^2}{\rho^2-\varepsilon^2}\right)\cos\theta \; . \tag{4.93}$$

Thus, the shape functional results in

$$\psi(\chi_\varepsilon) = \frac{\pi}{\log(\rho/\varepsilon)}a^2 + \frac{\pi}{2}\frac{\rho^2+\varepsilon^2}{\rho^2-\varepsilon^2} \; , \tag{4.94}$$

which can by expanded in powers of ε, such that

$$\psi(\chi_\varepsilon) = \frac{\pi}{2} + \frac{\pi}{\log(\rho/\varepsilon)}a^2 + \pi\varepsilon^2\frac{1}{\rho^2} + O(\varepsilon^4) \; . \tag{4.95}$$

Taking into account the final formula for the topological asymptotic expansion given by (4.70), we have

$$\begin{aligned}\psi(\chi_\varepsilon) &= \psi(\chi) - \frac{\pi}{\log\varepsilon + 2\pi g}u^2 + \pi\varepsilon^2\|\nabla u\|^2 + o(\varepsilon^2)\\ &= \frac{\pi}{2} + \frac{\pi}{\log(\rho/\varepsilon)}a^2 + \pi\varepsilon^2\frac{1}{\rho^2} + o(\varepsilon^2) \; ,\end{aligned} \tag{4.96}$$

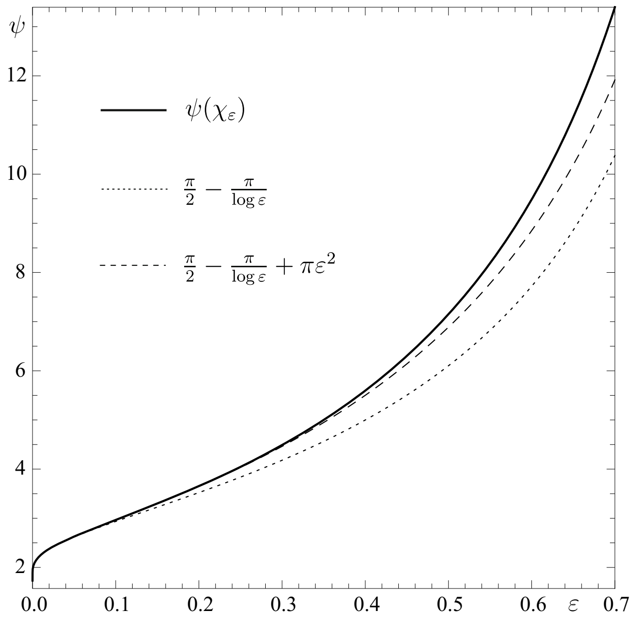


Fig. 4.6 Topological asymptotic expansions explicitly evaluated in the ring: the Dirichlet's case

that coincides with the above expansion in powers of ε, since $\|\nabla u\|^2 = 1/\rho^2$, where g is the solution to (4.35), that is

$$\begin{cases} \Delta g = 0 & \text{in } \Omega \\ g = -\frac{1}{2\pi}\log\rho & \text{on } \partial\Omega \end{cases} \Rightarrow g(\widehat{x}) = -\frac{1}{2\pi}\log\rho \,. \tag{4.97}$$

By choosing $\rho = a = 1$, we can compute the approximation for the shape functional taking into account only the first order topological derivative

$$\psi(\chi_\varepsilon) \approx \frac{\pi}{2} - \frac{\pi}{\log\varepsilon} \,. \tag{4.98}$$

Then we will compare it with the approximation considering both first and second order topological derivatives, that is

$$\psi(\chi_\varepsilon) \approx \frac{\pi}{2} - \frac{\pi}{\log\varepsilon} + \pi\varepsilon^2 \,. \tag{4.99}$$

These results are compared in the graphic of fig. 4.6, where we observe that the approximation (4.98) gives good results in comparison with (4.94) for small values for ε. In addition, we note that the second order topological derivative is an important correction factor in the expansion, since the expansion (4.99) remains precise even for large values of ε.

4.1.6 Additional Comments and Summary of the Results

In this section we have evaluated the topological derivatives for the energy shape functional associated to the Poisson equation in two-dimensional domains, taking into account homogeneous Neumann or Dirichlet conditions on the boundary of the hole.

In addition, we can also consider the Robin condition on the boundary of the hole. For that, we need to take $\beta = 0$ and add one more term to the total potential energy (4.8), namely

$$\frac{1}{2}\int_{\partial B_\varepsilon} u_\varepsilon^2 \,, \tag{4.100}$$

which leads the following condition on the boundary of the hole

$$u_\varepsilon + \partial_n u_\varepsilon = 0 \quad \text{on} \quad \partial B_\varepsilon \,. \tag{4.101}$$

The solution to the problem with the above boundary condition has the following *expansion*

$$u_\varepsilon(x) = u(x) + O(\varepsilon) = u(\widehat{x}) + O(\varepsilon) \,. \tag{4.102}$$

Therefore the shape derivative of the energy functional, taking into account the term associated to the Robin boundary condition on the hole (4.100), can be written as

$$\dot{\mathscr{J}}_{\Omega_\varepsilon}(u_\varepsilon) = \frac{1}{2}\int_{\partial B_\varepsilon} u_\varepsilon^2 \mathrm{div}_\Gamma \mathfrak{V} + O(\varepsilon) \,, \tag{4.103}$$

where $\mathrm{div}_\Gamma \mathfrak{V} = (\mathrm{I} - n \otimes n) \cdot \nabla \mathfrak{V}$, with $\mathfrak{V}$ standing for the shape change velocity field defined through (4.2). Since we are dealing with an uniform expansion of the circular hole, then by taking into account the associated velocity field, $\mathfrak{V} = -n$ on ∂B_ε, which implies $\mathrm{div}_\Gamma \mathfrak{V} = 1/\varepsilon$ on ∂B_ε, we obtain

$$\frac{d}{d\varepsilon}\psi(\chi_\varepsilon) = \dot{\mathscr{J}}_{\Omega_\varepsilon}(u_\varepsilon) = \frac{1}{2\varepsilon}\int_{\partial B_\varepsilon} u_\varepsilon^2 + O(\varepsilon) \,. \tag{4.104}$$

We note that on the boundary of the hole ∂B_ε, the velocity field can be written as

$$\mathfrak{V} = -n = \frac{x - \widehat{x}}{\varepsilon} \Rightarrow \nabla \mathfrak{V} = \frac{1}{\varepsilon}\mathrm{I} \,. \tag{4.105}$$

Therefore, the tangential divergence of the velocity on ∂B_ε is given by

$$\mathrm{div}_\Gamma \mathfrak{V} = (\mathrm{I} - n \otimes n) \cdot \nabla \mathfrak{V} = \frac{1}{\varepsilon}(\mathrm{I} - n \otimes n) \cdot \mathrm{I} = \frac{1}{\varepsilon}(\mathrm{tr}(\mathrm{I}) - n \cdot n) = \frac{1}{\varepsilon} \,, \tag{4.106}$$

with $\mathrm{tr}(\mathrm{I}) = 2$ and $n \cdot n = 1$. Considering the expansion (4.102) in (4.104) and after explicitly evaluating the integral on the boundary of the hole ∂B_ε, we obtain

$$\frac{d}{d\varepsilon}\psi(\chi_\varepsilon(\widehat{x})) = \frac{1}{2\varepsilon}\int_0^{2\pi} u(\widehat{x})^2 \varepsilon d\theta + O(\varepsilon) = \pi u(\widehat{x})^2 + O(\varepsilon) \, . \tag{4.107}$$

Therefore, the above result together with the relation between shape and topological derivatives given by (1.49) leads to

$$\mathcal{T}(\widehat{x}) = \lim_{\varepsilon \to 0} \frac{1}{f'(\varepsilon)} \left(\pi u(\widehat{x})^2 + O(\varepsilon) \right) \, . \tag{4.108}$$

Now, in order to identify the leading term of the above expansion, we choose

$$f(\varepsilon) = \pi\varepsilon \, , \tag{4.109}$$

which leads to the final formula for the *topological derivative*, namely [185]

$$\mathcal{T}(\widehat{x}) = u(\widehat{x})^2 \, . \tag{4.110}$$

Finally, the topological asymptotic expansion of the energy shape functional takes the form

$$\psi(\chi_\varepsilon(\widehat{x})) = \psi(\chi) + \pi\varepsilon u(\widehat{x})^2 + o(\varepsilon) \, . \tag{4.111}$$

Let us now summarize the results for *topological derivatives* obtained in this section, which are reported in Table 4.1. Recalling that u is the solution to (4.4) and g is the solution to (4.58), both defined in the unperturbed domain Ω.

Table 4.1 Topological derivatives for the energy shape functional associated to the Poisson equation in two-dimensional domains, taking into account homogeneous Neumann, Dirichlet or Robin conditions on the boundary of the hole

Boundary condition on ∂B_ε	$f(\varepsilon)$	$\mathcal{T}(\widehat{x})$
Neumann	$\pi\varepsilon^2$	$-\|\nabla u(\widehat{x})\|^2 + bu(\widehat{x})$
Dirichlet	$-\dfrac{\pi}{\log\varepsilon + 2\pi g(\widehat{x})}$	$u(\widehat{x})^2$
Robin	$\pi\varepsilon$	$u(\widehat{x})^2$

4.2 Second Order Elliptic System: The Navier Problem

In this section we evaluate the topological derivative of the total potential energy associated to plane stress linear elasticity problem, considering only homogeneous Neumann condition on the boundary of the hole ∂B_ε.

4.2.1 Problem Formulation

The shape functional in the unperturbed domain Ω is given by

$$\psi(\chi) := \mathscr{J}_\Omega(u) = \frac{1}{2}\int_\Omega \sigma(u)\cdot\nabla u^s - \int_\Omega b\cdot u - \int_{\Gamma_N} \overline{q}\cdot u\,, \tag{4.112}$$

where the vector function u is the solution to the variational problem:

$$\begin{cases} \text{Find } u \in \mathscr{U}\text{, such that} \\ \displaystyle\int_\Omega \sigma(u)\cdot\nabla\eta^s = \int_\Omega b\cdot\eta + \int_{\Gamma_N}\overline{q}\cdot\eta \quad \forall\eta\in\mathscr{V}\,, \\ \qquad\qquad\qquad\qquad \text{with} \quad \sigma(u) = \mathbb{C}\nabla u^s\,. \end{cases} \tag{4.113}$$

In the above equation, b is a constant body force distributed in the domain Ω and $\mathbb{C}$ is the constitutive tensor given by

$$\mathbb{C} = \frac{E}{1-\nu^2}((1-\nu)\mathbb{I} + \nu \mathrm{I}\otimes\mathrm{I})\,, \tag{4.114}$$

where I and $\mathbb{I}$ are the second and fourth order identity tensors, respectively, E is the Young modulus and ν the Poisson ratio, both considered constants everywhere. For the sake of simplicity, we also assume that the thickness of the elastic body is constant and equal to one. The set $\mathscr{U}$ and the space $\mathscr{V}$ are respectively defined as

$$\mathscr{U} := \{\varphi \in H^1(\Omega;\mathbb{R}^2) : \varphi_{|\Gamma_D} = \overline{u}\}\,, \tag{4.115}$$

$$\mathscr{V} := \{\varphi \in H^1(\Omega;\mathbb{R}^2) : \varphi_{|\Gamma_D} = 0\}\,. \tag{4.116}$$

In addition, $\partial\Omega = \overline{\Gamma}_D \cup \overline{\Gamma}_N$ with $\Gamma_D \cap \Gamma_N = \emptyset$, where Γ_D and Γ_N are Dirichlet and Neumann boundaries, respectively. Thus $\overline{u}$ is a Dirichlet data on Γ_D and $\overline{q}$ is a Neumann data on Γ_N, both assumed to be smooth enough. See the details in fig. 4.7. The strong system associated to the variational problem (4.113) reads:

$$\begin{cases} \text{Find } u\text{, such that} \\ -\mathrm{div}\sigma(u) = b & \text{in } \Omega\,, \\ \sigma(u) = \mathbb{C}\nabla u^s\,, \\ u = \overline{u} & \text{on } \Gamma_D\,, \\ \sigma(u)n = \overline{q} & \text{on } \Gamma_N\,. \end{cases} \tag{4.117}$$

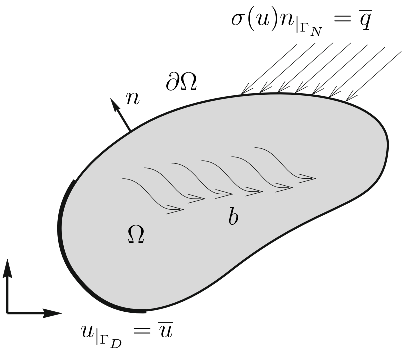


Fig. 4.7 The Navier problem defined in the unperturbed domain Ω

Remark 4.6. Since the Young modulus E and the Poisson ratio ν are constants, the above boundary value problem reduces itself to the well-known Navier system,

$$-\mu\Delta u - (\lambda+\mu)\nabla(\mathrm{div} u) = b \quad \text{in} \quad \Omega \,, \tag{4.118}$$

with the Lame's coefficients μ and λ respectively given by

$$\mu = \frac{E}{2(1+\nu)} \quad \text{and} \quad \lambda = \frac{\nu E}{1-\nu^2} \,. \tag{4.119}$$

Now, let us state the same problem in the perturbed domain Ω_ε. In this case, the total potential energy reads

$$\psi(\chi_\varepsilon) := \mathscr{J}_{\Omega_\varepsilon}(u_\varepsilon) = \frac{1}{2}\int_{\Omega_\varepsilon} \sigma(u_\varepsilon)\cdot\nabla u_\varepsilon^s - \int_{\Omega_\varepsilon} b\cdot u_\varepsilon - \int_{\Gamma_N} \overline{q}\cdot u_\varepsilon \,, \tag{4.120}$$

where the vector function u_ε solves the variational problem:

$$\begin{cases} \text{Find } u_\varepsilon \in \mathscr{U}_\varepsilon, \text{ such that} \\ \displaystyle\int_{\Omega_\varepsilon} \sigma(u_\varepsilon)\cdot\nabla\eta^s = \int_{\Omega_\varepsilon} b\cdot\eta + \int_{\Gamma_N} \overline{q}\cdot\eta \quad \forall\eta\in\mathscr{V}_\varepsilon \,, \\ \qquad\qquad\qquad\qquad \text{with} \quad \sigma(u_\varepsilon) = \mathbb{C}\nabla u_\varepsilon^s \,. \end{cases} \tag{4.121}$$

The set $\mathscr{U}_\varepsilon$ and the space $\mathscr{V}_\varepsilon$ are defined as

$$\mathscr{U}_\varepsilon := \{\varphi \in H^1(\Omega_\varepsilon;\mathbb{R}^2) : \varphi_{|\Gamma_D} = \overline{u}\} \,, \tag{4.122}$$

$$\mathscr{V}_\varepsilon := \{\varphi \in H^1(\Omega_\varepsilon;\mathbb{R}^2) : \varphi_{|\Gamma_D} = 0\} \,. \tag{4.123}$$

Since u_ε is free on ∂B_ε, then we have homogeneous Neumann condition on the boundary of the hole. It means that the hole is a void with the free boundary. See the details in fig. 4.8. The *strong system* associated to the variational problem (4.121) reads:

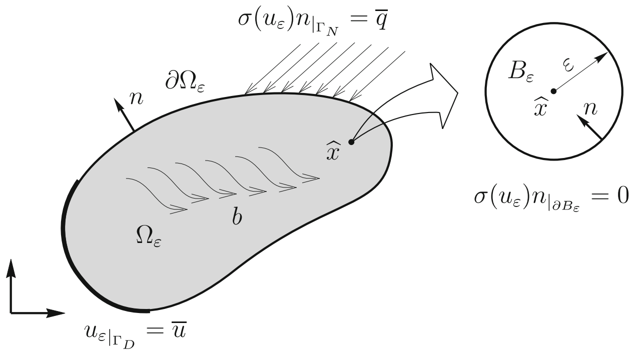


Fig. 4.8 The Navier problem defined in the perturbed domain Ω_ε

$$\begin{cases} \text{Find } u_\varepsilon, \text{ such that} \\ -\text{div}\sigma(u_\varepsilon) = b & \text{in } \Omega_\varepsilon \ , \\ \sigma(u_\varepsilon) = \mathbb{C}\nabla u_\varepsilon^s \ , \\ u_\varepsilon = \overline{u} & \text{on } \Gamma_D \ , \\ \sigma(u_\varepsilon)n = \overline{q} & \text{on } \Gamma_N \ , \\ \sigma(u_\varepsilon)n = 0 & \text{on } \partial B_\varepsilon \ . \end{cases} \tag{4.124}$$

4.2.2 Shape Sensitivity Analysis

In order to apply the result of Proposition 1.1, we need to evaluate the shape derivative of functional $\mathscr{J}_{\Omega_\varepsilon}(u_\varepsilon)$ with respect to an uniform expansion of the hole B_ε. Let us introduce the *Eshelby energy-momentum tensor* [57], which is given by

$$\Sigma_\varepsilon = \frac{1}{2}(\sigma(u_\varepsilon)\cdot\nabla u_\varepsilon^s - 2b\cdot u_\varepsilon)\mathrm{I} - \nabla u_\varepsilon^\top \sigma(u_\varepsilon) \ . \tag{4.125}$$

Therefore, we start by proving the following result:

Proposition 4.4. *Let $\mathscr{J}_{\Omega_\varepsilon}(u_\varepsilon)$ be the shape functional defined by (4.120). Then, the derivative of this functional with respect to the small parameter ε is given by*

$$\dot{\mathscr{J}}_{\Omega_\varepsilon}(u_\varepsilon) = \int_{\Omega_\varepsilon} \Sigma_\varepsilon \cdot \nabla\mathfrak{V} \ , \tag{4.126}$$

where $\mathfrak{V}$ is the shape change velocity field defined through (4.2) and Σ_ε is the Eshelby energy-momentum tensor given by (4.125).

Proof. By making use of the Reynolds' transport theorem through formula (2.84), the shape derivative (the material or total derivative with respect to the parameter ε) of the functional (4.120) is given by

$$\dot{\mathscr{J}}_{\Omega_\varepsilon}(u_\varepsilon) = \frac{1}{2}\int_{\Omega_\varepsilon}((\sigma(u_\varepsilon)\cdot\nabla u_\varepsilon^s)^{\cdot} + (\sigma(u_\varepsilon)\cdot\nabla u_\varepsilon^s)\mathrm{div}\mathfrak{V}) \\ - \int_{\Omega_\varepsilon} b\cdot(\dot{u}_\varepsilon + u_\varepsilon \mathrm{div}\mathfrak{V}) - \int_{\Gamma_N} \overline{q}\cdot\dot{u}_\varepsilon \ . \tag{4.127}$$

Next, by using the concept of material derivative of spatial fields through formula (2.92), we find that the first term of the above right hand side integral can be written as

$$(\sigma(u_\varepsilon)\cdot\nabla u_\varepsilon^s)^{\cdot} = 2\sigma(u_\varepsilon)\cdot\nabla\dot{u}_\varepsilon^s - 2\sigma(u_\varepsilon)\cdot(\nabla u_\varepsilon\nabla\mathfrak{V})^s \\ = 2\sigma(u_\varepsilon)\cdot\nabla\dot{u}_\varepsilon^s - 2\nabla u_\varepsilon^\top\sigma(u_\varepsilon)\cdot\nabla\mathfrak{V} \ , \tag{4.128}$$

since $\sigma(u_\varepsilon) = \mathbb{C}\nabla u_\varepsilon^s$. From the latter result we obtain

$$\dot{\mathscr{J}}_{\Omega_\varepsilon}(u_\varepsilon) = \frac{1}{2}\int_{\Omega_\varepsilon}((\sigma(u_\varepsilon)\cdot\nabla u_\varepsilon^s - 2b\cdot u_\varepsilon)\mathrm{I} - 2\nabla u_\varepsilon^\top\sigma(u_\varepsilon))\cdot\nabla\mathfrak{V} \\ + \int_{\Omega_\varepsilon}\sigma(u_\varepsilon)\cdot\nabla\dot{u}_\varepsilon^s - \int_{\Omega_\varepsilon} b\cdot\dot{u}_\varepsilon - \int_{\Gamma_N}\overline{q}\cdot\dot{u}_\varepsilon \ , \tag{4.129}$$

where we have made use of the identity $\mathrm{div}\mathfrak{V} = \mathrm{I}\cdot\nabla\mathfrak{V}$. Since $\dot{u}_\varepsilon$ is a variation of u_ε in the direction of the velocity field $\mathfrak{V}$, then $\dot{u}_\varepsilon \in \mathscr{V}_\varepsilon$ [210]. Finally, by taking $\dot{u}_\varepsilon$ as test function in the variational problem (4.121), we have that the last three terms of the above equation vanish. □

Now, we can prove that the shape derivative of the functional $\mathscr{J}_{\Omega_\varepsilon}(u_\varepsilon)$ can be written in terms of quantities concentrated on the boundary $\partial\Omega_\varepsilon$. In fact, the following result holds:

Proposition 4.5. *Let $\mathscr{J}_{\Omega_\varepsilon}(u_\varepsilon)$ be the shape functional defined by (4.120). Then, its derivative with respect to the small parameter ε is given by*

$$\dot{\mathscr{J}}_{\Omega_\varepsilon}(u_\varepsilon) = \int_{\partial\Omega_\varepsilon}\Sigma_\varepsilon n\cdot\mathfrak{V} \ , \tag{4.130}$$

with $\mathfrak{V}$ standing for the shape change velocity field defined through (4.2) and tensor Σ_ε is given by (4.125).

Proof. By making use of the other version of the Reynolds' transport theorem given by formula (2.85), we obtain the shape derivative of the functional (4.120)

$$\dot{\mathscr{J}}_{\Omega_\varepsilon}(u_\varepsilon) = \frac{1}{2}\int_{\Omega_\varepsilon}(\sigma(u_\varepsilon)\cdot\nabla u_\varepsilon^s)' + \frac{1}{2}\int_{\partial\Omega_\varepsilon}(\sigma(u_\varepsilon)\cdot\nabla u_\varepsilon^s)n\cdot\mathfrak{V} \\ - \int_{\Omega_\varepsilon} b\cdot u_\varepsilon' - \int_{\partial\Omega_\varepsilon}(b\cdot u_\varepsilon)n\cdot\mathfrak{V} - \int_{\Gamma_N}\overline{q}\cdot\dot{u}_\varepsilon \ . \tag{4.131}$$

Next, by using the concept of shape derivatives of spatial fields, we find that the first term of the above right hand side integral can be written as

$$(\sigma(u_\varepsilon)\cdot\nabla u_\varepsilon^s)' = 2\sigma(u_\varepsilon)\cdot(\nabla u_\varepsilon')^s \ , \tag{4.132}$$

since $\sigma(u_\varepsilon) = \sigma(u_\varepsilon)^\top$ and $(\cdot)'$ is the partial derivative of $(\cdot)$ with respect to ε. Now, let us use the relation between material and spatial derivatives of vector fields (2.83), namely $\varphi' = \dot{\varphi} - (\nabla\varphi)\mathfrak{V}$, which leads to

$$(\sigma(u_\varepsilon)\cdot\nabla u_\varepsilon^s)' = 2\sigma(u_\varepsilon)\cdot\nabla(\dot{u}_\varepsilon - (\nabla u_\varepsilon)\mathfrak{V})^s = 2\sigma(u_\varepsilon)\cdot\nabla\dot{u}_\varepsilon^s - 2\sigma(u_\varepsilon)\cdot\nabla((\nabla u_\varepsilon)\mathfrak{V})^s \,. \tag{4.133}$$

From this last result we obtain

$$\begin{aligned}\dot{\mathscr{J}}_{\Omega_\varepsilon}(u_\varepsilon) &= \frac{1}{2}\int_{\partial\Omega_\varepsilon}(\sigma(u_\varepsilon)\cdot\nabla u_\varepsilon^s - 2b\cdot u_\varepsilon)n\cdot\mathfrak{V} \\ &\quad - \int_{\Omega_\varepsilon}(\sigma(u_\varepsilon)\cdot\nabla((\nabla u_\varepsilon)\mathfrak{V})^s - b\cdot(\nabla u_\varepsilon)\mathfrak{V}) \\ &\quad + \int_{\Omega_\varepsilon}\sigma(u_\varepsilon)\cdot\nabla\dot{u}_\varepsilon^s - \int_{\Omega_\varepsilon} b\cdot\dot{u}_\varepsilon - \int_{\Gamma_N}\overline{q}\cdot\dot{u}_\varepsilon \,. \end{aligned} \tag{4.134}$$

Since $\dot{u}_\varepsilon$ is a variation of u_ε in the direction of the velocity field $\mathfrak{V}$, then $\dot{u}_\varepsilon \in \mathscr{V}_\varepsilon$. Now, by taking into account that u_ε is the solution to the variational problem (4.121), we have that the last three terms of the above equation vanish. By using the tensor relation (G.23) and after applying the divergence theorem (G.33), we have

$$\begin{aligned}\dot{\mathscr{J}}_{\Omega_\varepsilon}(u_\varepsilon) &= \frac{1}{2}\int_{\partial\Omega_\varepsilon}(\sigma(u_\varepsilon)\cdot\nabla u_\varepsilon^s - 2b\cdot u_\varepsilon)n\cdot\mathfrak{V} - \int_{\partial\Omega_\varepsilon}(\nabla u_\varepsilon)\mathfrak{V}\cdot\sigma(u_\varepsilon)^\top n \\ &\quad + \int_{\Omega_\varepsilon}(\operatorname{div}\sigma(u_\varepsilon) + b)\cdot(\nabla u_\varepsilon)\mathfrak{V} \,. \end{aligned} \tag{4.135}$$

Then, since $\sigma(u_\varepsilon)^\top = \sigma(u_\varepsilon)$, we can rewrite the above equation in the compact form

$$\dot{\mathscr{J}}_{\Omega_\varepsilon}(u_\varepsilon) = \int_{\partial\Omega_\varepsilon}\Sigma_\varepsilon n\cdot\mathfrak{V} + \int_{\Omega_\varepsilon}(\operatorname{div}\sigma(u_\varepsilon) + b)\cdot(\nabla u_\varepsilon)\mathfrak{V} \,. \tag{4.136}$$

The last term of the above equation vanishes provided that u_ε is also solution to the strong system (4.124), namely $-\operatorname{div}\sigma(u_\varepsilon) = b$, which leads to the result. □

Corollary 4.2. *From the tensor relation (G.23) and after applying the divergence theorem (G.32) to the right hand side of (4.126), we obtain*

$$\dot{\mathscr{J}}_{\Omega_\varepsilon}(u_\varepsilon) = \int_{\partial\Omega_\varepsilon}\Sigma_\varepsilon n\cdot\mathfrak{V} - \int_{\Omega_\varepsilon}\operatorname{div}\Sigma_\varepsilon\cdot\mathfrak{V} \,. \tag{4.137}$$

Since the above equation and (4.130) remain valid for all velocity fields $\mathfrak{V}$, we have that the second term of the above equation satisfies

$$\int_{\Omega_\varepsilon}\operatorname{div}\Sigma_\varepsilon\cdot\mathfrak{V} = 0 \quad \forall\mathfrak{V} \quad \Rightarrow \quad \operatorname{div}\Sigma_\varepsilon = 0 \,, \tag{4.138}$$

that is, Σ_ε is a divergence free tensor field.

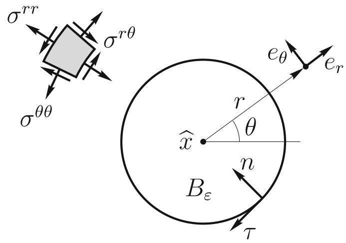


Fig. 4.9 Polar coordinate system (r,θ) centered at the point $\widehat{x} \in \Omega$

Corollary 4.3. *According to Proposition 4.5, we have*

$$\dot{\mathscr{J}}_{\Omega_\varepsilon}(u_\varepsilon) = \int_{\partial\Omega_\varepsilon} \Sigma_\varepsilon n \cdot \mathfrak{V} = \int_{\partial B_\varepsilon} \Sigma_\varepsilon n \cdot \mathfrak{V} + \int_{\partial\Omega} \Sigma_\varepsilon n \cdot \mathfrak{V} \,. \tag{4.139}$$

Since we are dealing with an uniform expansion of the circular hole B_ε, then in view of the associated velocity field (4.2), namely, $\mathfrak{V} = -n$ on ∂B_ε and $\mathfrak{V} = 0$ on $\partial\Omega$, we finally obtain

$$\frac{d}{d\varepsilon}\psi(\chi_\varepsilon) = \dot{\mathscr{J}}_{\Omega_\varepsilon}(u_\varepsilon) = -\int_{\partial B_\varepsilon} \Sigma_\varepsilon n \cdot n \,. \tag{4.140}$$

It means that the shape derivative of the cost functional is represented either by a boundary integral of the shape gradient given by a function or by the duality pairing with the shape gradient given by a distribution concentrated (supported) on ∂B_ε.

From the above corollary, we observe that the distributed shape gradient originally defined in the whole domain Ω_ε leads to the boundary shape gradient and to an integral defined only on the boundary of the hole ∂B_ε. In particular, the shape derivative of functional $\mathscr{J}_{\Omega_\varepsilon}(u_\varepsilon)$, given by the final formula (4.140), is written in terms of quantities supported on ∂B_ε. It means that we need to know the asymptotic behavior of the solution u_ε with respect to ε in the neighborhood of the hole B_ε. We will see later that this result simplifies enormously the next steps of the topological derivative calculation.

4.2.3 Asymptotic Analysis of the Solution

The shape derivative of functional $\mathscr{J}_{\Omega_\varepsilon}(u_\varepsilon)$ is given exclusively in terms of an integral over the boundary of the hole ∂B_ε (4.140). Therefore, in order to apply the result of Proposition 1.1, we need to know the behavior of the function u_ε with respect to ε in the neighborhood of the hole B_ε. In particular, once we know this behavior explicitly, we can identify function $f(\varepsilon)$ and perform the limit passage $\varepsilon \to 0$ in (1.49) to obtain the final formula for the topological derivative $\mathscr{T}$ of the shape functional ψ. Therefore, we need to perform the asymptotic analysis of u_ε with respect to ε.

In this section, we present the formal calculation of the expansions of the solution u_ε associated to homogeneous Neumann condition on the boundary of the hole. For a rigorous justification of the asymptotic expansions of u_ε, the reader may refer to [120, 148], for instance. Let us start with an *ansätz* for the expansion of u_ε in the form [120]

$$u_\varepsilon(x) = u(x) + w_\varepsilon(x) + \widetilde{u}_\varepsilon(x) . \tag{4.141}$$

After applying the operator σ we have

$$\begin{aligned}\sigma(u_\varepsilon(x)) &= \sigma(u(x)) + \sigma(w_\varepsilon(x)) + \sigma(\widetilde{u}_\varepsilon(x)) \\ &= \sigma(u(\widehat{x})) + \nabla\sigma(u(y))(x-\widehat{x}) + \sigma(w_\varepsilon(x)) + \sigma(\widetilde{u}_\varepsilon(x)) ,\end{aligned} \tag{4.142}$$

where y is an intermediate point between x and $\widehat{x}$. On the boundary of the hole ∂B_ε we have $\sigma(u_\varepsilon)n_{|_{\partial B_\varepsilon}} = 0$. Thus, the normal projection of the above expansion, evaluated on ∂B_ε, leads to

$$\sigma(u(\widehat{x}))n - \varepsilon(\nabla\sigma(u(y))n)n + \sigma(w_\varepsilon(x))n + \sigma(\widetilde{u}_\varepsilon(x))n = 0 . \tag{4.143}$$

Thus, we can choose $\sigma(w_\varepsilon)$ such that

$$\sigma(w_\varepsilon(x))n = -\sigma(u(\widehat{x}))n \quad \text{on} \quad \partial B_\varepsilon . \tag{4.144}$$

Now, the following exterior boundary value problem is considered and formally obtained as $\varepsilon \to 0$:

$$\begin{cases} \text{Find } \sigma(w_\varepsilon), \text{ such that} \\ \operatorname{div}\sigma(w_\varepsilon) = 0 & \text{in } \mathbb{R}^2 \setminus \overline{B_\varepsilon} , \\ \quad \sigma(w_\varepsilon) \to 0 & \text{at } \infty , \\ \quad \sigma(w_\varepsilon)n = -\sigma(u(\widehat{x}))n & \text{on } \partial B_\varepsilon . \end{cases} \tag{4.145}$$

The above boundary value problem admits an explicit solution (see, for instance, the book by Little 1973 [139]), which can be written in a polar coordinate system (r,θ) centered at the point $\widehat{x}$ as (see fig. 4.9)

$$\sigma^{rr}(w_\varepsilon(r,\theta)) = -\varphi_1\frac{\varepsilon^2}{r^2} - \varphi_2\left(4\frac{\varepsilon^2}{r^2} - 3\frac{\varepsilon^4}{r^4}\right)\cos 2\theta , \tag{4.146}$$

$$\sigma^{\theta\theta}(w_\varepsilon(r,\theta)) = \varphi_1\frac{\varepsilon^2}{r^2} - 3\varphi_2\frac{\varepsilon^4}{r^4}\cos 2\theta , \tag{4.147}$$

$$\sigma^{r\theta}(w_\varepsilon(r,\theta)) = -\varphi_2\left(2\frac{\varepsilon^2}{r^2} - 3\frac{\varepsilon^4}{r^4}\right)\sin 2\theta . \tag{4.148}$$

Some terms in the above formulae require explanations. The coefficients φ_1 and φ_2 are given by

$$\varphi_1 = \frac{1}{2}(\sigma_1(u(\widehat{x})) + \sigma_2(u(\widehat{x}))) , \quad \varphi_2 = \frac{1}{2}(\sigma_1(u(\widehat{x})) - \sigma_2(u(\widehat{x}))) , \tag{4.149}$$

where $\sigma_1(u(\widehat{x}))$ and $\sigma_2(u(\widehat{x}))$ are the eigenvalues of tensor $\sigma(u(\widehat{x}))$, which can be expressed as

$$\sigma_{1,2}(u(\widehat{x})) = \frac{1}{2}\left(\mathrm{tr}\,\sigma(u(\widehat{x})) \pm \sqrt{2\sigma^D(u(\widehat{x}))\cdot\sigma^D(u(\widehat{x}))}\right), \tag{4.150}$$

with $\sigma^D(u(\widehat{x}))$ standing for the deviatory part of the stress tensor $\sigma(u(\widehat{x}))$, namely

$$\sigma^D(u(\widehat{x})) = \sigma(u(\widehat{x})) - \frac{1}{2}\mathrm{tr}\,\sigma(u(\widehat{x}))\mathrm{I}\,. \tag{4.151}$$

In addition, $\sigma^{rr}(\varphi)$, $\sigma^{\theta\theta}(\varphi)$ and $\sigma^{r\theta}(\varphi)$ are the components of tensor $\sigma(\varphi)$ in the polar coordinate system, namely, $\sigma^{rr}(\varphi) = e^r\cdot\sigma(\varphi)e^r$, $\sigma^{\theta\theta}(\varphi) = e^\theta\cdot\sigma(\varphi)e^\theta$ and $\sigma^{r\theta}(\varphi) = \sigma^{\theta r}(\varphi) = e^r\cdot\sigma(\varphi)e^\theta$, with e^r and e^θ used to denote the canonical basis associated to the polar coordinate system (r,θ), such that, $\|e^r\| = \|e^\theta\| = 1$ and $e^r\cdot e^\theta = 0$. See fig. 4.9.

Now we can construct $\widetilde{u}_\varepsilon$ in such a way that it compensates the discrepancies introduced by the higher-order terms in ε as well as by the boundary-layer w_ε on the exterior boundary $\partial\Omega$. It means that the remainder $\widetilde{u}_\varepsilon$ must be solution to the following boundary value problem:

$$\left\{\begin{array}{rcll} \multicolumn{4}{l}{\text{Find } \widetilde{u}_\varepsilon, \text{ such that}} \\ \mathrm{div}\,\sigma(\widetilde{u}_\varepsilon) &=& 0 & \text{in } \Omega_\varepsilon\,, \\ \sigma(\widetilde{u}_\varepsilon) &=& \mathbb{C}\nabla\widetilde{u}^s_\varepsilon\,, & \\ \widetilde{u}_\varepsilon &=& -w_\varepsilon & \text{on } \Gamma_D\,, \\ \sigma(\widetilde{u}_\varepsilon)n &=& -\sigma(w_\varepsilon)n & \text{on } \Gamma_N\,, \\ \sigma(\widetilde{u}_\varepsilon)n &=& \varepsilon h & \text{on } \partial B_\varepsilon\,, \end{array}\right. \tag{4.152}$$

where clearly $\widetilde{u}_\varepsilon = O(\varepsilon)$, since h is independent of ε and $w_\varepsilon = O(\varepsilon^2)$ on the exterior boundary $\partial\Omega$. Nevertheless, according to [120, 148], this estimate can be improved, namely, $\widetilde{u}_\varepsilon = O(\varepsilon^2)$. Finally, the *expansion* for $\sigma(u_\varepsilon)$ in polar coordinate system (r,θ) reads (see fig. 4.9)

$$\sigma^{rr}(u_\varepsilon(r,\theta)) = \varphi_1\left(1-\frac{\varepsilon^2}{r^2}\right) + \varphi_2\left(1-4\frac{\varepsilon^2}{r^2}+3\frac{\varepsilon^4}{r^4}\right)\cos 2\theta + O(\varepsilon^2)\,, \tag{4.153}$$

$$\sigma^{\theta\theta}(u_\varepsilon(r,\theta)) = \varphi_1\left(1+\frac{\varepsilon^2}{r^2}\right) - \varphi_2\left(1+3\frac{\varepsilon^4}{r^4}\right)\cos 2\theta + O(\varepsilon^2)\,, \tag{4.154}$$

$$\sigma^{r\theta}(u_\varepsilon(r,\theta)) = -\varphi_2\left(1+2\frac{\varepsilon^2}{r^2}-3\frac{\varepsilon^4}{r^4}\right)\sin 2\theta + O(\varepsilon^2)\,, \tag{4.155}$$

where we have used the fact that $\sigma^{rr}(u(\widehat{x})) = \varphi_1 + \varphi_2\cos 2\theta$, $\sigma^{\theta\theta}(u(\widehat{x})) = \varphi_1 - \varphi_2\cos 2\theta$ and $\sigma^{r\theta}(u(\widehat{x})) = -\varphi_2\sin 2\theta$.

4.2.4 Topological Derivative Evaluation

From an orthonormal curvilinear coordinate system n and τ defined on the boundary ∂B_ε (see fig. 4.9), the tensors $\sigma(u_\varepsilon)$ and ∇u_ε can be decomposed as

$$\begin{aligned}\sigma(u_\varepsilon)_{|\partial B_\varepsilon} &= \sigma^{nn}(u_\varepsilon)(n\otimes n)+\sigma^{n\tau}(u_\varepsilon)(n\otimes\tau)\\ &+\sigma^{\tau n}(u_\varepsilon)(\tau\otimes n)+\sigma^{\tau\tau}(u_\varepsilon)(\tau\otimes\tau)\,, \end{aligned}\tag{4.156}$$

$$\begin{aligned}\nabla u_{\varepsilon}{}_{|\partial B_\varepsilon} &= \partial_n u_\varepsilon^n(n\otimes n)+\partial_\tau u_\varepsilon^n(n\otimes\tau)\\ &+\partial_n u_\varepsilon^\tau(\tau\otimes n)+\partial_\tau u_\varepsilon^\tau(\tau\otimes\tau)\,. \end{aligned}\tag{4.157}$$

Therefore, we observe that

$$\sigma(u_\varepsilon)n_{|\partial B_\varepsilon} = \sigma^{nn}(u_\varepsilon)n+\sigma^{\tau n}(u_\varepsilon)\tau = 0\,,\tag{4.158}$$

which implies

$$\sigma^{nn}(u_\varepsilon)=\sigma^{\tau n}(u_\varepsilon)=\sigma^{n\tau}(u_\varepsilon)=0 \quad \text{on} \quad \partial B_\varepsilon\,,\tag{4.159}$$

since $\sigma(u_\varepsilon)=\sigma(u_\varepsilon)^\top$. In addition,

$$\begin{aligned}\Sigma_\varepsilon n\cdot n_{|\partial B_\varepsilon} &= \frac{1}{2}(\sigma(u_\varepsilon)\cdot\nabla u_\varepsilon^s-2b\cdot u_\varepsilon)\mathrm{I}n\cdot n-\nabla u_\varepsilon^\top\sigma(u_\varepsilon)n\cdot n\\ &= \frac{1}{2}(\sigma(u_\varepsilon)\cdot\nabla u_\varepsilon^s-2b\cdot u_\varepsilon)n\cdot n-\sigma(u_\varepsilon)n\cdot(\nabla u_\varepsilon)n\\ &= \frac{1}{2}(\sigma(u_\varepsilon)\cdot\nabla u_\varepsilon^s-2b\cdot u_\varepsilon)\\ &= \frac{1}{2}(\sigma^{\tau\tau}(u_\varepsilon)\partial_\tau u_\varepsilon^\tau-2b\cdot u_\varepsilon)\,. \end{aligned}\tag{4.160}$$

On the other hand, the constitutive tensor $\mathbb{C}$ is invertible, namely,

$$\mathbb{C}^{-1}=\frac{1}{E}((1+\nu)\mathbb{I}-\nu\mathrm{I}\otimes\mathrm{I})\,,\tag{4.161}$$

which implies

$$\begin{aligned}\nabla u_\varepsilon^s &= \mathbb{C}^{-1}\sigma(u_\varepsilon)\\ &\Rightarrow \partial_\tau u_\varepsilon^\tau = \frac{1}{E}(\sigma^{\tau\tau}(u_\varepsilon)-\nu\sigma^{nn}(u_\varepsilon))=\frac{1}{E}\sigma^{\tau\tau}(u_\varepsilon) \quad \text{on} \quad \partial B_\varepsilon\,. \end{aligned}\tag{4.162}$$

Therefore, we have

$$\Sigma_\varepsilon n\cdot n_{|\partial B_\varepsilon}=\frac{1}{2}\left(\frac{1}{E}\left(\sigma^{\tau\tau}(u_\varepsilon)\right)^2-2b\cdot u_\varepsilon\right)\,.\tag{4.163}$$

The shape derivative of the cost functional (4.140) reads

$$\frac{d}{d\varepsilon}\psi(\chi_\varepsilon) = \dot{\mathscr{J}}_{\Omega_\varepsilon}(u_\varepsilon) = -\frac{1}{2}\int_{\partial B_\varepsilon}\left(\frac{1}{E}(\sigma^{\tau\tau}(u_\varepsilon))^2 - 2b\cdot u_\varepsilon\right), \tag{4.164}$$

where we have used (4.163). From formula (4.154), we have that the following expansion for $\sigma^{\tau\tau}(u_\varepsilon)$ holds in the neighborhood of the hole

$$\begin{aligned}\sigma^{\tau\tau}(u_\varepsilon(x)) &= \sigma^{\theta\theta}(u_\varepsilon(r,\theta))\\ &= \varphi_1\left(1+\frac{\varepsilon^2}{r^2}\right) - \varphi_2\left(1+3\frac{\varepsilon^4}{r^4}\right)\cos 2\theta + O(\varepsilon)\\ &\Rightarrow \sigma^{\tau\tau}(u_\varepsilon(x))_{|\partial B_\varepsilon} = 2\varphi_1 - 4\varphi_2\cos 2\theta + O(\varepsilon)\,.\end{aligned} \tag{4.165}$$

In addition, the following expansion for the displacement field u_ε holds on the boundary of the hole

$$u_\varepsilon(x)_{|\partial B_\varepsilon} = \varphi_0 + O(\varepsilon)\,, \tag{4.166}$$

where $\varphi_0 = u(\widehat{x})$. Considering the above expansions in (4.164) and after solving the integral on the boundary of the hole ∂B_ε, we obtain

$$\begin{aligned}\frac{d}{d\varepsilon}\psi(\varepsilon) &= -\frac{1}{2}\int_0^{2\pi}\left(\frac{1}{E}(2\varphi_1 - 4\varphi_2\cos 2\theta)^2 - 2b\cdot\varphi_0\right)\varepsilon d\theta + O(\varepsilon^2)\\ &= -2\pi\varepsilon\left(\frac{2}{E}(\varphi_1^2 + 2\varphi_2^2) - b\cdot\varphi_0\right) + O(\varepsilon^2)\,.\end{aligned} \tag{4.167}$$

Therefore, the above result together with the relation between shape and topological derivatives given by (1.49) results in

$$\mathscr{T} = -\lim_{\varepsilon\to 0}\frac{1}{f'(\varepsilon)}\left[2\pi\varepsilon\left(\frac{2}{E}(\varphi_1^2 + 2\varphi_2^2) - b\cdot\varphi_0\right) + O(\varepsilon^2)\right]. \tag{4.168}$$

Now, in order to extract the leading term of the above expansion, the correction function is set as

$$f(\varepsilon) = \pi\varepsilon^2\,. \tag{4.169}$$

Therefore, the limit passage $\varepsilon \to 0$ in (4.168) leads to the final formula for the topological derivative, that is

$$\mathscr{T} = -\frac{2}{E}(\varphi_1^2 + 2\varphi_2^2) + b\cdot\varphi_0\,. \tag{4.170}$$

Recalling that $\varphi_1 = (\sigma_1(u(\widehat{x})) + \sigma_2(u(\widehat{x})))/2$, $\varphi_2 = (\sigma_1(u(\widehat{x})) - \sigma_2(u(\widehat{x})))/2$ and $\varphi_0 = u(\widehat{x})$, the *topological derivative* evaluated at $\widehat{x}\in\Omega$ can be written as follows [70, 135, 204]:

- In terms of the principal stresses $\sigma_1(\widehat{x}) = \sigma_1(u(\widehat{x}))$ and $\sigma_2(\widehat{x}) = \sigma_2(u(\widehat{x}))$

$$\mathscr{T}(\widehat{x}) = -\frac{1}{2E}\left[(\sigma_1(\widehat{x}) + \sigma_2(\widehat{x}))^2 + 2(\sigma_1(\widehat{x}) - \sigma_2(\widehat{x}))^2\right] + b \cdot u(\widehat{x}) . \tag{4.171}$$

- In terms of the stress tensor $\sigma(u(\widehat{x}))$

$$\mathscr{T}(\widehat{x}) = -\frac{1}{2E}\left[4\sigma(u(\widehat{x})) \cdot \sigma(u(\widehat{x})) - \mathrm{tr}^2\sigma(u(\widehat{x}))\right] + b \cdot u(\widehat{x}) . \tag{4.172}$$

- In terms of the stress tensor $\sigma(u(\widehat{x}))$ and the strain tensor $\nabla u^s(\widehat{x})$

$$\mathscr{T}(\widehat{x}) = -\mathbb{P}\sigma(u(\widehat{x})) \cdot \nabla u^s(\widehat{x}) + b \cdot u(\widehat{x}) , \tag{4.173}$$

  where $\mathbb{P}$ is the *Pólya-Szegö polarization tensor*, given in this particular case by the following isotropic fourth order tensor

$$\mathbb{P} = \frac{2}{1+\nu}\mathbb{I} - \frac{1-3\nu}{2(1-\nu^2)}\mathrm{I} \otimes \mathrm{I} . \tag{4.174}$$

Finally, the topological asymptotic expansion of the energy shape functional reads

$$\psi(\chi_\varepsilon(\widehat{x})) = \psi(\chi) - \pi\varepsilon^2(\mathbb{P}\sigma(u(\widehat{x})) \cdot \nabla u^s(\widehat{x}) - b \cdot u(\widehat{x})) + o(\varepsilon^2) . \tag{4.175}$$

The full mathematical justification for the above expansion follows the same steps to be presented in Chapter 10 for another problem.

Remark 4.7. In the case of plane strain linear elasticity, the elasticity tensor is given by

$$\mathbb{C} = \frac{E}{1+\nu}\left(\mathbb{I} + \frac{\nu}{1-2\nu}\mathrm{I} \otimes \mathrm{I}\right) . \tag{4.176}$$

Therefore, the polarization tensor leads to

$$\mathbb{P} = \frac{1-\nu}{2}\left(4\mathbb{I} - \frac{1-4\nu}{1-2\nu}\mathrm{I} \otimes \mathrm{I}\right) , \tag{4.177}$$

and the topological asymptotic expansion of the energy shape functional is given by (4.175), with the above formula for the polarization tensor.

4.3 Fourth Order Elliptic Equation: The Kirchhoff Problem

In this section we evaluate the topological derivative of the total potential energy associated to linear and elastic Kirchhoff plate bending problem, considering only homogeneous Neumann condition on the boundary of the hole B_ε.

4.3.1 Problem Formulation

The shape functional in the unperturbed domain Ω is given by

$$\psi(\chi) := \mathscr{J}_\Omega(u) = -\frac{1}{2}\int_\Omega M(u)\cdot\nabla\nabla u + \int_\Omega bu \\ - \int_{\Gamma_{N_q}} \overline{q}u + \int_{\Gamma_{N_m}} \overline{m}\partial_n u + \sum_{i=1}^{ns} \overline{Q}_i u(x_i)\,, \tag{4.178}$$

where the scalar function u is the solution to the variational problem:

$$\begin{cases} \text{Find } u \in \mathscr{U}, \text{ such that} \\ -\int_\Omega M(u)\cdot\nabla\nabla\eta = -\int_\Omega b\eta + \int_{\Gamma_{N_q}} \overline{q}\eta \\ \qquad - \int_{\Gamma_{N_m}} \overline{m}\partial_n\eta - \sum_{i=1}^{ns} \overline{Q}_i\eta(x_i) \quad \forall\eta\in\mathscr{V}, \\ \qquad \text{with} \quad M(u) = -\mathbb{C}\nabla\nabla u\,. \end{cases} \tag{4.179}$$

In the above equation, $\mathbb{C}$ is the constitutive tensor given by

$$\mathbb{C} = \frac{E}{1-\nu^2}((1-\nu)\mathbb{I} + \nu\mathrm{I}\otimes\mathrm{I})\,, \tag{4.180}$$

where I and $\mathbb{I}$ are the second and fourth order identity tensors, respectively, E is the Young modulus and ν the Poisson ratio, both considered constants everywhere. For the sake of simplicity, we have assumed that the plate thickness is constant and equal to $12^{1/3}$. The set $\mathscr{U}$ and the space $\mathscr{V}$ are respectively defined as

$$\mathscr{U} := \{\varphi \in H^2(\Omega) : \varphi_{|_{\Gamma_{D_u}}} = \overline{u},\ \partial_n\varphi_{|_{\Gamma_{D_\rho}}} = \overline{\rho}\}\,, \tag{4.181}$$

$$\mathscr{V} := \{\varphi \in H^2(\Omega) : \varphi_{|_{\Gamma_{D_u}}} = 0,\ \partial_n\varphi_{|_{\Gamma_{D_\rho}}} = 0\}\,. \tag{4.182}$$

In addition, b is a constant body force distributed in the domain Ω, $\overline{q}$ is a shear load distributed on the boundary Γ_{N_q}, $\overline{m}$ is a moment distributed on the boundary Γ_{N_m} and $\overline{Q}_i$ is a concentrated shear load supported at the points x_i where there are some geometrical singularities, with $i = 1,\ldots,ns$, and ns the number of such singularities. The displacement field u has to satisfy $u_{|_{\Gamma_{D_u}}} = \overline{u}$ and $\partial_n u_{|_{\Gamma_{D_\rho}}} = \overline{\rho}$, where $\overline{u}$ and $\overline{\rho}$ are a displacement and a rotation respectively prescribed on the boundaries Γ_{D_u} and Γ_{D_ρ}. Furthermore, $\Gamma_D = \overline{\Gamma}_{D_u} \cup \overline{\Gamma}_{D_\rho}$ and $\Gamma_N = \overline{\Gamma}_{N_q} \cup \overline{\Gamma}_{N_m}$ are such that $\Gamma_{D_u} \cap \Gamma_{N_q} = \varnothing$ and $\Gamma_{D_\rho} \cap \Gamma_{N_m} = \varnothing$. See the details in fig. 4.10. The strong formulation associated to the variational problem (4.179) reads:

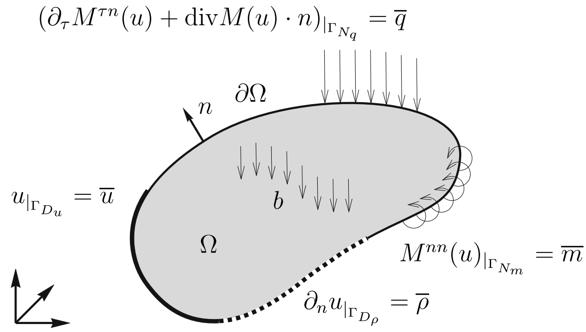


Fig. 4.10 The Kirchhoff problem defined in the unperturbed domain Ω

$$
\begin{cases}
\text{Find } u \text{, such that} \\
\qquad \mathrm{div}(\mathrm{div} M(u)) = b \quad \text{in } \Omega\,, \\
\qquad M(u) = -\mathbb{C}\nabla\nabla u\,, \\
\qquad u = \overline{u} \quad \text{on } \Gamma_{D_u}\,, \\
\qquad \partial_n u = \overline{\rho} \quad \text{on } \Gamma_{D_\rho}\,, \\
\qquad M^{nn}(u) = \overline{m} \quad \text{on } \Gamma_{N_m}\,, \\
\partial_\tau M^{\tau n}(u) + \mathrm{div} M(u) \cdot n = \overline{q} \quad \text{on } \Gamma_{N_q}\,, \\
\qquad [\![M^{\tau n}(u(x_i))]\!] = \overline{Q}_i \quad \text{on } x_i \in \Gamma_{N_q}\,.
\end{cases}
\tag{4.183}
$$

Remark 4.8. Since the Young modulus E, the Poisson ratio ν and the plate thickness are assumed to be constants, the above boundary value problem reduces itself to the well-known Kirchhoff equation, namely

$$
-k\Delta^2 u = b \quad \text{in} \quad \Omega\,, \quad \text{with} \quad k = \frac{Eh^3}{12(1-\nu^2)}\,,
\tag{4.184}
$$

where h is the plate thickness given by $h = 12^{1/3}$.

Now, let us state the problem associated to the perturbed domain Ω_ε. In this case, the total potential energy reads

$$
\begin{aligned}
\psi(\chi_\varepsilon) := \mathscr{J}_{\Omega_\varepsilon}(u_\varepsilon) = & -\frac{1}{2}\int_{\Omega_\varepsilon} M(u_\varepsilon) \cdot \nabla\nabla u_\varepsilon + \int_{\Omega_\varepsilon} b u_\varepsilon \\
& - \int_{\Gamma_{N_q}} \overline{q} u_\varepsilon + \int_{\Gamma_{N_m}} \overline{m}\partial_n u_\varepsilon + \sum_{i=1}^{ns} \overline{Q}_i u_\varepsilon(x_i)\,,
\end{aligned}
\tag{4.185}
$$

where the scalar function u_ε solves the variational problem:

$$
\begin{cases}
\text{Find } u_\varepsilon \in \mathscr{U}_\varepsilon \text{, such that} \\
-\displaystyle\int_{\Omega_\varepsilon} M(u_\varepsilon) \cdot \nabla\nabla\eta = -\int_{\Omega_\varepsilon} b\eta + \int_{\Gamma_{N_q}} \overline{q}\eta \\
\qquad\qquad - \displaystyle\int_{\Gamma_{N_m}} \overline{m}\partial_n \eta - \sum_{i=1}^{ns} \overline{Q}_i \eta(x_i) \quad \forall \eta \in \mathscr{V}_\varepsilon\,, \\
\qquad\qquad \text{with} \quad M(u_\varepsilon) = -\mathbb{C}\nabla\nabla u_\varepsilon\,.
\end{cases}
\tag{4.186}
$$

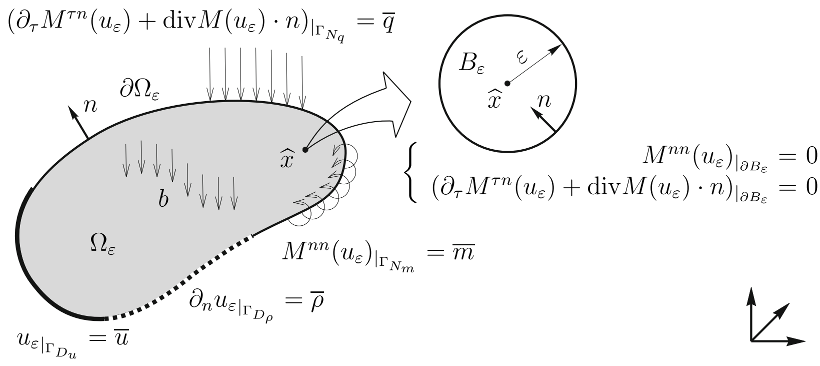


Fig. 4.11 The Kirchhoff problem defined in the perturbed domain Ω_ε

The set $\mathscr{U}_\varepsilon$ and the space $\mathscr{V}_\varepsilon$ are defined as

$$\mathscr{U}_\varepsilon := \{\varphi \in H^2(\Omega_\varepsilon) : \varphi_{|\Gamma_{D_u}} = \overline{u},\ \partial_n \varphi_{|\Gamma_{D_\rho}} = \overline{\rho}\}\ , \tag{4.187}$$

$$\mathscr{V}_\varepsilon := \{\varphi \in H^2(\Omega_\varepsilon) : \varphi_{|\Gamma_{D_u}} = 0,\ \partial_n \varphi_{|\Gamma_{D_\rho}} = 0\}\ . \tag{4.188}$$

Since u_ε and $\partial_n u_\varepsilon$ are free on ∂B_ε, then we have homogeneous Neumann condition on the boundary of the hole. It means that the hole is a free boundary representing a void. See the details in fig. 4.11. The *strong formulation* associated to the variational problem (4.186) reads:

$$\begin{cases} \text{Find } u_\varepsilon, \text{ such that} & \\ \text{div}(\text{div}M(u_\varepsilon)) = b & \text{in } \Omega_\varepsilon\ , \\ M(u_\varepsilon) = -\mathbb{C}\nabla\nabla u_\varepsilon\ , & \\ u_\varepsilon = \overline{u} & \text{on } \Gamma_{D_u}\ , \\ \partial_n u_\varepsilon = \overline{\rho} & \text{on } \Gamma_{D_\rho}\ , \\ M^{nn}(u_\varepsilon) = \overline{m} & \text{on } \Gamma_{N_m}\ , \\ \partial_\tau M^{\tau n}(u_\varepsilon) + \text{div}M(u_\varepsilon)\cdot n = \overline{q} & \text{on } \Gamma_{N_q}\ , \\ [\![M^{\tau n}(u_\varepsilon(x_i))]\!] = \overline{Q}_i & \text{on } x_i \in \Gamma_{N_q}\ , \\ \left.\begin{array}{r} M^{nn}(u_\varepsilon) = 0 \\ \partial_\tau M^{\tau n}(u_\varepsilon) + \text{div}M(u_\varepsilon)\cdot n = 0 \end{array}\right\} & \text{on } \partial B_\varepsilon\ . \end{cases} \tag{4.189}$$

4.3.2 Shape Sensitivity Analysis

In order to apply the result presented in Proposition 1.1, we need to evaluate the shape derivative of functional $\mathscr{J}_{\Omega_\varepsilon}(u_\varepsilon)$ with respect to an uniform expansion of the hole B_ε. Therefore, let us introduce the *Eshelby energy-momentum tensor* [57] of the form

$$\Sigma_\varepsilon = -\frac{1}{2}(M(u_\varepsilon)\cdot\nabla\nabla u_\varepsilon - 2bu_\varepsilon)\mathrm{I} + (\nabla\nabla u_\varepsilon)M(u_\varepsilon) - \nabla u_\varepsilon \otimes \mathrm{div}M(u_\varepsilon) \qquad (4.190)$$

and state the following result:

Proposition 4.6. *Let $\mathscr{J}_{\Omega_\varepsilon}(u_\varepsilon)$ be the shape functional defined by (4.185). Then, the derivative of this functional with respect to the small parameter ε is given by*

$$\dot{\mathscr{J}}_{\Omega_\varepsilon}(u_\varepsilon) = \int_{\Omega_\varepsilon}\Sigma_\varepsilon\cdot\nabla\mathfrak{V} + \int_{\partial\Omega_\varepsilon}\nabla\mathfrak{V}^\top\nabla u_\varepsilon\cdot M(u_\varepsilon)n\,, \qquad (4.191)$$

where $\mathfrak{V}$ is the shape change velocity field defined trough (4.2) and Σ_ε is the Eshelby energy-momentum tensor given by (4.190).

Proof. By making use of the Reynolds' transport theorem through formula (2.84), the shape derivative (the material or total derivative with respect to the parameter ε) of the functional (4.185) is given by

$$\begin{aligned}\dot{\mathscr{J}}_{\Omega_\varepsilon}(u_\varepsilon) = &-\frac{1}{2}\int_{\Omega_\varepsilon}((M(u_\varepsilon)\cdot\nabla\nabla u_\varepsilon)^\cdot + M(u_\varepsilon)\cdot\nabla\nabla u_\varepsilon\mathrm{div}\mathfrak{V})\\ &+\int_{\Omega_\varepsilon}b(\dot{u}_\varepsilon + u_\varepsilon\mathrm{div}\mathfrak{V}) - \int_{\Gamma_{N_q}}\overline{q}\dot{u}_\varepsilon\\ &+\int_{\Gamma_{N_m}}\overline{m}(\partial_n u_\varepsilon)^\cdot + \sum_{i=1}^{ns}\overline{Q}_i\dot{u}_\varepsilon(x_i)\,, \end{aligned} \qquad (4.192)$$

where $(\partial_n u_\varepsilon)^\cdot = \partial_n\dot{u}_\varepsilon$ since $\mathfrak{V}=0$ on $\partial\Omega$. Next, by using the concept of material derivative of spatial fields through formulae (2.89) and (2.90), we find that the first term of the above right hand side integral can be written as

$$\begin{aligned}(M(u_\varepsilon)\cdot\nabla\nabla u_\varepsilon)^\cdot &= 2M(u_\varepsilon)\cdot\nabla(\nabla u_\varepsilon)^\cdot - 2M(u_\varepsilon)\cdot(\nabla\nabla u_\varepsilon)\nabla\mathfrak{V}\\ &= 2M(u_\varepsilon)\cdot\nabla\nabla\dot{u}_\varepsilon - 2M(u_\varepsilon)\cdot\nabla(\nabla\mathfrak{V}^\top\nabla u_\varepsilon)\\ &- 2(\nabla\nabla u_\varepsilon)M(u_\varepsilon)\cdot\nabla\mathfrak{V}\\ &= 2M(u_\varepsilon)\cdot\nabla\nabla\dot{u}_\varepsilon - 2(\nabla\nabla u_\varepsilon)M(u_\varepsilon)\cdot\nabla\mathfrak{V}\\ &+ 2\mathrm{div}M(u_\varepsilon)\cdot\nabla\mathfrak{V}^\top\nabla u_\varepsilon - 2\mathrm{div}(M(u_\varepsilon)\nabla\mathfrak{V}^\top\nabla u_\varepsilon)\,, \end{aligned} \qquad (4.193)$$

since $M(u_\varepsilon) = -\mathbb{C}\nabla\nabla u_\varepsilon$. From these last results we obtain

$$\begin{aligned}\dot{\mathscr{J}}_{\Omega_\varepsilon}(u_\varepsilon) = &-\frac{1}{2}\int_{\Omega_\varepsilon}\Sigma_\varepsilon\cdot\nabla\mathfrak{V} + \int_{\partial\Omega_\varepsilon}\nabla\mathfrak{V}^\top\nabla u_\varepsilon\cdot M(u_\varepsilon)n\\ &-\int_{\Omega_\varepsilon}M(u_\varepsilon)\cdot\nabla\nabla\dot{u}_\varepsilon + \int_{\Omega_\varepsilon}b\dot{u}_\varepsilon\\ &-\int_{\Gamma_{N_q}}\overline{q}\dot{u}_\varepsilon + \int_{\Gamma_{N_m}}\overline{m}\partial_n\dot{u}_\varepsilon + \sum_{i=1}^{ns}\overline{Q}_i\dot{u}_\varepsilon(x_i)\,, \end{aligned} \qquad (4.194)$$

with $\operatorname{div}\mathfrak{V} = \mathrm{I} \cdot \nabla\mathfrak{V}$. Since $\dot{u}_\varepsilon$ is a variation of u_ε in the direction of the velocity field $\mathfrak{V}$, then $\dot{u}_\varepsilon \in \mathscr{V}_\varepsilon$ [210]. Finally, by taking $\dot{u}_\varepsilon$ as test function in the variational problem (4.186), we have that the last five terms of the above equation vanish. □

Now, we can prove that the shape derivative of the functional $\mathscr{J}_{\Omega_\varepsilon}(u_\varepsilon)$ can be written in terms of quantities concentrated on the boundary $\partial\Omega_\varepsilon$. In fact, the following result also holds:

Proposition 4.7. *Let $\mathscr{J}_{\Omega_\varepsilon}(u_\varepsilon)$ be the shape functional defined by (4.185). Then, the derivative of this functional with respect to the small parameter ε is given by*

$$\dot{\mathscr{J}}_{\Omega_\varepsilon}(u_\varepsilon) = \int_{\partial\Omega_\varepsilon} \Sigma_\varepsilon n \cdot \mathfrak{V} + \int_{\partial\Omega_\varepsilon} \nabla\mathfrak{V}^\top \nabla u_\varepsilon \cdot M(u_\varepsilon) n \,, \tag{4.195}$$

where $\mathfrak{V}$ is the shape change velocity field defined through (4.2) and tensor Σ_ε is given by (4.190).

Proof. By making use of the other version of the Reynolds' transport theorem given by formula (2.85), the shape derivative of the functional (4.185) results in

$$\begin{aligned} \dot{\mathscr{J}}_{\Omega_\varepsilon}(u_\varepsilon) = & -\frac{1}{2}\int_{\Omega_\varepsilon} (M(u_\varepsilon)\cdot\nabla\nabla u_\varepsilon)' - \frac{1}{2}\int_{\partial\Omega_\varepsilon} (M(u_\varepsilon)\cdot\nabla\nabla u_\varepsilon) n \cdot \mathfrak{V} \\ & + \int_{\Omega_\varepsilon} b u_\varepsilon' + \int_{\partial\Omega_\varepsilon} (b u_\varepsilon) n \cdot \mathfrak{V} - \int_{\Gamma_{N_q}} \overline{q}\dot{u}_\varepsilon \\ & + \int_{\Gamma_{N_m}} \overline{m}(\partial_n u_\varepsilon)^{\cdot} + \sum_{i=1}^{ns} \overline{Q}_i \dot{u}_\varepsilon(x_i) \,, \end{aligned} \tag{4.196}$$

where $(\partial_n u_\varepsilon)^{\cdot} = \partial_n \dot{u}_\varepsilon$, provided that $\mathfrak{V}$ vanishes on $\partial\Omega$. Next, by using the concept of shape derivatives of spatial fields, we find that the first term of the above right hand side integral can be written as follows

$$(M(u_\varepsilon)\cdot\nabla\nabla u_\varepsilon)' = 2M(u_\varepsilon)\cdot\nabla\nabla u_\varepsilon' \,, \tag{4.197}$$

since $M(u_\varepsilon) = M(u_\varepsilon)^\top$ and u_ε' is the partial derivative of u_ε with respect to ε. Now, let us use the relation between material and spatial derivatives of scalar fields (2.82), namely $\varphi' = \dot{\varphi} - \nabla\varphi \cdot \mathfrak{V}$, which leads to

$$\begin{aligned} (M(u_\varepsilon)\cdot\nabla\nabla u_\varepsilon)' &= 2M(u_\varepsilon)\cdot\nabla\nabla(\dot{u}_\varepsilon - \nabla u_\varepsilon \cdot \mathfrak{V}) \\ &= 2M(u_\varepsilon)\cdot\nabla\nabla\dot{u}_\varepsilon - 2M(u_\varepsilon)\cdot\nabla\nabla(\nabla u_\varepsilon\cdot\mathfrak{V}) \,. \end{aligned} \tag{4.198}$$

From the latter result we obtain

$$\dot{\mathscr{J}}_{\Omega_\varepsilon}(u_\varepsilon) = -\frac{1}{2}\int_{\partial\Omega_\varepsilon}(M(u_\varepsilon)\cdot\nabla\nabla u_\varepsilon - 2bu_\varepsilon)n\cdot\mathfrak{V} + \int_{\Omega_\varepsilon}(M(u_\varepsilon)\cdot\nabla\nabla(\nabla u_\varepsilon\cdot\mathfrak{V}) - b(\nabla u_\varepsilon\cdot\mathfrak{V})) - \int_{\Omega_\varepsilon}M(u_\varepsilon)\cdot\nabla\nabla\dot{u}_\varepsilon + \int_{\Omega_\varepsilon}b\dot{u}_\varepsilon - \int_{\Gamma_{N_q}}\overline{q}\dot{u}_\varepsilon + \int_{\Gamma_{N_m}}\overline{m}\partial_n\dot{u}_\varepsilon + \sum_{i=1}^{ns}\overline{Q}_i\dot{u}_\varepsilon(x_i)\,. \tag{4.199}$$

Since $\dot{u}_\varepsilon$ is a variation of u_ε in the direction of the velocity field $\mathfrak{V}$, then $\dot{u}_\varepsilon \in \mathscr{V}_\varepsilon$. Now, by taking $\dot{u}_\varepsilon$ as test function in the variational problem (4.186), we have that the last five terms of the above equation vanish. By using the tensor relations (G.18,G.20,G.23) and after applying twice the divergence theorem (G.33,G.35), we have

$$\int_{\Omega_\varepsilon}M(u_\varepsilon)\cdot\nabla\nabla(\nabla u_\varepsilon\cdot\mathfrak{V}) = \int_{\partial\Omega_\varepsilon}\nabla(\nabla u_\varepsilon\cdot\mathfrak{V})\cdot M(u_\varepsilon)n - \int_{\Omega_\varepsilon}\mathrm{div}M(u_\varepsilon)\cdot\nabla(\nabla u_\varepsilon\cdot\mathfrak{V}) = \int_{\partial\Omega_\varepsilon}((\nabla\nabla u_\varepsilon)^\top\mathfrak{V} + \nabla\mathfrak{V}^\top\nabla u_\varepsilon)\cdot M(u_\varepsilon)n - \int_{\partial\Omega_\varepsilon}(\mathrm{div}M(u_\varepsilon)\cdot n)(\nabla u_\varepsilon\cdot\mathfrak{V}) + \int_{\Omega_\varepsilon}\mathrm{div}(\mathrm{div}M(u_\varepsilon))(\nabla u_\varepsilon\cdot\mathfrak{V})\,. \tag{4.200}$$

Therefore, the shape derivative of functional $\mathscr{J}_{\Omega_\varepsilon}(u_\varepsilon)$ leads to

$$\dot{\mathscr{J}}_{\Omega_\varepsilon}(u_\varepsilon) = -\frac{1}{2}\int_{\partial\Omega_\varepsilon}(M(u_\varepsilon)\cdot\nabla\nabla u_\varepsilon - 2bu_\varepsilon)n\cdot\mathfrak{V} + \int_{\partial\Omega_\varepsilon}(\nabla\nabla u_\varepsilon)^\top\mathfrak{V}\cdot M(u_\varepsilon)n - \int_{\partial\Omega_\varepsilon}(\mathrm{div}M(u_\varepsilon)\cdot n)(\nabla u_\varepsilon\cdot\mathfrak{V}) + \int_{\partial\Omega_\varepsilon}\nabla\mathfrak{V}^\top\nabla u_\varepsilon\cdot M(u_\varepsilon)n + \int_{\Omega_\varepsilon}(\mathrm{div}(\mathrm{div}M(u_\varepsilon)) - b)(\nabla u_\varepsilon\cdot\mathfrak{V})\,. \tag{4.201}$$

Then, after some rearrangements we obtain

$$\dot{\mathscr{J}}_{\Omega_\varepsilon}(u_\varepsilon) = \int_{\partial\Omega_\varepsilon}\Sigma_\varepsilon n\cdot\mathfrak{V} + \int_{\partial\Omega_\varepsilon}\nabla\mathfrak{V}^\top\nabla u_\varepsilon\cdot M(u_\varepsilon)n + \int_{\Omega_\varepsilon}(\mathrm{div}(\mathrm{div}M(u_\varepsilon)) - b)(\nabla u_\varepsilon\cdot\mathfrak{V})\,. \tag{4.202}$$

Since $\operatorname{div}(\operatorname{div} M(u_\varepsilon)) = b$ provided that u_ε is also solution to the boundary value problem (4.189), the last term of the above equation vanishes, which completes the proof. □

Corollary 4.4. *From the tensor relation (G.23) and after applying the divergence theorem (G.32) to the right hand side of (4.191), we obtain*

$$\dot{\mathscr{J}}_{\Omega_\varepsilon}(u_\varepsilon) = \int_{\partial\Omega_\varepsilon} \Sigma_\varepsilon n \cdot \mathfrak{V} - \int_{\Omega_\varepsilon} \operatorname{div}\Sigma_\varepsilon \cdot \mathfrak{V} + \int_{\partial\Omega_\varepsilon} \nabla\mathfrak{V}^\top \nabla u_\varepsilon \cdot M(u_\varepsilon) n \, . \tag{4.203}$$

Since equations (4.195) and (4.203) remain valid for all velocity fields $\mathfrak{V}$, the domain integral in the above equation satisfies

$$\int_{\Omega_\varepsilon} \operatorname{div}\Sigma_\varepsilon \cdot \mathfrak{V} = 0 \quad \forall \mathfrak{V} \quad \Rightarrow \quad \operatorname{div}\Sigma_\varepsilon = 0 \, , \tag{4.204}$$

that is, Σ_ε is a divergence free tensor field.

Corollary 4.5. *According to Proposition 4.7, the shape derivative for $\varepsilon \geqslant 0$ is given by*

$$\begin{aligned} \dot{\mathscr{J}}_{\Omega_\varepsilon}(u_\varepsilon) &= \int_{\partial B_\varepsilon} \Sigma_\varepsilon n \cdot \mathfrak{V} + \int_{\partial\Omega} \Sigma_\varepsilon n \cdot \mathfrak{V} \\ &+ \int_{\partial\Omega} \nabla\mathfrak{V}^\top \nabla u_\varepsilon \cdot M(u_\varepsilon) n + \int_{\partial B_\varepsilon} \nabla\mathfrak{V}^\top \nabla u_\varepsilon \cdot M(u_\varepsilon) n \, . \end{aligned} \tag{4.205}$$

Since it concerns an uniform expansion of the circular hole, then in view of the associated velocity field defined through (4.2), $\mathfrak{V} = -n$ on ∂B_ε and $\mathfrak{V} = 0$ on $\partial\Omega$. Therefore, the derivative with respect to ε of the energy shape functional is given by

$$\frac{d}{d\varepsilon}\psi(\chi_\varepsilon) = \dot{\mathscr{J}}_{\Omega_\varepsilon}(u_\varepsilon) = -\int_{\partial B_\varepsilon} \Sigma_\varepsilon n \cdot n - \int_{\partial B_\varepsilon} M(u_\varepsilon) n \cdot \nabla n^\top \nabla u_\varepsilon \, . \tag{4.206}$$

From the above corollary, we observe that the shape gradient originally defined in the whole domain Ω_ε leads to an integral defined only on the boundary of the hole ∂B_ε. In particular, the shape derivative of functional $\mathscr{J}_{\Omega_\varepsilon}(u_\varepsilon)$, given by the formula (4.206), is written in terms of quantities supported on ∂B_ε. It means that we need to know the asymptotic behavior of the solution u_ε with respect to ε in the neighborhood of the hole B_ε. We will see later that this result simplifies enormously the next steps of the topological derivative evaluation.

4.3.3 Asymptotic Analysis of the Solution

The shape derivative of functional $\mathscr{J}_{\Omega_\varepsilon}(u_\varepsilon)$ is given exclusively in terms of an integral over the boundary of the hole ∂B_ε (4.206). Therefore, in order to apply the result of Proposition 1.1, we need to investigate the behavior of the function u_ε with

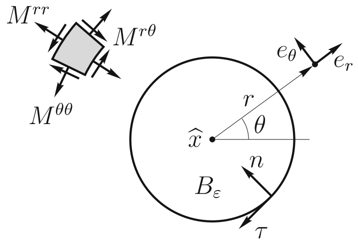


Fig. 4.12 Polar coordinate system (r,θ) centered at the point $\widehat{x} \in \Omega$

respect to ε in the neighborhood of the hole B_ε. In particular, once this behavior is explicitly known, the function $f(\varepsilon)$ can be identified and the limit passage $\varepsilon \to 0$ in (1.49) can be performed, leading to the final formula for the topological derivative $\mathscr{T}$ of the shape functional ψ. However, in general this is not a trivial procedure. In fact, we need to perform the asymptotic analysis of u_ε with respect to ε.

In this section, we establish formally the expansions of the solution u_ε for the problem with homogeneous Neumann condition on the boundary of the hole. For a rigorous justification of the asymptotic expansions of u_ε, the reader may refer to [120, 148], for instance. Let us start with an *ansätz* for the expansion of u_ε in the form [120]

$$u_\varepsilon(x) = u(x) + w_\varepsilon(x) + \widetilde{u}_\varepsilon(x) \ . \tag{4.207}$$

After applying the operator M we have

$$\begin{aligned} M(u_\varepsilon(x)) &= M(u(x)) + M(w_\varepsilon(x)) + M(\widetilde{u}_\varepsilon(x)) \\ &= M(u(\widehat{x})) + \nabla M(u(y))(x - \widehat{x}) \\ &+ M(w_\varepsilon(x)) + M(\widetilde{u}_\varepsilon(x)) \ , \end{aligned} \tag{4.208}$$

where y is an intermediate point between x and $\widehat{x}$. On the boundary of the hole ∂B_ε we have $\partial_\tau M^{\tau n}(u_\varepsilon) + \operatorname{div} M(u_\varepsilon) \cdot n = 0$ and $M^{nn}(u_\varepsilon) = 0$ on ∂B_ε. The above expansion, evaluated on ∂B_ε, leads to

$$M(u(\widehat{x}))n \cdot n - \varepsilon(\nabla M(u(y))n)n \cdot n + M^{nn}(w_\varepsilon(x)) + M^{nn}(\widetilde{u}_\varepsilon(x)) = 0 \ , \tag{4.209}$$

and

$$\begin{aligned} &(\partial_\tau M(u(\widehat{x}))n \cdot \tau + \operatorname{div} M(u(\widehat{x})) \cdot n) - \\ &\quad \varepsilon(\partial_\tau(\nabla M(u(y))n)n \cdot \tau + \operatorname{div}(\nabla M(u(y))n) \cdot n) + \\ &\quad (\partial_\tau M^{\tau n}(w_\varepsilon(x)) + \operatorname{div} M(w_\varepsilon(x)) \cdot n) + \\ &\quad (\partial_\tau M^{\tau n}(\widetilde{u}_\varepsilon(x)) + \operatorname{div} M(\widetilde{u}_\varepsilon(x)) \cdot n) = 0 \ . \end{aligned} \tag{4.210}$$

Thus, we can choose $M(w_\varepsilon)$ such that on the boundary of the hole ∂B_ε the relations hold

$$M^{nn}(w_\varepsilon(x)) = -M(u(\widehat{x}))n \cdot n \ , \tag{4.211}$$

$$\partial_\tau M^{\tau n}(w_\varepsilon(x)) + \operatorname{div} M(w_\varepsilon(x)) \cdot n = -(\partial_\tau M(u(\widehat{x}))n \cdot \tau + \operatorname{div} M(u(\widehat{x})) \cdot n) \ . \tag{4.212}$$

Now, the following exterior problem is considered, and formally obtained as $\varepsilon \to 0$:

$$\begin{cases} \text{Find } M(w_\varepsilon), \text{ such that} \\ \qquad \operatorname{div}(\operatorname{div} M(w_\varepsilon)) = 0 & \text{in } \mathbb{R}^2 \setminus \overline{B_\varepsilon}\,, \\ \qquad M(w_\varepsilon) \to 0 & \text{at } \infty\,, \\ \qquad M^{nn}(w_\varepsilon) = \widehat{u}_1 & \\ \partial_\tau M^{\tau n}(w_\varepsilon) + \operatorname{div} M(w_\varepsilon)\cdot n = \widehat{u}_2 & \end{cases} \Bigg\} \text{ on } \partial B_\varepsilon\,, \tag{4.213}$$

with

$$\widehat{u}_1 = -M(u(\widehat{x}))n\cdot n\,, \tag{4.214}$$

$$\widehat{u}_2 = -(\partial_\tau M(u(\widehat{x}))n\cdot\tau + \operatorname{div} M(u(\widehat{x}))\cdot n)\,. \tag{4.215}$$

The above boundary value problem admits an explicit solution (see, for instance, the book by Little 1973 [139]), which can be written in a polar coordinate system (r,θ) centered at the point $\widehat{x}$ as (see fig. 4.12)

$$M^{rr}(w_\varepsilon(r,\theta)) = -\varphi_1\frac{\varepsilon^2}{r^2} - \varphi_2\left(\frac{4\nu}{3+\nu}\frac{\varepsilon^2}{r^2} + 3\frac{1-\nu}{3+\nu}\frac{\varepsilon^4}{r^4}\right)\cos 2\theta\,, \tag{4.216}$$

$$M^{\theta\theta}(w_\varepsilon(r,\theta)) = \varphi_1\frac{\varepsilon^2}{r^2} - \varphi_2\left(\frac{4}{3+\nu}\frac{\varepsilon^2}{r^2} - 3\frac{1-\nu}{3+\nu}\frac{\varepsilon^4}{r^4}\right)\cos 2\theta\,, \tag{4.217}$$

$$M^{r\theta}(w_\varepsilon(r,\theta)) = \varphi_2\frac{1-\nu}{3+\nu}\left(2\frac{\varepsilon^2}{r^2} - 3\frac{\varepsilon^4}{r^4}\right)\sin 2\theta\,. \tag{4.218}$$

Some terms in the above formulae require explanations. The coefficients φ_1 and φ_2 are given by

$$\varphi_1 = \frac{1}{2}(m_1(u(\widehat{x})) + m_2(u(\widehat{x}))),\ \varphi_2 = \frac{1}{2}(m_1(u(\widehat{x})) - m_2(u(\widehat{x}))), \tag{4.219}$$

where $m_1(u(\widehat{x}))$ and $m_2(u(\widehat{x}))$ are the eigenvalues of the tensor $M(u(\widehat{x}))$, which can be expressed as

$$m_{1,2}(u(\widehat{x})) = \frac{1}{2}\left(\operatorname{tr} M(u(\widehat{x})) \pm \sqrt{2M^D(u(\widehat{x}))\cdot M^D(u(\widehat{x}))}\right)\,, \tag{4.220}$$

with $M^D(u(\widehat{x}))$ standing for the deviatory part of the moment tensor $M(u(\widehat{x}))$, namely

$$M^D(u(\widehat{x})) = M(u(\widehat{x})) - \frac{1}{2}\operatorname{tr} M(u(\widehat{x}))\mathrm{I}\,. \tag{4.221}$$

In addition, $M^{rr}(\varphi)$, $M^{\theta\theta}(\varphi)$ and $M^{r\theta}(\varphi)$ are the components of tensor $M(\varphi)$ in the polar coordinate system, namely, $M^{rr}(\varphi) = e^r\cdot M(\varphi)e^r$, $M^{\theta\theta}(\varphi) = e^\theta\cdot M(\varphi)e^\theta$ and $M^{r\theta}(\varphi) = M^{\theta r}(\varphi) = e^r\cdot M(\varphi)e^\theta$, where e^r and e^θ are the unit vectors in the canonical basis of the polar coordinate system (r,θ), such that, $\|e^r\| = \|e^\theta\| = 1$ and $e^r\cdot e^\theta = 0$. See fig. 4.12.

Now we can construct the remainder $\widetilde{u}_\varepsilon$ in such a way that it compensates the discrepancies introduced by the higher-order terms in ε as well as by the boundary-layer w_ε on the exterior boundary $\partial\Omega$. It means that the remainder $\widetilde{u}_\varepsilon$ must be the solution to the following boundary value problem:

$$\left\{\begin{array}{l} \text{Find } M(\widetilde{u}_\varepsilon), \text{ such that} \\ \begin{array}{rcll} \operatorname{div}(\operatorname{div} M(\widetilde{u}_\varepsilon)) &=& 0 & \text{in } \Omega_\varepsilon , \\ M(\widetilde{u}_\varepsilon) &=& -M(w_\varepsilon) & \text{on } \partial\Omega , \\ M^{nn}(\widetilde{u}_\varepsilon) &=& \varepsilon g_1 & \\ \partial_\tau M^{\tau n}(\widetilde{u}_\varepsilon) + \operatorname{div} M(\widetilde{u}_\varepsilon)\cdot n &=& \varepsilon g_2 & \end{array} \left.\right\} \text{on } \partial B_\varepsilon , \end{array}\right. \tag{4.222}$$

with

$$g_1 = (\nabla M(u(y))n)n\cdot n , \tag{4.223}$$

$$g_2 = \partial_\tau(\nabla M(u(y))n)n\cdot\tau + \operatorname{div}(\nabla M(u(y))n)\cdot n . \tag{4.224}$$

Clearly $\widetilde{u}_\varepsilon = O(\varepsilon)$, since g_1 and g_2 are independent of ε and $w_\varepsilon = O(\varepsilon^2)$ on the exterior boundary $\partial\Omega$. According to [120, 148], we can obtain an estimation for the remainder $\widetilde{u}_\varepsilon$ of the form $\widetilde{u}_\varepsilon = O(\varepsilon^2)$. Finally, the *expansion* for $M(u_\varepsilon)$ in the polar coordinate system (r,θ) reads (see fig. 4.12)

$$\begin{aligned} M^{rr}(u_\varepsilon(r,\theta)) &= \varphi_1\left(1-\frac{\varepsilon^2}{r^2}\right) \\ &\quad + \varphi_2\left(1-\frac{4\nu}{3+\nu}\frac{\varepsilon^2}{r^2} - 3\frac{1-\nu}{3+\nu}\frac{\varepsilon^4}{r^4}\right)\cos 2\theta + O(\varepsilon^2) , \end{aligned} \tag{4.225}$$

$$\begin{aligned} M^{\theta\theta}(u_\varepsilon(r,\theta)) &= \varphi_1\left(1+\frac{\varepsilon^2}{r^2}\right) \\ &\quad - \varphi_2\left(1+\frac{4}{3+\nu}\frac{\varepsilon^2}{r^2} - 3\frac{1-\nu}{3+\nu}\frac{\varepsilon^4}{r^4}\right)\cos 2\theta + O(\varepsilon^2) , \end{aligned} \tag{4.226}$$

$$M^{r\theta}(u_\varepsilon(r,\theta)) = -\varphi_2\left(1-2\frac{1-\nu}{3+\nu}\frac{\varepsilon^2}{r^2} + 3\frac{1-\nu}{3+\nu}\frac{\varepsilon^4}{r^4}\right)\sin 2\theta + O(\varepsilon^2) , \tag{4.227}$$

where we have used the fact that $M^{rr}(u(\widehat{x})) = \varphi_1 + \varphi_2\cos 2\theta$, $M^{\theta\theta}(u(\widehat{x})) = \varphi_1 - \varphi_2\cos 2\theta$ and $M^{r\theta}(u(\widehat{x})) = -\varphi_2\sin 2\theta$.

4.3.4 Topological Derivative Evaluation

From an orthonormal curvilinear coordinate system n and τ defined on the boundary ∂B_ε (see fig. 4.12), the tensors $M(u_\varepsilon)$ and $\nabla\nabla u_\varepsilon$ can be decomposed as

$$
\begin{aligned}
M(u_\varepsilon)_{|\partial B_\varepsilon} &= M^{nn}(u_\varepsilon)(n\otimes n)+M^{n\tau}(u_\varepsilon)(n\otimes\tau)\\
&+ M^{\tau n}(u_\varepsilon)(\tau\otimes n)+M^{\tau\tau}(u_\varepsilon)(\tau\otimes\tau)\,, &(4.228)\\
\nabla\nabla u_{\varepsilon}{}_{|\partial B_\varepsilon} &= \partial^2_{nn}u_\varepsilon(n\otimes n)+\partial^2_{n\tau}u_\varepsilon(n\otimes\tau)\\
&+ \partial^2_{\tau n}u_\varepsilon(\tau\otimes n)+\partial^2_{\tau\tau}u_\varepsilon(\tau\otimes\tau)\,. &(4.229)
\end{aligned}
$$

In addition,

$$
\begin{aligned}
\Sigma_\varepsilon n\cdot n = &-\frac{1}{2}(M(u_\varepsilon)\cdot\nabla\nabla u_\varepsilon-2bu_\varepsilon)\\
&+M(u_\varepsilon)n\cdot(\nabla\nabla u_\varepsilon)^\top n-(\nabla u_\varepsilon\cdot n)(\operatorname{div}M(u_\varepsilon)\cdot n)\,. \qquad (4.230)
\end{aligned}
$$

However, the identity below

$$
\nabla(\nabla u_\varepsilon\cdot n)=(\nabla\nabla u_\varepsilon)^\top n+\nabla n^\top\nabla u_\varepsilon\,, \qquad (4.231)
$$

implies

$$
M(u_\varepsilon)n\cdot(\nabla\nabla u_\varepsilon)^\top n = M(u_\varepsilon)n\cdot\nabla(\nabla u_\varepsilon\cdot n)-M(u_\varepsilon)n\cdot\nabla n^\top\nabla u_\varepsilon\,, \qquad (4.232)
$$

which leads to

$$
\begin{aligned}
\Sigma_\varepsilon n\cdot n_{|\partial B_\varepsilon} = &-\frac{1}{2}(M^{nn}(u_\varepsilon)\partial^2_{nn}u_\varepsilon+2M^{\tau n}(u_\varepsilon)\partial^2_{\tau n}u_\varepsilon+M^{\tau\tau}(u_\varepsilon)\partial^2_{\tau\tau}u_\varepsilon-2bu_\varepsilon)\\
&-M(u_\varepsilon)n\cdot\nabla n^\top\nabla u_\varepsilon+M^{nn}(u_\varepsilon)\partial^2_{nn}u_\varepsilon\\
&+M^{\tau n}(u_\varepsilon)\partial_\tau(\partial_n u_\varepsilon)-\partial_n u_\varepsilon(\operatorname{div}M(u_\varepsilon)\cdot n)\,. \qquad (4.233)
\end{aligned}
$$

From integration by parts of the first term in the integral below, we obtain

$$
\begin{aligned}
&\int_{\partial B_\varepsilon}(M^{\tau n}(u_\varepsilon)\partial_\tau(\partial_n u_\varepsilon)-\partial_n u_\varepsilon(\operatorname{div}M(u_\varepsilon)\cdot n)) =\\
&\qquad -\int_{\partial B_\varepsilon}(\partial_\tau M^{\tau n}(u_\varepsilon)+\operatorname{div}M(u_\varepsilon)\cdot n)(\partial_n u_\varepsilon)\,. \qquad (4.234)
\end{aligned}
$$

Therefore, since $\partial_\tau M^{\tau n}(u_\varepsilon)+\operatorname{div}M(u_\varepsilon)\cdot n=0$ and $M^{nn}(u_\varepsilon)=0$ on ∂B_ε, we have

$$
\begin{aligned}
\Sigma_\varepsilon n\cdot n_{|\partial B_\varepsilon} = &-\frac{1}{2}(M^{\tau\tau}(u_\varepsilon)\partial^2_{\tau\tau}u_\varepsilon+2M^{\tau n}(u_\varepsilon)\partial^2_{\tau n}u_\varepsilon-2bu_\varepsilon)\\
&-M(u_\varepsilon)n\cdot\nabla n^\top\nabla u_\varepsilon\,. \qquad (4.235)
\end{aligned}
$$

Note that the integral on the boundary ∂B_ε of the last term in the above equation cancels with the last term in (4.206), leading to

$$
\dot{\mathscr{J}}_{\Omega_\varepsilon}(u_\varepsilon)=\frac{1}{2}\int_{\partial B_\varepsilon}(M^{\tau\tau}(u_\varepsilon)\partial^2_{\tau\tau}u_\varepsilon+2M^{\tau n}(u_\varepsilon)\partial^2_{\tau n}u_\varepsilon-2bu_\varepsilon)\,. \qquad (4.236)
$$

On the other hand, the constitutive tensor $\mathbb{C}$ is invertible, namely,

$$\mathbb{C}^{-1} = \frac{1}{E}((1+\nu)\mathbb{I} - \nu \mathrm{I} \otimes \mathrm{I}) , \quad (4.237)$$

which implies $\nabla\nabla u_\varepsilon = -\mathbb{C}^{-1} M(u_\varepsilon)$. In particular, on the boundary of the hole ∂B_ε we have

$$\partial^2_{\tau\tau} u_\varepsilon = -\frac{1}{E}(M^{\tau\tau}(u_\varepsilon) - \nu M^{nn}(u_\varepsilon)) = -\frac{1}{E} M^{\tau\tau}(u_\varepsilon) , \quad (4.238)$$

$$\partial^2_{\tau n} u_\varepsilon = -\frac{1}{E}(1+\nu) M^{\tau n}(u_\varepsilon) , \quad (4.239)$$

since $M^{nn}(u_\varepsilon) = 0$ on ∂B_ε. Therefore, the shape derivative of the cost functional (4.206) reads

$$\frac{d}{d\varepsilon}\psi(\chi_\varepsilon) = \dot{\mathscr{J}}_{\Omega_\varepsilon}(u_\varepsilon) = \\ -\frac{1}{2}\int_{\partial B_\varepsilon}\left[\frac{1}{E}\left((M^{\tau\tau}(u_\varepsilon))^2 + 2(1+\nu)(M^{\tau n}(u_\varepsilon))^2\right) + 2bu_\varepsilon\right] . \quad (4.240)$$

From formulae (4.226) and (4.227), we have that the following expansions for $M^{\tau\tau}(u_\varepsilon)$ and $M^{\tau n}(u_\varepsilon)$ hold in the neighborhood of the hole

$$\begin{aligned} M^{\tau\tau}(u_\varepsilon(x)) &= M^{\theta\theta}(u_\varepsilon(r,\theta)) \\ &= \varphi_1\left(1+\frac{\varepsilon^2}{r^2}\right) - \varphi_2\left(1+\frac{4}{3+\nu}\frac{\varepsilon^2}{r^2} - 3\frac{1-\nu}{3+\nu}\frac{\varepsilon^4}{r^4}\right)\cos 2\theta + O(\varepsilon) \\ &\Rightarrow M^{\tau\tau}(u_\varepsilon(x))_{|\partial B_\varepsilon} = 2\varphi_1 - 4\frac{1+\nu}{3+\nu}\varphi_2 \cos 2\theta + O(\varepsilon), \end{aligned} \quad (4.241)$$

$$\begin{aligned} M^{\tau n}(u_\varepsilon(x)) &= M^{r\theta}(u_\varepsilon(r,\theta)) \\ &= -\varphi_2\left(1 - 2\frac{1-\nu}{3+\nu}\frac{\varepsilon^2}{r^2} + 3\frac{1-\nu}{3+\nu}\frac{\varepsilon^4}{r^4}\right)\sin 2\theta + O(\varepsilon) \\ &\Rightarrow M^{\tau n}(u_\varepsilon(x))_{|\partial B_\varepsilon} = -\frac{4}{3+\nu}\varphi_2 \sin 2\theta + O(\varepsilon). \end{aligned} \quad (4.242)$$

In addition, the following expansion for the displacement field u_ε holds on the boundary of the hole

$$u_\varepsilon(x)_{|\partial B_\varepsilon} = \varphi_0 + O(\varepsilon) , \quad (4.243)$$

where $\varphi_0 = u(\widehat{x})$. Considering the above expansions in (4.240)

$$\frac{d}{d\varepsilon}\psi(\chi_\varepsilon) = -\frac{1}{2}\int_0^{2\pi}\left(\frac{1}{E}\varphi + 2b\varphi_0\right)\varepsilon d\theta + O(\varepsilon^2) , \quad (4.244)$$

where

$$\varphi := \left(2\varphi_1 - 4\frac{1+\nu}{3+\nu}\varphi_2\cos 2\theta\right)^2 + 2(1+\nu)\left(\frac{4}{3+\nu}\varphi_2 \sin 2\theta\right)^2 , \quad (4.245)$$

and after analytically solving the integral on the boundary of the hole ∂B_ε, we obtain

$$\frac{d}{d\varepsilon}\psi(\chi_\varepsilon) = -2\pi\varepsilon\left(\frac{2}{E}\left(\varphi_1^2 + 2\frac{1+\nu}{3+\nu}\varphi_2^2\right) + b\varphi_0\right) + O(\varepsilon^2)\,. \tag{4.246}$$

Therefore, the above result together with the relation between shape and topological derivatives given by (1.49) leads to

$$\mathscr{T} = -\lim_{\varepsilon\to 0}\frac{1}{f'(\varepsilon)}\left[2\pi\varepsilon\left(\frac{2}{E}\left(\varphi_1^2 + 2\frac{1+\nu}{3+\nu}\varphi_2^2\right) + b\varphi_0\right) + O(\varepsilon^2)\right]\,. \tag{4.247}$$

Now, in order to extract the leading term of the above expansion, we choose

$$f(\varepsilon) = \pi\varepsilon^2\,, \tag{4.248}$$

which results in

$$\mathscr{T} = -\frac{2}{E}\left(\varphi_1^2 + 2\frac{1+\nu}{3+\nu}\varphi_2^2\right) - b\varphi_0\,, \tag{4.249}$$

where $\varphi_1 = (m_1(u(\widehat{x})) + m_2(u(\widehat{x})))/2$, $\varphi_2 = (m_1(u(\widehat{x})) - m_2(u(\widehat{x})))/2$ and $\varphi_0 = u(\widehat{x})$. Therefore, the final formula for the *topological derivative* evaluated at $\widehat{x} \in \Omega$ becomes [20, 186]:

- In terms of the principal moments $m_1(\widehat{x}) = m_1(u(\widehat{x}))$ and $m_2(\widehat{x}) = m_2(u(\widehat{x}))$

$$\mathscr{T}(\widehat{x}) = -\frac{1}{2E}\left[(m_1(\widehat{x}) + m_2(\widehat{x}))^2 + 2\tfrac{1+\nu}{3+\nu}(m_1(\widehat{x}) - m_2(\widehat{x}))^2\right] - bu(\widehat{x})\,. \tag{4.250}$$

- In terms of the moment tensor $M(u(\widehat{x}))$

$$\mathscr{T}(\widehat{x}) = -\frac{1}{2E}\left[4\tfrac{1+\nu}{3+\nu}M(u(\widehat{x}))\cdot M(u(\widehat{x})) + \tfrac{1-\nu}{3+\nu}\mathrm{tr}^2 M(u(\widehat{x}))\right] - bu(\widehat{x})\,. \tag{4.251}$$

- In terms of the moment tensor $M(u(\widehat{x}))$ and the curvature tensor $\nabla\nabla u(\widehat{x})$

$$\mathscr{T}(\widehat{x}) = \mathbb{P}M(u(\widehat{x}))\cdot\nabla\nabla u(\widehat{x}) - bu(\widehat{x})\,, \tag{4.252}$$

  where $\mathbb{P}$ is the *Pólya-Szegö polarization tensor*, given in this particular case by the following isotropic fourth order tensor

$$\mathbb{P} = \frac{2}{3+\nu}\mathbb{I} + \frac{1+3\nu}{2(1-\nu)(3+\nu)}\mathrm{I}\otimes\mathrm{I}\,. \tag{4.253}$$

Finally, the topological asymptotic expansion of the energy shape functional reads

$$\psi(\chi_\varepsilon(\widehat{x})) = \psi(\chi) + \pi\varepsilon^2(\mathbb{P}M(u(\widehat{x}))\cdot\nabla\nabla u(\widehat{x}) - bu(\widehat{x})) + o(\varepsilon^2)\,. \tag{4.254}$$

The complete mathematical justification for the above expansion follows the same steps to be presented in Chapter 10 for another problem.

4.4 Exercises

1. Consider the Poisson problem described in Section 4.1:

    a. From (4.8), derive (4.9) and (4.12).
    b. Take into account Remark 4.1.
    c. By using separation of variables, find the explicit solution to the boundary value problem (4.27).
    d. Consider the problem defined in a ring as presented in Section 4.1.5.1. By taking into account a shape functional of the form

    $$\psi(\chi_\varepsilon) = \frac{1}{2}\int_{\Omega_\varepsilon} \|\nabla u_\varepsilon\|^2 + \frac{1}{2}\int_{\partial B_\varepsilon} u_\varepsilon^2 \ ,$$

    where u_ε is solution to:

    $$\begin{cases} \text{Find } u_\varepsilon, \text{ such that} \\ \qquad \Delta u_\varepsilon = 0 \quad \text{in } \Omega_\varepsilon \ , \\ \qquad u_\varepsilon = a + \cos\theta \quad \text{on } \partial\Omega \ , \\ u_\varepsilon + \partial_n u_\varepsilon = 0 \quad \text{on } \partial B_\varepsilon \ . \end{cases}$$

    Develop $\psi(\chi_\varepsilon)$ in powers of ε around the origin to obtain

    $$\psi(\chi_\varepsilon) = \frac{\pi}{2} + \pi\varepsilon a^2 + o(\varepsilon^2) \ ,$$

    and compare it with the topological asymptotic expansion (4.111).

2. Consider the Navier problem described in Section 4.2:

    a. From (4.117), derive the Navier system as presented in Remark 4.6.
    b. From (4.120), derive (4.121) and (4.124).
    c. By using separation of variables, find the stress distribution around the hole explicitly, which is solution to the boundary value problem (4.145). Hint: take a look on the book by Little 1973 [139] and look for the Airy functions in polar coordinates.

3. Consider the Kirchhoff problem described in Section 4.3:

    a. From (4.183), derive the Kirchhoff equation as presented in Remark 4.8.
    b. From (4.185), derive (4.186) and (4.189).
    c. By using separation of variables, find the moment distribution around the hole explicitly, which is solution to the boundary value problem (4.213). Hint: take a look on the book by Little 1973 [139] and look for the Airy functions in polar coordinates.

Chapter 5
Configurational Perturbations of Energy Functionals

The evaluation of the topological derivatives for the energy shape functionals associated to the representative boundary value problems for the scalar (Laplace) and the vectorial (Navier) second-order partial differential equations and for the scalar fourth-order (Kirchhoff) partial differential equation is presented in this chapter. In contrast with Chapter 4, here the domain is topologically perturbed by the nucleation of a small inclusion, instead of a hole.

More precisely, the perturbed domain is obtained if a circular hole $B_\varepsilon(\widehat{x})$ is introduced inside $\Omega \subset \mathbb{R}^2$, where $\overline{B_\varepsilon(\widehat{x})} \Subset \Omega$ denotes a ball of radius ε and center at $\widehat{x} \in \Omega$. Then, $B_\varepsilon(\widehat{x})$ is filled by an inclusion with different material property compared to the unperturbed domain Ω, as it shown in fig. 5.1. The material properties are characterized by a piecewise constant function γ_ε of the form

$$\gamma_\varepsilon = \gamma_\varepsilon(x) := \begin{cases} 1 \text{ if} x \in \Omega \setminus \overline{B_\varepsilon} \,, \\ \gamma \text{ if } x \in B_\varepsilon \,, \end{cases} \tag{5.1}$$

where $\gamma \in \mathbb{R}_+$ is the contrast coefficient.

In the same way as in Chapter 4 the shape change velocity field $\mathfrak{V} \in \mathscr{S}_\varepsilon$ that represents an uniform expansion of the circular inclusion $B_\varepsilon(\widehat{x})$ is constructed, with the set $\mathscr{S}_\varepsilon$ defined in (4.2). Such a velocity field $\mathfrak{V}$ is the key point when using Proposition 1.1 leading to a simple and constructive method for evaluation of the topological derivative through formula (1.49). Note that in this case the topologies of the original and perturbed domains are preserved. However, we are introducing a nonsmooth perturbation in the coefficients of the differential operator through the contrast γ_ε, by changing the material property of the background in a small region $B_\varepsilon \subset \Omega$. This procedure is called the configurational perturbation. Since we are dealing with a nonsmooth perturbation of the material properties, the sensitivity of the shape functional with respect to the nucleation of an inclusion can also be studied through the topological asymptotic analysis concept, which is, in fact, the most appropriate approach for such a problem.

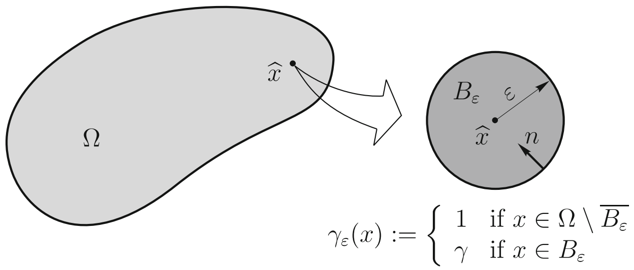


Fig. 5.1 Topologically perturbed domain by the nucleation of a small circular inclusion

5.1 Second Order Elliptic Equation: The Laplace Problem

In this section we evaluate the topological derivative of the total potential energy associated to the steady-state heat conduction problem, considering the nucleation of a small inclusion, represented by $B_\varepsilon \subset \Omega$, as the topological perturbation.

5.1.1 Problem Formulation

The shape functional associated to the unperturbed domain which we are dealing with is defined as

$$\psi(\chi) := \mathscr{J}_\Omega(u) = -\frac{1}{2}\int_\Omega q(u)\cdot\nabla u + \int_{\Gamma_N} \overline{q}u \,, \tag{5.2}$$

where the scalar function u is the solution to the variational problem:

$$\begin{cases} \text{Find } u \in \mathscr{U}, \text{ such that} \\ \displaystyle\int_\Omega q(u)\cdot\nabla\eta = \int_{\Gamma_N} \overline{q}\eta \quad \forall \eta \in \mathscr{V} \,, \\ \qquad\qquad \text{with} \quad q(u) = -k\nabla u \,. \end{cases} \tag{5.3}$$

In the above equation, k is the thermal conductivity of the medium, assumed to be constant everywhere. The set $\mathscr{U}$ and the space $\mathscr{V}$ are respectively defined as

$$\mathscr{U} := \{\varphi \in H^1(\Omega) : \varphi_{|\Gamma_D} = \overline{u}\} \,, \tag{5.4}$$

$$\mathscr{V} := \{\varphi \in H^1(\Omega) : \varphi_{|\Gamma_D} = 0\} \,. \tag{5.5}$$

In addition, $\partial\Omega = \overline{\Gamma}_D \cup \overline{\Gamma}_N$ with $\Gamma_D \cap \Gamma_N = \varnothing$, where Γ_D and Γ_N are Dirichlet and Neumann boundaries, respectively. Thus $\overline{u}$ is a Dirichlet data on Γ_D and $\overline{q}$ is a

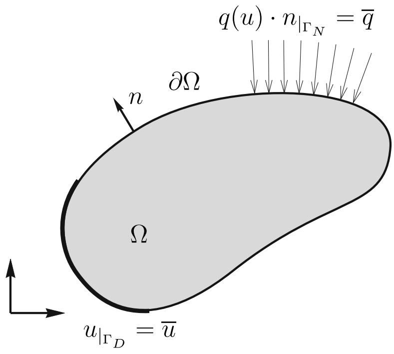


Fig. 5.2 The Laplace problem defined in the unperturbed domain

Neumann data on Γ_N, both assumed to be smooth enough. See the details in fig. 5.2. The strong equation associated to the above variational problem (5.3) reads:

$$\begin{cases} \text{Find } u, \text{ such that} \\ \operatorname{div} q(u) = 0 & \text{in } \Omega \,, \\ q(u) = -k\nabla u \,, \\ u = \overline{u} & \text{on } \Gamma_D \,, \\ q(u)\cdot n = \overline{q} & \text{on } \Gamma_N \,. \end{cases} \tag{5.6}$$

Remark 5.1. Since the thermal conductivity k is assumed to be constant, the above boundary value problem reduces itself to the well-known Laplace equation, namely

$$-\Delta u = 0 \quad \text{in} \quad \Omega \,. \tag{5.7}$$

Now, let us state the same problem in the perturbed domain. In this case, the total potential energy reads

$$\psi(\chi_\varepsilon) := \mathscr{J}_{\chi_\varepsilon}(u_\varepsilon) = -\frac{1}{2}\int_\Omega q_\varepsilon(u_\varepsilon)\cdot\nabla u_\varepsilon + \int_{\Gamma_N} \overline{q} u_\varepsilon \,, \tag{5.8}$$

where the scalar function u_ε solves the variational problem:

$$\begin{cases} \text{Find } u_\varepsilon \in \mathscr{U}_\varepsilon, \text{ such that} \\ \displaystyle\int_\Omega q_\varepsilon(u_\varepsilon)\cdot\nabla\eta = \int_{\Gamma_N} \overline{q}\eta \quad \forall \eta \in \mathscr{V}_\varepsilon \,, \\ \qquad \text{with} \quad q_\varepsilon(u_\varepsilon) = -\gamma_\varepsilon k \nabla u_\varepsilon \,, \end{cases} \tag{5.9}$$

with γ_ε defined by (5.1). The set $\mathscr{U}_\varepsilon$ and the space $\mathscr{V}_\varepsilon$ are defined as

$$\mathscr{U}_\varepsilon := \{\varphi \in \mathscr{U} : [\![\varphi]\!] = 0 \text{ on } \partial B_\varepsilon\} \,, \tag{5.10}$$

$$\mathscr{V}_\varepsilon := \{\varphi \in \mathscr{V} : [\![\varphi]\!] = 0 \text{ on } \partial B_\varepsilon\} \,, \tag{5.11}$$

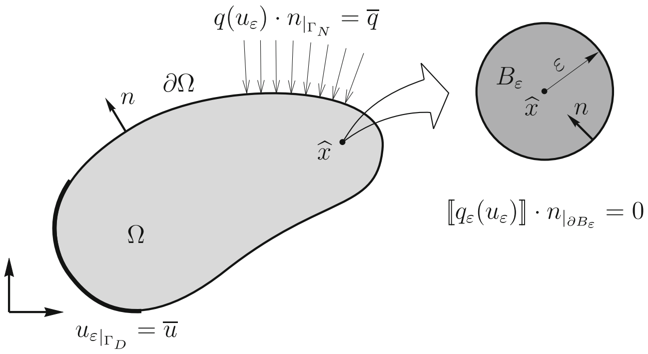


Fig. 5.3 The Laplace problem defined in the perturbed domain

where the operator $[\![\varphi]\!]$ is used to denote the jump of function φ on the boundary of the inclusion ∂B_ε, namely $[\![\varphi]\!] := \varphi_{|_{\Omega\setminus\overline{B_\varepsilon}}} - \varphi_{|_{B_\varepsilon}}$ on ∂B_ε. See the details in fig. 5.3. The *strong equation* associated to the variational problem (5.9) reads:

$$\begin{cases} \text{Find } u_\varepsilon \text{, such that} & \\ \operatorname{div} q_\varepsilon(u_\varepsilon) = 0 & \text{in } \Omega \,, \\ q_\varepsilon(u_\varepsilon) = -\gamma_\varepsilon k \nabla u_\varepsilon \,, & \\ u_\varepsilon = \overline{u} & \text{on } \Gamma_D \,, \\ q(u_\varepsilon)\cdot n = \overline{q} & \text{on } \Gamma_N \,, \\ \left.\begin{array}{r} [\![u_\varepsilon]\!] = 0 \\ [\![q_\varepsilon(u_\varepsilon)]\!]\cdot n = 0 \end{array}\right\} & \text{on } \partial B_\varepsilon \,. \end{cases} \tag{5.12}$$

The *transmission condition* on the boundary of the inclusion ∂B_ε comes out from the variation formulation (5.9).

5.1.2 Shape Sensitivity Analysis

Let us evaluate the shape derivative of functional $\mathscr{J}_{\chi_\varepsilon}(u_\varepsilon)$ with respect to an uniform expansion of the inclusion B_ε. We start by introducing the *Eshelby energy-momentum tensor* [57] of the form

$$\Sigma_\varepsilon = -\frac{1}{2}(q_\varepsilon(u_\varepsilon)\cdot\nabla u_\varepsilon)\mathrm{I} + \nabla u_\varepsilon \otimes q_\varepsilon(u_\varepsilon) \,. \tag{5.13}$$

After considering the constitutive relation $q_\varepsilon(u_\varepsilon) = -\gamma_\varepsilon k \nabla u_\varepsilon$ in (5.8), with the contrast γ_ε given by (5.1), we note that the shape functional $\mathscr{J}_{\chi_\varepsilon}(u_\varepsilon)$ can be written as follows

$$\mathscr{J}_{\chi_\varepsilon}(u_\varepsilon) = -\frac{1}{2}\left(\int_{\Omega\setminus\overline{B_\varepsilon}} q(u_\varepsilon)\cdot\nabla u_\varepsilon + \int_{B_\varepsilon} \gamma q(u_\varepsilon)\cdot\nabla u_\varepsilon\right) + \int_{\Gamma_N} \overline{q} u_\varepsilon \,, \tag{5.14}$$

where $q(u_\varepsilon) = -k\nabla u_\varepsilon$. Thus, we have an explicit dependence with respect to the parameter ε, which allows us to state the following result:

Proposition 5.1. *Let $\mathscr{J}_{\chi_\varepsilon}(u_\varepsilon)$ be the shape functional defined by (5.8). Then, the derivative of this functional with respect to the small parameter ε is given by*

$$\dot{\mathscr{J}}_{\chi_\varepsilon}(u_\varepsilon) = \int_\Omega \Sigma_\varepsilon \cdot \nabla\mathfrak{V} \,, \tag{5.15}$$

where $\mathfrak{V}$ stands for the shape change velocity field defined through (4.2) and Σ_ε is the Eshelby energy-momentum tensor given by (5.13).

Proof. Before starting, let us recall that the constitutive operator is defined as $q_\varepsilon(\varphi) = -\gamma_\varepsilon k\nabla\varphi$. Thus, by making use of the Reynolds' transport theorem given by the result (2.84) and the concept of material derivative of spatial fields through formula (2.89), the derivative with respect to ε of the shape functional (5.14) is given by

$$\begin{aligned}
\dot{\mathscr{J}}_{\chi_\varepsilon}(u_\varepsilon) &= -\frac{1}{2}\left(\int_{\Omega\setminus\overline{B_\varepsilon}} q(u_\varepsilon)\cdot\nabla u_\varepsilon + \int_{B_\varepsilon} \gamma q(u_\varepsilon)\cdot\nabla u_\varepsilon\right)^{\cdot} + \int_{\Gamma_N} \overline{q}\dot{u}_\varepsilon \\
&= -\int_{\Omega\setminus\overline{B_\varepsilon}} q(u_\varepsilon)\cdot\nabla\dot{u}_\varepsilon - \int_{B_\varepsilon} \gamma q(u_\varepsilon)\cdot\nabla\dot{u}_\varepsilon \\
&\quad -\frac{1}{2}\int_{\Omega\setminus\overline{B_\varepsilon}} ((q(u_\varepsilon)\cdot\nabla u_\varepsilon)\mathrm{I} - 2\nabla u_\varepsilon \otimes q(u_\varepsilon))\cdot\nabla\mathfrak{V} \\
&\quad -\frac{1}{2}\int_{B_\varepsilon} \gamma((q(u_\varepsilon)\cdot\nabla u_\varepsilon)\mathrm{I} - 2\nabla u_\varepsilon \otimes q(u_\varepsilon))\cdot\nabla\mathfrak{V} + \int_{\Gamma_N} \overline{q}\dot{u}_\varepsilon \\
&= -\frac{1}{2}\int_\Omega ((q_\varepsilon(u_\varepsilon)\cdot\nabla u_\varepsilon)\mathrm{I} - 2\nabla u_\varepsilon \otimes q_\varepsilon(u_\varepsilon))\cdot\nabla\mathfrak{V} \\
&\quad -\int_\Omega q_\varepsilon(u_\varepsilon)\cdot\nabla\dot{u}_\varepsilon + \int_{\Gamma_N} \overline{q}\dot{u}_\varepsilon \,.
\end{aligned} \tag{5.16}$$

Since $\dot{u}_\varepsilon$ is a variation of u_ε in the direction of the velocity field $\mathfrak{V}$, then $\dot{u}_\varepsilon \in \mathscr{V}_\varepsilon$ [210]. Finally, by taking $\dot{u}_\varepsilon$ as test function in the variational problem (5.9), we have that the last two terms of the above equation vanish. □

Proposition 5.2. *Let $\mathscr{J}_{\chi_\varepsilon}(u_\varepsilon)$ be the shape functional defined by (5.8). Then, its derivative with respect to the small parameter ε is given by*

$$\dot{\mathscr{J}}_{\chi_\varepsilon}(u_\varepsilon) = \int_{\partial\Omega} \Sigma_\varepsilon n\cdot\mathfrak{V} + \int_{\partial B_\varepsilon} [\![\Sigma_\varepsilon]\!] n\cdot\mathfrak{V} \,, \tag{5.17}$$

where $\mathfrak{V}$ is the shape change velocity field defined through (4.2) and tensor Σ_ε is given by (5.13).

Proof. Before starting, let us recall the constitutive operator $q_\varepsilon(\varphi) = -\gamma_\varepsilon k\nabla\varphi$ and the relation between material and spatial derivatives of scalar fields (2.82), namely

$\dot{\varphi} = \varphi' + \nabla\varphi \cdot \mathfrak{V}$. By making use of the other version of the Reynolds' transport theorem given by formula (2.85), the shape derivative of the functional (5.14) results in

$$\begin{aligned}\dot{\mathscr{J}}_{\chi_\varepsilon}(u_\varepsilon) &= -\frac{1}{2}\left(\int_\Omega q_\varepsilon(u_\varepsilon)\cdot\nabla u_\varepsilon\right)^{\cdot} + \int_{\Gamma_N} \overline{q}\dot{u}_\varepsilon \\ &= -\int_\Omega q_\varepsilon(u_\varepsilon)\cdot\nabla u'_\varepsilon - \frac{1}{2}\int_{\partial\Omega}(q_\varepsilon(u_\varepsilon)\cdot\nabla u_\varepsilon)n\cdot\mathfrak{V} \\ &\quad -\frac{1}{2}\int_{\partial B_\varepsilon}[\![q_\varepsilon(u_\varepsilon)\cdot\nabla u_\varepsilon]\!]n\cdot\mathfrak{V} + \int_{\Gamma_N}\overline{q}\dot{u}_\varepsilon\,. \end{aligned} \tag{5.18}$$

In addition, we have

$$\begin{aligned}\dot{\mathscr{J}}_{\chi_\varepsilon}(u_\varepsilon) &= -\frac{1}{2}\int_{\partial\Omega}(q_\varepsilon(u_\varepsilon)\cdot\nabla u_\varepsilon)n\cdot\mathfrak{V} - \frac{1}{2}\int_{\partial B_\varepsilon}[\![q_\varepsilon(u_\varepsilon)\cdot\nabla u_\varepsilon]\!]n\cdot\mathfrak{V} \\ &\quad + \int_\Omega q_\varepsilon(u_\varepsilon)\cdot\nabla(\nabla u_\varepsilon\cdot\mathfrak{V}) - \int_\Omega q_\varepsilon(u_\varepsilon)\cdot\nabla\dot{u}_\varepsilon + \int_{\Gamma_N}\overline{q}\dot{u}_\varepsilon\,. \end{aligned} \tag{5.19}$$

Since $\dot{u}_\varepsilon$ is a variation of u_ε in the direction of the velocity field $\mathfrak{V}$, then $\dot{u}_\varepsilon \in \mathscr{V}_\varepsilon$ [210]. Now, by taking into account that u_ε is the solution to the variational problem (5.9), we have that the last two terms of the above equation vanish. From integration by parts

$$\begin{aligned}\dot{\mathscr{J}}_{\chi_\varepsilon}(u_\varepsilon) &= -\frac{1}{2}\int_{\partial\Omega}(q_\varepsilon(u_\varepsilon)\cdot\nabla u_\varepsilon)n\cdot\mathfrak{V} - \frac{1}{2}\int_{\partial B_\varepsilon}[\![q_\varepsilon(u_\varepsilon)\cdot\nabla u_\varepsilon]\!]n\cdot\mathfrak{V} \\ &\quad + \int_{\partial\Omega}(\nabla u_\varepsilon\otimes q_\varepsilon(u_\varepsilon))n\cdot\mathfrak{V} + \int_{\partial B_\varepsilon}[\![\nabla u_\varepsilon\otimes q_\varepsilon(u_\varepsilon))]\!]n\cdot\mathfrak{V} \\ &\quad - \int_\Omega \operatorname{div}(q_\varepsilon(u_\varepsilon))\nabla u_\varepsilon\cdot\mathfrak{V}\,, \end{aligned} \tag{5.20}$$

and rewriting the above equation in the compact form, we obtain

$$\dot{\mathscr{J}}_{\chi_\varepsilon}(u_\varepsilon) = \int_{\partial\Omega}\Sigma_\varepsilon n\cdot\mathfrak{V} + \int_{\partial B_\varepsilon}[\![\Sigma_\varepsilon]\!]n\cdot\mathfrak{V} - \int_\Omega \operatorname{div}(q_\varepsilon(u_\varepsilon))\nabla u_\varepsilon\cdot\mathfrak{V}\,. \tag{5.21}$$

Finally, taking into account that u_ε is the solution to the state equation (5.12), namely $\operatorname{div} q_\varepsilon(u_\varepsilon) = 0$, we have that the last term in the above equation vanishes, which leads to the result. □

Corollary 5.1. *From the tensor relation (G.23) and after applying the divergence theorem (G.32) to the right hand side of (5.15), we obtain*

$$\dot{\mathscr{J}}_{\chi_\varepsilon}(u_\varepsilon) = \int_{\partial\Omega}\Sigma_\varepsilon n\cdot\mathfrak{V} + \int_{\partial B_\varepsilon}[\![\Sigma_\varepsilon]\!]n\cdot\mathfrak{V} - \int_\Omega \operatorname{div}\Sigma_\varepsilon\cdot\mathfrak{V}\,. \tag{5.22}$$

Since the above equation and (5.17) remain valid for all velocity fields $\mathfrak{V}$, we have that the last term of the above equation must satisfy

$$\int_\Omega \operatorname{div}\Sigma_\varepsilon\cdot\mathfrak{V} = 0 \quad \forall\mathfrak{V} \quad \Rightarrow \quad \operatorname{div}\Sigma_\varepsilon = 0\,. \tag{5.23}$$

Corollary 5.2. *Since we are dealing with an uniform expansion of the circular inclusion, then by taking into account the associated velocity field defined through (4.2), $\mathfrak{V} = -n$ on ∂B_ε and $\mathfrak{V} = 0$ on $\partial\Omega$. Therefore, according to Proposition 5.2, we have*

$$\frac{d}{d\varepsilon}\psi(\chi_\varepsilon) = \dot{\mathscr{J}}_{\chi_\varepsilon}(u_\varepsilon) = -\int_{\partial B_\varepsilon} [\![\Sigma_\varepsilon]\!] n \cdot n \,. \tag{5.24}$$

5.1.3 Asymptotic Analysis of the Solution

The shape derivative of functional $\mathscr{J}_{\chi_\varepsilon}(u_\varepsilon)$ is given in terms of an integral over the boundary of the inclusion ∂B_ε (5.24). Therefore, in order to apply the result of Proposition 1.1, we need to know the behavior of the function u_ε with respect to ε. In particular, once we know this behavior explicitly, we can identify function $f(\varepsilon)$ and evaluate the limit passage $\varepsilon \to 0$ in (1.49), leading to the final formula for the topological derivative $\mathscr{T}$ of the shape functional ψ. However, in general this procedure is quite involved. In fact, we need to perform an asymptotic analysis of u_ε with respect to ε. In this section we obtain the asymptotic expansion of the solution u_ε associated to the transmission condition on the inclusion. In particular, let us propose an *ansätz* for the expansion of u_ε in the form [120]

$$\begin{aligned} u_\varepsilon(x) &= u(x) + w_\varepsilon(x) + \widetilde{u}_\varepsilon(x) \\ &= u(\widehat{x}) + \nabla u(\widehat{x}) \cdot (x - \widehat{x}) + \frac{1}{2}\nabla\nabla u(y)(x - \widehat{x}) \cdot (x - \widehat{x}) \\ &+ w_\varepsilon(x) + \widetilde{u}_\varepsilon(x) \,, \end{aligned} \tag{5.25}$$

where y is an intermediate point between x and $\widehat{x}$. On the boundary of the inclusion ∂B_ε we have

$$[\![q_\varepsilon(u_\varepsilon)]\!] \cdot n = 0 \quad \Rightarrow \quad \partial_n u_\varepsilon|_{\Omega\setminus\overline{B_\varepsilon}} - \gamma\partial_n u_\varepsilon|_{B_\varepsilon} = 0 \,, \tag{5.26}$$

with $q_\varepsilon(\varphi) = -\gamma_\varepsilon k \nabla\varphi$. Therefore, the normal derivative of the above expansion, evaluated on ∂B_ε, leads to

$$\begin{aligned} &(1-\gamma)\nabla u(\widehat{x}) \cdot n - \varepsilon(1-\gamma)\nabla\nabla u(y) n \cdot n + \\ &\qquad \partial_n w_\varepsilon(x)|_{\Omega\setminus\overline{B_\varepsilon}} - \gamma\partial_n w_\varepsilon(x)|_{B_\varepsilon} + \\ &\qquad\qquad \partial_n \widetilde{u}_\varepsilon(x)|_{\Omega\setminus\overline{B_\varepsilon}} - \gamma\partial_n \widetilde{u}_\varepsilon(x)|_{B_\varepsilon} = 0 \,. \end{aligned} \tag{5.27}$$

Thus, we can choose w_ε such that

$$\partial_n w_\varepsilon(x)|_{\Omega\setminus\overline{B_\varepsilon}} - \gamma\partial_n w_\varepsilon(x)|_{B_\varepsilon} = -(1-\gamma)\nabla u(\widehat{x}) \cdot n \quad \text{on} \quad \partial B_\varepsilon \,. \tag{5.28}$$

Now, the following exterior problem is considered, and formally obtained as $\varepsilon \to 0$:

$$\begin{cases} \text{Find } w_\varepsilon \text{, such that} \\ \qquad \operatorname{div}(\gamma_\varepsilon \nabla w_\varepsilon) = 0 \quad \text{in } \mathbb{R}^2 , \\ \qquad w_\varepsilon \to 0 \quad \text{at } \infty , \\ \left. \begin{aligned} w_\varepsilon|_{\Omega\setminus\overline{B_\varepsilon}} - w_\varepsilon|_{B_\varepsilon} &= 0 \\ \partial_n w_\varepsilon|_{\Omega\setminus\overline{B_\varepsilon}} - \gamma\partial_n w_\varepsilon|_{B_\varepsilon} &= \widehat{u} \end{aligned} \right\} \text{on } \partial B_\varepsilon , \end{cases} \tag{5.29}$$

with $\widehat{u} = -(1-\gamma)\nabla u(\widehat{x}) \cdot n$. The above boundary value problem admits an explicit solution, namely

$$w_\varepsilon(x)_{|\Omega\setminus\overline{B_\varepsilon}} = \frac{1-\gamma}{1+\gamma}\frac{\varepsilon^2}{\|x-\widehat{x}\|^2}\nabla u(\widehat{x}) \cdot (x-\widehat{x}) , \tag{5.30}$$

$$w_\varepsilon(x)_{|B_\varepsilon} = \frac{1-\gamma}{1+\gamma}\nabla u(\widehat{x}) \cdot (x-\widehat{x}) . \tag{5.31}$$

Now we can construct $\widetilde{u}_\varepsilon$ in such a way that it compensates the discrepancies introduced by the higher order terms in ε as well as by the boundary layer w_ε on the exterior boundary $\partial\Omega$. It means that the remainder $\widetilde{u}_\varepsilon$ must be solution to the following boundary value problem:

$$\begin{cases} \text{Find } \widetilde{u}_\varepsilon \text{, such that} \\ \operatorname{div} q_\varepsilon(\widetilde{u}_\varepsilon) = 0 \quad \text{in } \Omega , \\ q_\varepsilon(\widetilde{u}_\varepsilon) = -\gamma_\varepsilon k \nabla \widetilde{u}_\varepsilon , \\ \widetilde{u}_\varepsilon = -w_\varepsilon \quad \text{on } \Gamma_D , \\ q(\widetilde{u}_\varepsilon)\cdot n = -q(w_\varepsilon)\cdot n \text{ on } \Gamma_N , \\ \left. \begin{aligned} [\![\widetilde{u}_\varepsilon]\!] &= 0 \\ [\![q_\varepsilon(\widetilde{u}_\varepsilon)]\!]\cdot n &= -\varepsilon h \end{aligned} \right\} \text{ on } \partial B_\varepsilon , \end{cases} \tag{5.32}$$

where $h = k(1-\gamma)\nabla\nabla u(y)n\cdot n$. Clearly $\widetilde{u}_\varepsilon = O(\varepsilon)$, since h doesn't depend on ε and $w_\varepsilon = O(\varepsilon^2)$ on the exterior boundary $\partial\Omega$. However, this estimate can be improved [120, 148], namely $\|\widetilde{u}_\varepsilon\|_{H^1(\Omega)} = O(\varepsilon^2)$, and the *expansion* for u_ε reads

$$u_\varepsilon(x)_{|\Omega\setminus\overline{B_\varepsilon}} = u(x) + \frac{1-\gamma}{1+\gamma}\frac{\varepsilon^2}{\|x-\widehat{x}\|^2}\nabla u(\widehat{x}) \cdot (x-\widehat{x}) + O(\varepsilon^2) , \tag{5.33}$$

$$u_\varepsilon(x)_{|B_\varepsilon} = u(x) + \frac{1-\gamma}{1+\gamma}\nabla u(\widehat{x}) \cdot (x-\widehat{x}) + O(\varepsilon^2) . \tag{5.34}$$

In fact, before proceeding, let us state the following result:

Lemma 5.1. *Let $\widetilde{u}_\varepsilon$ be the solution to (5.32) or equivalently the solution to the following variational problem:*

$$\begin{cases} \text{Find } \widetilde{u}_\varepsilon \in \widetilde{\mathscr{U}_\varepsilon} \text{, such that} \\ -\int_\Omega q_\varepsilon(\widetilde{u}_\varepsilon)\cdot\nabla\eta = \varepsilon^2\int_{\Gamma_N} q(g)\cdot n\,\eta + \varepsilon\int_{\partial B_\varepsilon} h\eta \quad \forall\eta\in\widetilde{\mathscr{V}_\varepsilon} , \\ \qquad\qquad \text{with} \quad q_\varepsilon(\widetilde{u}_\varepsilon) = -\gamma_\varepsilon k\nabla\widetilde{u}_\varepsilon , \end{cases} \tag{5.35}$$

where the set $\widetilde{\mathscr{U}_\varepsilon}$ *and the space* $\widetilde{\mathscr{V}_\varepsilon}$ *are defined as*

$$\widetilde{\mathscr{U}_\varepsilon} := \{\varphi \in H^1(\Omega) : [\![\varphi]\!] = 0 \text{ on } \partial B_\varepsilon,\ \varphi_{|\Gamma_D} = -\varepsilon^2 g\}\ ,$$
$$\widetilde{\mathscr{V}_\varepsilon} := \{\varphi \in H^1(\Omega) : [\![\varphi]\!] = 0 \text{ on } \partial B_\varepsilon,\ \varphi_{|\Gamma_D} = 0\}\ ,$$

with functions $g = \varepsilon^{-2} w_\varepsilon$ *and* $h = k(1-\gamma)\nabla\nabla u(y) n \cdot n$ *independent of the small parameter* ε*. Then, we have the estimate* $\|\widetilde{u}_\varepsilon\|_{H^1(\Omega)} = O(\varepsilon^2)$ *for the remainder.*

Proof. By taking $\eta = \widetilde{u}_\varepsilon - \varphi_\varepsilon$ in (5.35), where φ_ε is the lifting of the Dirichlet boundary data $\varepsilon^2 g$ on Γ_D, we have

$$-\int_\Omega q_\varepsilon(\widetilde{u}_\varepsilon) \cdot \nabla \widetilde{u}_\varepsilon = \varepsilon^2 \int_{\Gamma_N} q(g) \cdot n\, \widetilde{u}_\varepsilon + \varepsilon^2 \int_{\Gamma_D} g\, q(\widetilde{u}_\varepsilon) \cdot n + \varepsilon \int_{\partial B_\varepsilon} h\, \widetilde{u}_\varepsilon\ . \tag{5.36}$$

From the *Cauchy-Schwarz inequality* we obtain

$$\begin{aligned} -\int_\Omega q_\varepsilon(\widetilde{u}_\varepsilon) \cdot \nabla \widetilde{u}_\varepsilon \leqslant\ & \varepsilon^2 \|q(g) \cdot n\|_{H^{-1/2}(\Gamma_N)} \|\widetilde{u}_\varepsilon\|_{H^{1/2}(\Gamma_N)} \\ & + \varepsilon^2 \|g\|_{H^{1/2}(\Gamma_D)} \|q(\widetilde{u}_\varepsilon) \cdot n\|_{H^{-1/2}(\Gamma_D)} \\ & + \varepsilon \|h\|_{H^{-1/2}(\partial B_\varepsilon)} \|\widetilde{u}_\varepsilon\|_{H^{1/2}(\partial B_\varepsilon)}\ . \end{aligned} \tag{5.37}$$

Taking into account the *trace theorem*, we have

$$\begin{aligned} -\int_\Omega q_\varepsilon(\widetilde{u}_\varepsilon) \cdot \nabla \widetilde{u}_\varepsilon &\leqslant \varepsilon^2 C_1 \|\widetilde{u}_\varepsilon\|_{H^1(\Omega)} + \varepsilon^2 C_2 \|\nabla \widetilde{u}_\varepsilon\|_{L^2(\Omega)} + \varepsilon \|h\|_{L^2(B_\varepsilon)} \|\widetilde{u}_\varepsilon\|_{H^1(B_\varepsilon)} \\ &\leqslant \varepsilon^2 C_1 \|\widetilde{u}_\varepsilon\|_{H^1(\Omega)} + \varepsilon^2 C_3 \|\widetilde{u}_\varepsilon\|_{H^1(\Omega)} + \varepsilon^2 C_4 \|\widetilde{u}_\varepsilon\|_{H^1(\Omega)} \\ &\leqslant \varepsilon^2 C_5 \|\widetilde{u}_\varepsilon\|_{H^1(\Omega)}\ , \end{aligned} \tag{5.38}$$

where we have used the interior *elliptic regularity* of function u. Finally, from the *coercivity* of the bilinear form on the left hand side of (5.35), namely,

$$c \|\widetilde{u}_\varepsilon\|^2_{H^1(\Omega)} \leqslant -\int_\Omega q_\varepsilon(\widetilde{u}_\varepsilon) \cdot \nabla \widetilde{u}_\varepsilon\ , \tag{5.39}$$

we obtain

$$\|\widetilde{u}_\varepsilon\|_{H^1(\Omega)} \leqslant C\varepsilon^2\ , \tag{5.40}$$

which leads to the result, with $C = C_5/c$. □

5.1.4 Topological Derivative Evaluation

Now, we need to evaluate the integral in formula (5.24) to collect the terms in power of ε and recognize function $f(\varepsilon)$. With this result, we can perform the limit passage $\varepsilon \to 0$. The integral in (5.24) can be evaluated in the same way as shown in

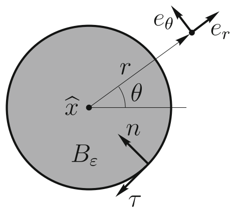


Fig. 5.4 Polar coordinate system (r,θ) centered at the point $\widehat{x} \in \Omega$

Section 4.1 by using the expansion for the solution u_ε given by (5.33) and (5.34). The idea is to introduce a polar coordinate system (r,θ) with center at $\widehat{x}$ (see fig. 5.4). Then, we can write u_ε in this coordinate system and evaluate the integral explicitly. In particular, the integral in (5.24) yields

$$-\int_{\partial B_\varepsilon} [\![\Sigma_\varepsilon]\!] n \cdot n = 2\pi\varepsilon P_\gamma q(u(\widehat{x})) \cdot \nabla u(\widehat{x}) + o(\varepsilon) \,. \tag{5.41}$$

Finally, the topological derivative given by (1.49) leads to

$$\mathscr{T}(\widehat{x}) = \lim_{\varepsilon\to 0} \frac{1}{f'(\varepsilon)} \left(2\pi\varepsilon P_\gamma q(u(\widehat{x})) \cdot \nabla u(\widehat{x}) + o(\varepsilon)\right) \,, \tag{5.42}$$

where the *polarization tensor* P_γ is given by the following second order isotropic tensor

$$P_\gamma = \frac{1-\gamma}{1+\gamma} \mathrm{I} \,. \tag{5.43}$$

Now, in order to extract the leading term of the above expansion, we choose

$$f(\varepsilon) = \pi\varepsilon^2 \,, \tag{5.44}$$

which leads to the final formula for the *topological derivative*, namely [13, 49]

$$\mathscr{T}(\widehat{x}) = P_\gamma q(u(\widehat{x})) \cdot \nabla u(\widehat{x}) \,. \tag{5.45}$$

Finally, the topological asymptotic expansion of the energy shape functional takes the form

$$\psi(\chi_\varepsilon(\widehat{x})) = \psi(\chi) + \pi\varepsilon^2 P_\gamma q(u(\widehat{x})) \cdot \nabla u(\widehat{x}) + o(\varepsilon^2) \,, \tag{5.46}$$

whose mathematical justification will be given at the end of this chapter through Theorem 5.1.

Remark 5.2. We note that the obtained polarization tensor is isotropic because we are dealing with circular inclusions. For the polarization tensor associated to arbitrary shaped inclusions the reader may refer to [10], for instance.

Remark 5.3. Formally, we can take the limit cases $\gamma \to 0$ and $\gamma \to \infty$. For $\gamma \to 0$, the inclusion leads to an ideal thermal insulator and the transmission condition on the boundary of the inclusion degenerates to homogeneous Neumann boundary condition. In fact, in this case the polarization tensor is given by

$$P_0 = \mathrm{I} \,, \tag{5.47}$$

which, together with (5.45), corroborates with the obtained formula (4.54) for $b = 0$ and $k = 1$, since $q(u(\widehat{x})) = -k\nabla u(\widehat{x})$. In addition, for $\gamma \to \infty$, the inclusion leads to an ideal thermal conductor and the polarization tensor is given by

$$P_\infty = -\mathrm{I} \,. \tag{5.48}$$

5.1.5 Numerical Example

Let us present a simple numerical example consisting in the design of a heat conductor. For that, we propose the following shape functional

$$\Psi_\Omega(u) := -\mathscr{J}_\Omega(u) + \beta\,|\Omega| \ , \tag{5.49}$$

where $|\Omega|$ is the Lebesgue measure of Ω and $\beta > 0$ is a fixed Lagrange multiplier. It means that the shape functional to be minimized is the energy stored in the body with a volume constraint. The topological derivative of $\Psi_\Omega(u)$ is given by

$$\mathscr{T} = -P_0 q(u) \cdot \nabla u - \beta \,, \tag{5.50}$$

with $q(u) = -k\nabla u$, where we have used formula (5.45) with $\gamma = 0$ and the fact that the topological derivative of the term $\beta\,|\Omega|$ is trivial. In addition, the temperature field u is evaluated by solving problem (5.3) numerically.

In the numerical example shown in fig. 5.5, the initial domain is represented by a 1×1 square, with thermal conductivity $k = 1$. The temperature $\overline{u} = 0$ is prescribed on the thick lines of length 0.2 and the body is submitted to a uniformly distributed heat flux $\bar{q} = 1$ on the left and $\bar{q} = -1$ on the right of the square. Each heat flux is applied in a region of length 0.2. The remainder part of the boundary of the square remains insulated. The Lagrange multiplier is fixed as $\beta = 0.8$ and the contrast $\gamma \to 0$.

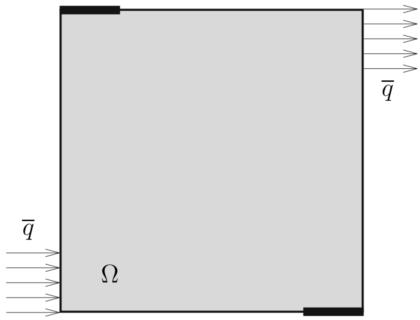
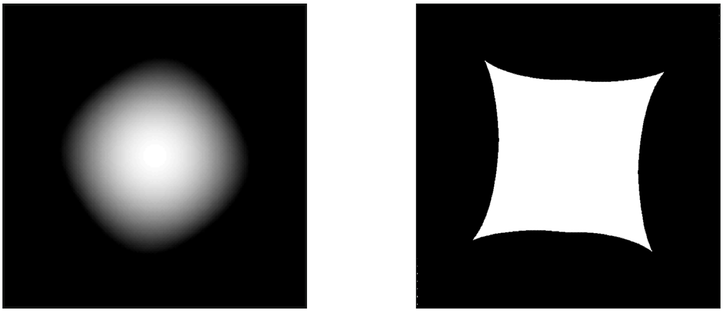


Fig. 5.5 Hold-all-domain



(a) topological derivative (b) final topology

Fig. 5.6 Topological derivative in the hold-all domain and optimal shape design [185]

The topological derivative of the shape functional $\Psi_\Omega(u)$ which is obtained in the first iteration of the shape and topology optimization numerical procedure is shown in fig. 5.6(a), where white to black levels mean smaller (negative) to higher (positive) values. This picture induces a level-set domain representation for the optimal shape, as proposed in [16]. The resulting topology design in the form of a heat conductor is shown in fig. 5.6(b).

5.2 Second Order Elliptic System: The Navier Problem

In this section we evaluate the topological derivative of the total potential energy associated to the plane stress linear elasticity problem, considering the nucleation of a small inclusion, represented by $B_\varepsilon \subset \Omega$, as the topological perturbation.

5.2.1 Problem Formulation

The shape functional associated to the unperturbed domain which we are dealing with is defined as

$$\psi(\chi) := \mathscr{J}_\Omega(u) = \frac{1}{2}\int_\Omega \sigma(u)\cdot\nabla u^s - \int_{\Gamma_N} \overline{q}\cdot u\,, \tag{5.51}$$

where the vector function u is the solution to the variational problem:

$$\begin{cases} \text{Find } u \in \mathscr{U}, \text{ such that} \\ \displaystyle\int_\Omega \sigma(u)\cdot\nabla\eta^s = \int_{\Gamma_N} \overline{q}\cdot\eta \quad \forall\eta\in\mathscr{V}\,, \\ \qquad\qquad\qquad \text{with} \quad \sigma(u) = \mathbb{C}\nabla u^s\,. \end{cases} \tag{5.52}$$

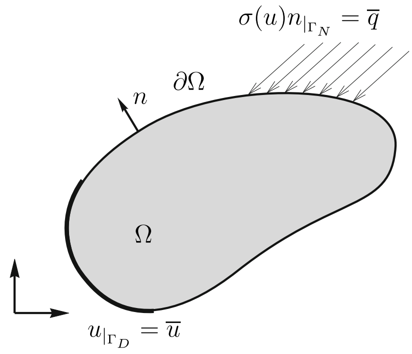


Fig. 5.7 The Navier problem defined in the unperturbed domain

In the above equation, $\mathbb{C}$ is the constitutive tensor given by

$$\mathbb{C} = \frac{E}{1-\nu^2}((1-\nu)\mathbb{I} + \nu \mathrm{I} \otimes \mathrm{I}) , \tag{5.53}$$

where I and $\mathbb{I}$ are the second and fourth order identity tensors, respectively, E is the Young modulus and ν the Poisson ratio, both considered constants everywhere. For the sake of simplicity, we also assume that the thickness of the elastic body is constant and equal to one. The set $\mathscr{U}$ and the space $\mathscr{V}$ are respectively defined as

$$\mathscr{U} := \{\varphi \in H^1(\Omega;\mathbb{R}^2) : \varphi_{|\Gamma_D} = \overline{u}\} , \tag{5.54}$$

$$\mathscr{V} := \{\varphi \in H^1(\Omega;\mathbb{R}^2) : \varphi_{|\Gamma_D} = 0\} . \tag{5.55}$$

In addition, $\partial\Omega = \overline{\Gamma}_D \cup \overline{\Gamma}_N$ with $\Gamma_D \cap \Gamma_N = \varnothing$, where Γ_D and Γ_N are Dirichlet and Neumann boundaries, respectively. Thus $\overline{u}$ is a Dirichlet data on Γ_D and $\overline{q}$ is a Neumann data on Γ_N, both assumed to be smooth enough. See the details in fig. 5.7. The strong system associated to the variational problem (5.52) reads:

$$\begin{cases} \text{Find } u \text{, such that} \\ \operatorname{div}\sigma(u) = 0 & \text{in } \Omega , \\ \sigma(u) = \mathbb{C}\nabla u^s , \\ u = \overline{u} & \text{on } \Gamma_D , \\ \sigma(u)n = \overline{q} & \text{on } \Gamma_N . \end{cases} \tag{5.56}$$

Remark 5.4. Since the Young modulus E and the Poisson ratio ν are constants, the above boundary value problem reduces itself to the well-known Navier system, namely

$$-\mu\Delta u - (\lambda+\mu)\nabla(\operatorname{div} u) = 0 \quad \text{in} \quad \Omega , \tag{5.57}$$

with the Lame's coefficients μ and λ respectively given by

$$\mu = \frac{E}{2(1+\nu)} \quad \text{and} \quad \lambda = \frac{\nu E}{1-\nu^2} . \tag{5.58}$$

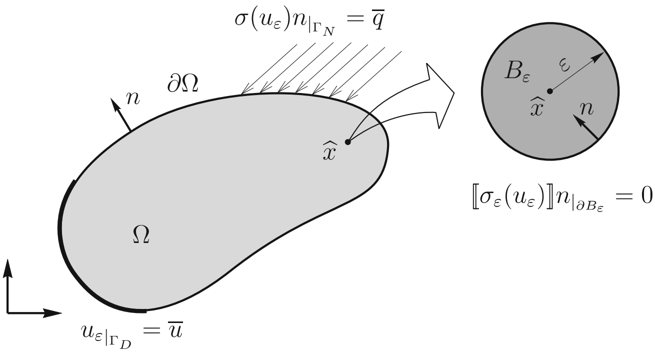


Fig. 5.8 The Navier problem defined in the perturbed domain

Now, let us state the same problem in the perturbed domain. In this case, the shape functional reads

$$\psi(\chi_\varepsilon) := \mathscr{J}_{\chi_\varepsilon}(u_\varepsilon) = \frac{1}{2}\int_\Omega \sigma_\varepsilon(u_\varepsilon)\cdot\nabla u_\varepsilon^s - \int_{\Gamma_N} \overline{q}\cdot u_\varepsilon \ , \tag{5.59}$$

where the vector function u_ε solves the variational problem:

$$\left\{\begin{array}{l} \text{Find } u_\varepsilon \in \mathscr{U}_\varepsilon, \text{ such that} \\ \displaystyle\int_\Omega \sigma_\varepsilon(u_\varepsilon)\cdot\nabla\eta^s = \int_{\Gamma_N} \overline{q}\cdot\eta \quad \forall\eta\in\mathscr{V}_\varepsilon \ , \\ \qquad\qquad\text{with} \quad \sigma_\varepsilon(u_\varepsilon) = \gamma_\varepsilon\mathbb{C}\nabla u_\varepsilon^s \ , \end{array}\right. \tag{5.60}$$

with γ_ε given by (5.1). The set $\mathscr{U}_\varepsilon$ and the space $\mathscr{V}_\varepsilon$ are defined as

$$\mathscr{U}_\varepsilon := \{\varphi\in\mathscr{U} : [\![\varphi]\!] = 0 \text{ on } \partial B_\varepsilon\} \ , \tag{5.61}$$

$$\mathscr{V}_\varepsilon := \{\varphi\in\mathscr{V} : [\![\varphi]\!] = 0 \text{ on } \partial B_\varepsilon\} \ , \tag{5.62}$$

where the operator $[\![\varphi]\!]$ is used to denote the jump of function φ on the boundary of the inclusion ∂B_ε, namely $[\![\varphi]\!] := \varphi_{|\Omega\setminus\overline{B_\varepsilon}} - \varphi_{|B_\varepsilon}$ on ∂B_ε. See the details in fig. 5.8. The *strong system* associated to the variational problem (5.60) reads:

$$\left\{\begin{array}{rcll} \multicolumn{4}{l}{\text{Find } u_\varepsilon, \text{ such that}} \\ \operatorname{div}\sigma_\varepsilon(u_\varepsilon) &=& 0 & \text{in } \Omega \ , \\ \sigma_\varepsilon(u_\varepsilon) &=& \gamma_\varepsilon\mathbb{C}\nabla u_\varepsilon^s \ , & \\ u_\varepsilon &=& \overline{u} & \text{on } \Gamma_D \ , \\ \sigma(u_\varepsilon)n &=& \overline{q} & \text{on } \Gamma_N \ , \\ \left.\begin{array}{r} [\![u_\varepsilon]\!] = 0 \\ [\![\sigma_\varepsilon(u_\varepsilon)]\!]n = 0 \end{array}\right\} & & & \text{on } \partial B_\varepsilon \ . \end{array}\right. \tag{5.63}$$

The *transmission condition* on the boundary of the inclusion ∂B_ε comes out from the variation formulation (5.60).

5.2.2 Shape Sensitivity Analysis

The next step consists in evaluating the shape derivative of functional $\mathscr{J}_{\chi_\varepsilon}(u_\varepsilon)$ with respect to an uniform expansion of the inclusion B_ε. Before starting, let us introduce the *Eshelby energy-momentum tensor* [57], namely

$$\Sigma_\varepsilon = \frac{1}{2}(\sigma_\varepsilon(u_\varepsilon)\cdot\nabla u_\varepsilon^s)\mathrm{I} - \nabla u_\varepsilon^\top \sigma_\varepsilon(u_\varepsilon) \ . \tag{5.64}$$

In addition, we note that after considering the constitutive relation $\sigma_\varepsilon(u_\varepsilon) = \gamma_\varepsilon \mathbb{C}\nabla u_\varepsilon^s$ in (5.59), with the contrast γ_ε given by (5.1), the shape functional $\mathscr{J}_{\chi_\varepsilon}(u_\varepsilon)$ can be written as follows

$$\mathscr{J}_{\chi_\varepsilon}(u_\varepsilon) = \frac{1}{2}\left(\int_{\Omega\setminus\overline{B_\varepsilon}} \sigma(u_\varepsilon)\cdot\nabla u_\varepsilon^s + \int_{B_\varepsilon} \gamma\sigma(u_\varepsilon)\cdot\nabla u_\varepsilon^s\right) - \int_{\Gamma_N} \overline{q}\cdot u_\varepsilon \ , \tag{5.65}$$

where $\sigma(u_\varepsilon) = \mathbb{C}\nabla u_\varepsilon^s$. Therefore, the explicit dependence with respect to the parameter ε arises, with allows us to state the following result:

Proposition 5.3. *Let $\mathscr{J}_{\chi_\varepsilon}(u_\varepsilon)$ be the shape functional defined by (5.59). Then, the derivative of $\mathscr{J}_{\chi_\varepsilon}(u_\varepsilon)$ with respect to the small parameter ε is given by*

$$\dot{\mathscr{J}}_{\chi_\varepsilon}(u_\varepsilon) = \int_\Omega \Sigma_\varepsilon\cdot\nabla\mathfrak{V} \ , \tag{5.66}$$

where $\mathfrak{V}$ is the shape change velocity field defined through (4.2) and Σ_ε is the Eshelby energy-momentum tensor given by (5.64).

Proof. Before starting, let us recall that the constitutive operator is defined as $\sigma_\varepsilon(\varphi) = \gamma_\varepsilon\mathbb{C}\nabla\varphi^s$. Thus, by making use of the Reynolds' transport theorem given by the result (2.84) and the concept of material derivative of spatial fields through formula (2.92), the derivative with respect to ε of the shape functional (5.65) is given by

$$\begin{aligned}
\dot{\mathscr{J}}_{\chi_\varepsilon}(u_\varepsilon) &= \frac{1}{2}\left(\int_{\Omega\setminus\overline{B_\varepsilon}} \sigma(u_\varepsilon)\cdot\nabla u_\varepsilon^s + \int_{B_\varepsilon}\gamma\sigma(u_\varepsilon)\cdot\nabla u_\varepsilon^s\right)^{\cdot} - \int_{\Gamma_N}\overline{q}\cdot\dot{u}_\varepsilon \\
&= \int_{\Omega\setminus\overline{B_\varepsilon}} \sigma(u_\varepsilon)\cdot\nabla\dot{u}_\varepsilon^s + \int_{B_\varepsilon}\gamma\sigma(u_\varepsilon)\cdot\nabla\dot{u}_\varepsilon^s \\
&+ \frac{1}{2}\int_{\Omega\setminus\overline{B_\varepsilon}}((\sigma(u_\varepsilon)\cdot\nabla u_\varepsilon^s)\mathrm{I} - 2\nabla u_\varepsilon^\top\sigma(u_\varepsilon))\cdot\nabla\mathfrak{V} \\
&+ \frac{1}{2}\int_{B_\varepsilon}\gamma((\sigma(u_\varepsilon)\cdot\nabla u_\varepsilon^s)\mathrm{I} - 2\nabla u_\varepsilon^\top\sigma(u_\varepsilon))\cdot\nabla\mathfrak{V} - \int_{\Gamma_N}\overline{q}\cdot\dot{u}_\varepsilon \ .
\end{aligned} \tag{5.67}$$

Then,

$$\dot{\mathscr{J}}_{\chi_\varepsilon}(u_\varepsilon) = \frac{1}{2}\int_\Omega ((\sigma_\varepsilon(u_\varepsilon)\cdot\nabla u_\varepsilon^s)\mathrm{I} - 2\nabla u_\varepsilon^\top \sigma_\varepsilon(u_\varepsilon))\cdot\nabla\mathfrak{V} + \int_\Omega \sigma_\varepsilon(u)\cdot\nabla\dot{u}_\varepsilon^s - \int_{\Gamma_N}\overline{q}\cdot\dot{u}_\varepsilon\,. \tag{5.68}$$

Since $\dot{u}_\varepsilon$ is a variation of u_ε in the direction of the velocity field $\mathfrak{V}$, then $\dot{u}_\varepsilon \in \mathscr{V}_\varepsilon$ [210]. Finally, by taking $\dot{u}_\varepsilon$ as test function in the variational problem (5.60), we have that the last two terms of the above equation vanish. □

Proposition 5.4. *Let $\mathscr{J}_{\chi_\varepsilon}(u_\varepsilon)$ be the shape functional defined by (5.59). Then, its derivative with respect to the small parameter ε is given by*

$$\dot{\mathscr{J}}_{\chi_\varepsilon}(u_\varepsilon) = \int_{\partial\Omega}\Sigma_\varepsilon n\cdot\mathfrak{V} + \int_{\partial B_\varepsilon}[\![\Sigma_\varepsilon]\!]n\cdot\mathfrak{V}\,, \tag{5.69}$$

with $\mathfrak{V}$ standing for the shape change velocity field defined through (4.2) and tensor Σ_ε given by (5.64).

Proof. Before starting, let us recall the constitutive operator $\sigma_\varepsilon(\varphi) = \gamma_\varepsilon\mathbb{C}\nabla\varphi^s$ and the relation between material and spatial derivatives of vector fields (2.83), namely $\dot{\varphi} = \varphi' + (\nabla\varphi)\mathfrak{V}$. By making use of the other version of the Reynolds' transport theorem given by formula (2.85), the shape derivative of the functional (5.59) results in

$$\begin{aligned}\dot{\mathscr{J}}_{\chi_\varepsilon}(u_\varepsilon) &= \left(\frac{1}{2}\int_\Omega \sigma_\varepsilon(u_\varepsilon)\cdot\nabla u_\varepsilon^s\right)^{\cdot} - \int_{\Gamma_N}\overline{q}\cdot\dot{u}_\varepsilon \\ &= \int_\Omega \sigma_\varepsilon(u_\varepsilon)\cdot(\nabla u_\varepsilon')^s + \frac{1}{2}\int_{\partial\Omega}(\sigma_\varepsilon(u_\varepsilon)\cdot\nabla u_\varepsilon^s)n\cdot\mathfrak{V} \\ &\quad + \frac{1}{2}\int_{\partial B_\varepsilon}[\![\sigma_\varepsilon(u_\varepsilon)\cdot\nabla u_\varepsilon^s]\!]n\cdot\mathfrak{V} - \int_{\Gamma_N}\overline{q}\cdot\dot{u}_\varepsilon\,.\end{aligned} \tag{5.70}$$

In addition, we have

$$\begin{aligned}\dot{\mathscr{J}}_{\chi_\varepsilon}(u_\varepsilon) &= \frac{1}{2}\int_{\partial\Omega}(\sigma_\varepsilon(u_\varepsilon)\cdot\nabla u_\varepsilon^s)n\cdot\mathfrak{V} + \frac{1}{2}\int_{\partial B_\varepsilon}[\![\sigma_\varepsilon(u_\varepsilon)\cdot\nabla u_\varepsilon^s]\!]n\cdot\mathfrak{V} \\ &\quad - \int_\Omega \sigma_\varepsilon(u_\varepsilon)\cdot\nabla((\nabla u_\varepsilon)\mathfrak{V})^s + \int_\Omega \sigma_\varepsilon(u)\cdot\nabla\dot{u}_\varepsilon^s - \int_{\Gamma_N}\overline{q}\cdot\dot{u}_\varepsilon\,.\end{aligned} \tag{5.71}$$

Since $\dot{u}_\varepsilon$ is a variation of u_ε in the direction of the velocity field $\mathfrak{V}$, then $\dot{u}_\varepsilon \in \mathscr{V}_\varepsilon$ [210]. Now, by taking into account that u_ε is the solution to the variational problem (5.60), we have that the last two terms of the above equation vanish. From integration by parts

$$
\begin{aligned}
\dot{\mathscr{J}}_{\chi_\varepsilon}(u_\varepsilon) &= \frac{1}{2}\int_{\partial\Omega}(\sigma_\varepsilon(u_\varepsilon)\cdot\nabla u_\varepsilon^s)n\cdot\mathfrak{V} + \frac{1}{2}\int_{\partial B_\varepsilon}[\![\sigma_\varepsilon(u_\varepsilon)\cdot\nabla u_\varepsilon^s]\!]n\cdot\mathfrak{V} \\
&\quad - \int_{\partial\Omega}(\nabla u_\varepsilon^\top\sigma_\varepsilon(u_\varepsilon))n\cdot\mathfrak{V} - \int_{\partial B_\varepsilon}[\![\nabla u_\varepsilon^\top\sigma_\varepsilon(u_\varepsilon)]\!]n\cdot\mathfrak{V} \\
&\quad + \int_\Omega \operatorname{div}(\sigma_\varepsilon(u_\varepsilon))\cdot(\nabla u_\varepsilon)\mathfrak{V}\,, \qquad (5.72)
\end{aligned}
$$

and rewriting the above equation in the compact form, we obtain

$$
\dot{\mathscr{J}}_{\chi_\varepsilon}(u_\varepsilon) = \int_{\partial\Omega}\Sigma_\varepsilon n\cdot\mathfrak{V} + \int_{\partial B_\varepsilon}[\![\Sigma_\varepsilon]\!]n\cdot\mathfrak{V} + \int_\Omega \operatorname{div}(\sigma_\varepsilon(u_\varepsilon))\cdot(\nabla u_\varepsilon)\mathfrak{V}\,. \quad (5.73)
$$

Finally, taking into account that u_ε is the solution to the state equation (5.63), namely $\operatorname{div}\sigma_\varepsilon(u_\varepsilon)=0$, we have that the last term in the above equation vanishes, which leads to the result. □

Corollary 5.3. *From the tensor relation (G.23) and after applying the divergence theorem (G.32) to the right hand side of (5.66), we obtain*

$$
\dot{\mathscr{J}}_{\chi_\varepsilon}(u_\varepsilon) = \int_{\partial\Omega}\Sigma_\varepsilon n\cdot\mathfrak{V} + \int_{\partial B_\varepsilon}[\![\Sigma_\varepsilon]\!]n\cdot\mathfrak{V} - \int_\Omega \operatorname{div}\Sigma_\varepsilon\cdot\mathfrak{V}\,. \quad (5.74)
$$

Since the above equation and (5.69) remain valid for all velocity fields $\mathfrak{V}$, we have that the last term of the above equation must satisfy

$$
\int_\Omega \operatorname{div}\Sigma_\varepsilon\cdot\mathfrak{V} = 0 \quad \forall\mathfrak{V} \quad \Rightarrow \quad \operatorname{div}\Sigma_\varepsilon = 0\,. \quad (5.75)
$$

Corollary 5.4. *Since we are dealing with an uniform expansion of the circular inclusion, then by taking into account the associated velocity field defined through (4.2), $\mathfrak{V}=-n$ on ∂B_ε and $\mathfrak{V}=0$ on $\partial\Omega$. Therefore, according to the obtained result in Proposition 5.4, we have*

$$
\frac{d}{d\varepsilon}\psi(\chi_\varepsilon) = \dot{\mathscr{J}}_{\chi_\varepsilon}(u_\varepsilon) = -\int_{\partial B_\varepsilon}[\![\Sigma_\varepsilon]\!]n\cdot n\,. \quad (5.76)
$$

5.2.3 Asymptotic Analysis of the Solution

The shape derivative of functional $\mathscr{J}_{\chi_\varepsilon}(u_\varepsilon)$ is given in terms of an integral over the boundary of the inclusion ∂B_ε (5.76). Therefore, in order to apply the result of Proposition 1.1, we need to know the behavior of the function u_ε with respect to ε. In particular, once we know this behavior explicitly, we can identify function $f(\varepsilon)$ and perform the limit passage $\varepsilon\to 0$ in (1.49) to obtain the final formula for the topological derivative $\mathscr{T}$ of the shape functional ψ. However, in general this is not a trivial procedure. In fact, we need to perform an asymptotic analysis of u_ε with respect to ε. In this section we obtain the asymptotic expansion of the solution

u_ε associated to the transmission condition on the inclusion. Thus, let us start by proposing an *ansätz* for u_ε of the form [120]

$$u_\varepsilon(x) = u(x) + w_\varepsilon(x) + \widetilde{u}_\varepsilon(x) \, . \tag{5.77}$$

After applying the operator σ_ε we have

$$\begin{aligned} \sigma_\varepsilon(u_\varepsilon(x)) &= \sigma_\varepsilon(u(x)) + \sigma_\varepsilon(w_\varepsilon(x)) + \sigma_\varepsilon(\widetilde{u}_\varepsilon(x)) \\ &= \sigma_\varepsilon(u(\widehat{x})) + \nabla\sigma_\varepsilon(u(y))(x-\widehat{x}) + \sigma_\varepsilon(w_\varepsilon(x)) + \sigma_\varepsilon(\widetilde{u}_\varepsilon(x)) \, , \end{aligned} \tag{5.78}$$

where y is an intermediate point between x and $\widehat{x}$. On the boundary of the inclusion ∂B_ε we have

$$[\![\sigma_\varepsilon(u_\varepsilon)]\!]n = 0 \quad \Rightarrow \quad (\sigma(u_\varepsilon)_{|_{\Omega\setminus\overline{B_\varepsilon}}} - \gamma\sigma(u_\varepsilon)_{|_{B_\varepsilon}})n = 0 \, , \tag{5.79}$$

with $\sigma_\varepsilon(\varphi) = \gamma_\varepsilon \mathbb{C}\nabla\varphi^s$ and $\sigma(\varphi) = \mathbb{C}\nabla\varphi^s$. The above expansion, evaluated on ∂B_ε, leads to

$$\begin{aligned} &(1-\gamma)\sigma(u(\widehat{x}))n - \varepsilon(1-\gamma)(\nabla\sigma(u(y))n)n + \\ &\qquad\qquad [\![\sigma_\varepsilon(w_\varepsilon(x))]\!]n + [\![\sigma_\varepsilon(\widetilde{u}_\varepsilon(x))]\!]n = 0 \, . \end{aligned} \tag{5.80}$$

Thus, we can choose $\sigma_\varepsilon(w_\varepsilon)$ such that

$$[\![\sigma_\varepsilon(w_\varepsilon(x))]\!]n = -(1-\gamma)\sigma(u(\widehat{x}))n \quad \text{on} \quad \partial B_\varepsilon \, . \tag{5.81}$$

Now, the following exterior problem is considered, and formally obtained as $\varepsilon \to 0$:

$$\begin{cases} \text{Find } \sigma_\varepsilon(w_\varepsilon), \text{ such that} \\ \operatorname{div}\sigma_\varepsilon(w_\varepsilon) = 0 \text{ in } \mathbb{R}^2 \, , \\ \sigma_\varepsilon(w_\varepsilon) \to 0 \text{ at } \infty \, , \\ [\![\sigma_\varepsilon(w_\varepsilon)]\!]n = \widehat{u} \text{ on } \partial B_\varepsilon \, , \end{cases} \tag{5.82}$$

with $\widehat{u} = -(1-\gamma)\sigma(u(\widehat{x}))n$. The above boundary value problem admits an explicit solution, which will be used later to construct the expansion for $\sigma_\varepsilon(u_\varepsilon)$. Now we can construct $\sigma_\varepsilon(\widetilde{u}_\varepsilon)$ in such a way that it compensates the discrepancies introduced by the higher order terms in ε as well as by the boundary layer $\sigma_\varepsilon(w_\varepsilon)$ on the exterior boundary $\partial\Omega$. It means that the remainder $\widetilde{u}_\varepsilon$ must be solution to the following boundary value problem:

$$\begin{cases} \text{Find } \widetilde{u}_\varepsilon, \text{ such that} \\ \operatorname{div}\sigma_\varepsilon(\widetilde{u}_\varepsilon) = 0 \quad \text{in } \Omega \, , \\ \sigma_\varepsilon(\widetilde{u}_\varepsilon) = \gamma_\varepsilon \mathbb{C}\nabla\widetilde{u}_\varepsilon^s \, , \\ \widetilde{u}_\varepsilon = -w_\varepsilon \quad \text{on } \Gamma_D \, , \\ \sigma(\widetilde{u}_\varepsilon)n = -\sigma(w_\varepsilon)n \text{ on } \Gamma_N \, , \\ \left.\begin{aligned} [\![\widetilde{u}_\varepsilon]\!] &= 0 \\ [\![\sigma_\varepsilon(\widetilde{u}_\varepsilon)]\!]n &= \varepsilon h \end{aligned}\right\} \quad \text{on } \partial B_\varepsilon \, , \end{cases} \tag{5.83}$$

with $h = (1-\gamma)(\nabla\sigma(u(y))n)n$. Analogously to the Section 5.1 (see Theorem 5.1 and the references [120, 148]), we can obtain an estimate for the remainder $\widetilde{u}_\varepsilon$ of the form $\|\widetilde{u}_\varepsilon\|_{H^1(\Omega;\mathbb{R}^2)} = O(\varepsilon^2)$. In fact, before proceeding, let us state the following result:

Lemma 5.2. *Let $\widetilde{u}_\varepsilon$ be the solution to (5.83) or equivalently the solution to the following variational problem:*

$$\begin{cases} \text{Find } \widetilde{u}_\varepsilon \in \widetilde{\mathscr{U}_\varepsilon}, \text{ such that} \\ \displaystyle\int_\Omega \sigma_\varepsilon(\widetilde{u}_\varepsilon)\cdot\nabla\eta^s = \varepsilon^2\int_{\Gamma_N}\sigma(g)n\cdot\eta + \varepsilon\int_{\partial B_\varepsilon} h\cdot\eta \quad \forall\eta\in\widetilde{\mathscr{V}_\varepsilon}\,, \\ \qquad\qquad\qquad\qquad\qquad \text{with}\quad \sigma_\varepsilon(\widetilde{u}_\varepsilon) = \gamma_\varepsilon\mathbb{C}\nabla\widetilde{u}_\varepsilon^s\,, \end{cases} \tag{5.84}$$

where the set $\widetilde{\mathscr{U}_\varepsilon}$ and the space $\widetilde{\mathscr{V}_\varepsilon}$ are defined as

$$\widetilde{\mathscr{U}_\varepsilon} := \{\varphi\in H^1(\Omega;\mathbb{R}^2) : [\![\varphi]\!] = 0 \text{ on } \partial B_\varepsilon,\ \varphi_{|\Gamma_D} = \varepsilon^2 g\}\,,$$
$$\widetilde{\mathscr{V}_\varepsilon} := \{\varphi\in H^1(\Omega;\mathbb{R}^2) : [\![\varphi]\!] = 0 \text{ on } \partial B_\varepsilon,\ \varphi_{|\Gamma_D} = 0\}\,,$$

with functions $g = -\varepsilon^{-2}w_\varepsilon$ and $h = (1-\gamma)(\nabla\sigma(u(y))n)n$ independent of the small parameter ε. Then, we have the estimate $\|\widetilde{u}_\varepsilon\|_{H^1(\Omega;\mathbb{R}^2)} = O(\varepsilon^2)$ for the remainder.

Proof. By taking $\eta = \widetilde{u}_\varepsilon - \varphi_\varepsilon$ in (5.84), where φ_ε is the lifting of the Dirichlet boundary data $\varepsilon^2 g$ on Γ_D, we have

$$\int_\Omega \sigma_\varepsilon(\widetilde{u}_\varepsilon)\cdot\nabla\widetilde{u}_\varepsilon^s = \varepsilon^2\int_{\Gamma_N}\sigma(g)n\cdot\widetilde{u}_\varepsilon + \varepsilon^2\int_{\Gamma_D} g\cdot\sigma(\widetilde{u}_\varepsilon)n + \varepsilon\int_{\partial B_\varepsilon} h\cdot\widetilde{u}_\varepsilon\,. \tag{5.85}$$

From the *Cauchy-Schwarz inequality* we obtain

$$\begin{aligned}\int_\Omega \sigma_\varepsilon(\widetilde{u}_\varepsilon)\cdot\nabla\widetilde{u}_\varepsilon^s \leqslant{}& \varepsilon^2\|\sigma(g)n\|_{H^{-1/2}(\Gamma_N;\mathbb{R}^2)}\|\widetilde{u}_\varepsilon\|_{H^{1/2}(\Gamma_N;\mathbb{R}^2)} \\ &+ \varepsilon^2\|g\|_{H^{1/2}(\Gamma_D;\mathbb{R}^2)}\|\sigma(\widetilde{u}_\varepsilon)n\|_{H^{-1/2}(\Gamma_D;\mathbb{R}^2)} \\ &+ \varepsilon\|h\|_{H^{-1/2}(\partial B_\varepsilon;\mathbb{R}^2)}\|\widetilde{u}_\varepsilon\|_{H^{1/2}(\partial B_\varepsilon;\mathbb{R}^2)}\,.\end{aligned} \tag{5.86}$$

Taking into account the *trace theorem*, we have

$$\begin{aligned}\int_\Omega \sigma_\varepsilon(\widetilde{u}_\varepsilon)\cdot\nabla\widetilde{u}_\varepsilon^s &\leqslant (\varepsilon^2 C_1 + \varepsilon\|h\|_{L^2(B_\varepsilon;\mathbb{R}^2)})\|\widetilde{u}_\varepsilon\|_{H^1(\Omega;\mathbb{R}^2)} \\ &\leqslant \varepsilon^2 C_2\|\widetilde{u}_\varepsilon\|_{H^1(\Omega;\mathbb{R}^2)}\,,\end{aligned} \tag{5.87}$$

where we have used the interior *elliptic regularity* of function u. Finally, from the *coercivity* of the bilinear form on the left hand side of (5.84), namely,

$$c\|\widetilde{u}_\varepsilon\|^2_{H^1(\Omega;\mathbb{R}^2)} \leqslant \int_\Omega \sigma_\varepsilon(\widetilde{u}_\varepsilon)\cdot\nabla\widetilde{u}_\varepsilon^s\,, \tag{5.88}$$

we obtain

$$\|\widetilde{u}_\varepsilon\|_{H^1(\Omega;\mathbb{R}^2)} \leqslant C\varepsilon^2 , \tag{5.89}$$

which leads to the result, with $C = C_2/c$. □

Therefore, the *expansion* for $\sigma_\varepsilon(u_\varepsilon)$ (see, for instance, the book by Little 1973 [139]) can be written in a polar coordinate system (r,θ) centered at the point $\widehat{x}$ (see fig. 5.9) as:

- For $r \geqslant \varepsilon$ (outside the inclusion)

$$\sigma_\varepsilon^{rr}(u_\varepsilon(r,\theta)) = \varphi_1\left(1 - \tfrac{1-\gamma}{1+\gamma\alpha}\tfrac{\varepsilon^2}{r^2}\right) + \varphi_2\left(1 - 4\tfrac{1-\gamma}{1+\gamma\beta}\tfrac{\varepsilon^2}{r^2} + 3\tfrac{1-\gamma}{1+\gamma\beta}\tfrac{\varepsilon^4}{r^4}\right)\cos 2\theta + O(\varepsilon^2), \tag{5.90}$$

$$\sigma_\varepsilon^{\theta\theta}(u_\varepsilon(r,\theta)) = \varphi_1\left(1 + \tfrac{1-\gamma}{1+\gamma\alpha}\tfrac{\varepsilon^2}{r^2}\right) - \varphi_2\left(1 + 3\tfrac{1-\gamma}{1+\gamma\beta}\tfrac{\varepsilon^4}{r^4}\right)\cos 2\theta + O(\varepsilon^2), \tag{5.91}$$

$$\sigma_\varepsilon^{r\theta}(u_\varepsilon(r,\theta)) = -\varphi_2\left(1 + 2\tfrac{1-\gamma}{1+\gamma\beta}\tfrac{\varepsilon^2}{r^2} - 3\tfrac{1-\gamma}{1+\gamma\beta}\tfrac{\varepsilon^4}{r^4}\right)\sin 2\theta + O(\varepsilon^2). \tag{5.92}$$

- For $0 < r < \varepsilon$ (inside the inclusion)

$$\sigma_\varepsilon^{rr}(u_\varepsilon(r,\theta)) = \varphi_1\left(\tfrac{2}{1-\nu}\tfrac{\gamma}{1+\gamma\alpha}\right) + \varphi_2\left(\tfrac{4}{1+\nu}\tfrac{\gamma}{1+\gamma\beta}\right)\cos 2\theta + O(\varepsilon^2), \tag{5.93}$$

$$\sigma_\varepsilon^{\theta\theta}(u_\varepsilon(r,\theta)) = \varphi_1\left(\tfrac{2}{1-\nu}\tfrac{\gamma}{1+\gamma\alpha}\right) - \varphi_2\left(\tfrac{4}{1+\nu}\tfrac{\gamma}{1+\gamma\beta}\right)\cos 2\theta + O(\varepsilon^2), \tag{5.94}$$

$$\sigma_\varepsilon^{r\theta}(u_\varepsilon(r,\theta)) = -\varphi_2\left(\tfrac{4}{1+\nu}\tfrac{\gamma}{1+\gamma\beta}\right)\sin 2\theta + O(\varepsilon^2). \tag{5.95}$$

Some terms in the above formulae require explanations. The coefficients φ_1 and φ_2 are given by

$$\varphi_1 = \frac{1}{2}(\sigma_1(u(\widehat{x})) + \sigma_2(u(\widehat{x}))) , \quad \varphi_2 = \frac{1}{2}(\sigma_1(u(\widehat{x})) - \sigma_2(u(\widehat{x}))) , \tag{5.96}$$

where $\sigma_1(u(\widehat{x}))$ and $\sigma_2(u(\widehat{x}))$ are the eigenvalues of tensor $\sigma(u(\widehat{x}))$, which can be expressed as

$$\sigma_{1,2}(u(\widehat{x})) = \frac{1}{2}\left(\operatorname{tr}\sigma(u(\widehat{x})) \pm \sqrt{2\sigma^D(u(\widehat{x}))\cdot\sigma^D(u(\widehat{x}))}\right) , \tag{5.97}$$

with $\sigma^D(u(\widehat{x}))$ standing for the deviatory part of the stress tensor $\sigma(u(\widehat{x}))$, namely

$$\sigma^D(u(\widehat{x})) = \sigma(u(\widehat{x})) - \frac{1}{2}\operatorname{tr}\sigma(u(\widehat{x}))\mathrm{I} . \tag{5.98}$$

In addition, the constants α and β are given by

$$\alpha = \frac{1+\nu}{1-\nu} \quad \text{and} \quad \beta = \frac{3-\nu}{1+\nu} . \tag{5.99}$$

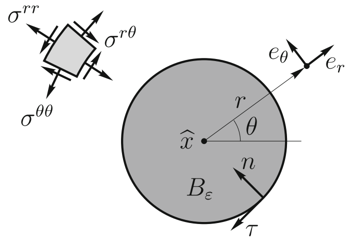


Fig. 5.9 Polar coordinate system (r,θ) centered at the point $\widehat{x} \in \Omega$

Finally, $\sigma_\varepsilon^{rr}(u_\varepsilon)$, $\sigma_\varepsilon^{\theta\theta}(u_\varepsilon)$ and $\sigma_\varepsilon^{r\theta}(u_\varepsilon)$ are the components of tensor $\sigma_\varepsilon(u_\varepsilon)$ in the polar coordinate system, namely $\sigma_\varepsilon^{rr}(u_\varepsilon) = e^r \cdot \sigma_\varepsilon(u_\varepsilon)e^r$, $\sigma_\varepsilon^{\theta\theta}(u_\varepsilon) = e^\theta \cdot \sigma_\varepsilon(u_\varepsilon)e^\theta$ and $\sigma_\varepsilon^{r\theta}(u_\varepsilon) = \sigma_\varepsilon^{\theta r}(u_\varepsilon) = e^r \cdot \sigma_\varepsilon(u_\varepsilon)e^\theta$, with e^r and e^θ used to denote the canonical basis associated to the polar coordinate system (r,θ), such that, $\|e^r\| = \|e^\theta\| = 1$ and $e^r \cdot e^\theta = 0$. See fig. 5.9.

Note 5.1 (Eshelby's theorem). According to (5.93), (5.94) and (5.95), we observe that the strain tensor field associated to the solution of the exterior problem (5.82) is uniform inside the inclusion $B_\varepsilon(\widehat{x})$. It means that the strain acting in the inclusion embedded in the whole two-dimensional space $\mathbb{R}^2$ can be written in the following compact form

$$\nabla w_\varepsilon^s|_{B_\varepsilon(\widehat{x})} = \mathbb{T}\nabla u^s(\widehat{x}) \;, \tag{5.100}$$

where $\mathbb{T}$ is a fourth order uniform (constant) tensor. Therefore, the above result fits the famous Eshelby's problem. This problem, formulated by Eshelby in 1957 [55] and 1959 [56], represents one of the major advances in the continuum mechanics theory of the 20th century [104]. It plays a central role in the theory of elasticity involving the determination of effective elastic properties of materials with multiple inhomogeneities. For more details, see the book by Mura 1987 [159], for instance. The Eshelby's problem, also referred as the Eshelby's theorem, is also related to the Polarization tensor in asymptotic analysis of the strain energy with respect to singular domain perturbations [168]. In fact, tensor $\mathbb{T}$ represents one term contribution to the Polarization tensor coming from the solution to the exterior problem (5.82). In the next section we will apply the Eshelby's theorem to the derivation of the polarization tensor and to the topological derivative evaluation as well. Concerning applications of the Eshelby's theorem to the problem of optimal patch in elasticity, see [132, 169].

5.2.4 Topological Derivative Evaluation

Now, we can evaluate the integral in formula (5.76) to collect the terms in power of ε and recognize function $f(\varepsilon)$. With this result, we can perform the limit passage $\varepsilon \to 0$. The integral in (5.76) can be evaluated in the same way as shown in Section 4.2 by using the expansion for $\sigma_\varepsilon(u_\varepsilon)$ given by (5.90)-(5.95). The idea is to introduce a polar coordinate system (r,θ) with center at $\widehat{x}$ (see fig. 5.9). Then, we can write u_ε in this coordinate system to evaluate the integral explicitly. In particular, the integral in (5.76) yields

$$\int_{\partial B_\varepsilon} [\![\Sigma_\varepsilon]\!] n \cdot n = 2\pi\varepsilon \mathbb{P}_\gamma \sigma(u(\widehat{x})) \cdot \nabla u^s(\widehat{x}) + o(\varepsilon) \,. \tag{5.101}$$

Finally, the topological derivative given by (1.49) leads to

$$\mathscr{T}(\widehat{x}) = -\lim_{\varepsilon\to 0} \frac{1}{f'(\varepsilon)} \left(2\pi\varepsilon \mathbb{P}_\gamma \sigma(u(\widehat{x})) \cdot \nabla u^s(\widehat{x}) + o(\varepsilon)\right) \,, \tag{5.102}$$

where the *polarization tensor* $\mathbb{P}_\gamma$ is given by the following fourth order isotropic tensor

$$\mathbb{P}_\gamma = \frac{1}{2}\frac{1-\gamma}{1+\gamma\beta}\left((1+\beta)\mathbb{I} + \frac{1}{2}(\alpha-\beta)\frac{1-\gamma}{1+\gamma\alpha}\mathrm{I}\otimes\mathrm{I}\right) \,, \tag{5.103}$$

with the parameters α and β given by (5.99). Now, in order to extract the leading term of the above expansion, we choose

$$f(\varepsilon) = \pi\varepsilon^2 \,, \tag{5.104}$$

which leads to the final formula for the *topological derivative*, namely [13, 77]

$$\mathscr{T}(\widehat{x}) = -\mathbb{P}_\gamma \sigma(u(\widehat{x})) \cdot \nabla u^s(\widehat{x}) \,. \tag{5.105}$$

Finally, the topological asymptotic expansion of the energy shape functional takes the form

$$\psi(\chi_\varepsilon(\widehat{x})) = \psi(\chi) - \pi\varepsilon^2 \mathbb{P}_\gamma \sigma(u(\widehat{x})) \cdot \nabla u^s(\widehat{x}) + o(\varepsilon^2) \,, \tag{5.106}$$

whose mathematical justification will be given at the end of this chapter.

Remark 5.5. We note that the obtained polarization tensor is isotropic because we are dealing with circular inclusions. For the polarization tensor associated to arbitrary shaped inclusions the reader may refer to [10], for instance.

Remark 5.6. Formally, we can consider the limit cases $\gamma \to 0$ and $\gamma \to \infty$. For $\gamma \to 0$, the inclusion leads to a void and the transmission condition on the boundary of the inclusion degenerates to homogeneous Neumann boundary condition. In fact, in this case the polarization tensor is given by

$$\mathbb{P}_0 = \frac{1}{2}(1+\beta)\mathbb{I} + \frac{1}{4}(\alpha-\beta)\mathrm{I}\otimes\mathrm{I} = \frac{2}{1+\nu}\mathbb{I} - \frac{1-3\nu}{2(1-\nu^2)}\mathrm{I}\otimes\mathrm{I} \,, \tag{5.107}$$

which, together with (5.105), corroborates with the obtained formula (4.173) for $b=0$. In addition, for $\gamma \to \infty$, the elastic inclusion leads to a rigid one and the polarization tensor is given by

$$\mathbb{P}_\infty = -\frac{1+\beta}{2\beta}\mathbb{I} + \frac{\alpha-\beta}{4\alpha\beta}\mathrm{I}\otimes\mathrm{I} = -\frac{2}{3-\nu}\mathbb{I} - \frac{1-3\nu}{2(1+\nu)(3-\nu)}\mathrm{I}\otimes\mathrm{I} \,. \tag{5.108}$$

5.2.5 Numerical Example

We start with the description of the model in the hold-all domain and compute the topological derivative of the compliance to be minimized with a volume constraint, and finally present the optimal shape. It is clear from the numerical experiments that the topological derivative reflects an optimal topology for the shape optimization problem. Thus, in three figures below we present the initial guess of the structure to be optimized, the contour plot of the topological derivative of the goal functional obtained for the hold-all geometrical domain, and finally the optimal shape in the form of the bridge structure, which is well known from the literature on the subject. We start by proposing the following shape functional

$$\Psi_\Omega(u) := -\mathscr{J}_\Omega(u) + \beta\,|\Omega| \ , \tag{5.109}$$

where $|\Omega|$ is the Lebesgue measure of Ω and $\beta > 0$ is a fixed Lagrange multiplier. It means that the shape functional to be minimized is the strain energy stored in the structure with a volume constraint. The topological derivative of $\Psi_\Omega(u)$ is given by

$$\mathscr{T} = \mathbb{P}_0\sigma(u)\cdot\nabla u^s - \beta \ , \tag{5.110}$$

with $\sigma(u) = \mathbb{C}\nabla u^s$, where we have used formula (5.105) with $\gamma = 0$ and the fact that the topological derivative of the term $\beta\,|\Omega|$ is trivial. In addition, the displacement vector field u is evaluated by solving problem (5.52) numerically.

In the numerical example shown in fig. 5.10, the initial domain is represented by a rectangular panel $180\times 60\ m^2$, with Young modulus $E = 210\times 10^9 N/m^2$ and Poisson ratio $\nu = 1/3$, clamped on the region $a = 9m$ and submitted to an uniformly distributed traffic loading $\bar{q} = 250\times 10^3\ N/m^2$. This load is applied on the dark strip of height $h = 3m$, which is placed at the distance $c = 30m$ from the top of the design domain. The dark strip will not be optimized. The Lagrange multiplier is fixed as $\beta = 10\times 10^6\ N/m^2$ and the contrast $\gamma\to 0$.

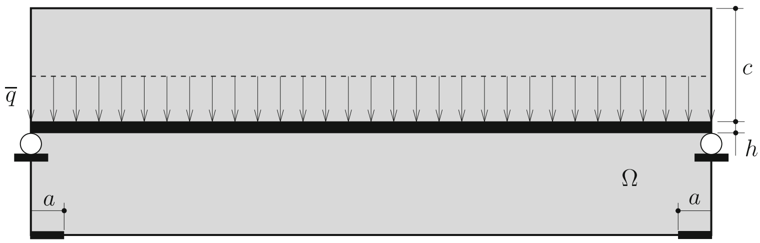


Fig. 5.10 Hold-all-domain

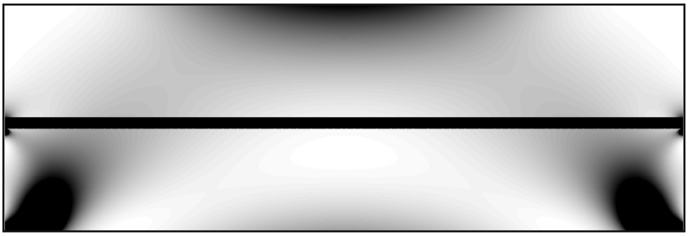


Fig. 5.11 Topological derivative in the hold-all domain

The topological derivative of the shape functional $\Psi_\Omega(u)$ which is obtained in the first iteration of the shape and topology optimization numerical procedure is shown in fig. 5.11, where white to black levels mean smaller (negative) to higher (positive) values. This picture induces a level-set domain representation for the optimal shape, as proposed in [16].

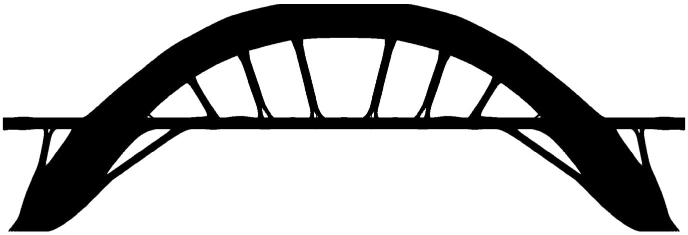


Fig. 5.12 Optimal shape design [97]

The resulting topology design in the form of a well-known tie-arch bridge structure, which is acceptable from practical point of view, is shown in fig. 5.12. Usually it is a local minimizer obtained numerically for the compliance minimization with volume constraint. Indeed, there is a lack of sufficient optimality conditions for such shape optimization problems.

5.3 Fourth Order Elliptic Equation: The Kirchhoff Problem

In this section we evaluate the topological derivative of the total potential energy associated to the Kirchhoff plate bending problem, considering the nucleation of a small inclusion, represented by $B_\varepsilon \subset \Omega$, as the topological perturbation.

5.3.1 Problem Formulation

The shape functional associated to the unperturbed domain which we are dealing with is defined as

$$\psi(\chi) := \mathscr{J}_\Omega(u) = -\frac{1}{2}\int_\Omega M(u)\cdot\nabla\nabla u - \int_{\Gamma_{N_q}} \overline{q}u + \int_{\Gamma_{N_m}} \overline{m}\partial_n u + \sum_{i=1}^{ns}\overline{Q}_i u(x_i)\,. \tag{5.111}$$

The scalar function u is the solution to the variational problem:

$$\begin{cases} \text{Find } u\in\mathscr{U}\text{, such that} \\ -\displaystyle\int_\Omega M(u)\cdot\nabla\nabla\eta = \int_{\Gamma_{N_q}}\overline{q}\eta \\ \qquad -\displaystyle\int_{\Gamma_{N_m}}\overline{m}\partial_n\eta - \sum_{i=1}^{ns}\overline{Q}_i\eta(x_i) \quad \forall\eta\in\mathscr{V}, \\ \qquad \text{with} \quad M(u) = -\mathbb{C}\nabla\nabla u\,. \end{cases} \tag{5.112}$$

In the above equation, $\mathbb{C}$ is the constitutive tensor given by

$$\mathbb{C} = \frac{E}{1-\nu^2}((1-\nu)\mathbb{I}+\nu\mathrm{I}\otimes\mathrm{I})\,, \tag{5.113}$$

where I and $\mathbb{I}$ are the second and fourth order identity tensors, respectively, E is the Young modulus and ν the Poisson ratio, both considered constants everywhere. For the sake of simplicity, we have assumed that the plate thickness is constant and equal to $12^{1/3}$. The set $\mathscr{U}$ and the space $\mathscr{V}$ are respectively defined as

$$\mathscr{U} := \{\varphi\in H^2(\Omega) : \varphi_{|_{\Gamma_{D_u}}} = \overline{u},\ \partial_n\varphi_{|_{\Gamma_{D_\rho}}} = \overline{\rho}\}\,, \tag{5.114}$$

$$\mathscr{V} := \{\varphi\in H^2(\Omega) : \varphi_{|_{\Gamma_{D_u}}} = 0,\ \partial_n\varphi_{|_{\Gamma_{D_\rho}}} = 0\}\,. \tag{5.115}$$

In addition, $\overline{q}$ is a shear load distributed on the boundary Γ_{N_q}, $\overline{m}$ is a moment distributed on the boundary Γ_{N_m} and $\overline{Q}_i$ is a concentrated shear load supported at the points x_i where there are some geometrical singularities, with $i = 1,...,ns$, and ns the number of such singularities. The displacement field u has to satisfy $u_{|_{\Gamma_{D_u}}} = \overline{u}$ and $\partial_n u_{|_{\Gamma_{D_\rho}}} = \overline{\rho}$, where $\overline{u}$ and $\overline{\rho}$ are a displacement and a rotation respectively prescribed on the boundaries Γ_{D_u} and Γ_{D_ρ}. Furthermore, $\Gamma_D = \overline{\Gamma}_{D_u}\cup\overline{\Gamma}_{D_\rho}$ and $\Gamma_N = \overline{\Gamma}_{N_q}\cup\overline{\Gamma}_{N_m}$ are such that $\Gamma_{D_u}\cap\Gamma_{N_q} = \varnothing$ and $\Gamma_{D_\rho}\cap\Gamma_{N_m} = \varnothing$. See the details in fig. 5.13. The strong formulation associated to the variational problem (5.112) reads:

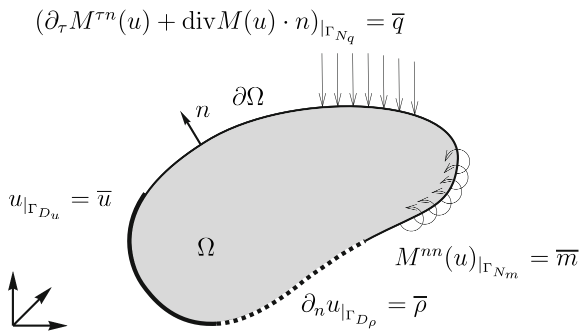


Fig. 5.13 The Kirchhoff problem defined in the unperturbed domain

$$\begin{cases} \text{Find } u, \text{ such that} \\ \qquad \mathrm{div}(\mathrm{div} M(u)) = 0 & \text{in } \Omega\ , \\ \qquad M(u) = -\mathbb{C}\nabla\nabla u\ , \\ \qquad u = \overline{u} & \text{on } \Gamma_{D_u}\ , \\ \qquad \partial_n u = \overline{\rho} & \text{on } \Gamma_{D_\rho}\ , \\ \qquad M^{nn}(u) = \overline{m} & \text{on } \Gamma_{N_m}\ , \\ \qquad \partial_\tau M^{\tau n}(u) + \mathrm{div} M(u) \cdot n = \overline{q} & \text{on } \Gamma_{N_q}\ , \\ \qquad [\![M^{\tau n}(u(x_i))]\!] = \overline{Q}_i & \text{on } x_i \in \Gamma_{N_q}\ . \end{cases} \tag{5.116}$$

Remark 5.7. Since the Young modulus E, the Poisson ratio ν and the plate thickness are assumed to be constants, the above boundary value problem reduces itself to the well-known Kirchhoff equation, namely

$$-k\Delta^2 u = 0 \quad \text{in} \quad \Omega\ , \quad \text{with} \quad k = \frac{Eh^3}{12(1-\nu^2)}\ , \tag{5.117}$$

where h is the plate thickness given by $h = 12^{1/3}$.

Now, let us state the same problem in the perturbed domain. In this case, the shape functional reads

$$\begin{aligned} \psi(\chi_\varepsilon) := \mathscr{J}_{\chi_\varepsilon}(u_\varepsilon) = & -\frac{1}{2}\int_\Omega M_\varepsilon(u_\varepsilon) \cdot \nabla\nabla u_\varepsilon \\ & - \int_{\Gamma_{N_q}} \overline{q} u_\varepsilon + \int_{\Gamma_{N_m}} \overline{m}\partial_n u_\varepsilon + \sum_{i=1}^{ns} \overline{Q}_i u_\varepsilon(x_i)\ , \end{aligned} \tag{5.118}$$

where the scalar function u_ε solves the variational problem:

$$\begin{cases} \text{Find } u_\varepsilon \in \mathscr{U}_\varepsilon, \text{ such that} \\ -\displaystyle\int_\Omega M_\varepsilon(u_\varepsilon) \cdot \nabla\nabla\eta = \int_{\Gamma_{N_q}} \overline{q}\eta \\ \qquad\qquad - \displaystyle\int_{\Gamma_{N_m}} \overline{m}\partial_n\eta - \sum_{i=1}^{ns} \overline{Q}_i \eta(x_i) \quad \forall \eta \in \mathscr{V}_\varepsilon, \\ \qquad\qquad \text{with} \quad M_\varepsilon(u_\varepsilon) = -\gamma_\varepsilon \mathbb{C}\nabla\nabla u_\varepsilon\ , \end{cases} \tag{5.119}$$

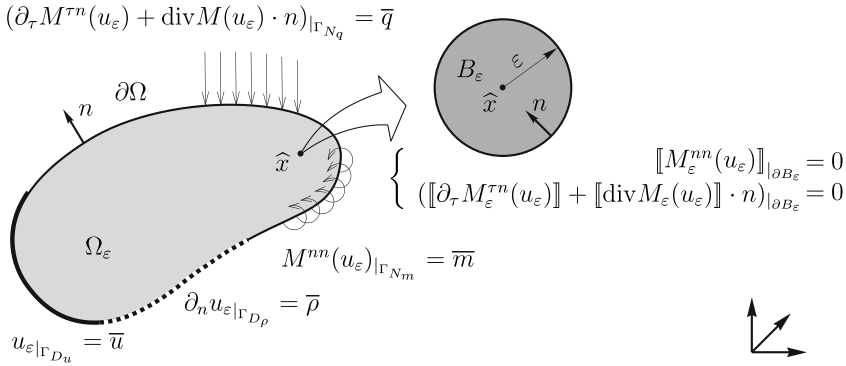


Fig. 5.14 The Kirchhoff problem defined in the perturbed domain

with γ_ε defined by (5.1). The set $\mathscr{U}_\varepsilon$ and the space $\mathscr{V}_\varepsilon$ are defined as

$$\mathscr{U}_\varepsilon := \{\varphi \in \mathscr{U} : [\![\varphi]\!] = [\![\partial_n \varphi]\!] = 0 \text{ on } \partial B_\varepsilon\} \,, \tag{5.120}$$

$$\mathscr{V}_\varepsilon := \{\varphi \in \mathscr{V} : [\![\varphi]\!] = [\![\partial_n \varphi]\!] = 0 \text{ on } \partial B_\varepsilon\} \,, \tag{5.121}$$

where the operator $[\![\varphi]\!]$ is used to denote the jump of function φ on the boundary of the inclusion ∂B_ε, namely $[\![\varphi]\!] := \varphi_{|_{\Omega \setminus \overline{B_\varepsilon}}} - \varphi_{|_{B_\varepsilon}}$ on ∂B_ε. See the details in fig. 5.14. The *strong formulation* associated to the variational problem (5.119) reads:

$$\left\{ \begin{array}{l} \text{Find } u_\varepsilon \text{, such that} \\ \begin{array}{rcll} \mathrm{div}(\mathrm{div} M_\varepsilon(u_\varepsilon)) &=& 0 & \text{in } \Omega \,, \\ M_\varepsilon(u_\varepsilon) &=& -\gamma_\varepsilon \mathbb{C} \nabla\nabla u_\varepsilon \,, & \\ u_\varepsilon &=& \overline{u} & \text{on } \Gamma_{D_u} \,, \\ \partial_n u_\varepsilon &=& \overline{\rho} & \text{on } \Gamma_{D_\rho} \,, \\ M^{nn}(u_\varepsilon) &=& \overline{m} & \text{on } \Gamma_{N_m} \,, \\ \partial_\tau M^{\tau n}(u_\varepsilon) + \mathrm{div} M(u_\varepsilon) \cdot n &=& \overline{q} & \text{on } \Gamma_{N_q} \,, \\ [\![M^{\tau n}(u_\varepsilon(x_i))]\!] &=& \overline{Q}_i & \text{on } x_i \in \Gamma_{N_q} \,, \\ \left. \begin{array}{r} [\![u_\varepsilon]\!] = 0 \\ [\![\partial_n u_\varepsilon]\!] = 0 \\ [\![M_\varepsilon^{nn}(u_\varepsilon)]\!] = 0 \\ [\![\partial_\tau M_\varepsilon^{\tau n}(u_\varepsilon)]\!] + [\![\mathrm{div} M_\varepsilon(u_\varepsilon)]\!] \cdot n = 0 \end{array} \right\} & & & \text{on } \partial B_\varepsilon \,. \end{array} \end{array} \right. \tag{5.122}$$

The *transmission condition* on the boundary of the inclusion ∂B_ε comes out from the variation formulation (4.186).

5.3.2 Shape Sensitivity Analysis

The next step consists in evaluating the shape derivative of functional $\mathscr{J}_{\chi_\varepsilon}(u_\varepsilon)$ with respect to an uniform expansion of the inclusion B_ε. Before starting, let us introduce the *Eshelby energy-momentum tensor* [57], that is

$$\Sigma_\varepsilon = -\frac{1}{2}(M_\varepsilon(u_\varepsilon)\cdot\nabla\nabla u_\varepsilon)\mathrm{I} + (\nabla\nabla u_\varepsilon)M_\varepsilon(u_\varepsilon) - \nabla u_\varepsilon \otimes \operatorname{div}(M_\varepsilon(u_\varepsilon)) \ . \tag{5.123}$$

Furthermore, we note that after considering the constitutive relation $M_\varepsilon(u_\varepsilon) = -\gamma_\varepsilon \mathbb{C}\nabla\nabla u_\varepsilon$ in (5.118), with the contrast γ_ε given by (5.1), the shape functional $\mathscr{J}_{\chi_\varepsilon}(u_\varepsilon)$ can be written as follows

$$\begin{aligned}\mathscr{J}_{\chi_\varepsilon}(u_\varepsilon) = &-\frac{1}{2}\left(\int_{\Omega\setminus\overline{B_\varepsilon}} M(u_\varepsilon)\cdot\nabla\nabla u_\varepsilon + \int_{B_\varepsilon}\gamma M(u_\varepsilon)\cdot\nabla\nabla u_\varepsilon\right)\\ &-\int_{\Gamma_{N_q}}\overline{q}u_\varepsilon + \int_{\Gamma_{N_m}}\overline{m}\partial_n u_\varepsilon + \sum_{i=1}^{ns}\overline{Q}_i u_\varepsilon(x_i) \ ,\end{aligned} \tag{5.124}$$

where $M(u_\varepsilon) = -\mathbb{C}\nabla\nabla u_\varepsilon$. Thus, we have an explicit dependence with respect to the parameter ε. Therefore, let us start by proving the following result:

Proposition 5.5. *Let $\mathscr{J}_{\chi_\varepsilon}(u_\varepsilon)$ be the shape functional defined by (5.118). Then, its derivative with respect to the small parameter ε is given by*

$$\begin{aligned}\dot{\mathscr{J}}_{\chi_\varepsilon}(u_\varepsilon) = &\int_\Omega \Sigma_\varepsilon\cdot\nabla\mathfrak{V}\\ &+\int_{\partial\Omega} M_\varepsilon(u_\varepsilon)n\cdot\nabla\mathfrak{V}^\top\nabla u_\varepsilon + \int_{\partial B_\varepsilon}[\![M_\varepsilon(u_\varepsilon)]\!]n\cdot\nabla\mathfrak{V}^\top\nabla u_\varepsilon \ ,\end{aligned} \tag{5.125}$$

where $\mathfrak{V}$ is the shape change velocity field defined through (4.2) and Σ_ε is the Eshelby energy-momentum tensor given by (5.123).

Proof. Before starting, let us recall that the constitutive operator is defined as $M_\varepsilon(\varphi) = -\gamma_\varepsilon\mathbb{C}\nabla\nabla\varphi$. Thus, by making use of the Reynolds' transport theorem given by the result (2.84) and the concept of material derivative of spatial fields through formulae (2.89) and (2.90), the derivative with respect to ε of the shape functional (5.124) is given by

$$\begin{aligned}\dot{\mathscr{J}}_{\chi_\varepsilon}(u_\varepsilon) = &-\frac{1}{2}\left(\int_{\Omega\setminus\overline{B_\varepsilon}} M(u_\varepsilon)\cdot\nabla\nabla u_\varepsilon + \int_{B_\varepsilon}\gamma M(u_\varepsilon)\cdot\nabla\nabla u_\varepsilon\right)^{\cdot}\\ &-\int_{\Gamma_{N_q}}\overline{q}\dot{u}_\varepsilon + \int_{\Gamma_{N_m}}\overline{m}\partial_n\dot{u}_\varepsilon + \sum_{i=1}^{ns}\overline{Q}_i\dot{u}_\varepsilon(x_i) \ .\end{aligned} \tag{5.126}$$

In addition, we have

$$\begin{aligned}\dot{\mathscr{J}}_{\chi_\varepsilon}(u_\varepsilon) = &-\int_{\Omega\setminus\overline{B_\varepsilon}} M(u_\varepsilon)\cdot\nabla\nabla\dot{u}_\varepsilon - \int_{B_\varepsilon}\gamma M(u_\varepsilon)\cdot\nabla\nabla\dot{u}_\varepsilon \\ &-\frac{1}{2}\int_\Omega [(M_\varepsilon(u_\varepsilon)\cdot\nabla\nabla u_\varepsilon)\mathrm{I} \\ &\quad -2(\nabla\nabla u_\varepsilon)M_\varepsilon(u_\varepsilon) + 2\nabla u_\varepsilon\otimes\operatorname{div}(M_\varepsilon(u_\varepsilon))]\cdot\nabla\mathfrak{V} \\ &+\int_{\partial\Omega} M_\varepsilon(u_\varepsilon)n\cdot\nabla\mathfrak{V}^\top\nabla u_\varepsilon + \int_{\partial B_\varepsilon}[\![M_\varepsilon(u_\varepsilon)]\!]n\cdot\nabla\mathfrak{V}^\top\nabla u_\varepsilon \\ &-\int_{\Gamma_{N_q}}\overline{q}\dot{u}_\varepsilon + \int_{\Gamma_{N_m}}\overline{m}\partial_n\dot{u}_\varepsilon + \sum_{i=1}^{ns}\overline{Q}_i\dot{u}_\varepsilon(x_i)\ , \end{aligned} \tag{5.127}$$

which leads to

$$\begin{aligned}\dot{\mathscr{J}}_{\chi_\varepsilon}(u_\varepsilon) = &-\frac{1}{2}\int_\Omega [(M_\varepsilon(u_\varepsilon)\cdot\nabla\nabla u_\varepsilon)\mathrm{I} \\ &\quad -2(\nabla\nabla u_\varepsilon)M_\varepsilon(u_\varepsilon) + 2\nabla u_\varepsilon\otimes\operatorname{div}(M_\varepsilon(u_\varepsilon))]\cdot\nabla\mathfrak{V} \\ &+\int_{\partial\Omega} M_\varepsilon(u_\varepsilon)n\cdot\nabla\mathfrak{V}^\top\nabla u_\varepsilon + \int_{\partial B_\varepsilon}[\![M_\varepsilon(u_\varepsilon)]\!]n\cdot\nabla\mathfrak{V}^\top\nabla u_\varepsilon \\ &-\int_\Omega M_\varepsilon(u_\varepsilon)\cdot\nabla\nabla\dot{u}_\varepsilon - \int_{\Gamma_{N_q}}\overline{q}\dot{u}_\varepsilon + \int_{\Gamma_{N_m}}\overline{m}\partial_n\dot{u}_\varepsilon + \sum_{i=1}^{ns}\overline{Q}_i\dot{u}_\varepsilon(x_i)\ . \end{aligned} \tag{5.128}$$

Since $\dot{u}_\varepsilon$ is a variation of u_ε in the direction of the velocity field $\mathfrak{V}$, then $\dot{u}_\varepsilon \in \mathscr{V}_\varepsilon$ [210]. Finally, by taking $\dot{u}_\varepsilon$ as test function in the variational problem (5.119), we have that the last four terms of the above equation vanish. □

Proposition 5.6. *Let $\mathscr{J}_{\chi_\varepsilon}(u_\varepsilon)$ be the shape functional defined by (5.118). Then, the derivative of $\mathscr{J}_{\chi_\varepsilon}(u_\varepsilon)$ with respect to the small parameter ε is given by*

$$\begin{aligned}\dot{\mathscr{J}}_{\chi_\varepsilon}(u_\varepsilon) = &\int_{\partial\Omega}\Sigma_\varepsilon n\cdot\mathfrak{V} + \int_{\partial B_\varepsilon}[\![\Sigma_\varepsilon]\!]n\cdot\mathfrak{V} \\ &+\int_{\partial\Omega} M_\varepsilon(u_\varepsilon)n\cdot\nabla\mathfrak{V}^\top\nabla u_\varepsilon + \int_{\partial B_\varepsilon}[\![M_\varepsilon(u_\varepsilon)]\!]n\cdot\nabla\mathfrak{V}^\top\nabla u_\varepsilon\ , \end{aligned} \tag{5.129}$$

with $\mathfrak{V}$ standing for the shape change velocity field defined through (4.2) and tensor Σ_ε given by (5.123).

Proof. Before starting, let us recall the constitutive operator $M_\varepsilon(\varphi) = -\gamma_\varepsilon\mathbb{C}\nabla\nabla\varphi$ and the relation between material and spatial derivatives of scalar fields (2.82), namely $\dot{\varphi} = \varphi' + \nabla\varphi\cdot\mathfrak{V}$. By making use of the other version of the Reynolds' transport theorem given by formula (2.85), the shape derivative of the functional (5.118) results in

$$
\begin{aligned}
\dot{\mathscr{J}}_{\chi_\varepsilon}(u_\varepsilon) = &-\left(\frac{1}{2}\int_\Omega M_\varepsilon(u_\varepsilon)\cdot\nabla\nabla u_\varepsilon\right)^{\dot{}} \\
&-\int_{\Gamma_{N_q}} \overline{q}\dot{u}_\varepsilon + \int_{\Gamma_{N_m}} \overline{m}\partial_n \dot{u}_\varepsilon + \sum_{i=1}^{ns} \overline{Q}_i \dot{u}_\varepsilon(x_i) \\
= &-\int_\Omega M_\varepsilon(u_\varepsilon)\cdot\nabla\nabla u'_\varepsilon - \frac{1}{2}\int_{\partial\Omega}(M_\varepsilon(u_\varepsilon)\cdot\nabla\nabla u_\varepsilon)n\cdot\mathfrak{V} \\
&-\frac{1}{2}\int_{\partial B_\varepsilon} [\![M_\varepsilon(u_\varepsilon)\cdot\nabla\nabla u_\varepsilon]\!] n\cdot\mathfrak{V} \\
&-\int_{\Gamma_{N_q}} \overline{q}\dot{u}_\varepsilon + \int_{\Gamma_{N_m}} \overline{m}\partial_n \dot{u}_\varepsilon + \sum_{i=1}^{ns} \overline{Q}_i \dot{u}_\varepsilon(x_i)\,.
\end{aligned} \tag{5.130}
$$

In addition, we have

$$
\begin{aligned}
\dot{\mathscr{J}}_{\chi_\varepsilon}(u_\varepsilon) = &-\frac{1}{2}\int_{\partial\Omega}(M_\varepsilon(u_\varepsilon)\cdot\nabla\nabla u_\varepsilon)n\cdot\mathfrak{V} - \frac{1}{2}\int_{\partial B_\varepsilon} [\![M_\varepsilon(u_\varepsilon)\cdot\nabla\nabla u_\varepsilon]\!] n\cdot\mathfrak{V} \\
&+\int_\Omega M_\varepsilon(u_\varepsilon)\cdot\nabla\nabla(\nabla u_\varepsilon\cdot\mathfrak{V}) \\
&-\int_\Omega M_\varepsilon(u_\varepsilon)\cdot\nabla\nabla\dot{u}_\varepsilon - \int_{\Gamma_{N_q}} \overline{q}\dot{u}_\varepsilon + \int_{\Gamma_{N_m}} \overline{m}\partial_n \dot{u}_\varepsilon + \sum_{i=1}^{ns} \overline{Q}_i \dot{u}_\varepsilon(x_i)\,.
\end{aligned} \tag{5.131}
$$

Since $\dot{u}_\varepsilon$ is a variation of u_ε in the direction of the velocity field $\mathfrak{V}$, then $\dot{u}_\varepsilon \in \mathscr{V}_\varepsilon$ [210]. Now, by taking into account that u_ε is the solution to the variational problem (5.119), we have that the last four terms of the above equation vanish. From integration by parts, we obtain

$$
\begin{aligned}
\dot{\mathscr{J}}_{\chi_\varepsilon}(u_\varepsilon) = &-\frac{1}{2}\int_{\partial\Omega}(M_\varepsilon(u_\varepsilon)\cdot\nabla\nabla u_\varepsilon)n\cdot\mathfrak{V} - \frac{1}{2}\int_{\partial B_\varepsilon} [\![M_\varepsilon(u_\varepsilon)\cdot\nabla\nabla u_\varepsilon]\!] n\cdot\mathfrak{V} \\
&+\int_{\partial\Omega}(\nabla\nabla u_\varepsilon)M_\varepsilon(u_\varepsilon)n\cdot\mathfrak{V} + \int_{\partial\Omega} M_\varepsilon(u_\varepsilon)n\cdot\nabla\mathfrak{V}^\top\nabla u_\varepsilon \\
&+\int_{\partial B_\varepsilon} [\![(\nabla\nabla u_\varepsilon)M_\varepsilon(u_\varepsilon)]\!] n\cdot\mathfrak{V} + \int_{\partial B_\varepsilon} [\![M_\varepsilon(u_\varepsilon)]\!] n\cdot\nabla\mathfrak{V}^\top\nabla u_\varepsilon \\
&-\int_{\partial\Omega}(\nabla u_\varepsilon\otimes\operatorname{div}M_\varepsilon(u_\varepsilon))n\cdot\mathfrak{V} - \int_{\partial B_\varepsilon} [\![\nabla u_\varepsilon\otimes\operatorname{div}M_\varepsilon(u_\varepsilon)]\!] n\cdot\mathfrak{V} \\
&+\int_\Omega \operatorname{div}(\operatorname{div}(M_\varepsilon(u_\varepsilon)))\nabla u_\varepsilon\cdot\mathfrak{V}\,,
\end{aligned} \tag{5.132}
$$

and rewriting the above equation in the compact form, we obtain

$$
\begin{aligned}
\dot{\mathscr{J}}_{\chi_\varepsilon}(u_\varepsilon) = &\int_{\partial\Omega} \Sigma_\varepsilon n\cdot\mathfrak{V} + \int_{\partial B_\varepsilon} [\![\Sigma_\varepsilon]\!] n\cdot\mathfrak{V} \\
&+\int_{\partial\Omega} M_\varepsilon(u_\varepsilon)n\cdot\nabla\mathfrak{V}^\top\nabla u_\varepsilon + \int_{\partial B_\varepsilon} [\![M_\varepsilon(u_\varepsilon)]\!] n\cdot\nabla\mathfrak{V}^\top\nabla u_\varepsilon \\
&+\int_\Omega \operatorname{div}(\operatorname{div}(M_\varepsilon(u)))\nabla u_\varepsilon\cdot\mathfrak{V}\,.
\end{aligned} \tag{5.133}
$$

Finally, taking into account that u_ε is the solution to the state equation (5.122), namely $\mathrm{div}(\mathrm{div} M_\varepsilon(u_\varepsilon)) = 0$, we have that the last term in the above equation vanishes, which leads to the result. □

Corollary 5.5. *From the tensor relation (G.23) and after applying the divergence theorem (G.32) to the right hand side of (5.125), we obtain*

$$\begin{aligned}\dot{\mathscr{J}}_{\chi_\varepsilon}(u_\varepsilon) = &\int_{\partial\Omega} \Sigma_\varepsilon n \cdot \mathfrak{V} + \int_{\partial B_\varepsilon} [\![\Sigma_\varepsilon]\!] n \cdot \mathfrak{V} - \int_\Omega \mathrm{div}\Sigma_\varepsilon \cdot \mathfrak{V} \\ &+ \int_{\partial\Omega} M_\varepsilon(u_\varepsilon) n \cdot \nabla \mathfrak{V}^\top \nabla u_\varepsilon + \int_{\partial B_\varepsilon} [\![M_\varepsilon(u_\varepsilon)]\!] n \cdot \nabla \mathfrak{V}^\top \nabla u_\varepsilon \,. \end{aligned} \tag{5.134}$$

Since the above equation and (5.129) remain valid for all velocity fields $\mathfrak{V}$*, we have that the third term of the above equation must satisfy*

$$\int_\Omega \mathrm{div}\Sigma_\varepsilon \cdot \mathfrak{V} = 0 \quad \forall \mathfrak{V} \quad \Rightarrow \quad \mathrm{div}\Sigma_\varepsilon = 0 \,. \tag{5.135}$$

Corollary 5.6. *Since we are dealing with an uniform expansion of the circular inclusion, then by taking into account the associated velocity field defined through (4.2),* $\mathfrak{V} = -n$ *on* ∂B_ε *and* $\mathfrak{V} = 0$ *on* $\partial\Omega$*. Therefore, according to Proposition 5.6, we have*

$$\frac{d}{d\varepsilon}\psi(\chi_\varepsilon) = \dot{\mathscr{J}}_{\chi_\varepsilon}(u_\varepsilon) = -\int_{\partial B_\varepsilon} [\![\Sigma_\varepsilon]\!] n \cdot n - \int_{\partial B_\varepsilon} [\![M_\varepsilon(u_\varepsilon)]\!] n \cdot \nabla n^\top \nabla u_\varepsilon \,. \tag{5.136}$$

5.3.3 Asymptotic Analysis of the Solution

The shape derivative of functional $\mathscr{J}_{\chi_\varepsilon}(u_\varepsilon)$ is given in terms of an integral over the boundary of the inclusion ∂B_ε (5.136). Therefore, in order to apply the result of Proposition 1.1, we need to know the behavior of the function u_ε with respect to ε. In particular, once we know this behavior explicitly, we can identify function $f(\varepsilon)$ and perform the limit passage $\varepsilon \to 0$ in (1.49) to obtain the final formula for the topological derivative $\mathscr{T}$ of the shape functional ψ. It means that we need to perform an asymptotic analysis of u_ε with respect to ε. In this section we present a procedure to obtain the asymptotic expansion of the solution u_ε associated to the transmission condition on the inclusion. Therefore, let us start by proposing an *ansätz* for u_ε of the form [120]

$$u_\varepsilon(x) = u(x) + w_\varepsilon(x) + \widetilde{u}_\varepsilon(x) \,. \tag{5.137}$$

After applying the operator M_ε we have

$$\begin{aligned} M_\varepsilon(u_\varepsilon(x)) &= M_\varepsilon(u(x)) + M_\varepsilon(w_\varepsilon(x)) + M_\varepsilon(\widetilde{u}_\varepsilon(x)) \\ &= M_\varepsilon(u(\widehat{x})) + \nabla M_\varepsilon(u(y))(x - \widehat{x}) \\ &+ M_\varepsilon(w_\varepsilon(x)) + M_\varepsilon(\widetilde{u}_\varepsilon(x)) \,, \end{aligned} \tag{5.138}$$

where y is an intermediate point between x and $\widehat{x}$. On the boundary of the inclusion ∂B_ε we have

$$[\![M_\varepsilon^{nn}(u_\varepsilon)]\!]n = 0 \quad \Rightarrow \quad (M^{nn}(u_\varepsilon)_{|_{\Omega\setminus\overline{B_\varepsilon}}} - \gamma M^{nn}(u_\varepsilon)_{|_{B_\varepsilon}})n = 0\,, \tag{5.139}$$

and

$$\begin{aligned}&[\![\partial_\tau M_\varepsilon^{\tau n}(u_\varepsilon)]\!] + [\![\mathrm{div} M_\varepsilon(u_\varepsilon)]\!]\cdot n = 0 \\ &\qquad \Rightarrow (\partial_\tau M^{\tau n}(u_\varepsilon)_{|_{\Omega\setminus\overline{B_\varepsilon}}} - \gamma\partial_\tau M_\varepsilon^{\tau n}(u_\varepsilon)_{|_{B_\varepsilon}})+ \\ &\qquad\qquad (\mathrm{div}(M(u_\varepsilon)_{|_{\Omega\setminus\overline{B_\varepsilon}}} - \gamma M^{nn}(u_\varepsilon)_{|_{B_\varepsilon}}))\cdot n = 0\,,\end{aligned} \tag{5.140}$$

with $M_\varepsilon(\varphi) = -\gamma_\varepsilon \mathbb{C}\nabla\nabla\varphi$ and $M(\varphi) = -\mathbb{C}\nabla\nabla\varphi$. The above expansion, evaluated on ∂B_ε, leads to

$$\begin{aligned}&(1-\gamma)M(u(\widehat{x}))n\cdot n - \varepsilon(1-\gamma)(\nabla M(u(y))n)n\cdot n \\ &\qquad + [\![M_\varepsilon^{nn}(w_\varepsilon(x))]\!] + [\![M_\varepsilon^{nn}(\widetilde{u}_\varepsilon(x))]\!] = 0\end{aligned} \tag{5.141}$$

and

$$\begin{aligned}&(1-\gamma)(\partial_\tau M(u(\widehat{x}))n\cdot\tau + \mathrm{div}M(u(\widehat{x}))\cdot n)- \\ &\qquad \varepsilon(1-\gamma)(\partial_\tau(\nabla M(u(y))n)n\cdot\tau + \mathrm{div}(\nabla M(u(y))n)\cdot n)+ \\ &\qquad\qquad [\![\partial_\tau M_\varepsilon^{\tau n}(w_\varepsilon(x))]\!] + [\![\mathrm{div}M_\varepsilon(w_\varepsilon(x))]\!]\cdot n + \\ &\qquad\qquad\quad [\![\partial_\tau M_\varepsilon^{\tau n}(\widetilde{u}_\varepsilon(x))]\!] + [\![\mathrm{div}M_\varepsilon(\widetilde{u}_\varepsilon(x))]\!]\cdot n = 0\,.\end{aligned} \tag{5.142}$$

Thus, we can choose $M_\varepsilon(w_\varepsilon)$ such that

$$[\![M_\varepsilon^{nn}(w_\varepsilon(x))]\!] = -(1-\gamma)M(u(\widehat{x}))n\cdot n\,, \tag{5.143}$$

$$\begin{aligned}&[\![\partial_\tau M_\varepsilon^{\tau n}(w_\varepsilon(x))]\!] + [\![\mathrm{div}M_\varepsilon(w_\varepsilon(x))]\!]\cdot n = \\ &\qquad -(1-\gamma)(\partial_\tau M(u(\widehat{x}))n\cdot\tau + \mathrm{div}M(u(\widehat{x}))\cdot n)\,.\end{aligned} \tag{5.144}$$

Now, the following exterior problem is considered, and formally obtained as $\varepsilon \to 0$:

$$\left\{\begin{array}{l}\text{Find } M_\varepsilon(w_\varepsilon), \text{ such that} \\ \qquad \begin{array}{rcll}\mathrm{div}(\mathrm{div}M_\varepsilon(w_\varepsilon)) &=& 0 & \text{in } \mathbb{R}^2\,, \\ M_\varepsilon(w_\varepsilon) &\to& 0 & \text{at } \infty\,, \\ [\![M_\varepsilon^{nn}(w_\varepsilon)]\!] &=& \widehat{u}_1 & \\ [\![\partial_\tau M_\varepsilon^{\tau n}(w_\varepsilon)]\!] + [\![\mathrm{div}M_\varepsilon(w_\varepsilon)]\!]\cdot n &=& \widehat{u}_2 & \text{on } \partial B_\varepsilon\,,\end{array}\end{array}\right. \tag{5.145}$$

with

$$\begin{aligned}\widehat{u}_1 &= -(1-\gamma)M(u(\widehat{x}))n\cdot n\,, \\ \widehat{u}_2 &= -(1-\gamma)(\partial_\tau M(u(\widehat{x}))n\cdot\tau + \mathrm{div}M(u(\widehat{x}))\cdot n)\,.\end{aligned}$$

The above boundary value problem admits an explicit solution, which will be used later to construct the expansion for $M_\varepsilon(u_\varepsilon)$. Now we can construct $M_\varepsilon(\widetilde{u}_\varepsilon)$ in such a way that it compensates the discrepancies introduced by the higher order terms in ε as well as by the boundary layer $M_\varepsilon(w_\varepsilon)$ on the exterior boundary $\partial\Omega$. It means that the remainder $M_\varepsilon(\widetilde{u}_\varepsilon)$ must be solution to the following boundary value problem:

$$
\left\{
\begin{array}{rcll}
\text{Find } \widetilde{u}_\varepsilon, \text{ such that} & & & \\
\operatorname{div}(\operatorname{div} M_\varepsilon(\widetilde{u}_\varepsilon)) &=& 0 & \text{in } \Omega\,, \\
M_\varepsilon(\widetilde{u}_\varepsilon) &=& -\gamma_\varepsilon \mathbb{C}\nabla\nabla\widetilde{u}_\varepsilon\,, & \\
\widetilde{u}_\varepsilon &=& -w_\varepsilon & \text{on } \Gamma_{D_u}\,, \\
\partial_n \widetilde{u}_\varepsilon &=& -\partial_n w_\varepsilon & \text{on } \Gamma_{D_\rho}\,, \\
M^{nn}(\widetilde{u}_\varepsilon) &=& -M^{nn}(w_\varepsilon) & \text{on } \Gamma_{N_m}\,, \\
\partial_\tau M^{\tau n}(\widetilde{u}_\varepsilon) + \operatorname{div} M(\widetilde{u}_\varepsilon)\cdot n &=& -s(w_\varepsilon) & \text{on } \Gamma_{N_q}\,, \\
[\![M^{\tau n}(\widetilde{u}_\varepsilon(x_i))]\!] &=& -[\![M^{\tau n}(w_\varepsilon(x_i))]\!] & \text{on } x_i \in \Gamma_{N_q}\,, \\
[\![\widetilde{u}_\varepsilon]\!] &=& 0 & \\
[\![\partial_n \widetilde{u}_\varepsilon]\!] &=& 0 & \\
[\![M^{nn}_\varepsilon(\widetilde{u}_\varepsilon)]\!] &=& -\varepsilon h_1 & \text{on } \partial B_\varepsilon\,, \\
[\![\partial_\tau M^{\tau n}_\varepsilon(\widetilde{u}_\varepsilon)]\!] + [\![\operatorname{div} M_\varepsilon(\widetilde{u}_\varepsilon)]\!]\cdot n &=& +\varepsilon h_2 &
\end{array}
\right. \tag{5.146}
$$

where we have introduced the notation $s(\varphi) = \partial_\tau M^{\tau n}(\varphi) + \operatorname{div} M(\varphi)\cdot n$. In addition, the functions h_1 and h_2 are independent of ε, with

$$
\begin{aligned}
h_1 &= +(1-\gamma)(\nabla M(u(y))n)n\cdot n\,, \\
h_2 &= -(1-\gamma)(\partial_\tau(\nabla M(u(y))n)n\cdot\tau + \operatorname{div}(\nabla M(u(y))n)\cdot n)\,.
\end{aligned}
$$

Analogously to the Section 5.1 (see Theorem 5.1), $\widetilde{u}_\varepsilon$ has an estimate of the form $\|\widetilde{u}_\varepsilon\|_{H^2(\Omega)} = O(\varepsilon^2)$ [120, 148]. In fact, before proceeding, let us state the following result:

Lemma 5.3. *Let $\widetilde{u}_\varepsilon$ be the solution to (5.146) or equivalently the solution to the following variational problem:*

$$
\left\{
\begin{array}{l}
\textit{Find } \widetilde{u}_\varepsilon \in \widetilde{\mathscr{U}_\varepsilon}, \textit{ such that} \\
\displaystyle -\int_\Omega M_\varepsilon(\widetilde{u}_\varepsilon)\cdot\nabla\nabla\eta = \varepsilon^2\int_{\Gamma_{N_q}} s(g_2)\,\eta + \varepsilon^2\int_{\Gamma_{N_m}} M^{nn}(g_1)\,\partial_n\eta \\
\displaystyle \qquad\qquad + \varepsilon^2\sum_{i=1}^{ns} [\![M^{\tau n}(g_1(x_i))]\!]\,\eta(x_i) \\
\displaystyle \qquad\qquad + \varepsilon\int_{\partial B_\varepsilon} h_2\,\eta + \varepsilon\int_{\partial B_\varepsilon} h_1\,\partial_n\eta \quad \forall\eta\in\widetilde{\mathscr{V}}_\varepsilon\,, \\
\qquad\qquad\qquad \textit{with} \quad M_\varepsilon(\widetilde{u}_\varepsilon) = -\gamma_\varepsilon\mathbb{C}\nabla\nabla\widetilde{u}_\varepsilon\,,
\end{array}
\right. \tag{5.147}
$$

where the set $\widetilde{\mathscr{U}_\varepsilon}$ and the space $\widetilde{\mathscr{V}}_\varepsilon$ are defined as

$$
\widetilde{\mathscr{U}_\varepsilon} := \{\varphi\in H^2(\Omega) : [\![\varphi]\!] = [\![\partial_n\varphi]\!] = 0 \textit{ on } \partial B_\varepsilon,\ \varphi_{|_{\Gamma_{D_u}}} = \varepsilon^2 g_2, \partial_n\varphi_{|_{\Gamma_{D_\rho}}} = -\varepsilon^2\partial_n g_1\}\,,
$$

$$
\widetilde{\mathscr{V}}_\varepsilon := \{\varphi\in H^2(\Omega) : [\![\varphi]\!] = [\![\partial_n\varphi]\!] = 0 \textit{ on } \partial B_\varepsilon,\ \varphi_{|_{\Gamma_{D_u}}} = 0, \partial_n\varphi_{|_{\Gamma_{D_\rho}}} = 0\}\,,
$$

with functions $g_1 = \varepsilon^{-2} w_\varepsilon$, $g_2 = -\varepsilon^{-2} w_\varepsilon$, h_1 and h_2 independent of the small parameter ε. Then, we have the estimate $\|\widetilde{u}_\varepsilon\|_{H^2(\Omega)} = O(\varepsilon^2)$ for the remainder.

Proof. By taking $\eta = \widetilde{u}_\varepsilon - \varphi_\varepsilon$ in (5.147), where φ_ε is the lifting of the Dirichlet boundaries data $\varepsilon^2 g_2$ on Γ_{D_u} and $-\varepsilon^2 \partial_n g_1$ on Γ_{D_ρ}, we have

$$\begin{aligned} -\int_\Omega M_\varepsilon(\widetilde{u}_\varepsilon) \cdot \nabla\nabla \widetilde{u}_\varepsilon = {} & \varepsilon^2 \int_{\Gamma_{D_u}} g_2 \, s(\widetilde{u}_\varepsilon) + \varepsilon^2 \int_{\Gamma_{N_q}} s(g_2)\, \widetilde{u}_\varepsilon \\ & + \varepsilon^2 \int_{\Gamma_{D_\rho}} \partial_n g_1 \, M^{nn}(\widetilde{u}_\varepsilon) + \varepsilon^2 \int_{\Gamma_{N_m}} M^{nn}(g_1)\, \partial_n \widetilde{u}_\varepsilon \\ & + \varepsilon^2 \sum_{i=1}^{ns} [\![M^{\tau n}(g_1(x_i))]\!] \widetilde{u}_\varepsilon(x_i) \\ & + \varepsilon \int_{\partial B_\varepsilon} h_2 \, \widetilde{u}_\varepsilon + \varepsilon \int_{\partial B_\varepsilon} h_1 \, \partial_n \widetilde{u}_\varepsilon \, . \end{aligned} \tag{5.148}$$

From the *Cauchy-Schwarz inequality* we obtain

$$\begin{aligned} -\int_\Omega M_\varepsilon(\widetilde{u}_\varepsilon) \cdot \nabla\nabla \widetilde{u}_\varepsilon \leqslant {} & \varepsilon^2 \|g_2\|_{H^{3/2}(\Gamma_{D_u})} \|s(\widetilde{u}_\varepsilon)\|_{H^{-3/2}(\Gamma_{D_u})} \\ & + \varepsilon^2 \|s(g_2)\|_{H^{-3/2}(\Gamma_{N_q})} \|\widetilde{u}_\varepsilon\|_{H^{3/2}(\Gamma_{N_q})} \\ & + \varepsilon^2 \|\partial_n g_1\|_{H^{1/2}(\Gamma_{D_\rho})} \|M^{nn}(\widetilde{u}_\varepsilon)\|_{H^{-1/2}(\Gamma_{D_\rho})} \\ & + \varepsilon^2 \|M^{nn}(g_1)\|_{H^{-1/2}(\Gamma_{N_m})} \|\partial_n \widetilde{u}_\varepsilon\|_{H^{1/2}(\Gamma_{N_m})} \\ & + \varepsilon^2 \max_i (|M^{\tau n}(g_1(x_i))| \; |\widetilde{u}_\varepsilon(x_i)|) \\ & + \varepsilon \|h_2\|_{H^{-3/2}(\partial B_\varepsilon)} \|\widetilde{u}_\varepsilon\|_{H^{3/2}(\partial B_\varepsilon)} \\ & + \varepsilon \|h_1\|_{H^{-1/2}(\partial B_\varepsilon)} \|\partial_n \widetilde{u}_\varepsilon\|_{H^{1/2}(\partial B_\varepsilon)} \, . \end{aligned} \tag{5.149}$$

Taking into account the *trace theorem*, we have

$$-\int_\Omega M_\varepsilon(\widetilde{u}_\varepsilon) \cdot \nabla\nabla \widetilde{u}_\varepsilon \leqslant \varepsilon^2 C_1 \|\widetilde{u}_\varepsilon\|_{H^2(\Omega)} \, , \tag{5.150}$$

where we have used the interior *elliptic regularity* of function u. Finally, from the *coercivity* of the bilinear form on the left hand side of (5.147), namely,

$$c \|\widetilde{u}_\varepsilon\|^2_{H^2(\Omega)} \leqslant -\int_\Omega M_\varepsilon(\widetilde{u}_\varepsilon) \cdot \nabla\nabla \widetilde{u}_\varepsilon \, , \tag{5.151}$$

we obtain

$$\|\widetilde{u}_\varepsilon\|_{H^2(\Omega)} \leqslant C \varepsilon^2 \, , \tag{5.152}$$

which leads to the result, with $C = C_1 / c$. □

Therefore, the *expansion* for $M_\varepsilon(u_\varepsilon)$ (see, for instance, the book by Little 1973 [139]) can be written in a polar coordinate system (r, θ) centered at the point $\widehat{x}$ (see fig. 5.15) as:

- For $r \geqslant \varepsilon$ (outside the inclusion)

$$M_\varepsilon^{rr}(u_\varepsilon(r,\theta)) = \varphi_1\left(1 - \tfrac{1-\gamma}{1+\gamma\alpha}\tfrac{\varepsilon^2}{r^2}\right) + \varphi_2\left(1 - \tfrac{1-\gamma}{1+\gamma\beta}\left(\tfrac{4\nu}{3+\nu}\tfrac{\varepsilon^2}{r^2} + 3\beta\tfrac{\varepsilon^4}{r^4}\right)\right)\cos 2\theta + O(\varepsilon^2), \tag{5.153}$$

$$M_\varepsilon^{\theta\theta}(u_\varepsilon(r,\theta)) = \varphi_1\left(1 + \tfrac{1-\gamma}{1+\gamma\alpha}\tfrac{\varepsilon^2}{r^2}\right) - \varphi_2\left(1 + \tfrac{1-\gamma}{1+\gamma\beta}\left(\tfrac{4}{3+\nu}\tfrac{\varepsilon^2}{r^2} - 3\beta\tfrac{\varepsilon^4}{r^4}\right)\right)\cos 2\theta + O(\varepsilon^2), \tag{5.154}$$

$$M_\varepsilon^{r\theta}(u_\varepsilon(r,\theta)) = -\varphi_2\left(1 - \beta\tfrac{1-\gamma}{1+\gamma\beta}\left(2\tfrac{\varepsilon^2}{r^2} - 3\tfrac{\varepsilon^4}{r^4}\right)\right)\sin 2\theta + O(\varepsilon^2). \tag{5.155}$$

- For $0 < r < \varepsilon$ (inside the inclusion)

$$M_\varepsilon^{rr}(u_\varepsilon(r,\theta)) = \varphi_1\tfrac{2}{(1-\nu)(1+\gamma\alpha)} + \varphi_2\tfrac{4}{(3+\nu)(1+\gamma\beta)}\cos 2\theta + O(\varepsilon^2), \tag{5.156}$$

$$M_\varepsilon^{\theta\theta}(u_\varepsilon(r,\theta)) = \varphi_1\tfrac{2}{(1-\nu)(1+\gamma\alpha)} - \varphi_2\tfrac{4}{(3+\nu)(1+\gamma\beta)}\cos 2\theta + O(\varepsilon^2), \tag{5.157}$$

$$M_\varepsilon^{r\theta}(u_\varepsilon(r,\theta)) = -\varphi_2\tfrac{4}{(3+\nu)(1+\gamma\beta)}\sin 2\theta + O(\varepsilon^2). \tag{5.158}$$

Some terms in the above formulae require explanations. The coefficients φ_1 and φ_2 are given by

$$\varphi_1 = \frac{1}{2}(m_1(u(\widehat{x})) + m_2(u(\widehat{x}))), \quad \varphi_2 = \frac{1}{2}(m_1(u(\widehat{x})) - m_2(u(\widehat{x}))), \tag{5.159}$$

where $m_1(u(\widehat{x}))$ and $m_2(u(\widehat{x}))$ are the eigenvalues of tensor $M(u(\widehat{x}))$, which can be expressed as

$$m_{1,2}(u(\widehat{x})) = \frac{1}{2}\left(\operatorname{tr} M(u(\widehat{x})) \pm \sqrt{2M^D(u(\widehat{x}))\cdot M^D(u(\widehat{x}))}\right), \tag{5.160}$$

with $M^D(u(\widehat{x}))$ standing for the deviatory part of the momentum tensor $M(u(\widehat{x}))$, namely

$$M^D(u(\widehat{x})) = M(u(\widehat{x})) - \frac{1}{2}\operatorname{tr} M(u(\widehat{x}))\mathrm{I}. \tag{5.161}$$

In addition, the constants α and β are given by

$$\alpha = \frac{1+\nu}{1-\nu} \quad \text{and} \quad \beta = \frac{1-\nu}{3+\nu}. \tag{5.162}$$

Finally, $M_\varepsilon^{rr}(u_\varepsilon)$, $M_\varepsilon^{\theta\theta}(u_\varepsilon)$ and $M_\varepsilon^{r\theta}(u_\varepsilon)$ are the components of tensor $M_\varepsilon(u_\varepsilon)$ in the polar coordinate system, namely $M_\varepsilon^{rr}(u_\varepsilon) = e^r \cdot M_\varepsilon(u_\varepsilon)e^r$, $M_\varepsilon^{\theta\theta}(u_\varepsilon) = e^\theta \cdot M_\varepsilon(u_\varepsilon)e^\theta$ and $M_\varepsilon^{r\theta}(u_\varepsilon) = M_\varepsilon^{\theta r}(u_\varepsilon) = e^r \cdot M_\varepsilon(u_\varepsilon)e^\theta$, with e^r and e^θ used to denote the canonical basis associated to the polar coordinate system (r,θ), such that, $\|e^r\| = \|e^\theta\| = 1$ and $e^r \cdot e^\theta = 0$. See fig. 5.15.

Note 5.2. The obtained results in formulae (5.156), (5.157) and (5.158) are conform with the *Eshelby's theorem*. In fact, the curvature of the plate associated to the

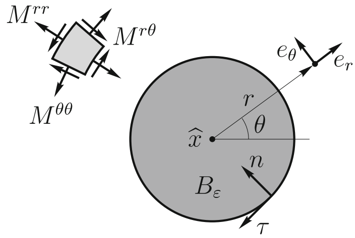


Fig. 5.15 Polar coordinate system (r,θ) centered at the point $\widehat{x} \in \Omega$

solution of the exterior problem (5.145) is uniform inside the inclusion $B_\varepsilon(\widehat{x})$ embedded in the whole two-dimensional space $\mathbb{R}^2$ and can be written in the following compact form

$$\nabla\nabla w_\varepsilon|_{B_\varepsilon(\widehat{x})} = \mathbb{T}\nabla\nabla u(\widehat{x}) \ , \tag{5.163}$$

where $\mathbb{T}$ is a fourth order uniform (constant) tensor. See Note 5.1 in Section 5.2 for more details on this important result.

5.3.4 *Topological Derivative Evaluation*

Now, we can evaluate the integrals in formula (5.136) to collect the terms in power of ε and recognize function $f(\varepsilon)$. With these results, we can perform the limit passage $\varepsilon \to 0$. The integrals in (5.136) can be evaluated in the same way as shown in Section 4.3 by using the expansions for $M_\varepsilon(u_\varepsilon)$ given by (5.153)-(5.158). The idea is to introduce a polar coordinate system (r,θ) with center at $\widehat{x}$ (see fig. 5.15). Then, we can write u_ε in this coordinate system to evaluate the integrals explicitly. In particular, the integrals in (5.136) yield

$$\begin{aligned} -\int_{\partial B_\varepsilon} [\![\Sigma_\varepsilon]\!] n \cdot n - \int_{\partial B_\varepsilon} [\![\nabla n^\top \nabla u_\varepsilon \cdot M_\varepsilon(u_\varepsilon) n]\!] \\ = 2\pi\varepsilon \mathbb{P}_\gamma M(u(\widehat{x})) \cdot \nabla\nabla u(\widehat{x}) + o(\varepsilon) \ . \end{aligned} \tag{5.164}$$

Finally, the topological derivative given by (1.49) leads to

$$\mathscr{T}(\widehat{x}) = \lim_{\varepsilon\to 0} \frac{1}{f'(\varepsilon)} \left(2\pi\varepsilon \mathbb{P}_\gamma M(u(\widehat{x})) \cdot \nabla\nabla u(\widehat{x}) + o(\varepsilon)\right) \ , \tag{5.165}$$

where the *polarization tensor* $\mathbb{P}_\gamma$ is given by the following fourth order isotropic tensor

$$\mathbb{P}_\gamma = \frac{1}{2} \frac{1-\gamma}{1+\gamma\beta} \left(\frac{4\beta}{1-\nu} \mathbb{I} + \alpha\beta \frac{1+3\nu}{1-\nu^2} \frac{1-\gamma}{1+\gamma\alpha} \mathrm{I} \otimes \mathrm{I} \right) \ , \tag{5.166}$$

with the parameters α and β given by (5.162). Now, in order to extract the leading term of the above expansion, we choose

$$f(\varepsilon) = \pi\varepsilon^2 \,, \tag{5.167}$$

which leads to the final formula for the *topological derivative*, namely [20, 186]

$$\mathscr{T}(\widehat{x}) = \mathbb{P}_\gamma M(u(\widehat{x})) \cdot \nabla\nabla u(\widehat{x}) \,. \tag{5.168}$$

Finally, the topological asymptotic expansion of the energy shape functional takes the form

$$\psi(\chi_\varepsilon(\widehat{x})) = \psi(\chi) + \pi\varepsilon^2 \mathbb{P}_\gamma M(u(\widehat{x})) \cdot \nabla\nabla u(\widehat{x}) + o(\varepsilon^2) \,, \tag{5.169}$$

whose mathematical justification will be given at the end of this chapter.

Remark 5.8. We note that the obtained polarization tensor is isotropic because we are dealing with circular inclusions. We claim however that in the case of arbitrary shaped inclusion, the form of the polarization tensor associated to the Kirchhoff plates has not been reported in the literature.

Remark 5.9. Formally, we can consider the limit cases $\gamma \to 0$ and $\gamma \to \infty$. For $\gamma \to 0$, the inclusion leads to a void and the transmission condition on the boundary of the inclusion degenerates to homogeneous Neumann boundary condition. In fact, in this case the polarization tensor is given by

$$\mathbb{P}_0 = \frac{2}{3+\nu}\mathbb{I} + \frac{1+3\nu}{2(1-\nu)(3+\nu)} \mathrm{I} \otimes \mathrm{I} \,, \tag{5.170}$$

which, together with (5.168), corroborates with the obtained formula (4.252) for $b = 0$. In addition, for $\gamma \to \infty$, the elastic inclusion leads to a rigid one and the polarization tensor is given by

$$\mathbb{P}_\infty = -\frac{2}{1-\nu}\mathbb{I} + \frac{1+3\nu}{2(1-\nu^2)} \mathrm{I} \otimes \mathrm{I} \,. \tag{5.171}$$

5.3.5 *Numerical Example*

Let us present a simple numerical example consisting in the design of a clamped beam. For that, we propose the following shape functional

$$\Psi_\Omega(u) := -\mathscr{J}_\Omega(u) + \beta\,|\Omega| \,, \tag{5.172}$$

where $|\Omega|$ is the Lebesgue measure of Ω and $\beta > 0$ is a fixed Lagrange multiplier. It means that the shape functional to be minimized is the energy stored in the body with a volume constraint. The topological derivative of $\Psi_\Omega(u)$ is given by

$$\mathscr{T} = -\mathbb{P}_0 M(u) \cdot \nabla\nabla u - \beta \,, \tag{5.173}$$

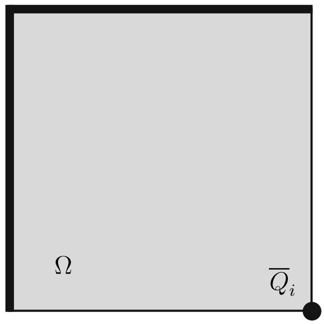
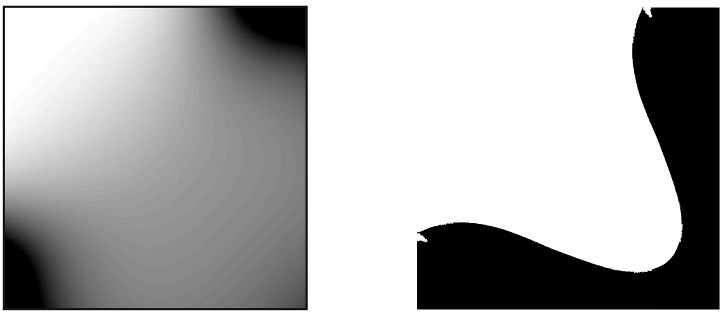


Fig. 5.16 Hold-all-domain

with $M(u) = -\mathbb{C}\nabla\nabla u$, where we have used formula (5.168) with $\gamma = 0$ and the fact that the topological derivative of the term $\beta\,|\Omega|$ is trivial. In addition, the displacement scalar field u is evaluated by solving problem (5.112) numerically.

In the numerical example shown in fig. 5.16, the initial domain is represented by a 1×1 square, with Young Modulus $E = 1$ and Poisson ratio $\nu = 0.3$. The square is clamped on the thick lines and the beam is submitted to a concentrated load $\bar{Q}_i = 1$ applied on the bottom-right corner of the square. The remainder part of the boundary of the square remains free. The Lagrange multiplier is fixed as $\beta = 4$ and the contrast $\gamma \to 0$.

The topological derivative of the shape functional $\Psi_\Omega(u)$ which is obtained in the first iteration of the shape and topology optimization numerical procedure is shown in fig. 5.17(a), where white to black levels mean smaller (negative) to higher (positive) values. This picture induces a level-set domain representation for the optimal shape, as proposed in [16]. The resulting topology design in the form of a beam is shown in fig. 5.17(b).



(a) topological derivative (b) final topology

Fig. 5.17 Topological derivative in the hold-all domain and optimal shape design [186]

5.4 Estimates for the Remainders

In this section we present an alternative procedure to compute the topological derivative for inclusions associated to the energy shape functional. We also provide the full mathematical justification for the expansions (5.46), (5.106) and (5.169) by using simple arguments. Thus, let us start by introducing the problem in an abstract setting. The energy shape functional associated to the unperturbed domain reads

$$\psi(\chi):=\frac{1}{2}a(u,u)-l(u)\ , \tag{5.174}$$

with u solution to the abstract variational problem of the form

$$u\in\mathscr{U}:a(u,\eta)=l(\eta)\quad\forall\eta\in\mathscr{V}\ , \tag{5.175}$$

where $\mathscr{U}$ is the set of admissible functions and $\mathscr{V}$ is the space of admissible variations, both associated to the unperturbed problem. The energy shape functional associated to the perturbed domain is defined as

$$\psi(\chi_\varepsilon):=\frac{1}{2}a_\varepsilon(u_\varepsilon,u_\varepsilon)-l(u_\varepsilon)\ , \tag{5.176}$$

with u_ε solution to the abstract variational problem of the form

$$u_\varepsilon\in\mathscr{U}_\varepsilon:a_\varepsilon(u_\varepsilon,\eta)=l(\eta)\quad\forall\eta\in\mathscr{V}_\varepsilon\ , \tag{5.177}$$

where $\mathscr{U}_\varepsilon$ is the set of admissible functions and $\mathscr{V}_\varepsilon$ is the space of admissible variations, both associated to the perturbed problem. In addition, $a:U(\Omega)\times V(\Omega)\to\mathbb{R}$ and $a_\varepsilon:U(\Omega)\times V(\Omega)\to\mathbb{R}$ are symmetrical bilinear forms and $l:V(\Omega)\to\mathbb{R}$ is a linear functional, with $U(\Omega)$ and $V(\Omega)$ used to denote affine and linear Hilbert subspaces, respectively. By taking $\eta=u_\varepsilon-u$ in the above variational problems we have

$$a(u,u_\varepsilon-u)=l(u_\varepsilon-u)\quad\text{and}\quad a_\varepsilon(u_\varepsilon,u_\varepsilon-u)=l(u_\varepsilon-u)\ . \tag{5.178}$$

From the above equalities, we can rewritten the shape functions as follows

$$\begin{aligned}\psi(\chi)&=\frac{1}{2}a(u,u)-l(u)+\frac{1}{2}a(u,u_\varepsilon-u)-\frac{1}{2}l(u_\varepsilon-u)\\&=\frac{1}{2}a(u,u_\varepsilon)-\frac{1}{2}l(u_\varepsilon+u)\ ,\end{aligned} \tag{5.179}$$

$$\begin{aligned}\psi(\chi_\varepsilon)&=\frac{1}{2}a_\varepsilon(u_\varepsilon,u_\varepsilon)-l(u_\varepsilon)-\frac{1}{2}a_\varepsilon(u_\varepsilon,u_\varepsilon-u)+\frac{1}{2}l(u_\varepsilon-u)\\&=\frac{1}{2}a_\varepsilon(u_\varepsilon,u)-\frac{1}{2}l(u_\varepsilon+u)\ .\end{aligned} \tag{5.180}$$

After subtracting both equations we get

$$\psi(\chi_\varepsilon) - \psi(\chi) = \frac{1}{2}(a_\varepsilon(u_\varepsilon, u) - a(u_\varepsilon, u)) \, . \tag{5.181}$$

Now, we will specify the bilinear forms $a(u_\varepsilon, u)$ and $a_\varepsilon(u_\varepsilon, u)$ for each problem under consideration, namely, Laplacian, Navier and Kirchhoff. Then, the full mathematical justification for the obtained topological asymptotical expansions (5.46), (5.106) and (5.169), will be respectively provided through the following three theorems:

Theorem 5.1. *Let us consider the Laplacian problem as presented in Section 5.1. Then, the bilinear forms $a(u_\varepsilon, u)$ and $a_\varepsilon(u_\varepsilon, u)$ are defined as*

$$a(u_\varepsilon, u) := -\int_\Omega q(u_\varepsilon) \cdot \nabla u \quad \text{and} \quad a_\varepsilon(u_\varepsilon, u) := -\int_\Omega q_\varepsilon(u_\varepsilon) \cdot \nabla u \, , \tag{5.182}$$

where $u \in \mathscr{U}$ and $u_\varepsilon \in \mathscr{U}_\varepsilon$ are solutions to (5.3) and (5.9), respectively. In addition, the sets $\mathscr{U}$ and $\mathscr{U}_\varepsilon$ are respectively defined through (5.5) and (5.11). Therefore, by taking into account (5.181) we have the following topological asymptotic expansion for the energy shape functional

$$\psi(\chi_\varepsilon(\widehat{x})) - \psi(\chi) = \pi\varepsilon^2 P_\gamma q(u(\widehat{x})) \cdot \nabla u(\widehat{x}) + o(\varepsilon^2) \, , \tag{5.183}$$

with the polarization tensor P_γ given by (5.43) and γ used to denote the contrast on the material properties.

Proof. We start by recalling that $q_\varepsilon(\varphi) = \gamma_\varepsilon q(\varphi)$ and $q(\varphi) = -k\nabla\varphi$, with γ_ε given by (5.1). Therefore, we have

$$\begin{aligned} a_\varepsilon(u_\varepsilon, u) - a(u_\varepsilon, u) &= -\int_{\Omega \setminus \overline{B_\varepsilon}} q(u_\varepsilon) \cdot \nabla u - \gamma \int_{B_\varepsilon} q(u_\varepsilon) \cdot \nabla u \\ &\quad + \int_{\Omega \setminus \overline{B_\varepsilon}} q(u_\varepsilon) \cdot \nabla u + \int_{B_\varepsilon} q(u_\varepsilon) \cdot \nabla u \\ &= (1-\gamma) \int_{B_\varepsilon} q(u) \cdot \nabla u_\varepsilon \, . \end{aligned} \tag{5.184}$$

The above integral can be rewritten as follows

$$\int_{B_\varepsilon} q(u) \cdot \nabla u_\varepsilon = \int_{B_\varepsilon} q(u) \cdot \nabla u + \int_{B_\varepsilon} q(u) \cdot \nabla (u_\varepsilon - u) \, . \tag{5.185}$$

The first integral on the right hand side of the above equation can be expanded in power of ε, which leads to

$$\int_{B_\varepsilon} q(u) \cdot \nabla u = \pi\varepsilon^2 q(u(\widehat{x})) \cdot \nabla u(\widehat{x}) + o(\varepsilon^2) \, , \tag{5.186}$$

where we have used the interior *elliptic regularity* of the solution u. By taking into account the expansion of the solution $u_{\varepsilon|_{B_\varepsilon}}$ given by (5.34), the second integral yields

$$\int_{B_\varepsilon} q(u) \cdot \nabla(u_\varepsilon - u) = \pi\varepsilon^2 \frac{1-\gamma}{1+\gamma} q(u(\widehat{x})) \cdot \nabla u(\widehat{x}) + o(\varepsilon^2) + \int_{B_\varepsilon} q(u) \cdot \nabla \widetilde{u}_\varepsilon \,, \tag{5.187}$$

where we have used again the interior elliptic regularity of the solution u. Finally, we have the following estimate for the last integral on the right hand side of the above equation

$$\int_{B_\varepsilon} q(u) \cdot \nabla(\widetilde{u}_\varepsilon) \leqslant \|q(u)\|_{L^2(B_\varepsilon)} \|\nabla \widetilde{u}_\varepsilon\|_{L^2(B_\varepsilon)} \leqslant \varepsilon C_1 \|\nabla \widetilde{u}_\varepsilon\|_{L^2(\Omega)} \leqslant \varepsilon C_2 \|\widetilde{u}_\varepsilon\|_{H^1(\Omega)} \leqslant \varepsilon^3 C \,, \tag{5.188}$$

where we have used once again the interior elliptic regularity of the solution u and the result of Lemma 5.1. □

Theorem 5.2. *Let us consider the Navier problem as presented in Section 5.2. Then, the bilinear forms $a(u_\varepsilon, u)$ and $a_\varepsilon(u_\varepsilon, u)$ are defined as*

$$a(u_\varepsilon, u) := \int_\Omega \sigma(u_\varepsilon) \cdot \nabla u^s \quad \text{and} \quad a_\varepsilon(u_\varepsilon, u) := \int_\Omega \sigma_\varepsilon(u_\varepsilon) \cdot \nabla u^s \,, \tag{5.189}$$

where $u \in \mathscr{U}$ and $u_\varepsilon \in \mathscr{U}_\varepsilon$ are solutions to (5.52) and (5.60), respectively, with the sets $\mathscr{U}$ and $\mathscr{U}_\varepsilon$ respectively defined through (5.55) and (5.62). Therefore, by taking into account (5.181) we have the following topological asymptotic expansion for the energy shape functional

$$\psi(\chi_\varepsilon(\widehat{x})) - \psi(\chi) = -\pi\varepsilon^2 \mathbb{P}_\gamma \sigma(u(\widehat{x})) \cdot \nabla u^s(\widehat{x}) + o(\varepsilon^2) \,, \tag{5.190}$$

with the polarization tensor $\mathbb{P}_\gamma$ given by (5.103) and γ used to denote the contrast on the material properties.

Proof. We start by recalling that $\sigma_\varepsilon(\varphi) = \gamma_\varepsilon \sigma(\varphi)$ and $\sigma(\varphi) = \mathbb{C}\nabla\varphi^s$, with γ_ε given by (5.1). Therefore, we have

$$\begin{aligned} a_\varepsilon(u_\varepsilon, u) - a(u_\varepsilon, u) &= \int_{\Omega\setminus\overline{B_\varepsilon}} \sigma(u_\varepsilon) \cdot \nabla u^s + \gamma \int_{B_\varepsilon} \sigma(u_\varepsilon) \cdot \nabla u^s \\ &\quad - \int_{\Omega\setminus\overline{B_\varepsilon}} \sigma(u_\varepsilon) \cdot \nabla u^s - \int_{B_\varepsilon} \sigma(u_\varepsilon) \cdot \nabla u^s \\ &= -(1-\gamma) \int_{B_\varepsilon} \sigma(u) \cdot \nabla u^s_\varepsilon \,. \end{aligned} \tag{5.191}$$

By taking into account the expansion for the stress tensor $\sigma_\varepsilon(u_\varepsilon)_{|B_\varepsilon}$ given by formulae (5.93)-(5.95), the above integral can be rewritten as follows

$$
\begin{aligned}
(1-\gamma)\int_{B_\varepsilon} \sigma(u)\cdot\nabla u_\varepsilon^s &= \frac{1-\gamma}{\gamma}\int_{B_\varepsilon} \sigma_\varepsilon(u_\varepsilon)\cdot\nabla u^s \\
&= 2\pi\varepsilon^2\mathbb{P}_\gamma\sigma(u(\widehat{x}))\cdot\nabla u^s(\widehat{x}) + o(\varepsilon^2) \\
&+ (1-\gamma)\int_{B_\varepsilon} \sigma(u)\cdot\nabla\widetilde{u}_\varepsilon^s \, , \qquad (5.192)
\end{aligned}
$$

where we have used the interior *elliptic regularity* of the solution u. Finally, we have the following estimate for the last integral on the right hand side of the above equation

$$
\begin{aligned}
\int_{B_\varepsilon} \sigma(u)\cdot\nabla\widetilde{u}_\varepsilon^s &\leqslant \|\sigma(u)\|_{L^2(B_\varepsilon;\mathbb{R}^2)}\|\nabla\widetilde{u}_\varepsilon^s\|_{L^2(B_\varepsilon;\mathbb{R}^2)} \\
&\leqslant \varepsilon C_1\|\nabla\widetilde{u}_\varepsilon^s\|_{L^2(\Omega;\mathbb{R}^2)} \leqslant \varepsilon C_2\|\widetilde{u}_\varepsilon\|_{H^1(\Omega;\mathbb{R}^2)} \leqslant \varepsilon^3 C \, , \qquad (5.193)
\end{aligned}
$$

where we have used again the interior elliptic regularity of the solution u and the result of Lemma 5.2. □

Theorem 5.3. *Let us consider the Kirchhoff problem as presented in Section 5.3. Then, the bilinear forms $a(u_\varepsilon,u)$ and $a_\varepsilon(u_\varepsilon,u)$ are defined as*

$$
a(u_\varepsilon,u) := -\int_\Omega M(u_\varepsilon)\cdot\nabla\nabla u \quad \textit{and} \quad a_\varepsilon(u_\varepsilon,u) := -\int_\Omega M_\varepsilon(u_\varepsilon)\cdot\nabla\nabla u \, , \qquad (5.194)
$$

where $u \in \mathscr{U}$ and $u_\varepsilon \in \mathscr{U}_\varepsilon$ are solutions to (5.112) and (5.119), respectively, with the sets $\mathscr{U}$ and $\mathscr{U}_\varepsilon$ respectively defined through (5.115) and (5.121). Therefore, by taking into account (5.181) we have the following topological asymptotic expansion for the energy shape functional

$$
\psi(\chi_\varepsilon(\widehat{x})) - \psi(\chi) = \pi\varepsilon^2\mathbb{P}_\gamma M(u(\widehat{x}))\cdot\nabla\nabla u(\widehat{x}) + o(\varepsilon^2) \, , \qquad (5.195)
$$

with the polarization tensor $\mathbb{P}_\gamma$ given by (5.166) and γ used to denote the contrast on the material properties.

Proof. We start by recalling that $M_\varepsilon(\varphi) = \gamma_\varepsilon M(\varphi)$ and $M(\varphi) = -\mathbb{C}\nabla\nabla\varphi$, with γ_ε given by (5.1). Therefore, we have

$$
\begin{aligned}
a_\varepsilon(u_\varepsilon,u) - a(u_\varepsilon,u) &= -\int_{\Omega\setminus\overline{B_\varepsilon}} M(u_\varepsilon)\cdot\nabla\nabla u - \gamma\int_{B_\varepsilon} M(u_\varepsilon)\cdot\nabla\nabla u \\
&\quad + \int_{\Omega\setminus\overline{B_\varepsilon}} M(u_\varepsilon)\cdot\nabla\nabla u + \int_{B_\varepsilon} M(u_\varepsilon)\cdot\nabla\nabla u \\
&= (1-\gamma)\int_{B_\varepsilon} M(u)\cdot\nabla\nabla u_\varepsilon \, . \qquad (5.196)
\end{aligned}
$$

By taking into account the expansion for the momentum tensor $M_\varepsilon(u_\varepsilon)_{|B_\varepsilon}$ given by formulae (5.156)-(5.158), the above integral can be rewritten as follows

$$
\begin{aligned}
(1-\gamma)\int_{B_\varepsilon} M(u)\cdot\nabla\nabla u_\varepsilon &= \frac{1-\gamma}{\gamma}\int_{B_\varepsilon} M_\varepsilon(u_\varepsilon)\cdot\nabla\nabla u \\
&= 2\pi\varepsilon^2\mathbb{P}_\gamma M(u(\widehat{x}))\cdot\nabla\nabla u(\widehat{x}) + o(\varepsilon^2) \\
&+ (1-\gamma)\int_{B_\varepsilon} M(u)\cdot\nabla\nabla\widetilde{u}_\varepsilon\ , \qquad (5.197)
\end{aligned}
$$

where we have used the interior *elliptic regularity* of the solution u. Finally, we have the following estimate for the last integral on the right hand side of the above equation

$$
\begin{aligned}
\int_{B_\varepsilon} M(u)\cdot\nabla\nabla(\widetilde{u}_\varepsilon) &\leqslant \|M(u)\|_{L^2(B_\varepsilon)}\|\nabla\nabla\widetilde{u}_\varepsilon\|_{L^2(B_\varepsilon)} \\
&\leqslant \varepsilon C_1\|\nabla\nabla\widetilde{u}_\varepsilon\|_{L^2(\Omega)} \leqslant \varepsilon C_2\|\widetilde{u}_\varepsilon\|_{H^2(\Omega)} \leqslant \varepsilon^3 C\ , \qquad (5.198)
\end{aligned}
$$

where we have used again the interior elliptic regularity of the solution u and the result of Lemma 5.3. □

Remark 5.10. The previous results can be slightly improved by using the *Hölder inequality* together with the *Sobolev embedding theorem* in the last step of the proofs. See for instance Example 1.8 in Chapter 1.

5.5 Exercises

1. Consider the Poisson problem described in Section 5.1:

   a. From (5.8), derive (5.9) and (5.12).
   b. By using separation of variables, find the explicit solution to the boundary value problem (5.29).
   c. Repeat the Example A presented in Section 4.1.5.1, by considering an inclusion with contrast γ instead of a hole.

2. Consider the Navier problem described in Section 5.2:

   a. From (5.56), derive the Navier system as presented in Remark 5.4.
   b. From (5.59), derive (5.60) and (5.63).
   c. By using separation of variables, find the stress distribution around the inclusion explicitly, which is solution to the boundary value problem (5.82). Hint: take a look on the book by Little 1973 [139] and look for the Airy functions in polar coordinates.
   d. Take into account Note 5.1 and derive a closed form for the isotropic and uniform tensor $\mathbb{T} = \alpha_1 \mathbb{I} + \alpha_2 \mathrm{I} \otimes \mathrm{I}$, by finding the constant coefficients α_1 and α_2 explicitly.

3. Consider the Kirchhoff problem described in Section 5.3:

   a. From (5.116), derive the Kirchhoff equation as presented in Remark 5.7.
   b. From (5.118), derive (5.119) and (5.122).
   c. By using separation of variables, find the moment distribution around the inclusion explicitly, which is solution to the boundary value problem (5.145). Hint: take a look on the book by Little 1973 [139] and look for the Airy functions in polar coordinates.
   d. Take into account Note 5.2 and derive a closed form for the isotropic and uniform tensor $\mathbb{T} = \alpha_1 \mathbb{I} + \alpha_2 \mathrm{I} \otimes \mathrm{I}$, by finding the constant coefficients α_1 and α_2 explicitly.

Chapter 6
Topological Derivative Evaluation with Adjoint States

The evaluation of the topological derivative for a general class of shape functionals is presented in this chapter. The method is applied to a modified energy shape functional associated with the steady-state heat conduction problem. The nucleation of a small circular hole, represented by $B_\varepsilon(\widehat{x})$, with $\widehat{x} \in \Omega \subset \mathbb{R}^2$ and $\overline{B_\varepsilon} \Subset \Omega$, is considered as the topological perturbation. Therefore, the topologically perturbed domain is obtained as $\Omega_\varepsilon = \Omega \setminus \overline{B_\varepsilon}$.

For the specific problem, some methods were proposed to evaluate the topological derivative [11, 130, 184]. In this chapter, we extend the approach of Chapter 4 (see also [184]) to deal with the modified adjoint method proposed in [11]. This leads to an alternative approach to calculate the topological derivative based on shape sensitivity analysis combined with the modified Lagrangian method.

Since we consider a general class of shape functionals, which are not necessarily associated with the energy, we will show later that the proposed approach simplifies the most delicate step of the topological derivative calculation, namely, the asymptotic analysis of the adjoint state.

6.1 Problem Formulation

The shape functional in the unperturbed domain which we are dealing with is defined as

$$\psi(\chi) := \mathscr{J}_\Omega(u) = \frac{1}{2}\int_\Omega B\nabla u \cdot \nabla u \,, \tag{6.1}$$

where B is a given second order symmetric constant tensor and the scalar function u is the solution to the variational problem:

$$\begin{cases} \text{Find } u \in \mathscr{U}, \text{ such that} \\ \displaystyle\int_\Omega \nabla u \cdot \nabla \eta + \int_{\Gamma_N} \overline{q}\eta = 0 \quad \forall \eta \in \mathscr{V} \,. \end{cases} \tag{6.2}$$

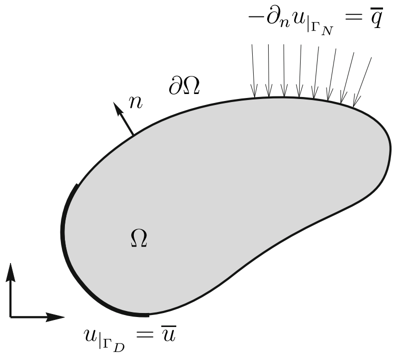


Fig. 6.1 The Laplace problem defined in the unperturbed domain Ω

The set $\mathscr{U}$ and the space $\mathscr{V}$ are respectively defined as

$$\mathscr{U} := \{\varphi \in H^1(\Omega) : \varphi_{|\Gamma_D} = \overline{u}\} , \tag{6.3}$$

$$\mathscr{V} := \{\varphi \in H^1(\Omega) : \varphi_{|\Gamma_D} = 0\} . \tag{6.4}$$

In addition, $\partial\Omega = \overline{\Gamma}_D \cup \overline{\Gamma}_N$ with $\Gamma_D \cap \Gamma_N = \varnothing$, where Γ_D and Γ_N are Dirichlet and Neumann boundaries, respectively. Thus $\overline{u}$ is a Dirichlet data on Γ_D and $\overline{q}$ is a Neumann data on Γ_N, both assumed to be smooth enough. See the details in fig. 6.1. The strong equation associated to the above variational problem (6.2) reads:

$$\left\{\begin{array}{l} \text{Find}\, u, \text{ such that} \\ -\Delta u = 0 \text{ in } \Omega , \\ \quad u = \overline{u} \text{ on } \Gamma_D , \\ -\partial_n u = \overline{q} \text{ on } \Gamma_N . \end{array}\right. \tag{6.5}$$

Remark 6.1. The functional (6.1) includes a large range of shape functions, which shall be useful for practical applications. In particular, when $B = \mathrm{I}$, the functional (6.1) degenerates to the energy. In addition, when $B \neq \mathrm{I}$, the analysis becomes much more involved, which justifies the introduction of a modified adjoint state, as already mentioned in the beginning of this chapter.

Now, let us state the same problem in the perturbed domain. In this case, the shape functional reads

$$\psi(\chi_\varepsilon) := \mathscr{J}_{\Omega_\varepsilon}(u_\varepsilon) = \frac{1}{2}\int_{\Omega_\varepsilon} B\nabla u_\varepsilon \cdot \nabla u_\varepsilon , \tag{6.6}$$

where the scalar function u_ε solves the variational problem:

$$\left\{\begin{array}{l} \text{Find}\, u_\varepsilon \in \mathscr{U}_\varepsilon, \text{ such that} \\ \displaystyle\int_{\Omega_\varepsilon} \nabla u_\varepsilon \cdot \nabla \eta + \int_{\Gamma_N} \overline{q}\eta = 0 \quad \forall \eta \in \mathscr{V}_\varepsilon . \end{array}\right. \tag{6.7}$$

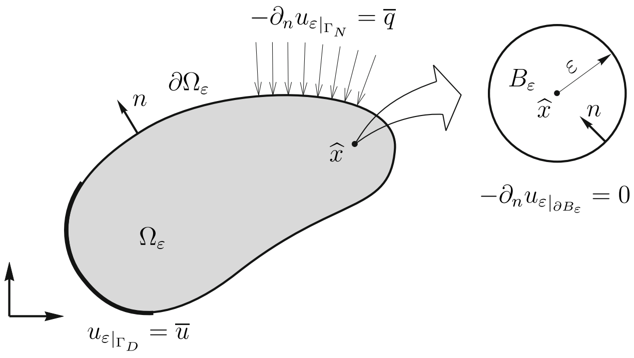


Fig. 6.2 The Laplace problem defined in the perturbed domain Ω_ε

The set $\mathscr{U}_\varepsilon$ and the space $\mathscr{V}_\varepsilon$ are defined as

$$\mathscr{U}_\varepsilon := \{\varphi \in H^1(\Omega_\varepsilon) : \varphi_{|\Gamma_D} = \overline{u}\} , \tag{6.8}$$

$$\mathscr{V}_\varepsilon := \{\varphi \in H^1(\Omega_\varepsilon) : \varphi_{|\Gamma_D} = 0\} . \tag{6.9}$$

See details in fig. 6.2. The *strong equation* associated to the variational problem (6.7) reads:

$$\begin{cases} \text{Find}\, u_\varepsilon, \text{ such that} \\ -\Delta u_\varepsilon = 0 \text{ in } \Omega_\varepsilon , \\ u_\varepsilon = \overline{u} \text{ on } \Gamma_D , \\ -\partial_n u_\varepsilon = \overline{q} \text{ on } \Gamma_N , \\ -\partial_n u_\varepsilon = 0 \text{ on } \partial B_\varepsilon . \end{cases} \tag{6.10}$$

Now, we need to introduce the adjoint state v_ε. In this particular case, v_ε is the solution to the adjoint equation of the form:

$$\begin{cases} \text{Find}\, v_\varepsilon \in \mathscr{V}_\varepsilon, \text{ such that} \\ \displaystyle\int_{\Omega_\varepsilon} \nabla v_\varepsilon \cdot \nabla \eta = -\langle D_u \mathscr{J}_{\Omega_\varepsilon}(u), \eta\rangle \\ \displaystyle\qquad = -\int_{\Omega_\varepsilon} B\nabla u \cdot \nabla \eta \quad \forall \eta \in \mathscr{V}_\varepsilon . \end{cases} \tag{6.11}$$

The strong equation associated to the variational problem (6.11) reads:

$$\begin{cases} \text{Find}\, v_\varepsilon, \text{ such that} \\ -\Delta v_\varepsilon = \operatorname{div}(B\nabla u) \text{ in } \Omega_\varepsilon , \\ v_\varepsilon = 0 \quad \text{on } \Gamma_D , \\ -\partial_n v_\varepsilon = B\nabla u \cdot n \quad \text{on } \Gamma_N , \\ -\partial_n v_\varepsilon = B\nabla u \cdot n \quad \text{on } \partial B_\varepsilon . \end{cases} \tag{6.12}$$

It means that with this construction, the right hand side of the adjoint equation does not depend on the parameter ε through the function u_ε. This feature will simplify the asymptotic analysis of the adjoint state v_ε. Finally, the adjoint state associated to the unperturbed domain is given by taking $\varepsilon = 0$ in (6.11), namely, v is the solution to the adjoint equation of the form:

$$\left\{\begin{array}{l} \text{Find}\, v \in \mathscr{V}, \text{ such that} \\ \displaystyle\int_\Omega \nabla v \cdot \nabla \eta = -\langle D_u \mathscr{J}_\Omega(u), \eta\rangle \\ \qquad\qquad\qquad \displaystyle = -\int_\Omega B\nabla u \cdot \nabla \eta \quad \forall \eta \in \mathscr{V} \ . \end{array}\right. \tag{6.13}$$

The strong equation associated to the variational problem (6.11) reads:

$$\left\{\begin{array}{l} \text{Find}\, v, \text{ such that} \\ \begin{array}{rcll} -\Delta v &=& \operatorname{div}(B\nabla u) & \text{in } \Omega \ , \\ v &=& 0 & \text{on } \Gamma_D \ , \\ -\partial_n v &=& B\nabla u \cdot n & \text{on } \Gamma_N \ . \end{array} \end{array}\right. \tag{6.14}$$

6.2 Shape Sensitivity Analysis

The next step consists in evaluating the shape derivative of functional $\mathscr{J}_{\Omega_\varepsilon}(u_\varepsilon)$ with respect to an uniform expansion of the hole B_ε. Therefore, let us start by introducing the following generalization of the classical *Eshelby energy-momentum tensor* [57]

$$\Sigma_\varepsilon = \frac{1}{2}(B\nabla u_\varepsilon \cdot \nabla u_\varepsilon + 2\nabla u_\varepsilon \cdot \nabla v_\varepsilon)\mathrm{I} - \\ (\nabla u_\varepsilon \otimes B\nabla u_\varepsilon + \nabla u_\varepsilon \otimes \nabla v_\varepsilon + \nabla v_\varepsilon \otimes \nabla u_\varepsilon) \ . \tag{6.15}$$

Thus, the following result holds true:

Proposition 6.1. *Let $\mathscr{J}_{\Omega_\varepsilon}(u_\varepsilon)$ be the shape functional defined by (6.6). Then, the derivative of $\mathscr{J}_{\Omega_\varepsilon}(u_\varepsilon)$ with respect to the small parameter ε is given by*

$$\dot{\mathscr{J}}_{\Omega_\varepsilon}(u_\varepsilon) = \int_{\Omega_\varepsilon} \Sigma_\varepsilon \cdot \nabla \mathfrak{V} + \int_{\Omega_\varepsilon} B\nabla(u_\varepsilon - u) \cdot \nabla \dot{u}_\varepsilon \ , \tag{6.16}$$

where $\mathfrak{V}$ is the shape change velocity field defined through (4.2) and Σ_ε is given by (6.15).

Proof. By making use of the Reynolds' transport theorem given by the result (2.84) and the concept of material derivative of spatial fields through formula (2.89), the derivative with respect to ε of the shape functional (6.6)

$$\dot{\mathscr{J}}_{\Omega_\varepsilon}(u_\varepsilon) = \frac{1}{2}\left(\int_{\Omega_\varepsilon} B\nabla u_\varepsilon \cdot \nabla u_\varepsilon\right)^{\cdot} \tag{6.17}$$

is given by

$$\dot{\mathscr{J}}_{\Omega_\varepsilon}(u_\varepsilon) = \int_{\Omega_\varepsilon} B\nabla u \cdot \nabla \dot{u}_\varepsilon + \int_{\Omega_\varepsilon} B\nabla (u_\varepsilon - u) \cdot \nabla \dot{u}_\varepsilon + \frac{1}{2}\int_{\Omega_\varepsilon} ((B\nabla u_\varepsilon \cdot \nabla u_\varepsilon)\mathrm{I} - 2\nabla u_\varepsilon \otimes B\nabla u_\varepsilon) \cdot \nabla \mathfrak{V} \,. \tag{6.18}$$

Now, let us differentiate both sides of the state equation (6.7) with respect to ε, which leads to

$$\int_{\Omega_\varepsilon} \nabla \dot{u}_\varepsilon \cdot \nabla \eta = -\int_{\Omega_\varepsilon} ((\nabla u_\varepsilon \cdot \nabla \eta)\mathrm{I} - \nabla u_\varepsilon \otimes \nabla \eta - \nabla \eta \otimes \nabla u_\varepsilon) \cdot \nabla \mathfrak{V} \,. \tag{6.19}$$

Since $\dot{u}_\varepsilon$ is a variation of u_ε in the direction of the velocity field $\mathfrak{V}$, then $\dot{u}_\varepsilon \in \mathscr{V}_\varepsilon$ [210]. In addition, the modified adjoint state $v_\varepsilon \in \mathscr{V}_\varepsilon$. Thus, let us respectively take $\eta = v_\varepsilon$ in the above equation and $\eta = \dot{u}_\varepsilon$ in the modified adjoint equation (6.11), which leads to

$$\int_{\Omega_\varepsilon} \nabla v_\varepsilon \cdot \nabla \dot{u}_\varepsilon = -\int_{\Omega_\varepsilon} B\nabla u \cdot \nabla \dot{u}_\varepsilon \tag{6.20}$$

and

$$\int_{\Omega_\varepsilon} \nabla \dot{u}_\varepsilon \cdot \nabla v_\varepsilon = -\int_{\Omega_\varepsilon} ((\nabla u_\varepsilon \cdot \nabla v_\varepsilon) - \nabla u_\varepsilon \otimes \nabla v_\varepsilon - \nabla v_\varepsilon \otimes \nabla u_\varepsilon) \cdot \nabla \mathfrak{V} . \tag{6.21}$$

Due the symmetry of the bilinear forms on the left hand sides of both equations, we have

$$\int_{\Omega_\varepsilon} B\nabla u \cdot \nabla \dot{u}_\varepsilon = \int_{\Omega_\varepsilon} ((\nabla u_\varepsilon \cdot \nabla v_\varepsilon)\mathrm{I} - \nabla u_\varepsilon \otimes \nabla v_\varepsilon - \nabla v_\varepsilon \otimes \nabla u_\varepsilon) \cdot \nabla \mathfrak{V} \,. \tag{6.22}$$

From this last equation we obtain

$$\dot{\mathscr{J}}_{\Omega_\varepsilon}(u_\varepsilon) = \frac{1}{2}\int_{\Omega_\varepsilon} [(B\nabla u_\varepsilon \cdot \nabla u_\varepsilon + 2\nabla u_\varepsilon \cdot \nabla v_\varepsilon)\mathrm{I} - 2(\nabla u_\varepsilon \otimes B\nabla u_\varepsilon + \nabla u_\varepsilon \otimes \nabla v_\varepsilon + \nabla v_\varepsilon \otimes \nabla u_\varepsilon)] \cdot \nabla \mathfrak{V} + \int_{\Omega_\varepsilon} B\nabla (u_\varepsilon - u) \cdot \nabla \dot{u}_\varepsilon \,, \tag{6.23}$$

which leads to the result. □

Proposition 6.2. *Let $\mathscr{J}_{\Omega_\varepsilon}(u_\varepsilon)$ be the shape functional defined by (6.6). Then, its derivative with respect to the small parameter ε is given by*

$$\dot{\mathscr{J}}_{\Omega_\varepsilon}(u_\varepsilon) = \int_{\partial\Omega_\varepsilon} \Sigma_\varepsilon n \cdot \mathfrak{V} + \int_{\Omega_\varepsilon} \mathrm{div}(B\nabla (u_\varepsilon - u))\nabla u_\varepsilon \cdot \mathfrak{V} + \int_{\Omega_\varepsilon} B\nabla (u_\varepsilon - u) \cdot \nabla \dot{u}_\varepsilon \,, \tag{6.24}$$

where $\mathfrak{V}$ is the shape change velocity field defined through (4.2) and tensor Σ_ε is given by (6.15).

Proof. Before starting, let us recall the relation between material and spatial derivatives of scalar fields (2.82), namely $\dot{\varphi} = \varphi' + \nabla\varphi \cdot \mathfrak{V}$. By making use of the other version of the Reynolds' transport theorem given by formula (2.85), the shape derivative of the functional (6.6) results in

$$\dot{\mathscr{J}}_{\Omega_\varepsilon}(u_\varepsilon) = \frac{1}{2}\left(\int_{\Omega_\varepsilon} B\nabla u_\varepsilon \cdot \nabla u_\varepsilon\right)^{\cdot} = \int_{\Omega_\varepsilon} B\nabla u_\varepsilon \cdot \nabla u_\varepsilon' + \frac{1}{2}\int_{\partial\Omega_\varepsilon} (B\nabla u_\varepsilon \cdot \nabla u_\varepsilon) n \cdot \mathfrak{V} \,. \tag{6.25}$$

In addition, we have

$$\dot{\mathscr{J}}_{\Omega_\varepsilon}(u_\varepsilon) = \int_{\Omega_\varepsilon} B\nabla u_\varepsilon \cdot \nabla \dot{u}_\varepsilon - \int_{\Omega_\varepsilon} B\nabla u_\varepsilon \cdot \nabla(\nabla u_\varepsilon \cdot \mathfrak{V}) + \frac{1}{2}\int_{\partial\Omega_\varepsilon} (B\nabla u_\varepsilon \cdot \nabla u_\varepsilon) n \cdot \mathfrak{V} \,. \tag{6.26}$$

From integration by parts, we obtain

$$\begin{aligned}\dot{\mathscr{J}}_{\Omega_\varepsilon}(u_\varepsilon) = &\int_{\Omega_\varepsilon} B\nabla u \cdot \nabla \dot{u}_\varepsilon + \int_{\Omega_\varepsilon} B\nabla (u_\varepsilon - u) \cdot \nabla \dot{u}_\varepsilon \\ &+ \int_{\Omega_\varepsilon} \operatorname{div}(B\nabla u_\varepsilon)\nabla u_\varepsilon \cdot \mathfrak{V} - \int_{\partial\Omega_\varepsilon} (\nabla u_\varepsilon \cdot \mathfrak{V}) B\nabla u_\varepsilon \cdot n \\ &+ \frac{1}{2}\int_{\partial\Omega_\varepsilon} (B\nabla u_\varepsilon \cdot \nabla u_\varepsilon) n \cdot \mathfrak{V} \,,\end{aligned} \tag{6.27}$$

and after some rearrangements

$$\begin{aligned}\dot{\mathscr{J}}_{\Omega_\varepsilon}(u_\varepsilon) = &\int_{\Omega_\varepsilon} B\nabla u \cdot \nabla \dot{u}_\varepsilon + \int_{\Omega_\varepsilon} B\nabla (u_\varepsilon - u) \cdot \nabla \dot{u}_\varepsilon \\ &+ \frac{1}{2}\int_{\partial\Omega_\varepsilon} ((B\nabla u_\varepsilon \cdot \nabla u_\varepsilon)\mathrm{I} - 2\nabla u_\varepsilon \otimes B\nabla u_\varepsilon) n \cdot \mathfrak{V} \\ &+ \int_{\Omega_\varepsilon} \operatorname{div}(B\nabla (u_\varepsilon - u))\nabla u_\varepsilon \cdot \mathfrak{V} + \int_{\Omega_\varepsilon} \operatorname{div}(B\nabla u)\nabla u_\varepsilon \cdot \mathfrak{V} \,.\end{aligned} \tag{6.28}$$

Now, let us differentiate both sides of the state equation (6.7) with respect to ε, which leads to

$$\int_{\Omega_\varepsilon} (\nabla u_\varepsilon \cdot \nabla \eta)' = -\int_{\partial\Omega_\varepsilon} (\nabla u_\varepsilon \cdot \nabla \eta) n \cdot \mathfrak{V} \,. \tag{6.29}$$

From the tensor relation (G.20)

$$\begin{aligned}\int_{\Omega_\varepsilon}(\nabla u_\varepsilon\cdot\nabla\eta)' &= \int_{\Omega_\varepsilon}(\nabla u_\varepsilon\cdot\nabla\eta)^{\cdot} - \int_{\Omega_\varepsilon}\nabla(\nabla u_\varepsilon\cdot\nabla\eta)\cdot\mathfrak{V}\\ &= \int_{\Omega_\varepsilon}\nabla\dot{u}_\varepsilon\cdot\nabla\eta - \int_{\Omega_\varepsilon}(\nabla\mathfrak{V}^\top\nabla u_\varepsilon\cdot\nabla\eta + \nabla\mathfrak{V}^\top\nabla\eta\cdot\nabla u_\varepsilon)\\ &\quad - \int_{\Omega_\varepsilon}((\nabla\nabla u_\varepsilon)^\top\nabla\eta\cdot\mathfrak{V} + (\nabla\nabla\eta)^\top\nabla u_\varepsilon\cdot\mathfrak{V})\,. \end{aligned} \tag{6.30}$$

After some rearrangements, we obtain

$$\begin{aligned}\int_{\Omega_\varepsilon}(\nabla u_\varepsilon\cdot\nabla\eta)' &= \int_{\Omega_\varepsilon}\nabla\dot{u}_\varepsilon\cdot\nabla\eta \qquad (6.31)\\ &\quad - \int_{\Omega_\varepsilon}((\nabla\nabla u_\varepsilon)\mathfrak{V}\cdot\nabla\eta + \nabla\mathfrak{V}^\top\nabla u_\varepsilon\cdot\nabla\eta)\\ &\quad - \int_{\Omega_\varepsilon}((\nabla\nabla\eta)\mathfrak{V}\cdot\nabla u_\varepsilon + \nabla\mathfrak{V}^\top\nabla\eta\cdot\nabla u_\varepsilon)\\ &= \int_{\Omega_\varepsilon}\nabla\dot{u}_\varepsilon\cdot\nabla\eta - \int_{\Omega_\varepsilon}\nabla(\nabla u_\varepsilon\cdot\mathfrak{V})\cdot\nabla\eta - \int_{\Omega_\varepsilon}\nabla(\nabla\eta\cdot\mathfrak{V})\cdot\nabla u_\varepsilon\,, \end{aligned}$$

where we have taken into account that $\nabla\nabla\varphi = (\nabla\nabla\varphi)^\top$. Therefore, we have

$$\begin{aligned}\int_{\Omega_\varepsilon}\nabla\dot{u}_\varepsilon\cdot\nabla\eta &= -\int_{\partial\Omega_\varepsilon}(\nabla u_\varepsilon\cdot\nabla\eta)n\cdot\mathfrak{V}\\ &\quad + \int_{\Omega_\varepsilon}\nabla\eta\cdot\nabla(\nabla u_\varepsilon\cdot\mathfrak{V}) + \int_{\Omega_\varepsilon}\nabla u_\varepsilon\cdot\nabla(\nabla\eta\cdot\mathfrak{V})\,. \end{aligned} \tag{6.32}$$

Since $\dot{u}_\varepsilon \in \mathscr{V}_\varepsilon$ and the modified adjoint state $v_\varepsilon \in \mathscr{V}_\varepsilon$, then we can take $\eta = v_\varepsilon$ in the above equation and $\eta = \dot{u}_\varepsilon$ in the modified adjoint equation (6.11), leading to

$$\int_{\Omega_\varepsilon}\nabla v_\varepsilon\cdot\nabla\dot{u}_\varepsilon = -\int_{\Omega_\varepsilon}B\nabla u\cdot\nabla\dot{u}_\varepsilon \tag{6.33}$$

and

$$\begin{aligned}\int_{\Omega_\varepsilon}\nabla\dot{u}_\varepsilon\cdot\nabla v_\varepsilon &= -\int_{\partial\Omega_\varepsilon}(\nabla u_\varepsilon\cdot\nabla v_\varepsilon)n\cdot\mathfrak{V}\\ &\quad + \int_{\Omega_\varepsilon}\nabla v_\varepsilon\cdot\nabla(\nabla u_\varepsilon\cdot\mathfrak{V}) + \int_{\Omega_\varepsilon}\nabla u_\varepsilon\cdot\nabla(\nabla v_\varepsilon\cdot\mathfrak{V})\,. \end{aligned} \tag{6.34}$$

By symmetry of the above bilinear forms, we have

$$\begin{aligned}\int_{\Omega_\varepsilon}B\nabla u\cdot\nabla\dot{u}_\varepsilon &= \int_{\partial\Omega_\varepsilon}(\nabla u_\varepsilon\cdot\nabla v_\varepsilon)n\cdot\mathfrak{V}\\ &\quad - \int_{\Omega_\varepsilon}\nabla v_\varepsilon\cdot\nabla(\nabla u_\varepsilon\cdot\mathfrak{V}) - \int_{\Omega_\varepsilon}\nabla u_\varepsilon\cdot\nabla(\nabla v_\varepsilon\cdot\mathfrak{V})\,. \end{aligned} \tag{6.35}$$

From integration by parts and some rearrangements, we obtain

$$\begin{aligned}\int_{\Omega_\varepsilon} B\nabla u\cdot\nabla\dot{u}_\varepsilon = &-\int_{\partial\Omega_\varepsilon}(\nabla u_\varepsilon\otimes\nabla v_\varepsilon)n\cdot\mathfrak{V}-\int_{\partial\Omega_\varepsilon}(\nabla v_\varepsilon\otimes\nabla u_\varepsilon)n\cdot\mathfrak{V}\\ &+\int_{\Omega_\varepsilon}\operatorname{div}(\nabla v_\varepsilon)\nabla u_\varepsilon\cdot\mathfrak{V}+\int_{\Omega_\varepsilon}\operatorname{div}(\nabla u_\varepsilon)\nabla v_\varepsilon\cdot\mathfrak{V}\\ &+\int_{\partial\Omega_\varepsilon}(\nabla u_\varepsilon\cdot\nabla v_\varepsilon)n\cdot\mathfrak{V}\,. \end{aligned}\tag{6.36}$$

After considering this last result, we obtain

$$\begin{aligned}\dot{\mathscr{J}}_{\Omega_\varepsilon}(u_\varepsilon) = &\int_{\partial\Omega_\varepsilon}\Sigma_\varepsilon n\cdot\mathfrak{V}\\ &+\int_{\Omega_\varepsilon}\operatorname{div}(B\nabla(u_\varepsilon-u))\nabla u_\varepsilon\cdot\mathfrak{V}+\int_{\Omega_\varepsilon}B\nabla(u_\varepsilon-u)\cdot\nabla\dot{u}_\varepsilon\\ &+\int_{\Omega_\varepsilon}(\Delta v_\varepsilon+\operatorname{div}(B\nabla u))\nabla u_\varepsilon\cdot\mathfrak{V}+\int_{\Omega_\varepsilon}(\Delta u_\varepsilon)\nabla v_\varepsilon\cdot\mathfrak{V}\,. \end{aligned}\tag{6.37}$$

Finally, taking into account that u_ε is the solution to the state equation (6.10) and that v_ε is the solution to the modified adjoint equation (6.12), namely, $-\Delta u_\varepsilon = 0$ and $-\Delta v_\varepsilon = \operatorname{div}(B\nabla u)$, respectively, we have that the last two terms in the above equation vanish, which leads to the result. □

Corollary 6.1. *From the tensor relation (G.23) and after applying the divergence theorem (G.32) to the right hand side of (6.16), we obtain*

$$\dot{\mathscr{J}}_{\Omega_\varepsilon}(u_\varepsilon) = \int_{\partial\Omega_\varepsilon}\Sigma_\varepsilon n\cdot\mathfrak{V}-\int_{\Omega_\varepsilon}\operatorname{div}\Sigma_\varepsilon\cdot\mathfrak{V}+\int_{\Omega_\varepsilon}B\nabla(u_\varepsilon-u)\cdot\nabla\dot{u}_\varepsilon\,.\tag{6.38}$$

Since the above equation and (6.24) remain valid for all velocity fields $\mathfrak{V}$, we have that the second term of the above equation must satisfy

$$\int_{\Omega_\varepsilon}(\operatorname{div}\Sigma_\varepsilon+\operatorname{div}(B\nabla(u_\varepsilon-u))\nabla u_\varepsilon)\cdot\mathfrak{V}=0\quad\forall\mathfrak{V}\,,\tag{6.39}$$

which implies

$$-\operatorname{div}\Sigma_\varepsilon=\operatorname{div}(B\nabla(u_\varepsilon-u))\nabla u_\varepsilon\,.\tag{6.40}$$

Corollary 6.2. *According to the obtained result in Proposition 6.2, we have*

$$\begin{aligned}\dot{\mathscr{J}}_{\Omega_\varepsilon}(u_\varepsilon) = &\int_{\partial\Omega_\varepsilon}\Sigma_\varepsilon n\cdot\mathfrak{V}+\int_{\Omega_\varepsilon}\operatorname{div}(B\nabla(u_\varepsilon-u))\nabla u_\varepsilon\cdot\mathfrak{V}\\ &+\int_{\Omega_\varepsilon}B\nabla(u_\varepsilon-u)\cdot\nabla u_\varepsilon'+\int_{\Omega_\varepsilon}B\nabla(u_\varepsilon-u)\cdot\nabla(\nabla u_\varepsilon\cdot\mathfrak{V})\,. \end{aligned}\tag{6.41}$$

Then,

$$\dot{\mathscr{J}}_{\Omega_\varepsilon}(u_\varepsilon) = \int_{\partial\Omega_\varepsilon} \Sigma_\varepsilon n \cdot \mathfrak{V} + \int_{\partial\Omega_\varepsilon} (\nabla u_\varepsilon \cdot \mathfrak{V}) B\nabla(u_\varepsilon - u) \cdot n + \int_{\Omega_\varepsilon} B\nabla(u_\varepsilon - u) \cdot \nabla u'_\varepsilon \,. \qquad (6.42)$$

Since we are dealing with an uniform expansion of the circular hole, then by taking into account the associated velocity field $\mathfrak{V} \in \mathscr{S}_\varepsilon$, with $\mathscr{S}_\varepsilon$ defined in (4.2), namely $\mathfrak{V} = -n$ on ∂B_ε and $\mathfrak{V} = 0$ on $\partial\Omega$, we obtain

$$\frac{d}{d\varepsilon}\psi(\chi_\varepsilon) = \dot{\mathscr{J}}_{\Omega_\varepsilon}(u_\varepsilon) = -\int_{\partial B_\varepsilon} (\Sigma_\varepsilon + \nabla u_\varepsilon \otimes B\nabla(u_\varepsilon - u))n \cdot n + \int_{\Omega_\varepsilon} B\nabla(u_\varepsilon - u) \cdot \nabla u'_\varepsilon \,. \qquad (6.43)$$

Remark 6.2. According to the obtained result in Proposition 6.1, we have

$$\dot{\mathscr{J}}_{\Omega_\varepsilon}(u_\varepsilon) = \int_{\partial\Omega_\varepsilon} \Sigma_\varepsilon n \cdot \mathfrak{V} - \int_{\Omega_\varepsilon} \mathrm{div}\Sigma_\varepsilon \cdot \mathfrak{V} + \int_{\partial\Omega_\varepsilon} (\nabla u_\varepsilon \cdot \mathfrak{V}) B\nabla(u_\varepsilon - u) \cdot n - \int_{\Omega_\varepsilon} \mathrm{div}(B\nabla(u_\varepsilon - u))\nabla u_\varepsilon \cdot \mathfrak{V} + \int_{\Omega_\varepsilon} B\nabla(u_\varepsilon - u) \cdot \nabla u'_\varepsilon \,. \qquad (6.44)$$

From (6.40) and taking into account the velocity field defined through (4.2), namely, $\mathfrak{V} = -n$ on ∂B_ε and $\mathfrak{V} = 0$ on $\partial\Omega$, we obtain (6.43).

6.3 Asymptotic Analysis of the Solution

The shape derivative of functional $\mathscr{J}_{\Omega_\varepsilon}(u_\varepsilon)$ is given in terms of an integral over the boundary of the hole ∂B_ε and also in terms of a domain integral associated to u'_ε (6.43). This domain integral comes out from the introduction of the modified adjoint state, solution to (6.11). Therefore, in order to apply the result of Proposition 1.1, we need to know the behavior of the functions u_ε and v_ε with respect to ε. In particular, once we know these behaviors explicitly, we can identify function $f(\varepsilon)$ and perform the limit passage $\varepsilon \to 0$ in (1.49) to obtain the final formula for the topological derivative $\mathscr{T}$ of the shape functional ψ. Therefore, we need to perform an asymptotic analysis of u_ε and v_ε with respect to ε. In this section we present the formal calculation of the expansions of the solutions u_ε and v_ε associated to homogeneous Neumann boundary condition on the hole. For a rigorous justification of the asymptotic expansions of u_ε and v_ε, the reader may refer to [120, 148], for instance.

6.3.1 Asymptotic Expansion of the Direct State

Let us propose an *ansätz* for the expansion of u_ε in the form [120]

$$\begin{aligned} u_\varepsilon(x) &= u(x) + w_\varepsilon(x) + \widetilde{u}_\varepsilon(x) \\ &= u(\widehat{x}) + \nabla u(\widehat{x}) \cdot (x - \widehat{x}) + \frac{1}{2} \nabla\nabla u(y)(x - \widehat{x}) \cdot (x - \widehat{x}) \\ &+ w_\varepsilon(x) + \widetilde{u}_\varepsilon(x) , \end{aligned} \tag{6.45}$$

where y is an intermediate point between x and $\widehat{x}$. On the boundary of the hole ∂B_ε we have $\partial_n u_\varepsilon = 0$. Thus, the normal derivative of the above expansion, evaluated on ∂B_ε, leads to

$$\nabla u(\widehat{x}) \cdot n - \varepsilon \nabla\nabla u(y) n \cdot n + \partial_n w_\varepsilon(x) + \partial_n \widetilde{u}_\varepsilon(x) = 0 . \tag{6.46}$$

In particular, we can choose w_ε such that

$$\partial_n w_\varepsilon(x) = -\nabla u(\widehat{x}) \cdot n \quad \text{on} \quad \partial B_\varepsilon . \tag{6.47}$$

Now, the following exterior problem is considered, and formally obtained as $\varepsilon \to 0$:

$$\begin{cases} \text{Find } w_\varepsilon, \text{ such that} \\ \Delta w_\varepsilon = 0 & \text{in } \mathbb{R}^2 \setminus \overline{B_\varepsilon} , \\ w_\varepsilon \to 0 & \text{at } \infty , \\ \partial_n w_\varepsilon = -\nabla u(\widehat{x}) \cdot n & \text{on } \partial B_\varepsilon . \end{cases} \tag{6.48}$$

The above boundary value problem admits an explicit solution, namely

$$w_\varepsilon(x) = \frac{\varepsilon^2}{\|x - \widehat{x}\|^2} \nabla u(\widehat{x}) \cdot (x - \widehat{x}) . \tag{6.49}$$

Now we can construct $\widetilde{u}_\varepsilon$ in such a way that it compensates the discrepancies introduced by the higher-order terms in ε as well as by the boundary-layer w_ε on the exterior boundary $\partial\Omega$. It means that the remainder $\widetilde{u}_\varepsilon$ must be solution to the following boundary value problem:

$$\begin{cases} \text{Find } \widetilde{u}_\varepsilon, \text{ such that} \\ \Delta \widetilde{u}_\varepsilon = 0 & \text{in } \Omega_\varepsilon , \\ \widetilde{u}_\varepsilon = -w_\varepsilon & \text{on } \Gamma_D , \\ \partial_n \widetilde{u}_\varepsilon = -\partial_n w_\varepsilon & \text{on } \Gamma_N , \\ \partial_n \widetilde{u}_\varepsilon = \varepsilon \nabla\nabla u(y) n \cdot n & \text{on } \partial B_\varepsilon . \end{cases} \tag{6.50}$$

Clearly $\widetilde{u}_\varepsilon = O(\varepsilon)$, since $w_\varepsilon = O(\varepsilon^2)$ on the exterior boundary $\partial\Omega$. However, this estimate can be improved [120, 148]. In fact, analogously to the Section 4.1, we have $\widetilde{u}_\varepsilon = O(\varepsilon^2)$. Finally, the *expansion* for u_ε reads

$$u_\varepsilon(x) = u(x) + \frac{\varepsilon^2}{\|x-\widehat{x}\|^2}\nabla u(\widehat{x}) \cdot (x-\widehat{x}) + O(\varepsilon^2)\ . \tag{6.51}$$

6.3.2 Asymptotic Expansion of the Adjoint State

Analogously to the asymptotic expansion of the direct state u_ε, let us propose an *ansätz* for the expansion of v_ε in the form [120]

$$\begin{aligned} v_\varepsilon(x) &= v(x) + w_\varepsilon(x) + \widetilde{v}_\varepsilon(x) \\ &= v(\widehat{x}) + \nabla v(\widehat{x}) \cdot (x-\widehat{x}) + \frac{1}{2}\nabla\nabla v(y)(x-\widehat{x}) \cdot (x-\widehat{x}) \\ &+ w_\varepsilon(x) + \widetilde{v}_\varepsilon(x)\ , \end{aligned} \tag{6.52}$$

where y is an intermediate point between x and $\widehat{x}$. On the boundary of the hole ∂B_ε we have $\partial_n v_\varepsilon = -B\nabla u \cdot n$. Thus, the normal derivative of the above expansion, evaluated on ∂B_ε, leads to

$$\nabla v(\widehat{x}) \cdot n - \varepsilon \nabla\nabla v(y) n \cdot n + \partial_n w_\varepsilon(x) + \partial_n \widetilde{v}_\varepsilon(x) = -B\nabla u \cdot n\ . \tag{6.53}$$

In particular, we can choose w_ε such that

$$\partial_n w_\varepsilon(x) = -(\nabla v(\widehat{x}) + B\nabla u(\widehat{x})) \cdot n \quad \text{on} \quad \partial B_\varepsilon\ , \tag{6.54}$$

where we have expanded $B\nabla u(x)$ in Taylor's series around the center $\widehat{x}$ of the hole. Note that from the construction of the adjoint state we have

$$-\Delta v_\varepsilon = \operatorname{div}(B\nabla u) \quad \text{in} \quad \Omega_\varepsilon \quad \text{and} \quad -\Delta v = \operatorname{div}(B\nabla u) \quad \text{in} \quad \Omega\ . \tag{6.55}$$

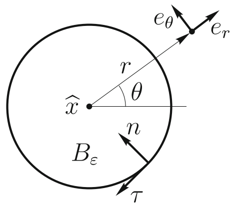
In addition, $v_\varepsilon = v = 0$ on Γ_D and $\partial_n v_\varepsilon = \partial_n v = -B\nabla u \cdot n$ on Γ_N. It means that both boundary value problems associated to v_ε and v have the same source-term and boundary data, except, of course, on the boundary of the hole ∂B_ε. In particular, the boundary condition $\partial_n v_\varepsilon = -B\nabla u \cdot n$ on ∂B_ε does not depend on the parameter ε through the solution u_ε. Now, the following exterior problem is considered, and formally obtained with $\varepsilon \to 0$:

$$\left\{ \begin{array}{lll} \text{Find}\, w_\varepsilon, \text{ such that} & & \\ \Delta w_\varepsilon &= 0 & \text{in } \mathbb{R}^2 \setminus \overline{B_\varepsilon}\ , \\ w_\varepsilon &\to 0 & \text{at } \infty\ , \\ \partial_n w_\varepsilon &= -(\nabla v(\widehat{x}) + B\nabla u(\widehat{x})) \cdot n & \text{on } \partial B_\varepsilon\ . \end{array} \right. \tag{6.56}$$

The above boundary value problem admits an explicit solution given by

$$w_\varepsilon(x) = \frac{\varepsilon^2}{\|x-\widehat{x}\|^2}(\nabla v(\widehat{x}) + B\nabla u(\widehat{x})) \cdot (x-\widehat{x})\ . \tag{6.57}$$

Fig. 6.3 Polar coordinate system (r,θ) centered at the point $\widehat{x} \in \Omega$



Now we can construct $\widetilde{v}_\varepsilon$ in such a way that it compensates the discrepancies introduced by the higher-order terms in ε as well as by the boundary-layer w_ε on the exterior boundary $\partial\Omega$. It means that the remainder $\widetilde{v}_\varepsilon$ must be solution to the following boundary value problem:

$$\begin{cases} \text{Find}\,\widetilde{v}_\varepsilon, \text{ such that} \\ \Delta\widetilde{v}_\varepsilon = 0 & \text{in } \Omega_\varepsilon\ , \\ \widetilde{v}_\varepsilon = -w_\varepsilon & \text{on } \Gamma_D\ , \\ \partial_n\widetilde{v}_\varepsilon = -\partial_n w_\varepsilon & \text{on } \Gamma_N\ , \\ \partial_n\widetilde{v}_\varepsilon = \varepsilon(\nabla\nabla v(y)n + B\nabla\nabla u(z)n)\cdot n & \text{on } \partial B_\varepsilon\ , \end{cases} \tag{6.58}$$

where z is an intermediate point between x and $\widehat{x}$. Once again, we clearly have $\widetilde{v}_\varepsilon = O(\varepsilon)$, since $w_\varepsilon = O(\varepsilon^2)$ on the exterior boundary $\partial\Omega$. However, this estimate can be improved. In fact, according to [120, 148], we have $\widetilde{v}_\varepsilon = O(\varepsilon^2)$. Finally, the *expansion* for v_ε reads

$$v_\varepsilon(x) = v(x) + \frac{\varepsilon^2}{\|x-\widehat{x}\|^2}(\nabla u(\widehat{x}) + B\nabla u(\widehat{x}))\cdot(x-\widehat{x}) + O(\varepsilon^2)\ . \tag{6.59}$$

6.4 Topological Derivative Evaluation

Now, we need to evaluate the integrals in formula (6.43) to collect the terms in power of ε and recognize function $f(\varepsilon)$. With these results, we can perform the limit passage $\varepsilon \to 0$. The integrals in (6.43) can be evaluated in the same way as shown in Section 4.1 by using the expansions for the direct u_ε and adjoint v_ε states, respectively given by (6.51) and (6.59). The idea is to introduce a polar coordinate system (r,θ) with center at $\widehat{x}$ (see fig. 6.3). Then, we can write u_ε, v_ε and also the tensor B in this coordinate system, and evaluate the integrals explicitly. In particular, the first integral in (6.43) leads to

$$\int_{\partial B_\varepsilon}(\Sigma_\varepsilon + \nabla u_\varepsilon \otimes B\nabla(u_\varepsilon - u))n\cdot n = \tag{6.60}$$
$$2\pi\varepsilon\left(2\nabla u(\widehat{x})\cdot\nabla v(\widehat{x}) + \frac{3}{2}B\nabla u(\widehat{x})\cdot\nabla u(\widehat{x}) + \frac{1}{4}\mathrm{tr}(B)\|\nabla u(\widehat{x})\|^2\right) + o(\varepsilon)\ .$$

The second integral in (6.43) becomes

$$\int_{\Omega_\varepsilon} B\nabla(u_\varepsilon - u)\cdot\nabla u'_\varepsilon = 2\pi\varepsilon\left(\frac{1}{2}\mathrm{tr}(B)\|\nabla u(\widehat{x})\|^2\right) + o(\varepsilon)\,, \tag{6.61}$$

where u'_ε is obtained simply by calculating the derivative of u_ε in (6.51) with respect to ε. Finally, the topological derivative given by (1.49) leads to

$$\mathscr{T}(\widehat{x}) = -\lim_{\varepsilon\to 0}\frac{1}{f'(\varepsilon)}\left(2\pi\varepsilon g(\widehat{x}) + o(\varepsilon)\right)\,. \tag{6.62}$$

Now, in order to extract the leading term of the above expansion, we choose

$$f(\varepsilon) = \pi\varepsilon^2\,, \tag{6.63}$$

which leads to the final formula for the *topological derivative*, with $\mathscr{T}(\widehat{x}) = -g(\widehat{x})$

$$\mathscr{T}(\widehat{x}) = -2\nabla u(\widehat{x})\cdot\nabla v(\widehat{x}) - \frac{3}{2}B\nabla u(\widehat{x})\cdot\nabla u(\widehat{x}) + \frac{1}{4}\mathrm{tr}(B)\|\nabla u(\widehat{x})\|^2\,. \tag{6.64}$$

Remark 6.3. We observe that for $B = \mathrm{I}$ we have the energy shape functional. In this case, the adjoint state reads $v = -(u+\varphi)$, where φ is the lifting of the Dirichlet boundary data $\overline{u}$ on Γ_D. Since we can construct φ such that $\widehat{x}\notin\mathrm{supp}(\varphi)$, then the topological derivative becomes

$$\mathscr{T}(\widehat{x}) = \|\nabla u(\widehat{x})\|^2\,, \tag{6.65}$$

which corroborates with the obtained formula (4.54) with $b = 0$, since the total potential energy has the opposite sign with respect to the energy.

6.5 Exercises

1. Derive expressions (6.60) and (6.61).
2. Repeat the development presented in this Chapter by taking into account the following shape functional

$$\psi(\chi) := \mathscr{J}_\Omega(u) = \frac{1}{2}\int_\Omega \mathbb{B}\sigma(u) \cdot \nabla u^s ,$$

where $\mathbb{B} = \beta_1 \mathbb{I} + \beta_2 \mathrm{I} \otimes \mathrm{I}$ is a fourth order isotropic tensor, with β_1 and β_2 used to denote given parameters. In addition, the vector function u is the solution to the following boundary value problem (see Section 4.2):

$$\begin{cases} \text{Find } u, \text{ such that} \\ -\mathrm{div}\sigma(u) = 0 \quad \text{in } \Omega , \\ \sigma(u) = \mathbb{C}\nabla u^s , \\ u = \overline{u} \quad \text{on } \Gamma_D , \\ \sigma(u)n = \overline{q} \quad \text{on } \Gamma_N . \end{cases}$$

3. Repeat the development presented in this Chapter by taking into account the following shape functional

$$\psi(\chi) := \mathscr{J}_\Omega(u) = -\frac{1}{2}\int_\Omega \mathbb{B}M(u) \cdot \nabla\nabla u ,$$

with $\mathbb{B} = \beta_1 \mathbb{I} + \beta_2 \mathrm{I} \otimes \mathrm{I}$ used to denote a fourth order isotropic tensor, where β_1 and β_2 are given parameters. In addition, the scalar function u is the solution to the following boundary value problem (see Section 4.3):

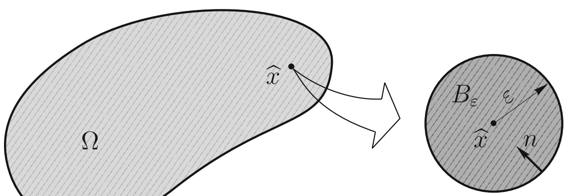
$$\begin{cases} \text{Find } u, \text{ such that} \\ \mathrm{div}(\mathrm{div}M(u)) = 0 \quad \text{in } \Omega , \\ M(u) = -\mathbb{C}\nabla\nabla u , \\ u = \overline{u} \quad \text{on } \Gamma_{D_u} , \\ \partial_n u = \overline{\rho} \quad \text{on } \Gamma_{D_\rho} , \\ M^{nn}(u) = \overline{m} \quad \text{on } \Gamma_{N_m} , \\ \partial_\tau M^{\tau n}(u) + \mathrm{div}M(u) \cdot n = \overline{q} \quad \text{on } \Gamma_{N_q} , \\ [\![M^{\tau n}(u(x_i))]\!] = \overline{Q}_i \quad \text{on } x_i \in \Gamma_{N_q} . \end{cases}$$

Chapter 7
Topological Derivative for Steady-State Orthotropic Heat Diffusion Problems

The topological derivative associated with the nucleation of a hole in the domain characterized by an orthotropic material was calculated in [204]. In order to simplify the analysis the domain was perturbed by introducing a specific elliptical hole, instead of a circular hole. The elliptical hole was oriented in the directions of the orthotropy and the semi-axis of the ellipse were proportional to the material properties coefficients in each orthogonal direction.

In this chapter, this result of [204] is extended to the configurational domain perturbations with a contrast parameter for the material properties (see Chapter 5 for the related results on topological derivatives for inclusions). The nucleation of a small circular inclusion is considered with the property that the bulk phase (matrix) is of the same nature as the topological perturbation (see fig. 7.1), hence a contrast parameter is employed for the material properties in our problem.

Therefore, the topological derivative of the total potential energy for the steady-state orthotropic heat diffusion problem in two spatial dimensions is evaluated with respect to the nucleation of a small circular inclusion made of an orthotropic material defined by a contrast parameter with respect to the orthotropic material of the bulk phase.



$$\gamma_\varepsilon(x) := \begin{cases} 1 & \text{if } x \in \Omega \setminus \overline{B_\varepsilon} \\ \gamma & \text{if } x \in B_\varepsilon \end{cases}$$

Fig. 7.1 Topologically perturbed domain by the nucleation of a small circular inclusion of the same nature as the bulk phase

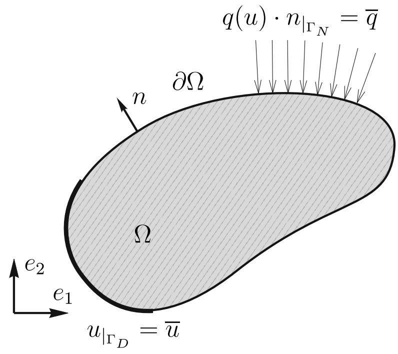


Fig. 7.2 Orthotropic steady-state heat diffusion problem defined in the unperturbed domain

7.1 Problem Formulation

The shape functional in the unperturbed domain Ω is given by

$$\psi(\chi) := \mathscr{J}_\Omega(u) = -\frac{1}{2}\int_\Omega q(u) \cdot \nabla u + \int_{\Gamma_N} \overline{q} u \,, \tag{7.1}$$

where the scalar function u is the solution to the variational problem:

$$\begin{cases} \text{Find}\, u \in \mathscr{U}, \text{ such that} \\ \displaystyle\int_\Omega q(u) \cdot \nabla \eta = \int_{\Gamma_N} \overline{q}\eta \quad \forall \eta \in \mathscr{V} \,, \\ \qquad\qquad \text{with} \quad q(u) = -K\nabla u \,. \end{cases} \tag{7.2}$$

In the above equation, K is the symmetric second order thermal conductivity tensor with eigenvalues k_1 and k_2, respectively associated to the orthogonal directions e_1 and e_2. The set $\mathscr{U}$ and the space $\mathscr{V}$ are respectively defined as

$$\mathscr{U} := \{\varphi \in H^1(\Omega) : \varphi_{|\Gamma_D} = \overline{u}\} \,, \tag{7.3}$$

$$\mathscr{V} := \{\varphi \in H^1(\Omega) : \varphi_{|\Gamma_D} = 0\} \,. \tag{7.4}$$

In addition, $\partial\Omega = \overline{\Gamma}_D \cup \overline{\Gamma}_N$ with $\Gamma_D \cap \Gamma_N = \varnothing$, where Γ_D and Γ_N are Dirichlet and Neumann boundaries, respectively. Thus $\overline{u}$ is a Dirichlet data on Γ_D and $\overline{q}$ is a Neumann data on Γ_N, both assumed to be smooth enough. See the details in fig. 7.2. The strong formulation associated to the variational problem (7.2) reads:

$$\begin{cases} \text{Find}\, u, \text{ such that} \\ \operatorname{div} q(u) = 0 & \text{in } \Omega \,, \\ \quad q(u) = -K\nabla u \,, \\ \qquad u = \overline{u} & \text{on } \Gamma_D \,, \\ q(u) \cdot n = \overline{q} & \text{on } \Gamma_N \,. \end{cases} \tag{7.5}$$

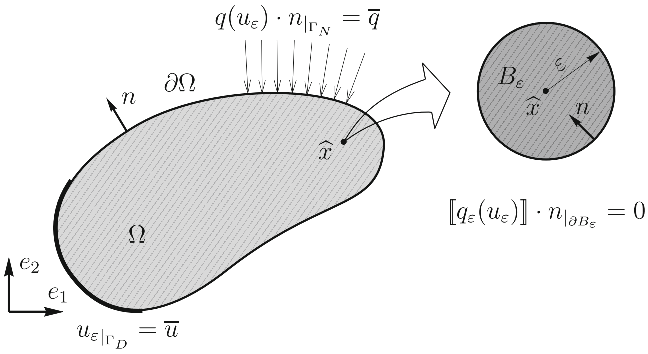


Fig. 7.3 Orthotropic steady-state heat diffusion problem defined in the perturbed domain

Now, let us state the same problem in the perturbed domain. In this case, the total potential energy reads

$$\psi(\chi_\varepsilon) := \mathscr{J}_{\chi_\varepsilon}(u_\varepsilon) = -\frac{1}{2}\int_\Omega q_\varepsilon(u_\varepsilon)\cdot\nabla u_\varepsilon + \int_{\Gamma_N} \overline{q} u_\varepsilon \ , \tag{7.6}$$

where the scalar function u_ε solves the variational problem:

$$\left\{\begin{array}{l} \text{Find } u_\varepsilon \in \mathscr{U}_\varepsilon, \text{ such that} \\ \displaystyle\int_\Omega q_\varepsilon(u_\varepsilon)\cdot\nabla\eta = \int_{\Gamma_N} \overline{q}\eta \quad \forall \eta \in \mathscr{V}_\varepsilon \ , \\ \qquad\qquad \text{with} \quad q_\varepsilon(u_\varepsilon) = -\gamma_\varepsilon K \nabla u_\varepsilon \ , \end{array}\right. \tag{7.7}$$

with γ_ε defined by (5.1). It means that the inclusion has the same nature as the bulk phase, but with a contrast γ. The set $\mathscr{U}_\varepsilon$ and the space $\mathscr{V}_\varepsilon$ are defined as

$$\mathscr{U}_\varepsilon := \{\varphi \in \mathscr{U} : [\![\varphi]\!] = 0 \text{ on } \partial B_\varepsilon\} \ , \tag{7.8}$$

$$\mathscr{V}_\varepsilon := \{\varphi \in \mathscr{V} : [\![\varphi]\!] = 0 \text{ on } \partial B_\varepsilon\} \ , \tag{7.9}$$

where the operator $[\![\varphi]\!]$ is used to denote the jump of function φ on the boundary of the inclusion ∂B_ε, namely, $[\![\varphi]\!] := \varphi_{|_{\Omega\setminus\overline{B_\varepsilon}}} - \varphi_{|_{B_\varepsilon}}$ on ∂B_ε. See the details in fig. 7.3. The *strong formulation* associated to the variational problem (7.7) reads:

$$\left\{\begin{array}{rcll} \multicolumn{4}{l}{\text{Find } u_\varepsilon, \text{ such that}} \\ \operatorname{div} q_\varepsilon(u_\varepsilon) &=& 0 & \text{in } \Omega \ , \\ q_\varepsilon(u_\varepsilon) &=& -\gamma_\varepsilon K \nabla u_\varepsilon \ , & \\ u_\varepsilon &=& \overline{u} & \text{on } \Gamma_D \ , \\ q_\varepsilon(u_\varepsilon)\cdot n &=& \overline{q} & \text{on } \Gamma_N \ , \\ \left.\begin{array}{r} [\![u_\varepsilon]\!] = 0 \\ [\![q_\varepsilon(u_\varepsilon)]\!]\cdot n = 0 \end{array}\right\} & & & \text{on } \partial B_\varepsilon \ . \end{array}\right. \tag{7.10}$$

The *transmission condition* on the boundary of the inclusion ∂B_ε comes out from the variation formulation (5.60).

7.2 Shape Sensitivity Analysis

In order to apply the result presented in Proposition 1.1, we need to evaluate the shape derivative of functional $\mathscr{J}_{\chi_\varepsilon}(u_\varepsilon)$ with respect to an uniform expansion of the inclusion B_ε. Therefore, by making use of the Reynolds' transport theorem given by formula (2.88), the shape derivative of the functional (7.6) results in

$$\dot{\mathscr{J}}_{\chi_\varepsilon}(u_\varepsilon) = -\int_\Omega q_\varepsilon(u_\varepsilon)\cdot\nabla u'_\varepsilon - \frac{1}{2}\int_{\partial\Omega}(q_\varepsilon(u_\varepsilon)\cdot\nabla u_\varepsilon)n\cdot\mathfrak{V} \\ -\frac{1}{2}\int_{\partial B_\varepsilon}[\![q_\varepsilon(u_\varepsilon)\cdot\nabla u_\varepsilon]\!]n\cdot\mathfrak{V} + \int_{\Gamma_N}\overline{q}\dot{u}_\varepsilon\ , \tag{7.11}$$

where $(\cdot)'$ is the partial derivative of $(\cdot)$ with respect to ε and $\mathfrak{V}$ is the shape change velocity field defined trough (4.2). Now, let us use the relation between material and spatial derivatives of scalar fields (2.82), namely $\varphi' = \dot{\varphi} - \nabla\varphi\cdot\mathfrak{V}$, which leads to

$$\dot{\mathscr{J}}_{\chi_\varepsilon}(u_\varepsilon) = -\frac{1}{2}\int_{\partial\Omega}(q_\varepsilon(u_\varepsilon)\cdot\nabla u_\varepsilon)n\cdot\mathfrak{V} - \frac{1}{2}\int_{\partial B_\varepsilon}[\![q_\varepsilon(u_\varepsilon)\cdot\nabla u_\varepsilon]\!]n\cdot\mathfrak{V} \\ +\int_\Omega q_\varepsilon(u_\varepsilon)\cdot\nabla(\nabla u_\varepsilon\cdot\mathfrak{V}) - \int_\Omega q_\varepsilon(u_\varepsilon)\cdot\nabla\dot{u}_\varepsilon + \int_{\Gamma_N}\overline{q}\dot{u}_\varepsilon\ . \tag{7.12}$$

Since $\dot{u}_\varepsilon$ is a variation of u_ε in the direction of the velocity field $\mathfrak{V}$, then $\dot{u}_\varepsilon \in \mathscr{V}_\varepsilon$. Now, by taking $\dot{u}_\varepsilon$ as test function in the variational problem (7.7), we have that the last two terms of the above equation vanish. By using the tensor relation (G.18) and after applying the divergence theorem, we have

$$\dot{\mathscr{J}}_{\chi_\varepsilon}(u_\varepsilon) = -\frac{1}{2}\int_{\partial\Omega}(q_\varepsilon(u_\varepsilon)\cdot\nabla u_\varepsilon)n\cdot\mathfrak{V} - \frac{1}{2}\int_{\partial B_\varepsilon}[\![q_\varepsilon(u_\varepsilon)\cdot\nabla u_\varepsilon]\!]n\cdot\mathfrak{V} \\ +\int_{\partial\Omega}(\nabla u_\varepsilon\cdot\mathfrak{V})q_\varepsilon(u_\varepsilon)\cdot n + \int_{\partial B_\varepsilon}[\![(\nabla u_\varepsilon\cdot\mathfrak{V})q_\varepsilon(u_\varepsilon)]\!]\cdot n \\ -\int_\Omega \operatorname{div} q_\varepsilon(u_\varepsilon)(\nabla u_\varepsilon\cdot\mathfrak{V})\ . \tag{7.13}$$

Considering that u_ε is also solution to the strong equation (7.10), namely, $\operatorname{div} q_\varepsilon(u_\varepsilon) = 0$ in Ω, the last term of the above equation vanishes. Then, we have

$$\dot{\mathscr{J}}_{\chi_\varepsilon}(u_\varepsilon) = -\frac{1}{2}\int_{\partial\Omega}(q_\varepsilon(u_\varepsilon)\cdot\nabla u_\varepsilon)n\cdot\mathfrak{V} - \frac{1}{2}\int_{\partial B_\varepsilon}[\![q_\varepsilon(u_\varepsilon)\cdot\nabla u_\varepsilon]\!]n\cdot\mathfrak{V} \\ +\int_{\partial\Omega}(\nabla u_\varepsilon\cdot\mathfrak{V})q_\varepsilon(u_\varepsilon)\cdot n + \int_{\partial B_\varepsilon}[\![(\nabla u_\varepsilon\cdot\mathfrak{V})q_\varepsilon(u_\varepsilon)]\!]\cdot n\ . \tag{7.14}$$

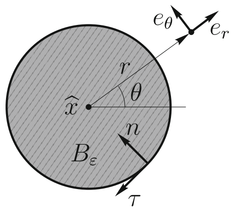


Fig. 7.4 Polar coordinate system (r,θ) centered at the point $\widehat{x} \in \Omega$

Since we are dealing with an uniform expansion on the circular inclusion B_ε, we recall that $\mathfrak{V}_{|\partial\Omega} = 0$ and $\mathfrak{V}_{|\partial B_\varepsilon} = -n$, which implies

$$\frac{d}{d\varepsilon}\psi(\chi_\varepsilon) = \dot{\mathscr{J}}_{\chi_\varepsilon}(u_\varepsilon) = \frac{1}{2}\int_{\partial B_\varepsilon} [\![q_\varepsilon^\tau(u_\varepsilon)\partial_\tau u_\varepsilon - q_\varepsilon^n(u_\varepsilon)\partial_n u_\varepsilon]\!] , \tag{7.15}$$

where, from an orthonormal curvilinear coordinate system n and τ on the boundary ∂B_ε (see fig. 7.4), the heat flux $q_\varepsilon(u_\varepsilon)$ and the gradient ∇u_ε were decomposed into their normal and tangential components, that is

$$\nabla u_{\varepsilon|\partial B_\varepsilon} = (\partial_n u_\varepsilon)n + (\partial_\tau u_\varepsilon)\tau , \tag{7.16}$$

$$q_\varepsilon(u_\varepsilon)_{|\partial B_\varepsilon} = q_\varepsilon^n(u_\varepsilon)n + q_\varepsilon^\tau(u_\varepsilon)\tau . \tag{7.17}$$

According to formula (7.15), the shape gradient originally defined in the whole domain Ω leads, once again, to an integral concentrated only on the boundary of the inclusion ∂B_ε. Therefore, in order to apply the result of Proposition 1.1, we need to know the behavior of the function u_ε with respect to ε in the neighborhood of the inclusion B_ε. In particular, once we know this behavior explicitly, we can identify function $f(\varepsilon)$ and perform the limit passage $\varepsilon \to 0$ in (1.49) to obtain the final formula for the topological derivative $\mathscr{T}$ of the shape functional ψ.

7.3 Asymptotic Analysis of the Solution

The problem given by (7.10), although linear, is not so easy to expand in power of ε. Initially, we consider a local coordinate system centered at $\widehat{x}$ and oriented along the eigenvectors of tensor K. Therefore, let us make the following change of variables

$$x_i = \sqrt{k_i}\, y_i \quad \text{for} \quad i = 1,2 \quad \Rightarrow \quad x = K^{\frac{1}{2}} y , \tag{7.18}$$

where $x = (x_1, x_2)$ and $y = (y_1, y_2)$ are points defined over the domain Ω and transformed domain $\widetilde{\Omega}$, respectively. Thus, the circular inclusion $B_\varepsilon(\widehat{x})$ is mapped into an ellipse $\mathscr{E}_\varepsilon(\widehat{y})$ with semi-major axis $\alpha = 1/\sqrt{k_1}$, semi-minor axis $\beta = 1/\sqrt{k_2}$ and centered at point $\widehat{y}$, as can be seen in fig. 7.5. The above mapping allows us to rewrite the boundary value problem (7.10) as

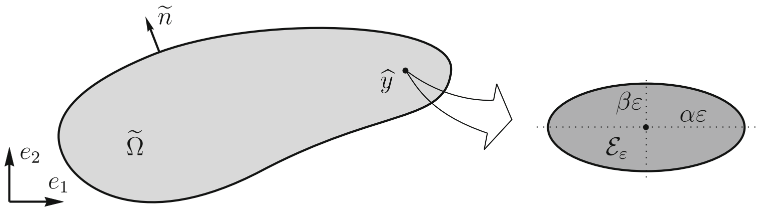


Fig. 7.5 Transformed domain $\widetilde{\Omega}$

$$\begin{cases} \text{Find } \widetilde{u}_\varepsilon, \text{ such that} \\ \operatorname{div}_y(\gamma_\varepsilon \nabla_y \widetilde{u}_\varepsilon) = 0 & \text{in } \widetilde{\Omega} , \\ \widetilde{u}_\varepsilon = \overline{u} & \text{on } \widetilde{\Gamma}_D , \\ -\partial_{\widetilde{n}} \widetilde{u}_\varepsilon = \overline{q} & \text{on } \widetilde{\Gamma}_N , \\ \left. \begin{array}{r} [\![\widetilde{u}_\varepsilon]\!] = 0 \\ [\![\gamma_\varepsilon \nabla_y \widetilde{u}_\varepsilon]\!] \cdot \widetilde{n} = 0 \end{array} \right\} & \text{on } \partial \mathscr{E}_\varepsilon , \end{cases} \tag{7.19}$$

where, according to (7.18), $y = K^{-\frac{1}{2}}x$, $\widetilde{n} = K^{-\frac{1}{2}}n$, $\widetilde{u}_\varepsilon(y) = u_\varepsilon(x)$ and, for the sake of simplicity, we are using the same notation for the boundary conditions $\overline{u}$ and $\overline{q}$. Then, the following asymptotic expansion of solution $\widetilde{u}_\varepsilon$ in $\widetilde{\Omega}$ holds [9, 39, 45, 176],

$$\widetilde{u}_\varepsilon(y)_{|_{\widetilde{\Omega} \setminus \overline{\mathscr{E}_\varepsilon}}} = \widetilde{u}(y) + \frac{\varepsilon^2}{\|y - \widehat{y}\|^2} P_\gamma \nabla u(\widehat{y}) \cdot (y - \widehat{y}) + O(\varepsilon^2) , \tag{7.20}$$

$$\widetilde{u}_\varepsilon(y)_{|_{\mathscr{E}_\varepsilon}} = \widetilde{u}(y) + P_\gamma \nabla u(\widehat{y}) \cdot (y - \widehat{y}) + O(\varepsilon^2) , \tag{7.21}$$

where $\widetilde{u}$ is the solution of the problem in the unperturbed domain $\widetilde{\Omega}$, namely $\widetilde{u}(y) = u(x)$, and P_γ is given by

$$P_\gamma = \frac{1}{2}(1-\gamma)\alpha\beta \begin{pmatrix} \frac{\alpha+\beta}{\alpha+\gamma\beta} & 0 \\ 0 & \frac{\alpha+\beta}{\beta+\gamma\alpha} \end{pmatrix} , \tag{7.22}$$

which has been derived from the polarization tensor for an elliptical inclusion [198].

Considering the inverse mapping $y = Jx$ in (7.20) and (7.21), where $J := K^{-\frac{1}{2}}$, we have that the asymptotic *expansion* for u_ε in Ω is given by

$$u_\varepsilon(x)_{|_{\Omega \setminus \overline{B_\varepsilon}}} = u(x) + \frac{\varepsilon^2}{\|J(x - \widehat{x})\|^2} P_\gamma \nabla u(\widehat{x}) \cdot (x - \widehat{x}) + O(\varepsilon^2) , \tag{7.23}$$

$$u_\varepsilon(x)_{|_{B_\varepsilon}} = u(x) + P_\gamma \nabla u(\widehat{x}) \cdot (x - \widehat{x}) + O(\varepsilon^2) . \tag{7.24}$$

It is well known that the asymptotic expansions can be differentiated term by term [148, 143]. Thus, by assuming a sufficient regularity of u in Ω and performing its Taylor's series expansion around point $\widehat{x}$, we obtain the following expansion for ∇u_ε in Ω,

$$\nabla u_\varepsilon(x)_{|_{\Omega\setminus\overline{B_\varepsilon}}} = \nabla u(\widehat{x}) + \frac{\varepsilon^2}{\|J(x-\widehat{x})\|^2} S P_\gamma \nabla u(\widehat{x}) + O(\varepsilon) \,, \tag{7.25}$$

$$\nabla u_\varepsilon(x)_{|_{B_\varepsilon}} = \nabla u(\widehat{x}) + P_\gamma \nabla u(\widehat{x}) + O(\varepsilon) \,, \tag{7.26}$$

with the tensor S given by

$$S := I - \frac{2}{\|J(x-\widehat{x})\|^2} J^2 (x-\widehat{x}) \otimes (x-\widehat{x}) \,. \tag{7.27}$$

7.4 Topological Derivative Evaluation

From expansions (7.25) and (7.26) written in a polar coordinate system (r,θ) with center at $\widehat{x}$ (see fig. 7.4), we can solve the integral (7.15) explicitly. This result together with the relation between shape and topological derivative given by (1.49) leads to

$$\mathscr{T}(\widehat{x}) = \lim_{\varepsilon\to 0} \frac{1}{f'(\varepsilon)} \left[2\pi\varepsilon \sqrt{\det K} P_\gamma q(u(\widehat{x})) \cdot \nabla u(\widehat{x}) + o(\varepsilon) \right] \,. \tag{7.28}$$

Now, in order to identify the leading term of the above expansion, we choose

$$f(\varepsilon) = \pi\varepsilon^2 \,, \tag{7.29}$$

which leads to the final expression of the *topological derivative* given by a scalar function that depends on the solution u associated to the original domain Ω (without inclusion), namely [13, 78]

$$\mathscr{T}(\widehat{x}) = \sqrt{\det K} P_\gamma q(u(\widehat{x})) \cdot \nabla u(\widehat{x}) \,. \tag{7.30}$$

Therefore, the topological asymptotic expansion of the energy shape functional associated to the steady-state orthotropic heat diffusion problem is given by

$$\psi(\chi_\varepsilon(\widehat{x})) = \psi(\chi) + \pi\varepsilon^2 \sqrt{\det K} P_\gamma q(u(\widehat{x})) \cdot \nabla u(\widehat{x}) + o(\varepsilon^2) \,. \tag{7.31}$$

The full mathematical justification for the above expansion follows the same steps presented in Chapter 5, Section 5.4.

Remark 7.1. It is interesting to observe that for isotropic material, we have $k_1 = k_2 = k$ and the final expression for the topological derivative (7.30) degenerates to the classical one given by [13],

$$\mathscr{T}(\widehat{x}) = \frac{1-\gamma}{1+\gamma} q(u(\widehat{x})) \cdot \nabla u(\widehat{x}) \,, \tag{7.32}$$

which corroborates with the formula (5.45).

Remark 7.2. From the final expression for the topological derivative (7.30), we can analyze the limits cases of the parameter γ, which are:

- Ideal thermal insulator ($\gamma \to 0$):

$$\mathscr{T}(\widehat{x}) = \frac{1}{2\sqrt{\det K}} \left(K + \sqrt{\det K} \mathrm{I} \right) q(u(\widehat{x})) \cdot \nabla u(\widehat{x}) \, . \tag{7.33}$$

- Ideal thermal conductor ($\gamma \to \infty$):

$$\mathscr{T}(\widehat{x}) = -\frac{1}{2} \left(\mathrm{I} + \sqrt{\det K} K^{-1} \right) q(u(\widehat{x})) \cdot \nabla u(\widehat{x}) \, . \tag{7.34}$$

Chapter 8
Topological Derivative for Three-Dimensional Linear Elasticity Problems

In this chapter the elasticity boundary value problems in three spatial dimensions are considered. The topological derivative of the total potential energy for the perturbation in the form of a small spherical cavity $B_\varepsilon(\widehat{x})$, with $\widehat{x} \in \Omega \subset \mathbb{R}^3$ and $\overline{B_\varepsilon} \Subset \Omega$, is obtained. Therefore, the topologically perturbed domain is given by $\Omega_\varepsilon = \Omega \setminus \overline{B_\varepsilon}$. The method for derivation of the topological derivative follows the same steps as presented in Chapter 4. We start by defining a shape change velocity field $\mathfrak{V}$ that represents an uniform expansion of the cavity $B_\varepsilon(\widehat{x})$. Thanks to this velocity field, together with Proposition 1.1, we can use the shape derivative of the energy functional as an intermediate step in the topological derivative calculation. In fact, after obtaining the (formal) asymptotic expansion of the solution to the elasticity system (defined in the perturbed domain Ω_ε) with respect to the small parameter ε, the singular limit $\varepsilon \to 0$ in formula (1.49) can be evaluated explicitly, leading to the closed form of the topological derivative.

In the second part of this chapter the multiscale constitutive modeling is introduced. The topological derivative of the macroscopic elasticity tensor with respect to topological perturbations on the micro level is obtained in its closed form. This part is a new and important direction of research in the field of shape and topology optimization in structural mechanics. In particular, the obtained topological derivatives of the effective material properties can be used in the synthesis and optimal design of microstructures.

8.1 Problem Formulation

The shape functional associated to the unperturbed domain Ω is given by

$$\psi(\chi) := \mathscr{J}_\Omega(u) = \frac{1}{2}\int_\Omega \sigma(u)\cdot\nabla u^s - \int_{\Gamma_N} \overline{q}\cdot u\,, \tag{8.1}$$

where the vector function u is the solution to the variational problem:

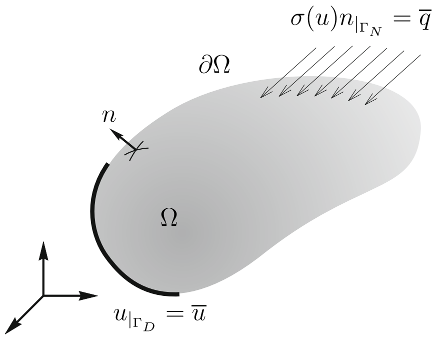


Fig. 8.1 Three-dimensional linear elasticity problem defined in the unperturbed domain Ω

$$\begin{cases} \text{Find } u \in \mathscr{U}, \text{ such that} \\ \displaystyle\int_\Omega \sigma(u) \cdot \nabla\eta^s = \int_{\Gamma_N} \overline{q} \cdot \eta \quad \forall \eta \in \mathscr{V}, \\ \qquad\qquad \text{with} \quad \sigma(u) = \mathbb{C}\nabla u^s . \end{cases} \tag{8.2}$$

In the above equation, $\mathbb{C}$ is the constitutive tensor given by

$$\mathbb{C} = \frac{E}{1+\nu}\left(\mathbb{I} + \frac{\nu}{1-2\nu}\mathrm{I} \otimes \mathrm{I}\right), \tag{8.3}$$

where I and $\mathbb{I}$ are the second and fourth order identity tensors, respectively, E is the Young modulus and ν the Poisson ratio, both considered constants everywhere. The set $\mathscr{U}$ and the space $\mathscr{V}$ are respectively defined as

$$\mathscr{U} := \{\varphi \in H^1(\Omega;\mathbb{R}^3) : \varphi_{|\Gamma_D} = \overline{u}\}, \tag{8.4}$$

$$\mathscr{V} := \{\varphi \in H^1(\Omega;\mathbb{R}^3) : \varphi_{|\Gamma_D} = 0\}. \tag{8.5}$$

In addition, $\partial\Omega = \overline{\Gamma}_D \cup \overline{\Gamma}_N$ with $\Gamma_D \cap \Gamma_N = \varnothing$, where Γ_D and Γ_N are Dirichlet and Neumann boundaries, respectively. Thus $\overline{u}$ is a Dirichlet data on Γ_D and $\overline{q}$ is a Neumann data on Γ_N, both assumed to be smooth enough. See the details in fig. 8.1. The strong system associated to the variational problem (8.2) reads:

$$\begin{cases} \text{Find } u, \text{ such that} \\ -\mathrm{div}\sigma(u) = 0 \quad \text{in } \Omega, \\ \sigma(u) = \mathbb{C}\nabla^s u, \\ u = \overline{u} \quad \text{on } \Gamma_D, \\ \sigma(u)n = \overline{q} \quad \text{on } \Gamma_N . \end{cases} \tag{8.6}$$

Remark 8.1. Since the Young modulus E and the Poisson ratio ν are considered constants, the above boundary value problem reduces itself to the well-known Navier system, namely

$$-\mu\Delta u - (\lambda+\mu)\nabla(\mathrm{div}u) = 0 \quad \text{in} \quad \Omega, \tag{8.7}$$

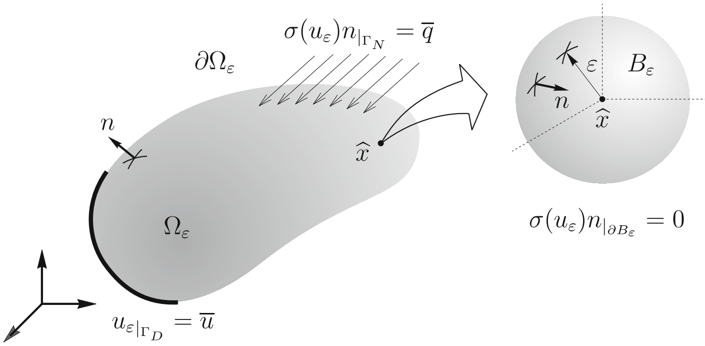


Fig. 8.2 Three-dimensional linear elasticity problem defined in the perturbed domain Ω_ε

with the Lame's coefficients μ and λ respectively given by

$$\mu = \frac{E}{2(1+\nu)} \quad \text{and} \quad \lambda = \frac{\nu E}{(1+\nu)(1-2\nu)} \,. \tag{8.8}$$

Now, let us state the same problem in the perturbed domain Ω_ε. In this case, the total potential energy reads

$$\psi(\chi_\varepsilon) := \mathscr{J}_{\Omega_\varepsilon}(u_\varepsilon) = \frac{1}{2}\int_{\Omega_\varepsilon} \sigma(u_\varepsilon)\cdot\nabla u_\varepsilon^s - \int_{\Gamma_N} \overline{q}\cdot u_\varepsilon \,, \tag{8.9}$$

where the vector function u_ε solves the variational problem:

$$\begin{cases} \text{Find}\, u_\varepsilon \in \mathscr{U}_\varepsilon, \text{ such that} \\ \displaystyle\int_{\Omega_\varepsilon} \sigma(u_\varepsilon)\cdot\nabla\eta^s = \int_{\Gamma_N} \overline{q}\cdot\eta \quad \forall\eta\in\mathscr{V}_\varepsilon \,, \\ \qquad\qquad \text{with} \quad \sigma(u_\varepsilon) = \mathbb{C}\nabla u_\varepsilon^s \,. \end{cases} \tag{8.10}$$

The set $\mathscr{U}_\varepsilon$ and the space $\mathscr{V}_\varepsilon$ are defined as

$$\mathscr{U}_\varepsilon := \{\varphi\in H^1(\Omega_\varepsilon;\mathbb{R}^3) : \varphi_{|\Gamma_D} = \overline{u}\} \,, \tag{8.11}$$

$$\mathscr{V}_\varepsilon := \{\varphi\in H^1(\Omega_\varepsilon;\mathbb{R}^3) : \varphi_{|\Gamma_D} = 0\} \,. \tag{8.12}$$

Since u_ε is free on ∂B_ε, then we have homogeneous Neumann boundary condition on the cavity. It means that the cavity is a free boundary representing a void. See the details in fig. 8.2. The *strong system* associated to the variational problem (8.10) reads:

$$\begin{cases} \text{Find}\, u_\varepsilon, \text{ such that} \\ -\text{div}\sigma(u_\varepsilon) = 0 & \text{in } \Omega_\varepsilon \,, \\ \sigma(u_\varepsilon) = \mathbb{C}\nabla u_\varepsilon^s \,, \\ u_\varepsilon = \overline{u} & \text{on } \Gamma_D \,, \\ \sigma(u_\varepsilon)n = \overline{q} & \text{on } \Gamma_N \,, \\ \sigma(u_\varepsilon)n = 0 & \text{on } \partial B_\varepsilon \,. \end{cases} \tag{8.13}$$

8.2 Shape Sensitivity Analysis

In order to apply the result presented in Proposition 1.1, we need to evaluate the shape derivative of functional $\mathscr{J}_{\Omega_\varepsilon}(u_\varepsilon)$ with respect to an uniform expansion of the cavity B_ε. In particular, we could use directly the result presented in Corollary 4.3 through formula (4.140), since it is independent of the spacial dimension of the problem. However, we will repeat the shape sensitivity analysis in order to show a faster way to obtain the shape derivative of $\mathscr{J}_{\Omega_\varepsilon}(u_\varepsilon)$ for the particular case associated to an uniform expansion of the spherical cavity.

Therefore, by making use of the Reynolds' transport theorem given by formula (2.85), the shape derivative of the functional (8.9) results in

$$\dot{\mathscr{J}}_{\Omega_\varepsilon}(u_\varepsilon) = \int_{\Omega_\varepsilon} \sigma(u_\varepsilon)\cdot(\nabla u_\varepsilon')^s + \frac{1}{2}\int_{\partial\Omega_\varepsilon} (\sigma(u_\varepsilon)\cdot\nabla u_\varepsilon^s)n\cdot\mathfrak{V} - \int_{\Gamma_N} \overline{q}\cdot\dot{u}_\varepsilon \,, \tag{8.14}$$

where $(\cdot)'$ is the partial derivative of $(\cdot)$ with respect to ε and $\mathfrak{V}$ is the shape change velocity field defined such that $\mathfrak{V}_{|\partial\Omega} = 0$ and $\mathfrak{V}_{|\partial B_\varepsilon} = -n$. Now, let us use the relation between material and spatial derivatives of vector fields (2.83), namely $\varphi' = \dot{\varphi} - (\nabla\varphi)\mathfrak{V}$, which leads to

$$\begin{aligned}\dot{\mathscr{J}}_{\Omega_\varepsilon}(u_\varepsilon) &= \frac{1}{2}\int_{\partial\Omega_\varepsilon} (\sigma(u_\varepsilon)\cdot\nabla u_\varepsilon^s)n\cdot\mathfrak{V} - \int_{\Omega_\varepsilon} \sigma(u_\varepsilon)\cdot\nabla((\nabla u_\varepsilon)\mathfrak{V})^s \\ &\quad + \int_{\Omega_\varepsilon} \sigma(u_\varepsilon)\cdot\nabla\dot{u}_\varepsilon^s - \int_{\Gamma_N} \overline{q}\cdot\dot{u}_\varepsilon \,. \end{aligned}\tag{8.15}$$

Since $\dot{u}_\varepsilon$ is a variation of u_ε in the direction of the velocity field $\mathfrak{V}$, then $\dot{u}_\varepsilon \in \mathscr{V}_\varepsilon$. Now, by taking $\dot{u}_\varepsilon$ as test function in the variational problem (8.10), we have that the last two terms of the above equation vanish. By using the tensor relation (G.23) and after applying the divergence theorem (G.33), we have

$$\begin{aligned}\dot{\mathscr{J}}_{\Omega_\varepsilon}(u_\varepsilon) &= \frac{1}{2}\int_{\partial\Omega_\varepsilon} (\sigma(u_\varepsilon)\cdot\nabla u_\varepsilon^s)n\cdot\mathfrak{V} \\ &\quad - \int_{\partial\Omega_\varepsilon} ((\nabla u_\varepsilon)\mathfrak{V})\cdot\sigma(u_\varepsilon)n + \int_{\Omega_\varepsilon} (\operatorname{div}\sigma(u_\varepsilon))\cdot(\nabla u_\varepsilon)\mathfrak{V} \,, \end{aligned}\tag{8.16}$$

where the fact that $\sigma(u_\varepsilon)^\top = \sigma(u_\varepsilon)$ has been considered. Since we are dealing with an uniform expansion on the spherical cavity B_ε, we recall that $\mathfrak{V}_{|\partial\Omega} = 0$ and $\mathfrak{V}_{|\partial B_\varepsilon} = -n$, which implies

$$\begin{aligned}\dot{\mathscr{J}}_{\Omega_\varepsilon}(u_\varepsilon) &= -\frac{1}{2}\int_{\partial B_\varepsilon} \sigma(u_\varepsilon)\cdot\nabla u_\varepsilon^s + \int_{\partial B_\varepsilon} ((\nabla u_\varepsilon)n)\cdot\sigma(u_\varepsilon)n \\ &\quad + \int_{\Omega_\varepsilon} (\operatorname{div}\sigma(u_\varepsilon))\cdot(\nabla u_\varepsilon)\mathfrak{V} \,, \end{aligned}\tag{8.17}$$

where $\partial\Omega_\varepsilon = \partial\Omega \cup \partial B_\varepsilon$. Considering that u_ε is also solution to the strong system (8.13), namely, $\operatorname{div}\sigma(u_\varepsilon) = 0$ in Ω_ε and $\sigma(u_\varepsilon)n = 0$ on ∂B_ε, the last two terms of the above equation vanish. Then, we finally have

$$\frac{d}{d\varepsilon}\psi(\chi_\varepsilon) = \dot{\mathscr{J}}_{\Omega_\varepsilon}(u_\varepsilon) = -\frac{1}{2}\int_{\partial B_\varepsilon} \sigma(u_\varepsilon)\cdot\nabla u_\varepsilon^s \,, \tag{8.18}$$

where the shape gradient originally defined in the whole domain Ω_ε leads, once again, to an integral defined only on the boundary of the cavity ∂B_ε. Therefore, in order to apply the result of Proposition 1.1, we need to know the behavior of the function u_ε with respect to ε in the neighborhood of the cavity B_ε. In particular, once we know this behavior explicitly, we can identify function $f(\varepsilon)$ and perform the limit passage $\varepsilon \to 0$ in (1.49), allowing to obtain the final formula for the topological derivative $\mathscr{T}$ of the shape functional ψ.

8.3 Asymptotic Analysis of the Solution

In this section, we present the formal calculation of the expansions of the solution u_ε associated to homogeneous Neumann condition on the boundary of the cavity. For a rigorous justification of the asymptotic expansions of u_ε, the reader may refer to [120, 148], for instance. Let us propose an *ansätz* for the expansion of u_ε in the form [120]

$$u_\varepsilon(x) = u(x) + w_\varepsilon(x) + \widetilde{u}_\varepsilon(x) \,. \tag{8.19}$$

After applying the operator σ we have

$$\begin{aligned}\sigma(u_\varepsilon(x)) &= \sigma(u(x)) + \sigma(w_\varepsilon(x)) + \sigma(\widetilde{u}_\varepsilon(x)) \\ &= \sigma(u(\widehat{x})) + \nabla\sigma(u(y))(x-\widehat{x}) + \sigma(w_\varepsilon(x)) + \sigma(\widetilde{u}_\varepsilon(x)) \,,\end{aligned} \tag{8.20}$$

where y is an intermediate point between x and $\widehat{x}$. On the boundary of the cavity ∂B_ε we have $\sigma(u_\varepsilon)n_{|_{\partial B_\varepsilon}} = 0$. Thus, the normal projection of the above expansion, evaluated on ∂B_ε, leads to

$$\sigma(u(\widehat{x}))n - \varepsilon(\nabla\sigma(u(y))n)n + \sigma(w_\varepsilon(x))n + \sigma(\widetilde{u}_\varepsilon(x))n = 0 \,. \tag{8.21}$$

In particular, we can choose $\sigma(w_\varepsilon)$ such that

$$\sigma(w_\varepsilon(x))n = -\sigma(u(\widehat{x}))n \quad \text{on} \quad \partial B_\varepsilon \,. \tag{8.22}$$

Now, the following exterior problem is considered, and formally obtained as $\varepsilon \to 0$:

$$\begin{cases} \text{Find } \sigma(w_\varepsilon), \text{ such that} \\ \operatorname{div}\sigma(w_\varepsilon) = 0 & \text{in } \mathbb{R}^3 \setminus \overline{B_\varepsilon} \,, \\ \sigma(w_\varepsilon) \to 0 & \text{at } \infty \,, \\ \sigma(w_\varepsilon)n = -\sigma(u(\widehat{x}))n & \text{on } \partial B_\varepsilon \,. \end{cases} \tag{8.23}$$

The above boundary value problem admits an explicit solution (see, for instance, the book by Little 1973 [139]), which will be used later to obtain the expansion for $\sigma(u_\varepsilon)$. Now we can construct $\sigma(\widetilde{u}_\varepsilon)$ in such a way that it compensates the discrepancies introduced by the higher-order terms in ε as well as by the boundary-layer $\sigma(w_\varepsilon)$ on the exterior boundary $\partial\Omega$. It means that the remainder $\sigma(\widetilde{u}_\varepsilon)$ must be solution to the following boundary value problem:

$$\begin{cases} \text{Find}\,\sigma(\widetilde{u}_\varepsilon),\text{ such that} \\ \operatorname{div}\sigma(\widetilde{u}_\varepsilon) = 0 & \text{in } \Omega_\varepsilon\ , \\ \quad\sigma(\widetilde{u}_\varepsilon) = -\sigma(w_\varepsilon) & \text{on } \partial\Omega\ , \\ \quad\sigma(\widetilde{u}_\varepsilon)n = \varepsilon(\nabla\sigma(u(y))n)n & \text{on } \partial B_\varepsilon\ , \end{cases} \tag{8.24}$$

where, according to [120, 148], $\sigma(\widetilde{u}_\varepsilon) = O(\varepsilon^3)$. Finally, the *expansion* for $\sigma(u_\varepsilon)$ in the spherical coordinate system (r,θ,ϕ) reads (see fig. 8.3)

$$\begin{aligned} \sigma^{rr}(u_\varepsilon) &= \sigma_1^{rr} + \sigma_2^{rr} + \sigma_3^{rr} + O(\varepsilon)\ , \\ \sigma^{r\theta}(u_\varepsilon) &= \sigma_1^{r\theta} + \sigma_2^{r\theta} + \sigma_3^{r\theta} + O(\varepsilon)\ , \\ \sigma^{r\phi}(u_\varepsilon) &= \sigma_1^{r\phi} + \sigma_2^{r\phi} + \sigma_3^{r\phi} + O(\varepsilon)\ , \\ \sigma^{\theta\theta}(u_\varepsilon) &= \sigma_1^{\theta\theta} + \sigma_2^{\theta\theta} + \sigma_3^{\theta\theta} + O(\varepsilon)\ , \\ \sigma^{\theta\phi}(u_\varepsilon) &= \sigma_1^{\theta\phi} + \sigma_2^{\theta\phi} + \sigma_3^{\theta\phi} + O(\varepsilon)\ , \\ \sigma^{\phi\phi}(u_\varepsilon) &= \sigma_1^{\phi\phi} + \sigma_2^{\phi\phi} + \sigma_3^{\phi\phi} + O(\varepsilon)\ , \end{aligned} \tag{8.25}$$

where σ_i^{rr}, $\sigma_i^{r\theta}$, $\sigma_i^{r\phi}$, $\sigma_i^{\theta\theta}$, $\sigma_i^{\theta\phi}$ and $\sigma_i^{\phi\phi}$, for $i = 1,2,3$, are written, as:

For $i = 1$

$$\sigma_1^{rr} = \frac{\sigma_1}{14-10\nu}\left[12\left(\frac{\varepsilon^3}{r^3} - \frac{\varepsilon^5}{r^5}\right) + \left(14 - 10\nu - 10(5-\nu)\frac{\varepsilon^3}{r^3} + 36\frac{\varepsilon^5}{r^5}\right)\sin^2\theta\sin^2\phi\right]\ , \tag{8.26}$$

$$\sigma_1^{r\theta} = \frac{\sigma_1}{14-10\nu}\left[7 - 5\nu + 5(1+\nu)\frac{\varepsilon^3}{r^3} - 12\frac{\varepsilon^5}{r^5}\right]\sin 2\theta\sin^2\phi\ , \tag{8.27}$$

$$\sigma_1^{r\phi} = \frac{\sigma_1}{14-10\nu}\left[7 - 5\nu + 5(1+\nu)\frac{\varepsilon^3}{r^3} - 12\frac{\varepsilon^5}{r^5}\right]\sin\theta\sin 2\phi\ , \tag{8.28}$$

$$\sigma_1^{\theta\theta} = \frac{\sigma_1}{56-40\nu}\left[14 - 10\nu + (1+10\nu)\frac{\varepsilon^3}{r^3} + 3\frac{\varepsilon^5}{r^5} - \left(14 - 10\nu + 25(1-2\nu)\frac{\varepsilon^3}{r^3} - 9\frac{\varepsilon^5}{r^5}\right)\cos 2\phi + \left(28 - 20\nu - 10(1-2\nu)\frac{\varepsilon^3}{r^3} + 42\frac{\varepsilon^5}{r^5}\right)\cos 2\theta\sin^2\phi\right]\ , \tag{8.29}$$

$$\sigma_1^{\theta\phi} = \frac{\sigma_1}{14-10\nu}\left[7-5\nu+5(1-2\nu)\frac{\varepsilon^3}{r^3}+3\frac{\varepsilon^5}{r^5}\right]\cos\theta\sin 2\phi\ , \tag{8.30}$$

$$\sigma_1^{\phi\phi} = \frac{\sigma_1}{56-40\nu}\left[28-20\nu+(11-10\nu)\frac{\varepsilon^3}{r^3}+9\frac{\varepsilon^5}{r^5}+\right.$$
$$\left(28-20\nu+5(1-2\nu)\frac{\varepsilon^3}{r^3}+27\frac{\varepsilon^5}{r^5}\right)\cos 2\phi-$$
$$\left.30\left((1-2\nu)\frac{\varepsilon^3}{r^3}-\frac{\varepsilon^5}{r^5}\right)\cos 2\theta\sin^2\phi\right]\ . \tag{8.31}$$

For $i=2$

$$\sigma_2^{rr} = \frac{\sigma_2}{14-10\nu}\left[12\left(\frac{\varepsilon^3}{r^3}-\frac{\varepsilon^5}{r^5}\right)+\right.$$
$$\left.\left(14-10\nu-10(5-\nu)\frac{\varepsilon^3}{r^3}+36\frac{\varepsilon^5}{r^5}\right)\sin^2\theta\cos^2\phi\right]\ , \tag{8.32}$$

$$\sigma_2^{r\theta} = \frac{\sigma_2}{14-10\nu}\left[7-5\nu+5(1+\nu)\frac{\varepsilon^3}{r^3}-12\frac{\varepsilon^5}{r^5}\right]\cos^2\phi\sin 2\theta\ , \tag{8.33}$$

$$\sigma_2^{r\phi} = \frac{-\sigma_2}{14-10\nu}\left[7-5\nu+5(1+\nu)\frac{\varepsilon^3}{r^3}-12\frac{\varepsilon^5}{r^5}\right]\sin\theta\sin 2\phi\ , \tag{8.34}$$

$$\sigma_2^{\theta\theta} = \frac{\sigma_2}{56-40\nu}\left[14-10\nu+(1+10\nu)\frac{\varepsilon^3}{r^3}+3\frac{\varepsilon^5}{r^5}+\right.$$
$$\left(14-10\nu+25(1-2\nu)\frac{\varepsilon^3}{r^3}-9\frac{\varepsilon^5}{r^5}\right)\cos 2\phi+$$
$$\left.\left(28-20\nu-10(1-2\nu)\frac{\varepsilon^3}{r^3}+42\frac{\varepsilon^5}{r^5}\right)\cos 2\theta\cos^2\phi\right]\ , \tag{8.35}$$

$$\sigma_2^{\theta\phi} = \frac{-\sigma_2}{14-10\nu}\left[7-5\nu+5(1-2\nu)\frac{\varepsilon^3}{r^3}+3\frac{\varepsilon^5}{r^5}\right]\cos\theta\sin 2\phi\ , \tag{8.36}$$

$$\sigma_2^{\phi\phi} = \frac{\sigma_2}{56-40\nu}\left[28-20\nu+(11-10\nu)\frac{\varepsilon^3}{r^3}+9\frac{\varepsilon^5}{r^5}-\right.$$
$$\left(28-20\nu+5(1-2\nu)\frac{\varepsilon^3}{r^3}+27\frac{\varepsilon^5}{r^5}\right)\cos 2\phi-$$
$$\left.30\left((1-2\nu)\frac{\varepsilon^3}{r^3}-\frac{\varepsilon^5}{r^5}\right)\cos 2\theta\cos^2\phi\right]\ . \tag{8.37}$$

For $i = 3$

$$\sigma_3^{rr} = \frac{\sigma_3}{14-10\nu}\left[14-10\nu-(38-10\nu)\frac{\varepsilon^3}{r^3}+24\frac{\varepsilon^5}{r^5}- \left(14-10\nu-10(5-\nu)\frac{\varepsilon^3}{r^3}+36\frac{\varepsilon^5}{r^5}\right)\sin^2\theta\right], \tag{8.38}$$

$$\sigma_3^{r\theta} = \frac{-\sigma_3}{14-10\nu}\left[14-10\nu+10(1+\nu)\frac{\varepsilon^3}{r^3}-24\frac{\varepsilon^5}{r^5}\right]\cos\theta\sin\theta, \tag{8.39}$$

$$\sigma_3^{r\phi} = 0, \tag{8.40}$$

$$\sigma_3^{\theta\theta} = \frac{\sigma_3}{14-10\nu}\left[(9-15\nu)\frac{\varepsilon^3}{r^3}-12\frac{\varepsilon^5}{r^5}+ \left(14-10\nu-5(1-2\nu)\frac{\varepsilon^3}{r^3}+21\frac{\varepsilon^5}{r^5}\right)\sin^2\theta\right], \tag{8.41}$$

$$\sigma_3^{\theta\phi} = 0, \tag{8.42}$$

$$\sigma_3^{\phi\phi} = \frac{\sigma_3}{14-10\nu}\left[(9-15\nu)\frac{\varepsilon^3}{r^3}-12\frac{\varepsilon^5}{r^5}- 15\left((1-2\nu)\frac{\varepsilon^3}{r^3}-\frac{\varepsilon^5}{r^5}\right)\sin^2\theta\right], \tag{8.43}$$

where $\sigma_1 = \sigma_1(u(\widehat{x}))$, $\sigma_2 = \sigma_2(u(\widehat{x}))$ and $\sigma_3 = \sigma_3(u(\widehat{x}))$ are the principal stress values of tensor $\sigma(u(\widehat{x}))$ associated to the original domain without cavity Ω. In other words, tensor $\sigma(u(\widehat{x}))$ was diagonalized in the following way:

$$\sigma(u(\widehat{x})) = \sum_{i=1}^{3}\sigma_i(e_i\otimes e_i), \tag{8.44}$$

where σ_i is the eigenvalue associated to the e_i eigenvector of tensor $\sigma(u(\widehat{x}))$. In addition, $\sigma^{rr}(\varphi)$, $\sigma^{r\theta}(\varphi)$, $\sigma^{r\phi}(\varphi)$, $\sigma^{\theta\theta}(\varphi)$, $\sigma^{\theta\phi}(\varphi)$ and $\sigma^{\phi\phi}(\varphi)$ are the components of tensor $\sigma(\varphi)$ in the spherical coordinate system, namely, $\sigma^{rr}(\varphi) = e^r\cdot\sigma(\varphi)e^r$, $\sigma^{r\theta}(\varphi) = \sigma^{\theta r}(\varphi) = e^r\cdot\sigma(\varphi)e^\theta$, $\sigma^{r\phi}(\varphi) = \sigma^{\phi r}(\varphi) = e^r\cdot\sigma(\varphi)e^\phi$, $\sigma^{\theta\theta}(\varphi) = e^\theta\cdot\sigma(\varphi)e^\theta$, $\sigma^{\theta\phi}(\varphi) = \sigma^{\phi\theta}(\varphi) = e^\theta\cdot\sigma(\varphi)e^\phi$ and $\sigma^{\phi\phi}(\varphi) = e^\phi\cdot\sigma(\varphi)e^\phi$, with $\|e^r\| = \|e^\theta\| = \|e^\phi\| = 1$ and $e^r\cdot e^\theta = e^r\cdot e^\phi = e^\theta\cdot e^\phi = 0$. See fig. 8.3.

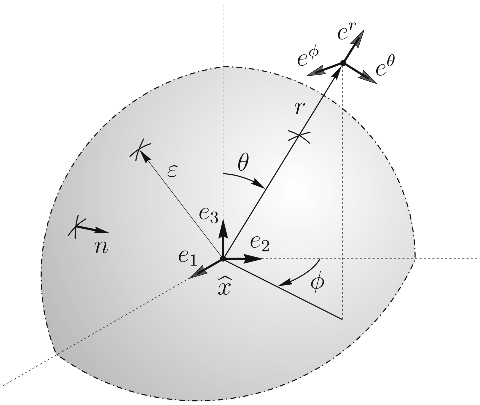


Fig. 8.3 Spherical coordinate system (r,θ,ϕ) centered at the point $\widehat{x} \in \Omega$

8.4 Topological Derivative Evaluation

From the spherical coordinate system (r,θ,ϕ) shown in fig. 8.3, the stress tensor $\sigma(u_\varepsilon) = \sigma(u_\varepsilon)^\top$ can be decomposed as

$$\begin{aligned}\sigma(u_\varepsilon)_{|\partial B_\varepsilon} &= \sigma^{rr}(u_\varepsilon)(e^r \otimes e^r) + \sigma^{r\theta}(u_\varepsilon)(e^r \otimes e^\theta) + \sigma^{r\phi}(u_\varepsilon)(e^r \otimes e^\phi) \\ &+ \sigma^{\theta\theta}(u_\varepsilon)(e^\theta \otimes e^\theta) + \sigma^{\theta\phi}(u_\varepsilon)(e^\theta \otimes e^\phi) + \sigma^{\phi\phi}(u_\varepsilon)(e^\phi \otimes e^\phi) \,. \end{aligned} \tag{8.45}$$

Since $n = -e^r$, we observe that $\sigma(u_\varepsilon)n_{|\partial B_\varepsilon} = -\sigma(u_\varepsilon)e^r{}_{|\partial B_\varepsilon}$. Therefore,

$$\sigma(u_\varepsilon)e^r_{|\partial B_\varepsilon} = \sigma^{rr}(u_\varepsilon)e^r + \sigma^{r\theta}(u_\varepsilon)e^\theta + \sigma^{r\phi}(u_\varepsilon)e^\phi = 0 \,, \tag{8.46}$$

with $e^r \perp e^\theta$, $e^r \perp e^\phi$ and $e^\theta \perp e^\phi$, which implies

$$\sigma^{rr}(u_\varepsilon) = \sigma^{r\theta}(u_\varepsilon) = \sigma^{\theta r}(u_\varepsilon) = \sigma^{r\phi}(u_\varepsilon) = \sigma^{\phi r}(u_\varepsilon) = 0 \quad \text{on} \quad \partial B_\varepsilon \,, \tag{8.47}$$

since $\sigma(u_\varepsilon) = \sigma(u_\varepsilon)^\top$. In addition, the constitutive tensor $\mathbb{C}$ is invertible,

$$\mathbb{C}^{-1} = \frac{1}{E}((1+\nu)\mathbb{I} - \nu \mathrm{I} \otimes \mathrm{I}) \,, \tag{8.48}$$

which implies $\nabla u^s_\varepsilon = \mathbb{C}^{-1}\sigma(u_\varepsilon)$. Therefore, we have

$$\sigma(u_\varepsilon) \cdot \nabla u^s_\varepsilon = \frac{1}{E}((1+\nu)\sigma(u_\varepsilon) \cdot \sigma(u_\varepsilon) - \nu \mathrm{tr}^2 \sigma(u_\varepsilon)) \,. \tag{8.49}$$

By using the above decomposition together with the boundary condition on ∂B_ε, the shape derivative of the cost functional (8.18) reads

$$\frac{d}{d\varepsilon}\psi(\chi_\varepsilon) = -\frac{1}{2E}\int_{\partial B_\varepsilon} g_\varepsilon \,, \tag{8.50}$$

where the auxiliary function g_ε is defined by

$$g_\varepsilon := \sigma^{\theta\theta}(u_\varepsilon)^2 + \sigma^{\phi\phi}(u_\varepsilon)^2 - 2\nu\sigma^{\theta\theta}(u_\varepsilon)\sigma^{\phi\phi}(u_\varepsilon) + 2(1+\nu)\sigma^{\theta\phi}(u_\varepsilon)^2 \ . \tag{8.51}$$

From formula (8.25), we have that the following expansion for $\sigma(u_\varepsilon)$ holds on the boundary the cavity, namely, for $r = \varepsilon$,

$$\begin{aligned}
\sigma^{\theta\theta}(u_\varepsilon)_{|\partial B_\varepsilon} = \frac{3}{4}\frac{1}{7-5\nu}\big[\sigma_1\left(3-5(1-2\nu)\cos 2\phi + 10\cos 2\theta \sin^2\phi\right) \\
+ \sigma_2\left(3+5(1-2\nu)\cos 2\phi + 10\cos 2\theta\cos^2\phi\right) \\
+\sigma_3\left(2(4-5\nu) - 10\cos 2\theta\right)\big] + O(\varepsilon) \ ,
\end{aligned} \tag{8.52}$$

$$\sigma^{\theta\phi}(u_\varepsilon)_{|\partial B_\varepsilon} = \frac{15}{2}\frac{1-\nu}{7-5\nu}(\sigma_1 - \sigma_2)\cos\theta\sin 2\phi + O(\varepsilon) \ , \tag{8.53}$$

$$\begin{aligned}
\sigma^{\phi\phi}(u_\varepsilon)_{|\partial B_\varepsilon} = \frac{3}{4}\frac{1}{7-5\nu}\big[\sigma_1\left(8-5\nu+5(2-\nu)\cos 2\phi + 10\nu\cos 2\theta\sin^2\phi\right) \\
+ \sigma_2\left(8-5\nu-5(2-\nu)\cos 2\phi + 10\nu\cos 2\theta\cos^2\phi\right) \\
-2\sigma_3\left(1+5\nu\cos 2\theta\right)\big] + O(\varepsilon) \ .
\end{aligned} \tag{8.54}$$

Considering the above expansions in (8.50) and by taking into account the identity below

$$\int_{\partial B_\varepsilon} \varphi = \int_0^{2\pi}\left(\int_0^{\pi} \varphi\varepsilon^2 \sin\theta d\theta\right) d\phi \ , \tag{8.55}$$

where φ is a given function, we have that after analytically solving the integral on the boundary of the cavity ∂B_ε, we obtain

$$\frac{d}{d\varepsilon}\psi(\chi_\varepsilon) = -4\pi\varepsilon^2 \frac{3}{4E}\frac{1-\nu}{7-5\nu}\left(10(1+\nu)\varphi_1 - (1+5\nu)\varphi_2\right) + O(\varepsilon^3) \ , \tag{8.56}$$

where φ_1 and φ_2 are respectively given by

$$\varphi_1 = \sigma_1^2 + \sigma_2^2 + \sigma_3^2 \quad \text{and} \quad \varphi_2 = (\sigma_1 + \sigma_2 + \sigma_3)^2 \ . \tag{8.57}$$

The above result together with the relation between shape and topological derivative given by (1.49) leads to

$$\mathscr{T} = -\lim_{\varepsilon\to 0}\frac{1}{f'(\varepsilon)}\left[4\pi\varepsilon^2 \frac{3}{4E}\frac{1-\nu}{7-5\nu}\left(10(1+\nu)\varphi_1 - (1+5\nu)\varphi_2\right) + O(\varepsilon^3)\right] . \tag{8.58}$$

Now, in order to extract the leading term of the above expansion, we choose

$$f(\varepsilon) = \frac{4}{3}\pi\varepsilon^3 \ , \tag{8.59}$$

which results in

$$\mathscr{T} = -\frac{3}{4E}\frac{1-\nu}{7-5\nu}\left(10(1+\nu)\varphi_1 - (1+5\nu)\varphi_2\right) \ . \tag{8.60}$$

Therefore, the final expression for the *topological derivative* becomes a scalar function that depends on solution u associated to the original domain Ω (without cavity), that is [70, 187]:

- In terms of the principal stresses $\sigma_i(\widehat{x}) = \sigma_i(u(\widehat{x}))$, $i = 1,2,3$

$$\mathscr{T}(\widehat{x}) = -\frac{3}{4E}\frac{1-\nu}{7-5\nu}\left[10(1+\nu)\sum_{i=1}^{3}\sigma_i(\widehat{x})^2 - (1+5\nu)\left(\sum_{i=1}^{3}\sigma_i(\widehat{x})\right)^2\right]. \quad (8.61)$$

- In terms of the stress tensor $\sigma(u(\widehat{x}))$

$$\mathscr{T}(\widehat{x}) = -\frac{3}{4E}\frac{1-\nu}{7-5\nu}\left[10(1+\nu)\sigma(u(\widehat{x}))\cdot\sigma(u(\widehat{x})) - (1+5\nu)\mathrm{tr}^2\sigma(u(\widehat{x}))\right]. \quad (8.62)$$

- In terms of the stress tensor $\sigma(u(\widehat{x}))$ and the strain tensor $\nabla u^s(\widehat{x})$

$$\mathscr{T}(\widehat{x}) = -\mathbb{P}\sigma(u(\widehat{x}))\cdot\nabla u^s(\widehat{x}) , \quad (8.63)$$

  where $\mathbb{P}$ is the *polarization tensor*, given in this particular case by the following isotropic fourth order tensor

$$\mathbb{P} = \frac{3}{4}\frac{1-\nu}{7-5\nu}\left(10\mathbb{I} - \frac{1-5\nu}{1-2\nu}\mathrm{I}\otimes\mathrm{I}\right). \quad (8.64)$$

Finally, the topological asymptotic expansion of the energy shape functional reads

$$\psi(\chi_\varepsilon(\widehat{x})) = \psi(\chi) - \pi\varepsilon^3\mathbb{P}\sigma(u(\widehat{x}))\cdot\nabla u^s(\widehat{x}) + o(\varepsilon^3) , \quad (8.65)$$

whose mathematical justification follows the same steps as it is presented in Chapter 10 for another problem.

8.5 Numerical Example

In order to explain briefly the significance of the topological derivative in shape optimization we present one example, with the well known solution obtained by numerical methods. We use a simple procedure consisting in a successive nucleation of cavities where the topological derivative is more negative. In particular, the topology is identified by the strong material distribution and the inclusions of weak material are use to mimic the cavities. In addition, the topological derivative is evaluated at the nodal points of the finite elements mesh. Then, we remove the elements that share the node where the topological derivative assumes its more negative values as shown in the sketching of fig. 8.4. This procedure is repeated until the topological derivative becomes positive everywhere. For more elaborated topology design algorithm, the reader may refer to the paper by Amstutz & Andrä 2006 [16].

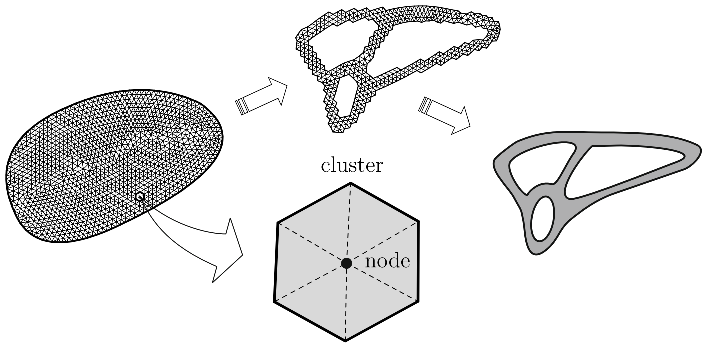


Fig. 8.4 Sketching of the procedure to nucleate inclusions in a finite element mesh. For more details on the adopted numerical procedure, see [185].

In particular, we consider the minimization of the strain energy stored in the elastic body with a volume constraint. Therefore, we propose the following shape functional

$$\Psi_\Omega(u) := -\mathscr{J}_\Omega(u) + \beta\,|\Omega| \ , \tag{8.66}$$

where $|\Omega|$ is the Lebesgue measure of Ω and $\beta > 0$ is a fixed Lagrange multiplier. It means that the shape functional to be minimized is the compliance with a volume constraint. The topological derivative of $\Psi_\Omega(u)$ is given by

$$\mathscr{T} = \mathbb{P}\sigma(u) \cdot \nabla u^s - \beta \ , \tag{8.67}$$

with $\sigma(u) = \mathbb{C}\nabla u^s$, where we have used formula (8.63) and the fact that the topological derivative of the term $\beta\,|\Omega|$ is trivial. In addition, the displacement vector field u is evaluated by solving problem (8.2) numerically.

Let us consider the design of a simply supported cube on the bottom under vertical load applied on the top, as shown in fig. 8.5. This cube has dimension $0.5 \times 0.5 \times 0.5\ m^3$. The load $\bar{q} = 10^3 N$ is distributed in a small centered circular region of radius equal to $0.03m$. The supports are circular and have radii equal to $0.02m$, with their centers at $0.035m$ from the edges of the cube. The material properties are given by Young's modulus $E = 210 \times 10^9 N/m^2$ and Poisson's ratio $\nu = 1/3$. The parameter β is chosen in such way that the required final volume $|\Omega^\star| = 0.02\,|\Omega|$ is attained . The cube is discretized using four-nodes tetrahedron finite elements and 5% of material is removed at each iteration.

Details of the obtained results are shown in fig. 8.6 and in fig. 8.7, where we can also observe the shape of the transversal sections of the bars obtained at the end of the process. The corresponding finite element mesh associated to the final configuration is presented in fig. 8.8 showing an intensification of the mesh in the regions of hard material, allowing a good identification of the topology. This numerical result is due to J.M. Marmo and can be found in [187].

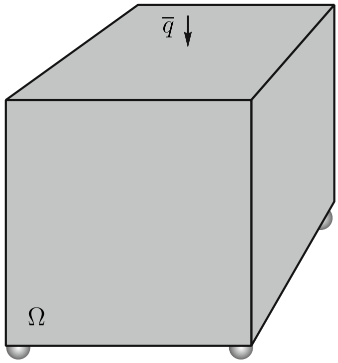
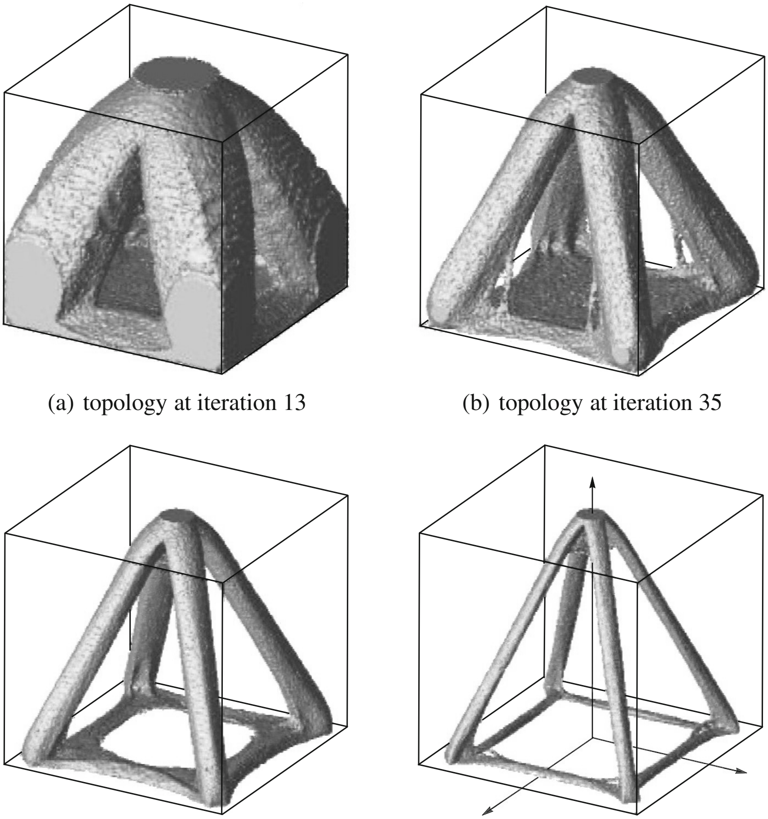


Fig. 8.5 Simply supported cube on the bottom under vertical load applied on the top



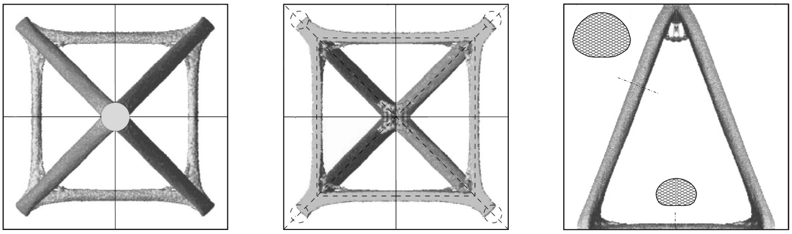
(a) topology at iteration 13

(b) topology at iteration 35

(c) topology at iteration 52

(d) topology at iteration 76

Fig. 8.6 History of the topology design process



(a) top (b) bottom (c) lateral

Fig. 8.7 Detail of the obtained final topology

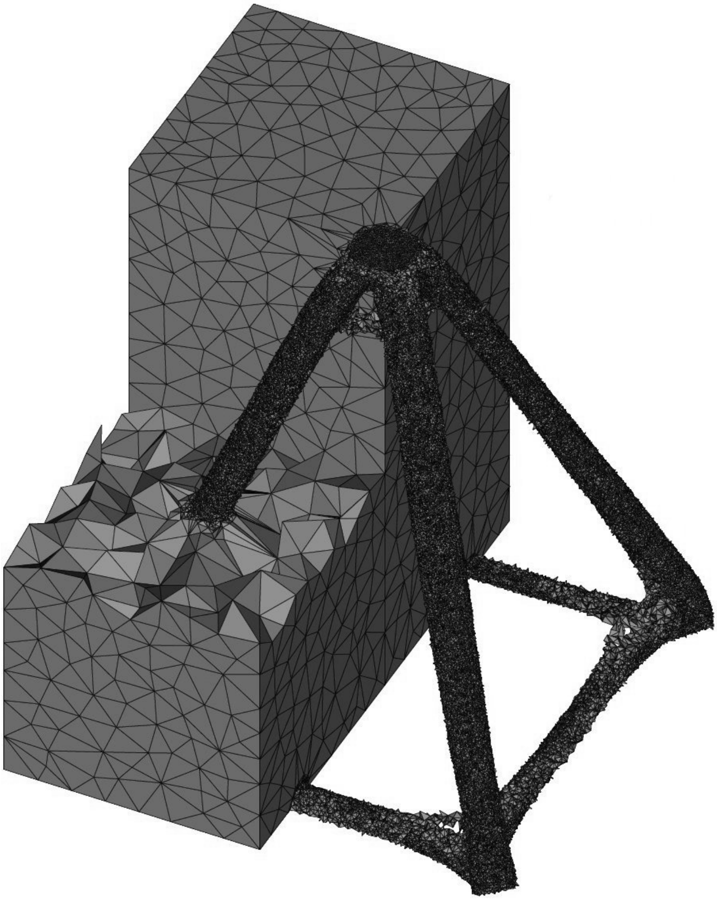


Fig. 8.8 Finite element mesh at the end of the topology design process

8.6 Multiscale Topological Derivatives

In this section we evaluate the topological derivative of the elasticity tensor obtained from a multiscale model with a periodic microstructure on the lower or micro level of the model for the purpose of synthesis and optimal design of microstructures. The macro behavior on the higher hierarchical or macro level of material model is obtained by asymptotic analysis with respect to the size of periodic cell which is commonly called *homogenization procedure* [137, 201]. The topological derivative of the homogenized elasticity tensor means that we find one term asymptotics of the components of the effective elasticity tensor which describes the resulting properties of the material which is influenced at the micro level by a small void or a small inclusion in the periodic cell. It turns out that the required result on the asymptotics and the form of the topological derivative of the effective elasticity tensor can be obtained in the same way as it is done in the previous chapters.

The material modeling in the framework of asymptotic analysis, with the parameters which is primarily the cell period, and secondary the size of the imperfection is the tool of our analysis. We recall that the procedure which translates the micro behavior of the material in the cell into the macro properties of the elastic body at the higher level is of common use. We refer the reader to [137] for an introduction from the point of view of solid mechanics, and to [201] for the mathematical description of such modeling. We are going to make use of the same concept and combine the presence of singular perturbations of the microstructure with the homogenization procedure to obtain the effective material properties at the macro level, this time depending on the parameter of singular perturbation of the cell, the void size.

Our goal is simple, we want to predict the behavior of an elastic material at the macro level when a small spherical cavity is introduced at the micro level. The predicted form of the elasticity tensor includes one term asymptotics and determines the topological derivatives of all components of the effective elasticity tensor. To this end we perform the formal asymptotic analysis of the effective or homogenized elasticity tensor of the material at the macro level for the singular perturbations of the periodic cells at the micro level by introduction of a small void into the cell. The components of the homogenized elasticity tensor is perturbed in a similar way as the energy shape functional with respect to the imperfection in the cell. Therefore our technique of derivation is applicable to this model and results in the topological derivatives of all components of the homogenized elasticity tensor in the presence of imperfections.

8.6.1 Multiscale Modeling in Solid Mechanics

The accurate prediction of the *constitutive behavior* of a continuum body under loading is of paramount importance in many areas of engineering and science. Until about a decade ago, this issue has been addressed mainly by means of conventional *phenomenological constitutive theories*. More recently, the increasing understanding of the microscopic mechanisms responsible for the macroscopic response, allied to the industrial demand for more accurate predictive tools, led to the development and use of so-called *multiscale constitutive theories*. Such theories are currently a subject of intensive research in applied mathematics and computational mechanics. Their starting point can be traced back to the pioneering developments reported in [35, 86, 92, 141, 201, 212]. Early applications were concerned with the description of relatively simple microscale phenomena often treated by analytical or semi-analytical methods [29, 30, 81, 182, 183, 190]. More recent applications rely often on finite element-based computational simulations [154, 155] and are frequently applied to more *complex material behavior* in areas such as the modeling of human arterial tissue [211], bone [191], the plastic behavior of porous metals [73] and the microstructural evolution and phase transition in the solidification of metals [46].

One interesting branching of such developments is the study of the sensitivity of the macroscopic response to changes in the underlying microstructure. The sensitivity information becomes essential in the analysis and potential purpose-design and optimization of heterogenous media. For instance, sensitivity information obtained by means of a relaxation-based technique has been successfully used in [7, 126, 127] to design microstructural topologies with negative macroscopic Poisson's ratio. Multi-scale models have also been applied with success to the topology optimization of load bearing structures in the context of the so-called homogenization approach to topology optimization (see, for instance, the review paper by Eschenauer and Olhoff 2001 [54] and the book by Allaire 2002 [4]) based on the fundamental papers by Żochowski 1988 [218] and Bendsøe & Kikuchi 1988 [34]. See also [47, 189]. In such cases, the microscale model acts as a regularization of the exact problem posed by a material point turning into a hole [33]. The homogenization approach has also been applied to microstructural topology optimization problems where the target is the design of topologies that yield pre-specified or extreme macroscopic response [114, 202, 203]. One of the drawbacks of this methodology, however, is that it often produces designs with large regions consisting of perforated material. To deal with this problem, a penalization of intermediate densities is commonly introduced.

In contrast to the regularized approaches, in this section we present a general *exact* analytical expression for the sensitivity of the three-dimensional macroscopic elasticity tensor to topological changes of the microstructure of the underlying material. We follow the ideas developed in [75] for two-dimensional elasticity. The obtained sensitivity is given by a symmetric fourth order tensor field over the Representative Volume Element (RVE) that measures how the macroscopic elasticity constants estimated within the multiscale framework changes when a small spherical void is introduced at the microscale. It is derived by making use of the notions of topological asymptotic analysis and topological derivative within the variational formulation of well-established multiscale constitutive theory fully developed in the book by Sanchez-Palencia 1980 [201] (see also [71, 154, 155]), where the macroscopic strain and stress tensors are volume averages of their microscopic counterparts over a Representative Volume Element (RVE) of material.

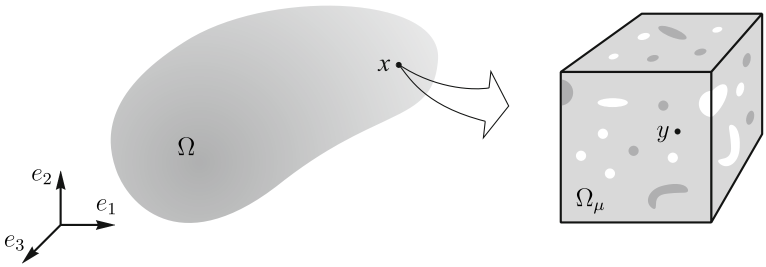


Fig. 8.9 Macroscopic continuum with a locally attached microstructure

The final format of the proposed analytical formula is strikingly simple and can be used in applications such as the synthesis and optimal design of microstructures to meet a specified macroscopic behavior [17].

8.6.2 The Homogenized Elasticity Tensor

The *homogenization-based multiscale constitutive framework* presented, among others, in [201], is adopted here in the estimation of the *macrostructure* elastic response from the knowledge of the underlying *microstructure*. The main idea behind this well-established family of constitutive theories is the assumption that any point x of the macroscopic continuum is associated to a local *Representative Volume Element* (RVE) whose domain is denoted by Ω_μ, with boundary $\partial\Omega_\mu$, as shown in fig. 8.9. Crucial to the developments presented in Section 8.6.3, is the closed form of the *homogenized elasticity tensor* $\mathbb{C}$ for the multiscale model defined in the above. The components of the homogenized elasticity tensor $\mathbb{C}$, in the orthonormal basis $\{e_i\}$, for $i = 1,2,3$, of the Euclidean space (refer to fig. 8.9), can be written as

$$(\mathbb{C})_{ijkl} = \frac{1}{V_\mu}\int_{\Omega_\mu} (\sigma_\mu(u_{\mu_{kl}}))_{ij} \ , \tag{8.68}$$

where V_μ denotes the total volume of the RVE, e.g. the volume of the cub in the sketch shown in fig. 8.9. The canonical microscopic displacement field $u_{\mu_{kl}}$ is solution to the equilibrium equation of the form [201]

$$\int_{\Omega_\mu} \sigma_\mu(u_{\mu_{kl}}) \cdot \nabla\eta^s = 0 \qquad \forall\eta \in \mathscr{V}_\mu \ . \tag{8.69}$$

We assume that the microscopic stress tensor field $\sigma_\mu(u_{\mu_{kl}})$ satisfies

$$\sigma_\mu(u_{\mu_{kl}}) = \mathbb{C}_\mu \nabla u^s_{\mu_{kl}} \ , \tag{8.70}$$

where $\mathbb{C}_\mu$ is the microscopic constitutive tensor given by

$$\mathbb{C}_\mu = \frac{E_\mu}{1+\nu_\mu}\left(\mathbb{I} + \frac{\nu_\mu}{1-2\nu_\mu}\mathrm{I}\otimes\mathrm{I}\right) , \tag{8.71}$$

with I and $\mathbb{I}$ the second and fourth order identity tensors, respectively, E_μ the Young modulus and ν_μ Poisson ratio of the RVE.

Without loss of generality, $u_{\mu_{kl}}(y)$, with $y \in \Omega_\mu$, may be decomposed into a sum

$$u_{\mu_{kl}}(y) := u + (e_k \otimes e_l)y + \widetilde{u}_{\mu_{kl}}(y) , \tag{8.72}$$

of a constant (rigid) RVE displacement coinciding with the macroscopic displacement field u at the point $x \in \Omega$, a linear field $(e_k \otimes e_l)y$, and a canonical microscopic displacement fluctuation field $\widetilde{u}_{\mu_{kl}}(y)$. The microscopic displacement fluctuation field $\widetilde{u}_{\mu_{kl}}$ is solution to the following *canonical set of variational problems* [201]:

$$\left\{\begin{array}{l} \text{Find}\, \widetilde{u}_{\mu_{kl}} \in \mathscr{V}_\mu \text{, such that} \\ \displaystyle\int_{\Omega_\mu} \sigma_\mu(\widetilde{u}_{\mu_{kl}}) \cdot \nabla\eta^s + \int_{\Omega_\mu} \mathbb{C}_\mu(e_k \otimes_s e_l) \cdot \nabla\eta^s = 0 \quad \forall \eta \in \mathscr{V}_\mu , \\ \qquad\qquad\qquad\qquad\qquad\qquad \text{with} \quad \sigma_\mu(u_{\mu_{kl}}) = \mathbb{C}_\mu \nabla u_{\mu_{kl}} . \end{array}\right. \tag{8.73}$$

The complete characterization of the multiscale constitutive model is obtained by defining the subspace $\mathscr{V}_\mu \subset \mathscr{U}_\mu$ of kinematically admissible displacement fluctuations. In general, different choices produce different macroscopic responses for the same RVE. In this section, the analysis will be focussed on media with periodic microstructure. In this case, the geometry of the RVE cannot be arbitrary and must represent a cell whose periodic repetition generates the macroscopic continuum. In addition, the displacement fluctuations must satisfy periodicity on the boundary of the RVE. Accordingly, we have

$$\mathscr{V}_\mu := \left\{\varphi \in \mathscr{U}_\mu : \varphi(y^+) = \varphi(y^-) \quad \forall\, (y^+, y^-) \in \mathfrak{P}\right\}, \tag{8.74}$$

where $\mathfrak{P}$ is the set of pairs of points, defined by a one-to-one periodicity correspondence, lying on opposing sides of the RVE boundary. Finally, the *minimally constrained space* of kinematically admissible displacements $\mathscr{U}_\mu$ is defined as

$$\mathscr{U}_\mu := \left\{\varphi \in H^1(\Omega_\mu; \mathbb{R}^3) : \int_{\Omega_\mu} \varphi = 0,\ \int_{\partial\Omega_\mu} \varphi \otimes_s n = 0\right\} , \tag{8.75}$$

where n is the outward unit normal to the boundary $\partial\Omega_\mu$ and $\otimes_s$ denotes the symmetric tensor product between vectors.

From the definition of the homogenized elasticity tensor (8.68), we have

$$(\mathbb{C})_{ijkl} = \frac{1}{V_\mu}\int_{\Omega_\mu} e_i \cdot \sigma_\mu(u_{\mu_{kl}})e_j = \frac{1}{V_\mu}\int_{\Omega_\mu} \sigma_\mu(u_{\mu_{kl}}) \cdot (e_i \otimes e_j) . \tag{8.76}$$

On the other hand, the additive decomposition (8.72) allows us to write

$$\begin{aligned} e_i \otimes e_j &= \nabla((e_i \otimes e_j)y)^s \\ &= \nabla(u_{\mu_{ij}}(y) - \widetilde{u}_{\mu_{ij}}(y) - u)^s \\ &= \nabla(u_{\mu_{ij}}(y) - \widetilde{u}_{\mu_{ij}}(y))^s \ , \end{aligned} \tag{8.77}$$

since $(e_i \otimes e_j)y = u_{\mu_{ij}}(y) - \widetilde{u}_{\mu_{ij}}(y) - u$. Therefore, by combining these two results, we obtain

$$\begin{aligned} (\mathbb{C})_{ijkl} &= \frac{1}{V_\mu} \int_{\Omega_\mu} \sigma_\mu(u_{\mu_{kl}}) \cdot \nabla(u_{\mu_{ij}} - \widetilde{u}_{\mu_{ij}})^s \\ &= \frac{1}{V_\mu} \int_{\Omega_\mu} \sigma_\mu(u_{\mu_{kl}}) \cdot \nabla u^s_{\mu_{ij}} \ , \end{aligned} \tag{8.78}$$

since $u_{\mu_{kl}}$ satisfies the equilibrium equation (8.69) and $\widetilde{u}_{\mu_{ij}} \in \mathscr{V}_\mu$.

8.6.3 Sensitivity of the Macroscopic Elasticity Tensor to Topological Microstructural Changes

A closed formula for the sensitivity of the homogenized elasticity tensor (8.68) to the nucleation of a spherical cavity within the RVE is presented in this section. We start by noting that each component of the homogenized elasticity tensor is defined by the energy based functional (8.78). Therefore, by taking into account the result (8.62), the topological derivative of (8.78) with respect to the nucleation of a spherical cavity at an arbitrary point $\widehat{y} \in \Omega_\mu$ is given by

$$\mathscr{T}_\mu(\widehat{y}) = -\mathbb{P}_\mu \sigma_\mu(u_{\mu_{ij}}(\widehat{y})) \cdot \sigma_\mu(u_{\mu_{kl}}(\widehat{y})) \quad \forall \widehat{y} \in \Omega_\mu \ , \tag{8.79}$$

with the *polarization tensor* $\mathbb{P}_\mu$ redefined as follows (see equation (8.62))

$$\mathbb{P}_\mu = \frac{3}{2V_\mu E_\mu} \left(10 \frac{1-\nu_\mu^2}{7-5\nu_\mu} \mathbb{I} - \frac{(1-\nu_\mu)(1+5\nu_\mu)}{7-5\nu_\mu} \mathrm{I} \otimes \mathrm{I} \right) . \tag{8.80}$$

From the result given by (8.79), we can recognize a fourth order tensor field over Ω_μ that represents the sensitivity of the macroscopic elasticity tensor $\mathbb{C}$ to topological microstructural changes resulting from the insertion of a spherical cavity within the RVE. Therefore, the *topological derivative* of the homogenized elasticity tensor reads

$$\mathbb{T}_\mu(\widehat{y}) = -\mathbb{P}_\mu \sigma_\mu(u_{\mu_{ij}}(\widehat{y})) \cdot \sigma_\mu(u_{\mu_{kl}}(\widehat{y})) e_i \otimes e_j \otimes e_k \otimes e_l \ , \tag{8.81}$$

where the fields $u_{\mu_{ij}}$ come out from the solutions to (8.73) for the unperturbed RVE domain Ω_μ together with the additive decomposition (8.72).

Remark 8.2. The remarkable simplicity of the closed form sensitivity given by (8.81) is to be noted. Once the vector fields $\widetilde{u}_{\mu_{ij}}$ have been obtained as solutions to the set of variational equations (8.73) for the *original* RVE domain, the sensitivity tensor $\mathbb{T}_\mu$ can be trivially assembled from the additive decomposition (8.72). The information provided by the fourth order topological derivative tensor field $\mathbb{T}_\mu$ given by (8.81) can be used in a number of practical applications such as the design of microstructures to match a specified macroscopic constitutive response.

Remark 8.3. Expression (8.81) allows the *exact* topological derivative of any differentiable function of $\mathbb{C}$ be calculated through the direct application of the conventional rules of differential calculus. That is, any such a function $\Psi(\mathbb{C})$ has exact topological derivative of the form

$$\mathscr{T}_\mu = \left\langle D\Psi(\mathbb{C}), \mathbb{T}_\mu \right\rangle \ , \tag{8.82}$$

with the brackets $\langle \cdot, \cdot \rangle$ denoting the appropriate product between the derivative of Ψ with respect to $\mathbb{C}$ and the topological derivative $\mathbb{T}_\mu$ of $\mathbb{C}$. Note, for example, that properties of interest such as the homogenized Young's, shear and bulk moduli as well as the Poisson ratio are all regular functions of $\mathbb{C}$. This observation together with Remark 8.2 point strongly to the suitability of the use of (8.82) in a topology algorithm for the synthesis and optimization of elastic micro-structures based on the minimization/maximization of cost functions defined in terms of homogenized properties. These features has been successfully explored in [17] in two-dimensional multiscale elasticity problem.

In order to fix theses ideas, let us present three examples concerning the topological derivatives of given functions $\Psi(\mathbb{C})$. Let $\varphi_1, \varphi_2 \in \mathbb{R}^3 \times \mathbb{R}^3$ be any pair of second order tensors. Then we obtain the following results, which can be used in numerical methods of synthesis and/or topology design of microstructures [17]:

Example 8.1. We consider a function $\Psi(\mathbb{C})$ of the form

$$\Psi(\mathbb{C}) := \mathbb{C}\varphi_1 \cdot \varphi_2 \ . \tag{8.83}$$

Therefore, according to (8.82), its topological derivative is given by

$$\mathscr{T}_\mu = \mathbb{T}_\mu \varphi_1 \cdot \varphi_2 \ . \tag{8.84}$$

If we set $\varphi_1 = e_i \otimes e_j$ and $\varphi_2 = e_k \otimes e_l$, for instance, we get $\Psi(\mathbb{C}) = (\mathbb{C})_{ijkl}$ and its topological derivative is given by $\mathscr{T}_\mu = (\mathbb{T}_\mu)_{ijkl}$. It means that $\mathscr{T}_\mu$ actually represents the topological derivative of the component $(\mathbb{C})_{ijkl}$ of the homogenized elasticity tensor $\mathbb{C}$.

Example 8.2. Now, let us consider a function $\Psi(\mathbb{C})$ of the form

$$\Psi(\mathbb{C}) := \mathbb{C}^{-1}\varphi_1 \cdot \varphi_2 \ . \tag{8.85}$$

According again to (8.82), the topological derivative of $\Psi(\mathbb{C})$ is given by

$$\mathscr{T}_\mu = -(\mathbb{C}^{-1}\mathbb{T}_\mu\mathbb{C}^{-1})\varphi_1 \cdot \varphi_2 \,. \tag{8.86}$$

Thus, by setting tensors φ_1 and φ_2 properly, we can obtain the topological derivative in its explicit form of any component of the inverse of the homogenized elasticity tensor $\mathbb{C}^{-1}$. The above derivation requires some additional explanation. Note that we can differentiate the relation $\mathbb{C}\mathbb{C}^{-1} = \mathbb{I}$ with respect to $\mathbb{C}$, namely

$$\mathbb{T}_\mu\mathbb{C}^{-1} + \mathbb{C}D(\mathbb{C}^{-1}) = 0 \,. \tag{8.87}$$

After multiplying to the left by $\mathbb{C}^{-1}$ we get

$$\mathbb{C}^{-1}\mathbb{T}_\mu\mathbb{C}^{-1} + D(\mathbb{C}^{-1}) = 0 \,, \tag{8.88}$$

which leads to

$$D(\mathbb{C}^{-1}) = -\mathbb{C}^{-1}\mathbb{T}_\mu\mathbb{C}^{-1} \,. \tag{8.89}$$

Example 8.3. Finally, we consider a function $\Psi(\mathbb{C})$ of the form

$$\Psi(\mathbb{C}) := \frac{\mathbb{C}^{-1}\varphi_1 \cdot \varphi_2}{\mathbb{C}^{-1}\varphi_1 \cdot \varphi_1} + \frac{\mathbb{C}^{-1}\varphi_2 \cdot \varphi_1}{\mathbb{C}^{-1}\varphi_2 \cdot \varphi_2} \,. \tag{8.90}$$

From (8.82), the corresponding topological derivative is

$$\begin{aligned} \mathscr{T}_\mu = &- \frac{(\mathbb{C}^{-1}\mathbb{T}_\mu\mathbb{C}^{-1})\varphi_1 \cdot [(\mathbb{C}^{-1}\varphi_1 \cdot \varphi_1)\varphi_2 - (\mathbb{C}^{-1}\varphi_1 \cdot \varphi_2)\varphi_1]}{(\mathbb{C}^{-1}\varphi_1 \cdot \varphi_1)^2} \\ &- \frac{(\mathbb{C}^{-1}\mathbb{T}_\mu\mathbb{C}^{-1})\varphi_2 \cdot [(\mathbb{C}^{-1}\varphi_2 \cdot \varphi_2)\varphi_1 - (\mathbb{C}^{-1}\varphi_2 \cdot \varphi_1)\varphi_2]}{(\mathbb{C}^{-1}\varphi_2 \cdot \varphi_2)^2} \,. \end{aligned} \tag{8.91}$$

Chapter 9
Compound Asymptotic Expansions for Spectral Problems

In this chapter the *elliptic spectral problems* in singularly perturbed domains are analyzed. The asymptotic expansion of simple and multiple eigenvalues and of the associated eigenfunctions with respect to the small parameter which governs the size of singular perturbations are derived. The *compound asymptotic expansions* method [148, 170] is applied to this end. The singular and nonsmooth perturbations far and close to the boundary of a smooth reference domain are considered [131, 160, 177, 178, 179]. We point out that the specific asymptotic expansions cannot be derived by the classic shape sensitivity technique of [62, 196, 210]. However, the obtained results in the case of the boundary perturbations may be compared with the related results obtained by the speed method of the shape sensitivity analysis (cf. example for the topological derivative on the boundary associated with the energy functional in Section 1.2). We refer also to [8, 65, 66, 67, 68, 69] for the related results on the asymptotic analysis of spectral problems by the matched asymptotic expansions method of [100].

In shape optimization [62, 210] the case of multiple eigenvalues is considered in the framework of nonsmooth optimization and the directional derivative of a multiple eigenvalue is obtained in the direction of the velocity field. This fact is translated [131, 160, 177, 178, 179] in the asymptotic analysis of multiple eigenvalues in a one term asymptotics in Appendix B, Theorem B.1, and in Section 9.3.4, Theorem 9.2. The shape differentiability of a simple eigenvalue can be performed in the same way as of the energy functional [210]. This means that the shape derivatives of any order can be obtained in the framework of the speed method in smooth domains. This property is translated in the framework of asymptotic analysis in complete asymptotic expansions, see Section 9.2.3 for a representative example.

In Section 9.1 we begin with elementary examples of the second order scalar elliptic problems. The main results presented in this chapter concern the spectral problems in three spatial dimensions, which are listed here:

- Dirichlet Laplacian with cavities far from the boundary, Section 9.2.
- Neumann Laplacian with cavities close to the boundary (caverns), Section 9.3.
- Anisotropic elasticity with inclusions close to the boundary, Section 9.4.

Singular domain perturbations in three spatial dimensions take the form of small caverns or cavities in the perturbed domain. There are two specific cases, the first is considered in Section 9.2 with the cavities far from the boundary, and the second considered in Sections 9.3, 9.4 as well as in Appendices B, C, with the caverns close to the boundary. There are different small parameters for two cases. The small shape parameter which governs the size of singular perturbations close to the boundary is denoted by $h \to 0$, in contrast with the parameter $\varepsilon \to 0$ for the cavities located in the perturbed domain far from the boundary of unperturbed domain. In Section 9.2 an example is presented for a scalar spectral problem in domains with small cavities. The formal asymptotic expansion of a simple eigenvalue for the Dirichlet Laplacian is derived in great detail. Such a construction of asymptotic expansions is performed in [160, Chapter 3, pp. 55–72] as well as in [148, Chapter 9]. The multiple eigenvalues are considered in Sections 9.3 and 9.4. For the convenience of the reader the proofs of some results presented in this chapter are relegated to Appendices A, B and C with the arguments particularly of the papers [131, 179, 180]. Shape optimization problems for eigenvalues in classic setting are also considered in [90].

9.1 Preliminaries and Examples

Let Ω be a bounded domain in $\mathbb{R}^3$, with C^2–boundary $\partial\Omega$. Let us consider the compact operator $\Delta_x^{-1} : L^2(\Omega) \ni f \mapsto u \in L^2(\Omega)$, the inverse of the unbounded operator named Dirichlet Laplacian $\Delta_x : L^2(\Omega) \to L^2(\Omega)$. Hence Δ_x^{-1} is defined as the solution operator for the boundary value problem for the Laplacian with the homogeneous Dirichlet boundary conditions:

Problem 9.1. Find $u \in H_0^1(\Omega)$ such that

$$-\Delta_x u(x) = f(x), \quad x \in \Omega, \tag{9.1a}$$

$$u(x) = 0, \quad x \in \partial\Omega, \tag{9.1b}$$

where $f \in L^2(\Omega)$ is given.

Let us consider the spectral problem associated with the Dirichlet Laplacian in an abstract form:

Problem 9.2. Find $(u,\mu) \in \mathscr{H} \times \mathbb{R}_+$ such that

$$\mathfrak{K}u = \mu u.$$

In order to apply Proposition A.1 to Problem 9.2 we define a Hilbert space $\mathscr{H}$ such that $\mathfrak{K} : \mathscr{H} \to \mathscr{H}$ is compact. First, the scalar product in $\mathscr{H}$ is introduced,

$$\langle u,v\rangle := (\nabla_x u, \nabla_x v)_\Omega,$$

and the operator $\mathfrak{K}: \mathscr{H} \to \mathscr{H}$ defined by

$$\langle \mathfrak{K}f, v\rangle := (f, v)_\Omega \quad \forall v \in \mathscr{H},$$

then we find the variational formulation of Problem 9.1

$$(\nabla_x(\mathfrak{K}f), \nabla_x v)_\Omega = (f, v)_\Omega \quad \forall v \in \mathscr{H}.$$

Therefore, $\mathfrak{K}: H_0^1(\Omega) \to H_0^1(\Omega)$ is the restriction of Δ_x^{-1} to $\mathscr{H} := H_0^1(\Omega)$ with the norm in $\mathscr{H}$ induced by the scalar product $(u,v)_{\mathscr{H}} := \langle u, v\rangle = (\nabla_x u, \nabla_x v)_\Omega$. By the standard *elliptic regularity* for Problem 9.1 the solution $u \in H^2(\Omega) \cap H_0^1(\Omega)$, further the embedding $H^2(\Omega) \hookrightarrow H_0^1(\Omega)$ is compact, therefore the solution operator for problem (9.1) considered as an operator in the Sobolev space $H_0^1(\Omega)$ satisfies all assumptions of Proposition A.1.

The spectral problem for $\mathfrak{K}$ can be written in an equivalent form for the Dirichlet Laplacian:

Problem 9.3. Find $(u, \lambda) \in H_0^1(\Omega) \times \mathbb{R}_+$ such that

$$\Delta_x u(x) + \lambda u(x) = 0, \quad x \in \Omega, \tag{9.2a}$$

$$u(x) = 0, \quad x \in \partial\Omega. \tag{9.2b}$$

Remark 9.1. The eigenvalues λ_k, $k \in \mathbb{N}$, for (9.2) are related to the eigenvalues μ_k, $k \in \mathbb{N}$ of $\mathfrak{K}$ by relation

$$\mu^k := \frac{1}{\lambda_k}.$$

Again, the classic theory of spectral problems applies to Problem 9.3. Therefore, there are eigenvalues

$$0 < \lambda^1 < \lambda^2 \leqslant \cdots \leqslant \lambda^n \to \infty. \tag{9.3}$$

It is well known that the first eigenvalue λ^1 is simple.

Note 9.1. Since the eigenfunctions are determined in $\mathscr{H} = H_0^1(\Omega)$, the eigenfunctions can be normalized in $H_0^1(\Omega)$

$$(\nabla_x v^k, \nabla_x v^l)_\Omega = \delta_{kl}, \quad \delta_{kl} \quad \text{is the Kronecker symbol.}$$

However, the standard normalization in $L^2(\Omega)$ for the eigenfunctions $v^1, v^2, \ldots, v^n$, $\ldots$ in $H_0^1(\Omega) \cap H^2(\Omega)$ is used in this chapter.

Assume that there is given a simple eigenvalue λ for (9.2) and let $\mathfrak{v}$ be the associate eigenfunction. Consider the Helmholtz boundary value problem for the particular choice of λ:

Problem 9.4. Find $u \in H_0^1(\Omega)$ such that

$$(\mathscr{L}u)(x) := (\Delta_x + \lambda \mathsf{I})u(x) = \Delta_x u(x) + \lambda u(x) = f(x), \quad x \in \Omega, \tag{9.4a}$$

$$u(x) = g(x), \quad x \in \partial\Omega, \tag{9.4b}$$

where $f \in L^2(\Omega)$ and $g \in H^{3/2}(\partial\Omega)$ are given elements. In addition, I is the identity mapping.

The existence of a solution to Problem 9.4 follows by Fredholm alternative. The kernel of the unbounded operator $\mathscr{L} := \Delta_x + \lambda \mathsf{I} : L^2(\Omega) \to L^2(\Omega)$ is one dimensional since λ is a simple eigenvalue, the associated eigenfunction $\mathfrak{v}$ belongs to the kernel. In addition, its domain $\mathscr{D}(\mathscr{L}) = H^2(\Omega) \cap H^1_0(\Omega)$ is obtained by the standard *elliptic regularity*. It is not difficult to show that a necessary condition for the existence of a solution to Problem 9.4 is the compatibility condition,

$$\int_\Omega f(x)\mathfrak{v}(x)dx + \int_{\partial\Omega} g(x)\partial_n \mathfrak{v}(x)ds(x) = 0. \tag{9.5}$$

The proof is left as an exercise. The solution to (9.4) becomes unique after normalization,

$$\int_\Omega u(x)\mathfrak{v}(x)dx = 0. \tag{9.6}$$

9.2 Dirichlet Laplacian in Domains with Small Cavities

In this section the *Dirichlet spectral problem* is considered. The asymptotic analysis of a simple eigenvalue for the Dirichlet Laplacian in the domain with small cavities in three spatial dimensions is presented. Our presentation is inspired by [160, Chapter 3, pp. 55–72]. Related results and examples can be found in [105] within the framework of selfadjoint extensions for spectral problems with the full proof, however only for the first term of the eigenvalue expansion. Examples of asymptotics for eigenvalues and eigenfunctions are also derived in [148, Chapter 9, pp. 318–351] for scalar as well as the elasticity problems, where the list of relevant references can be found.

Let $\Omega, \omega \subset \mathbb{R}^3$ be two domains with smooth boundaries $\partial\Omega, \partial\omega$ and the compact closures $\overline{\Omega}, \overline{\omega}$, respectively. The origin $\mathscr{O}$ belongs to Ω and ω. We denote $\omega_\varepsilon := \{x \in \mathbb{R}^3 : \varepsilon^{-1}x \in \omega\}$ and $\Omega_\varepsilon := \Omega \setminus \overline{\omega_\varepsilon}$. Therefore, the origin $\mathscr{O}$ is the center of ω_ε. Then, the *Dirichlet Laplace spectral problem* in Ω_ε reads:

Problem 9.5. Find $(u^\varepsilon, \lambda^\varepsilon) \in H^1(\Omega_\varepsilon) \times \mathbb{R}_+$ such that

$$\Delta_x u^\varepsilon(x) + \lambda^\varepsilon u^\varepsilon(x) = 0, \quad x \in \Omega_\varepsilon, \tag{9.7a}$$

$$u^\varepsilon(x) = 0, \quad x \in \partial\Omega, \tag{9.7b}$$

$$u^\varepsilon(x) = 0, \quad x \in \partial\omega_\varepsilon. \tag{9.7c}$$

We consider the simple eigenvalue of Problem 9.5. In the construction of the asymptotic expansion of the eigenvalue two different families of boundary problems are employed.

- The first limit problem or the *inner problem* for the regular corrector of expansion v_0 is the Dirichlet problem for the operator $\Delta_x + \lambda \mathsf{I}$ in Ω, where I stands for the identity mapping.

- The subsequent regular correctors should be introduced in the punctured domain $\Omega \setminus \{\mathscr{O}\}$ instead of Ω to leave the possibility for developing the singularities of the data and of the solution at the origin, the centre of singular perturbation of Ω. However, we mainly use the notation Ω for the equations of regular correctors at the stage of formal asymptotic analysis.
- The second limit problem or the *outer problem*, for which condition (9.7c) is taken into account, is obtained by the change of variables $x \to \xi := \varepsilon^{-1}x$ and the limit passage $\varepsilon \to 0$. In view of the identity $\Delta_x + \lambda \mathsf{I} = \varepsilon^{-2}\Delta_\xi + \lambda \mathsf{I}$, the second term is neglected and we obtain $\Delta_\xi w = 0$ in $\mathbb{R}^3 \setminus \overline{\omega}$.

9.2.1 First Order Asymptotic Expansion

Let λ_0 denotes a simple eigenvalue and v_0 be the corresponding positive eigenfunction normalized in $L^2(\Omega)$. The function v_0 leaves a discrepancy in the boundary condition (9.7c) which can be compensated by the boundary layer

$$\Delta_\xi w_0(\xi) = 0, \quad \xi \in \mathbb{R}^3 \setminus \overline{\omega}, \tag{9.8a}$$

$$w_0(\xi) = -v_0(\mathscr{O}), \quad \xi \in \partial\omega, \tag{9.8b}$$

$$w_0(\xi) \to 0, \quad \text{for } \|\xi\| \to \infty. \tag{9.8c}$$

It is well known that (9.8) admits the unique solution which enjoys the asymptotic representation for $\|\xi\| \to \infty$

$$w_0(\xi) = -\|\xi\|^{-1}v_0(\mathscr{O})\mathrm{cap}(\omega) + O(\|\xi\|^{-2}), \tag{9.9}$$

where $\mathrm{cap}(\omega)$ is the *Bessel capacity* of ω.

Note 9.2. The explicit definition of Bessel capacity in three spatial dimensions is the following (cf. Definitions 2.2.1, 2.2.2, 2.2.4 in [1]):

- Let $K \subset \mathbb{R}^3$ be compact. Then

$$\mathrm{cap}(K) = \inf\{\|\varphi\|^2_{H^1(\mathbb{R}^3)} : \varphi \in C_0^\infty(\mathbb{R}^3),\ \varphi \geqslant 1 \text{ on } K\}.$$

- Let $G \subset \mathbb{R}^3$ be open. Then

$$\mathrm{cap}(G) = \sup\{\mathrm{cap}(K) : K \subset G,\ K \text{ compact}\}.$$

- Let $A \subset \mathbb{R}^3$ be arbitrary. Then

$$\mathrm{cap}(A) = \inf\{\mathrm{cap}(G) : G \supset A,\, G \text{ open}\}.$$

The definition is exactly the same in $\mathbb{R}^2$.

The sum $v_0(x) + w_0(\varepsilon^{-1}x)$ of the first regular corrector of the expansion and of the first boundary layer corrector as an approximation of the solution to Problem 9.5

leaves a discrepancy in equation (9.7a) and condition (9.7b). The error in boundary condition, in view of (9.9), is

$$\varepsilon \|x\|^{-1} \mathrm{cap}(\omega) + O(\varepsilon^2). \tag{9.10}$$

Therefore, the second regular corrector of expansion v_1 is introduced, and the error (9.10) is compensated by the approximation $u^\varepsilon(x) \sim v_0(x) + w_0(\varepsilon^{-1}x) + \varepsilon v_1(x)$, with the nonhomogeneous Dirichlet condition

$$v_1(x) = \|x\|^{-1} v_0(\mathscr{O}) \mathrm{cap}(\omega), \quad x \in \partial\Omega. \tag{9.11}$$

Let us turn now to the discrepancy $\lambda_0 w_0(\varepsilon^{-1}x)$ left in (9.7a) by the boundary layer. We refer the reader to [160] for an explanation of the difficulty associated with compensation of this term, which could lead to an unbounded boundary layer term. At this point, the method of compound asymptotic expansions combined with the specific procedure of *rearrangements of discrepancies*, which is proposed in [143], can be used. To this end the discrepancy is represented as follows

$$\lambda_0 w_0(\xi) = -\varepsilon \lambda_0 v_0(\mathscr{O}) \mathrm{cap}(\omega) \|x\|^{-1} + \lambda_0 \{ w_0(\xi) + v_0(\mathscr{O}) \mathrm{cap}(\omega) \|\xi\|^{-1} \}. \tag{9.12}$$

The first term in (9.12) is written in slow variable x and the second term in the fast variable ξ. Since the first term is multiplied by ε it is taken into account by the second regular corrector v_1. The first order approximation of the simple eigenvalue at this stage takes the form

$$\lambda^\varepsilon \sim \lambda_0 + \varepsilon \lambda_1. \tag{9.13}$$

Therefore, by taking into account in (9.12) only the first order terms with respect to ε, we obtain the following boundary value problem for the second regular corrector v_1 of expansion

$$\Delta_x v_1(x) + \lambda_0 v_1(x) + \lambda_1 v_0(x) = \lambda_0 v_0(\mathscr{O}) \mathrm{cap}(\omega) \|x\|^{-1}, \quad x \in \Omega \setminus \{\mathscr{O}\}, \tag{9.14a}$$

$$v_1(x) = \|x\|^{-1} v_0(\mathscr{O}) \mathrm{cap}(\omega), \quad x \in \partial\Omega. \tag{9.14b}$$

Since λ_0 is an eigenvalue of the Dirichlet Laplacian, the compatibility conditions are required in order to assure the existence of a solution to problem (9.14a). We rewrite (9.14) in the form

$$\Delta_x v_1(x) + \lambda_0 v_1(x) = f_1(x), \quad x \in \Omega \setminus \{\mathscr{O}\}, \tag{9.15a}$$

$$v_1(x) = g_1(x), \quad x \in \partial\Omega, \tag{9.15b}$$

then multiply (9.15a) by v_0 and integrate in Ω. Taking into account that

$$\int_\Omega v_0(x)^2 dx = 1 \quad \text{and} \quad v_0(x) = -\frac{1}{\lambda_0} \Delta_x v_0(x), \tag{9.16}$$

we determine λ_1

$$\begin{aligned}\lambda_1 &= v_0(\mathscr{O})\mathrm{cap}(\omega)\left\{\lambda_0\int_\Omega \frac{v_0(x)}{\|x\|}dx + \int_{\partial\Omega}\frac{\partial_n v_0(x)}{\|x\|}ds(x)\right\}\\ &= -v_0(\mathscr{O})\mathrm{cap}(\omega)\int_\Omega v_0(x)\Delta_x(\|x\|^{-1})dx\\ &= 4\pi v_0(\mathscr{O})\mathrm{cap}(\omega)\int_\Omega \delta(x)v_0(x)dx\\ &= 4\pi v_0(\mathscr{O})^2\mathrm{cap}(\omega), \end{aligned} \tag{9.17}$$

where the notation

$$\int_\Omega \delta(x)v_0(x)dx = v_0(\mathscr{O}) \tag{9.18}$$

has been introduced for the distribution named the *Dirac measure* (point mass) $\delta(x) \in \mathscr{D}'(\mathbb{R}^3)$.

Remark 9.2. In equation (9.17) we have used $-\Delta_x(\|x\|^{-1}) = 4\pi\delta(x)$ in $\mathscr{D}'(\mathbb{R}^3)$ or *in the sense of distributions.*

Formally we have obtained

$$\lambda^\varepsilon = \lambda_0 + 4\varepsilon\pi v_0(\mathscr{O})^2\mathrm{cap}(\omega) + O(\varepsilon^2). \tag{9.19}$$

The above choice for λ_1 leads to existence of the regular corrector v_1 which is determined up to the term cv_0 with a constant c. The constant is determined by the orthogonality condition

$$\int_\Omega v_0(x)v_1(x)dx = 0. \tag{9.20}$$

Therefore, we have the following result:

Proposition 9.1. *Let us consider the boundary value problem of the form*

$$\Delta_x \mathsf{G}(x) + \lambda_0\mathsf{G}(x) = -\delta(x) + \frac{v_0(x)}{v_0(\mathscr{O})}, \quad x \in \Omega, \tag{9.21}$$

$$\mathsf{G}(x) = 0, \quad x \in \partial\Omega, \tag{9.22}$$

and denote by $\mathsf{G}^{\mathfrak{r}}(x)$ *the regular part of the solution* $\mathsf{G}(x)$*, orthogonal to* $v_0(x)$*, i.e.,*

$$\mathsf{G}^{\mathfrak{r}}(x) = \mathsf{G}(x) - \frac{1}{4\pi\|x\|}, \quad x \in \Omega \quad \textit{and} \quad \int_\Omega \mathsf{G}^{\mathfrak{r}}(x)v_0(x)dx = 0. \tag{9.23}$$

Then the first order regular corrector in the asymptotics is given by

$$v_1(x) = 4\pi v_0(\mathscr{O})\mathrm{cap}(\omega)\mathsf{G}^{\mathfrak{r}}(x). \tag{9.24}$$

Proof. The boundary value problem for the regular part takes the form

$$\begin{aligned} \Delta_x \mathsf{G}^{\mathfrak{r}}(x) + \lambda_0 \mathsf{G}^{\mathfrak{r}}(x) &= \Delta_x \mathsf{G}(x) + \lambda_0 \mathsf{G}(x) - \Delta_x \left(\frac{1}{4\pi\|x\|} \right) - \frac{\lambda_0}{4\pi\|x\|} \\ &= -\delta(x) + \frac{v_0(x)}{v_0(\mathscr{O})} - \Delta_x \left(\frac{1}{4\pi\|x\|} \right) - \frac{\lambda_0}{4\pi\|x\|} \\ &= \frac{v_0(x)}{v_0(\mathscr{O})} - \frac{\lambda_0}{4\pi\|x\|}, \quad x \in \Omega, \qquad (9.25a) \\ \mathsf{G}^{\mathfrak{r}}(x) &= \mathsf{G}(x) - \frac{1}{4\pi\|x\|}, \quad x \in \partial\Omega. \qquad (9.25b) \end{aligned}$$

The unique solution $\mathsf{G}^{\mathfrak{r}}(x)$ of (9.25) is continuous in Ω [72]. □

Remark 9.3. Let us point out that the continuous function $x \mapsto \mathsf{G}^{\mathfrak{r}}(x)$ has no singularity at the origin, therefore the value $\mathsf{G}^{\mathfrak{r}}(\mathscr{O}) = \mathsf{G}^{\mathfrak{r}}(0)$ is well defined.

9.2.2 Second Order Asymptotic Expansion

We have found the approximation of solution

$$u^{\varepsilon}(x) \sim v_0(x) + w_0(\varepsilon^{-1}x) + \varepsilon v_1(x), \qquad (9.26)$$

which leads to the discrepancy $\varepsilon v_1(\mathscr{O}) + \ nabla_x v_0(\mathscr{O}) \cdot x$ in the boundary condition (9.7a). Therefore, the second boundary layer corrector is given by the exterior problem

$$\Delta_\xi w_1(\xi) = 0, \quad \xi \in \mathbb{R}^3 \setminus \overline{\omega}, \qquad (9.27a)$$
$$w_1(\xi) = -v_1(\mathscr{O}) - \nabla_x v_0(\mathscr{O}) \cdot \xi, \quad \xi \in \partial\omega. \qquad (9.27b)$$

The solution to (9.27) admits an expansion for $\|\xi\| \to \infty$ of the form

$$w_1(\xi) = -\frac{1}{\|\xi\|} \left\{ v_1(\mathscr{O}) \mathrm{cap}(\omega) + \frac{1}{4\pi} \nabla_x v_0(\mathscr{O}) \cdot p \right\} + O(\|\xi\|^{-2}), \qquad (9.28)$$

where the vector of coefficients $p = (p_1, p_2, p_3)^\top$ is determined from the expansions

$$P_j(\xi) = -\frac{p_j}{4\pi\|\xi\|} + O(\|\xi\|^{-2}), \qquad (9.29)$$

of solutions to the exterior problems

$$\Delta_\xi P_j(\xi) = 0, \quad \xi \in \mathbb{R}^3 \setminus \overline{\omega}, \qquad (9.30a)$$
$$P_j(\xi) = -\xi_j, \quad \xi \in \partial\omega. \qquad (9.30b)$$

Proposition 9.2. *The following asymptotic formula is obtained for solution $w_0(\xi)$ of* (9.8)*:*

$$-\frac{w_0(\xi)}{v_0(\mathscr{O})} = \frac{\operatorname{cap}(\omega)}{\|\xi\|} - \frac{1}{4\pi}\sum_{j=1}^{3} q_j \frac{\xi_j}{\|\xi\|^3} + O(\|\xi\|^{-3}), \tag{9.31}$$

where $q_j = -p_j$.

Proof. We determine the coefficients q_j, $j = 1,2,3$, using the method of [149, 151]. Let us note, that the left hand side of (9.31) is given by the *capacitary potential* $\wp(\xi)$ of ω, i.e., by the solution to the exterior problem

$$\Delta_\xi \wp(\xi) = 0, \quad \xi \in \mathbb{R}^3 \setminus \overline{\omega}, \tag{9.32a}$$

$$\wp(\xi) = 1, \quad \xi \in \partial\omega, \tag{9.32b}$$

$$\lim_{\|\xi\|\to\infty} \wp(\xi) = 0. \tag{9.32c}$$

Let us insert two functions P_j and $1 - \wp$ into the Green formula in the domain $B_R \setminus \overline{\omega} := \{\xi : \rho = \|\xi\| < R\} \setminus \overline{\omega}$. By taking into account the relations (9.29) and (9.31), it follows that for $R \to \infty$,

$$\begin{aligned}
&\int_{\partial\omega} P_j(\xi)\partial_{n_\xi}(1-\wp(\xi))ds(\xi) = \\
&\int_{\partial B_R} \{(1-\wp(\xi))\partial_\rho P_j(\xi) - P_j(\xi)\partial_\rho(1-\wp(\xi))\}\, ds(\xi) = \\
&\int_{\partial B_R} \left\{\frac{p_j}{4\pi R^2} + O(R^{-3})\right\} ds(\xi) = \\
&-\frac{p_j}{4\pi}\int_{\partial B_R} ds(\xi) + o(1) = -p_j + o(1).
\end{aligned} \tag{9.33}$$

In the same way we insert the harmonic functions $\wp$ and $\xi_j - P_j$ into the Green formula in the domain $B_R \setminus \overline{\omega}$ and perform the limit passage $R \to \infty$,

$$\begin{aligned}
&\int_{\partial\omega} \wp(\xi)\partial_{n_\xi}(P_j(\xi) - \xi_j)ds(\xi) = \\
&\int_{\partial B_R} \left\{2\operatorname{cap}(\omega)\frac{\xi_j}{\|\xi\|} - \frac{3}{4\pi R^2}\sum_{k=1}^{3} q_k \frac{\xi_k}{\|\xi\|}\frac{\xi_j}{\|\xi\|} + O(R^{-3})\right\} ds(\xi) = \\
&-\int_{\partial B_R} \left\{2R\operatorname{cap}(\omega)\xi_j - \frac{3}{4\pi}\sum_{k=1}^{3} q_k\xi_k\xi_j + o(1)\right\} ds(\xi) = \\
&\frac{3q_j}{4\pi}\int_{\partial B_R} \xi_j^2 ds(\xi) + o(1) = q_j + o(1).
\end{aligned} \tag{9.34}$$

Since the functions $\wp$, P_j are harmonic and

$$\int_{\partial\omega} \frac{\partial\xi_j}{\partial n_\xi} ds(\xi) = 0, \tag{9.35}$$

then the left hand sides in (9.33) and in (9.34) are equal. Therefore, the limit passage $R \to \infty$ in the right hand sides of (9.33) and (9.34) leads to the equality $-q_j = p_j$. □

Now, we are going to determine λ_2 in the approximation

$$\lambda^\varepsilon \sim \lambda_0 + \varepsilon\lambda_1 + \varepsilon^2\lambda_2. \tag{9.36}$$

We have in hand the approximation

$$u^\varepsilon(x) \sim v_0(x) + w_0(\varepsilon^{-1}x) + \varepsilon(v_1(x) + w_1(\varepsilon^{-1}x)) + \varepsilon^2(v_2(x) + w_2(\varepsilon^{-1}x)). \tag{9.37}$$

We insert the approximation into (9.7a), which leads to the relation

$$\begin{aligned}
&\Delta_x u^\varepsilon(x) + \lambda^\varepsilon u^\varepsilon(x) \sim \qquad (9.38)\\
&\varepsilon^0 \{\Delta_x v_0(x) + \lambda_0 v_0(x)\} + \varepsilon^{-2}\Delta_\xi w_0(\xi) + \\
&\varepsilon^1 \left\{\Delta_x v_1(x) + \lambda_0 v_1(x) + \lambda_1 v_0(x) - v_0(\mathscr{O})\mathrm{cap}(\omega)\|x\|^{-1}\right\} + \varepsilon^{-1}\Delta_\xi w_1(\xi) + \\
&\varepsilon^2 \left\{\Delta_x v_2(x) + \lambda_0 v_2(x) + \lambda_1 v_1(x) + \lambda_2 v_0(x) - \lambda_1 v_0(\mathscr{O})\mathrm{cap}(\omega)\|x\|^{-1}\right\} + \\
&\varepsilon^2 \left\{\frac{\lambda_0 v_0(\mathscr{O})x\cdot p}{4\pi\|x\|^3} - \frac{\lambda_0}{\|x\|}\left(v_1(\mathscr{O})\mathrm{cap}(\omega) + \frac{1}{4\pi}\nabla_x v_0(\mathscr{O})\cdot p\right)\right\} + \\
&\varepsilon^0 \left\{\Delta_\xi w_2(\xi) + \lambda_0\left(w_0(\xi) + v_0(\mathscr{O})\left(\frac{\mathrm{cap}(\omega)}{\|\xi\|} - \frac{\xi\cdot p}{4\pi\|\xi\|^3}\right)\right)\right\} + O\left(\varepsilon^3 + \frac{1}{\varepsilon\|\xi\|^2}\right).
\end{aligned}$$

The terms of order $O(\varepsilon^0)$ and order $O(\varepsilon^1)$ written in the variable x on the right hand side of relation (9.38) are null by the choice of functions v_0 and v_1. The terms of order $O(\varepsilon^2)$ vanish if the regular corrector $v_2(x)$ satisfies the equation

$$\begin{aligned}
&\Delta_x v_2(x) + \lambda_0 v_2(x) + \lambda_1 v_1(x) + \lambda_2 v_0(x) = \lambda_1 v_0(\mathscr{O})\mathrm{cap}(\omega)\|x\|^{-1} - \\
&\lambda_0 \frac{v_0(\mathscr{O})x\cdot p}{4\pi\|x\|^3} + \frac{\lambda_0}{\|x\|}\left(v_1(\mathscr{O})\mathrm{cap}(\omega) + \frac{1}{4\pi}\nabla_x v_0(\mathscr{O})\cdot p\right), \quad x \in \Omega. \qquad (9.39)
\end{aligned}$$

Now we insert (9.37) into (9.7b) and find

$$\begin{aligned}
&u^\varepsilon(x) \sim \varepsilon^0 v_0(x) + \varepsilon^1\left\{v_1(x) - \frac{v_0(\mathscr{O})\mathrm{cap}(\omega)}{\|x\|}\right\} + \qquad (9.40)\\
&\varepsilon^2\left\{v_2(x) + \frac{v_0(\mathscr{O})x\cdot p}{4\pi\|x\|^3} - \frac{1}{\|x\|}\left(v_1(\mathscr{O})\mathrm{cap}(\omega) + \frac{1}{4\pi}\nabla_x v_0(\mathscr{O})\cdot p\right)\right\} + O(\varepsilon^3).
\end{aligned}$$

The terms of orders $O(\varepsilon^0)$ and $O(\varepsilon^1)$ vanish in (9.40) in view of the boundary conditions for $v_0(x)$ and $v_1(x)$. To make the term of order $O(\varepsilon^2)$ vanish we must set

$$v_2(x) = \frac{1}{\|x\|}\left(v_1(\mathscr{O})\mathrm{cap}(\omega) + \frac{1}{4\pi}\nabla_x v_0(\mathscr{O})\cdot p\right) - \frac{v_0(\mathscr{O})x\cdot p}{4\pi\|x\|^3}, \quad x \in \partial\Omega. \tag{9.41}$$

The boundary value problem for v_2 is now completed, it contains (9.39) along with the boundary conditions (9.41). The boundary value problem can be rewritten as follows

$$\Delta_x v_2(x) + \lambda_0 v_2(x) = f_2(x), \quad x \in \Omega, \tag{9.42a}$$
$$v_2(x) = g_2(x), \quad x \in \partial\Omega, \tag{9.42b}$$

where f_2 and g_2 are respectively defined as

$$f_2(x) := -\lambda_1 v_1(x) - \lambda_2 v_0(x) + \lambda_1 v_0(\mathscr{O})\mathrm{cap}(\omega)\|x\|^{-1}$$
$$-\lambda_0 \frac{v_0(\mathscr{O})x\cdot p}{4\pi\|x\|^3} + \frac{\lambda_0}{\|x\|}\left(v_1(\mathscr{O})\mathrm{cap}(\omega) + \frac{1}{4\pi}\nabla_x v_0(\mathscr{O})\cdot p\right), \tag{9.43}$$
$$g_2(x) := \frac{1}{\|x\|}\left(v_1(\mathscr{O})\mathrm{cap}(\omega) + \frac{1}{4\pi}\nabla_x v_0(\mathscr{O})\cdot p\right) - \frac{v_0(\mathscr{O})x\cdot p}{4\pi\|x\|^3}. \tag{9.44}$$

The term λ_2 is determined from the compatibility conditions for problem (9.42). We take into account that

$$\int_\Omega v_0(x)^2 dx = 1, \quad \int_\Omega v_0(x)v_1(x)dx = 0, \tag{9.45}$$

and we evaluate

$$\begin{aligned}\lambda_2 &= \int_\Omega f_2(x)v_0(x)dx + \int_{\partial\Omega} g_2(x)\partial_n v_0(x)ds(x) \\ &= \lambda_1 v_0(\mathscr{O})\mathrm{cap}(\omega)\int_\Omega \frac{v_0(x)}{\|x\|}dx \\ &+ \frac{v_0(\mathscr{O})}{4\pi}\sum_{j=1}^{3} p_j\left[\int_\Omega \frac{x_j\Delta_x v_0(x)}{\|x\|^3}dx - \int_{\partial\Omega}\frac{x_j\partial_n v_0(x)}{\|x\|^3}ds(x)\right] \\ &- \left(v_1(\mathscr{O})\mathrm{cap}(\omega) + \frac{\nabla_x v_0(\mathscr{O})\cdot p}{4\pi}\right)\left\{\int_\Omega \frac{\Delta_x v_0(x)}{\|x\|}dx - \int_{\partial\Omega}\frac{\partial_n v_0(x)}{\|x\|}ds(x)\right\}.\end{aligned} \tag{9.46}$$

We find

$$\int_\Omega \frac{x_j\Delta_x v_0(x)}{\|x\|^3}dx - \int_{\partial\Omega}\frac{x_j\partial_n v_0(x)}{\|x\|^3}ds(x) = 4\pi\int_\Omega v_0(x)\partial_{x_j}\delta(x)dx = 4\pi\partial_{x_j}v_0(\mathscr{O}), \tag{9.47}$$

and

$$\int_\Omega \frac{\Delta_x v_0(x)}{\|x\|}dx - \int_{\partial\Omega}\frac{\partial_n v_0(x)}{\|x\|}ds(x) = -4\pi\int_\Omega v_0(x)\delta(x)dx = -4\pi v_0(\mathscr{O}). \tag{9.48}$$

Thus, we obtain the second corrector in the expansion of the eigenvalue λ^ε, namely

$$\lambda_2 = \lambda_1 v_0(\mathscr{O})\mathrm{cap}(\omega)\int_\Omega \frac{v_0(x)}{\|x\|}dx + 4\pi v_0(\mathscr{O})v_1(\mathscr{O})\mathrm{cap}(\omega). \tag{9.49}$$

In view of (9.19) and (9.24) the obtained formula takes the form

$$\lambda_2 = [4\pi v_0(\mathscr{O})\mathrm{cap}(\omega)]^2 \left(\frac{1}{4\pi} \int_\Omega \frac{v_0(x)}{\|x\|} dx - \mathsf{G}^{\mathfrak{r}}(\mathscr{O}) \right). \tag{9.50}$$

Proposition 9.3. *If* λ_2 *is given by* (9.50) *then there exists the unique bounded solution* v_2 *of problem* (9.42)*, orthogonal to* v_0*. The function looses its continuity at the origin because of the presence of the singular term*

$$\frac{v_0(\mathscr{O}) x \cdot p}{4\pi \|x\|^3} \tag{9.51}$$

in the right hand side of equation (9.42a)*. In addition, the function* v_2 *admits the representation for* $\|x\| \to 0$*,*

$$v_2(x) = c + \frac{v_0(\mathscr{O}) x \cdot p}{2\pi \|x\|} + O(\|x\|). \tag{9.52}$$

Remark 9.4. The relation (9.38) shows that the boundary layer w_2 in (9.37) should be given by the solution of Poisson problem

$$\Delta_\xi w_2(\xi) = -\lambda_0 \left(w_0(\xi) + v_0(\mathscr{O}) \left(\frac{\mathrm{cap}(\omega)}{\|\xi\|} - \frac{\xi \cdot p}{4\pi \|\xi\|^3} \right) \right), \quad \xi \in \mathbb{R}^3 \setminus \overline{\omega}. \tag{9.53}$$

In view of (9.31) the right hand side of (9.53) is of order $O(\|\xi\|^{-3})$. Therefore, in the same way as for w_0 and w_1, it follows that $w_2(\xi) = O(\|\xi\|^{-1})$.

9.2.3 Complete Asymptotic Expansion

We have seen already that for an arbitrary integer $N \in \mathbb{N}$ the N-th order asymptotic expansion with respect to small parameter $\varepsilon \to 0$ for solutions of Problem (9.5) can be found in the form of *ansätze*

$$\lambda^\varepsilon = \sum_{k=0}^{N} \varepsilon^k \lambda_k + \lambda_N^\varepsilon, \tag{9.54a}$$

$$u^\varepsilon(x) = \sum_{k=0}^{N} \varepsilon^k \left(v_k(x) + w_k\left(\frac{x}{\varepsilon}\right) \right) + u_N^\varepsilon(x), \tag{9.54b}$$

where v_k stand for the regular correctors of expansion of eigenfunction, and w_k are boundary layer correctors of the same expansion. The regular and boundary layer correctors of the expansion (9.54b) are supposed to have the form

$$v_k(x) = \sum_{j=0}^{J-1} \|x\|^j v_k^{(j)}\left(\frac{x}{\|x\|}\right) + v_{k,J}(x), \tag{9.55a}$$

$$w_k(\xi) = \sum_{j=0}^{J-1} \|\xi\|^{-j-1} w_k^{(j)}\left(\frac{\xi}{\|\xi\|}\right) + w_{k,J}(\xi). \tag{9.55b}$$

We denote by $v_k^{(j)}(x)$ and $w_k^{(j)}(\xi)$ smooth functions on the unit sphere ∂B_1. For the remainders, which can be *differentiated term by term*, the following relations are postulated and actually can be shown

$$v_{k,J}(x) = O\left(\|x\|^J\right) \quad \text{and} \quad w_{k,J}(\xi) = O\left(\|\xi\|^{-J-1}\right). \tag{9.56}$$

We insert expansion (9.54) into Problem 9.5 and apply the specific procedure of *rearrangements of discrepancies*. It means that we decompose terms $\lambda_n w_m$ in the following way,

$$\lambda_n w_m\left(\frac{x}{\varepsilon}\right) = \varepsilon \frac{\lambda_n}{\|x\|} w_m^{(0)}\left(\frac{x}{\|x\|}\right) + \varepsilon^2 \frac{\lambda_n}{\|x\|^2} w_m^{(1)}\left(\frac{x}{\|x\|}\right) + \lambda_n w_{m,2}\left(\frac{x}{\varepsilon}\right). \tag{9.57}$$

In the next step of the procedure, in the Dirichlet boundary conditions (9.7b) and (9.7c) on $\partial\Omega$ and $\partial\omega_\varepsilon$, the functions w_k and v_k are developed in infinite series with $J=\infty$, and the coordinates x are used on $\partial\Omega$, the coordinates ξ on $\partial\omega_\varepsilon$, here we take into account that $x \in \partial\omega_\varepsilon$ if $\xi \in \partial\omega$. Finally, the coordinates x are used on Ω_ε. Taking into account the decompositions (9.57) in the equations resulting from Problem 9.5, we select the coefficients of the same powers of ε. As a result, recurrent system of boundary value problems is obtained. The Dirichlet problems for regular correctors in (punctured) domain

$$\Delta_x v_k(x) + \sum_{n=0}^{k} \lambda_n v_{k-n}(x) = -\sum_{n=0}^{k-1} \lambda_n \left\{ \tfrac{1}{\|x\|} w_{k-n-1}^{(0)}\left(\tfrac{x}{\|x\|}\right) + \tfrac{1}{\|x\|^2} w_{k-n-2}^{(1)}\left(\tfrac{x}{\|x\|}\right)\right\}, x \in \Omega, \tag{9.58a}$$

$$v_k(x) = -\sum_{n=0}^{k-1} \tfrac{1}{\|x\|^{n+1}} w_{k-n-1}^{(n)}\left(\tfrac{x}{\|x\|}\right), \quad x \in \partial\Omega, \tag{9.58b}$$

and the exterior Dirichlet problem for boundary layer correctors

$$\Delta_\xi w_k(\xi) = -\sum_{n=0}^{k-2} \lambda_n w_{k-n-2,2}(\xi), \quad \xi \in \mathbb{R}^3 \setminus \overline{\omega}, \tag{9.59a}$$

$$w_k(\xi) = -\sum_{n=0}^{k} \|\xi\|^n v_{k-n}^{(n)}\left(\tfrac{\xi}{\|\xi\|}\right), \quad \xi \in \partial\omega, \tag{9.59b}$$

where only nonnegative indices are allowed i.e., with the convention that the functions with negative indices are simply null. We assume also the orthogonality conditions

$$\int_{\Omega} v_k(x) v_0(x) dx = 0 \quad \text{for } k = 1, 2, \ldots \tag{9.59c}$$

The compatibility conditions for problem (9.58) leads to the equalities for the coefficients of the expansion (9.54a), actually

$$\begin{aligned} \lambda_k = & -\sum_{n=0}^{k-1} \lambda_n \int_{\Omega} \left[\|x\| w_{k-n-1}^{(0)} \left(\frac{x}{\|x\|} \right) + w_{k-n-2}^{(1)} \left(\frac{x}{\|x\|} \right) \right] \frac{v_0(x)}{\|x\|^2} dx \\ & -\sum_{n=0}^{k-1} \int_{\partial\Omega} w_{k-n-1}^{(n)} \left(\frac{x}{\|x\|} \right) \frac{\partial_n v_0(x)}{\|x\|^{1+n}} ds(x). \end{aligned} \tag{9.59d}$$

The following result given in [160] is presented here without proof.

Theorem 9.1. *Let λ_0 be a simple eigenvalue for Problem 9.3. In a vicinity of λ_0 there is a unique simple eigenvalue λ^ε of Problem 9.5, with the associated eigenfunction $u^\varepsilon(x)$ that admits expansion* (9.54)*. The coefficients of the expansion are given by system* (9.59)*, with the estimates for remainders*

$$\lambda_N^\varepsilon = O\left(\varepsilon^{N+1}\right) \quad \text{and} \quad u_N^\varepsilon(x) = O\left(\varepsilon^{N+1} \left(1 + \frac{\varepsilon}{\|x\|} \right) \right). \tag{9.60}$$

In addition, the remainder $u_N^\varepsilon(x)$ in (9.60) *can be* differentiated term by term.

Note 9.3. By Theorem 9.1 combined with (9.19) and (9.50) it follows that

$$\begin{aligned} \lambda^\varepsilon = & \lambda_0 + 4\pi v_0(\mathscr{O})^2 \text{cap}(\omega_\varepsilon) \\ & - 16\pi^2 v_0(\mathscr{O})^2 \text{cap}(\omega_\varepsilon)^2 \left(\mathsf{G}^\mathfrak{r}(\mathscr{O}) - \frac{1}{4\pi} \int_{\Omega} \frac{v_0(x)}{\|x\|} dx \right) + O(\text{cap}(\omega_\varepsilon)^3). \end{aligned} \tag{9.61}$$

Hence, for $f(\varepsilon) := 4\pi\text{cap}(\omega_\varepsilon)$ we obtain the *two term* expansion of a simple eigenvalue

$$\lambda^\varepsilon = \lambda_0 + f(\varepsilon) v_0(\mathscr{O})^2 + f(\varepsilon)^2 v_0(\mathscr{O})^2 \left(\mathsf{G}^\mathfrak{r}(\mathscr{O}) - \frac{1}{4\pi} \int_{\Omega} \frac{v_0(x)}{\|x\|} dx \right) + O(f(\varepsilon)^3).$$

Therefore, we can identify

- the first order topological derivative of a simple eigenvalue

$$v_0(\mathscr{O})^2 = \lim_{\varepsilon \to 0} \frac{\lambda^\varepsilon - \lambda_0}{f(\varepsilon)};$$

- the second order topological derivative of a simple eigenvalue

$$v_0(\mathscr{O})^2 \left(\mathsf{G}^\mathfrak{r}(\mathscr{O}) - \frac{1}{4\pi} \int_{\Omega} \frac{v_0(x)}{\|x\|} dx \right) = \lim_{\varepsilon \to 0} \frac{\lambda^\varepsilon - \lambda_0 - f(\varepsilon) v_0(\mathscr{O})^2}{f(\varepsilon)^2}.$$

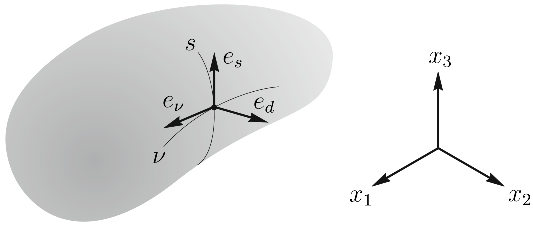


Fig. 9.1 Orthonormal curvilinear coordinate system (d,s,ν) in $\mathfrak{N}$

9.3 Neumann Laplacian in Domains with Small Caverns

In this section the *Neumann spectral problem* is considered. The asymptotic expansions of eigenvalues and eigenfunctions for the spectral problem defined in singularly perturbed domain are derived in the framework of the compound asymptotic expansions method. The cavities are close to the boundary (caverns). The size of the caverns is governed by a small parameter $h \to 0$.

Let $\Omega \subset \mathbb{R}^3$ be a bounded domain with a smooth boundary $\Gamma := \partial\Omega$, whose origin $\mathscr{O} \in \Gamma$. For a sufficiently small neighborhood $\mathfrak{N}$ of the point $\mathscr{O}$ there exists a conformal mapping which maps $\mathfrak{N}$ onto a neighborhood of the origin in the cartesian coordinate system. The associated orthonormal curvilinear coordinate system (d,s,ν) is introduced in $\mathfrak{N}$ (see fig. 9.1), where the *tangential coordinates* (s,ν) are the local surface coordinates on Γ at the origin $\mathscr{O}$, and coordinate d stands for the *oriented distance function* [50, 196] to Γ, with the convention that $d > 0$ in $\Omega^c = \mathbb{R}^3 \setminus \overline{\Omega}$. We denote (e_d, e_s, e_ν) the basis for the curvilinear coordinate system (d,s,ν). We assume that $\omega \subset \mathbb{R}^3_- = (-\infty,0)\times\mathbb{R}^2$ (see fig. 9.2), is a Lipschitz domain with the compact closure $\overline{\omega} = \omega \cup \partial\omega$. The boundary $\partial\Xi$ of unbounded domain $\Xi = \mathbb{R}^3_- \setminus \overline{\omega}$ is also Lipschitz. The singularly perturbed domain $\Omega_h = \Omega \setminus \overline{\omega_h}$ depends on the small parameter $h \to 0$, where

$$\omega_h = \{(d,s,\nu) : \xi = (\xi_1,\xi_2,\xi_3) := (h^{-1}d, h^{-1}s, h^{-1}\nu) \in \omega\}, \tag{9.62}$$

and the *Neumann Laplace spectral problem* in Ω_h is introduced:

Problem 9.6. Find $(u^h, \lambda^h) \in H^1(\Omega_h) \times \mathbb{R}_+$ such that

$$-\Delta_x u^h(x) = \lambda^h u^h(x), \quad x \in \Omega_h, \tag{9.63a}$$

$$\partial_{\mathfrak{n}} u^h(x) = 0, \quad x \in \Gamma_h := \partial\Omega_h, \tag{9.63b}$$

where $\partial_{\mathfrak{n}}\varphi = \nabla_x\varphi \cdot \mathfrak{n}$ denotes the normal derivative of φ along the outer normal $\mathfrak{n}$ on the boundary $\partial\Omega_h$.

The general theory applies (see Appendix A) and Problem 9.6 admits the sequence of eigenvalues

$$0 = \lambda_0^h < \lambda_1^h \leqslant \lambda_2^h \leqslant \cdots \leqslant \lambda_m^h \leqslant \cdots \to +\infty, \tag{9.64}$$

where the multiplicity is explicitly indicated. The orthonormal eigenfunctions u_0^h, u_1^h, $u_2^h, \ldots, u_m^h, \ldots$ satisfy

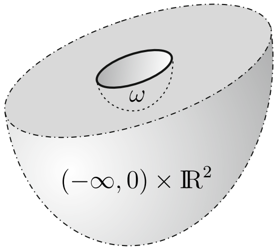


Fig. 9.2 The domain $\mathbb{R}^3_-$ with a cavern ω

$$(u_p^h, u_m^h)_{\Omega_h} = \delta_{pm}, \qquad p, m \in \mathbb{N}^* := \{0\} \cup \mathbb{N}. \tag{9.65}$$

We prove in Appendix B that for a fixed index m the eigenvalue λ_m^h of the perturbed problem in the sequence (9.64) converges with $h \to 0$ to the eigenvalue λ_m^0 in the sequence

$$0 = \lambda_0^0 < \lambda_1^0 \leqslant \lambda_2^0 \leqslant \cdots \leqslant \lambda_m^0 \leqslant \cdots \to +\infty, \tag{9.66}$$

for the limit spectral Neumann problem:

Problem 9.7. Find $(u^0, \lambda^0) \in H^1(\Omega) \times \mathbb{R}_+$ such that

$$-\Delta_x v^0(x) = \lambda^0 v^0(x), \quad x \in \Omega, \tag{9.67a}$$

$$\partial_n v^0(x) = 0, \quad x \in \Gamma := \partial\Omega. \tag{9.67b}$$

Therefore, an eigenfunction v^0 is used as the first approximation of u^h. The eigenfunctions of (9.67) are smooth in $\overline{\Omega}$ and satisfy the orthogonality and normalization conditions

$$(v_p^0, v_m^0)_\Omega = \delta_{pm}, \qquad p, m \in \mathbb{N}^*. \tag{9.68}$$

We propose the following asymptotic *ansätze* for λ_m^h and u_m^h

$$\lambda_m^h = \lambda_m^0 + h^3 \lambda_m' + \ldots \tag{9.69}$$

$$u_m^h(x) = v_m^0(x) + h\chi(x) w_m^1(\xi) + h^2 \chi(x) w_m^2(\xi) + h^3 v_m^3(x) + \ldots \tag{9.70}$$

Here $x \mapsto v_m^0(x), v_m^2(x)$ are *regular correctors* and $\xi \mapsto w_m^1(\xi), w_m^2(\xi)$ are *boundary layer correctors*, which depend on the *fast variables* $\xi = (\xi_1, \xi_2, \xi_3)$. The cut-off function $\chi \in C^\infty(\overline{\Omega})$, $0 \leqslant \chi \leqslant 1$, satisfies $\chi(x) = 1$ in a small neighborhood of $\mathscr{O}$, i.e., for $x \in B_\varepsilon = \{x : \|x - \mathscr{O}\| < \varepsilon\} \cap \overline{\Omega}$, with $\varepsilon > 0$ sufficiently small, and $\chi(x) = 0$ outside of a larger neighborhood $\mathfrak{N}$ of $\mathscr{O}$.

Remark 9.5. Let us observe the absence of terms $O(h^1)$ and $O(h^2)$ in (9.69) and of the regular correctors of the same order in (9.70).

Note 9.4. We present a formal preliminary description of the asymptotic procedure of construction the compound asymptotic expansion of the solution to Problem 9.6, which is summarized below:

- Inserting v_m^0 and λ_m^0 into Problem 9.6 causes a discrepancy in the boundary condition on the surface $\partial\Omega_h \cap \partial\omega_h$ of the cavern $\overline{\omega_h}$. This discrepancy cannot be compensated by a smooth function of the variables (d,s,ν). Hence, using the stretched curvilinear coordinates ξ defined in (9.62), we arrive at the first boundary layer corrector given by a solution to the exterior Neumann problem in the unbounded (infinite) domain Ξ (fig. 9.2). The solution decays at infinity as a linear combination of derivatives of the *fundamental solution* for the Laplacian,

$$h\left(c_1\partial_{\xi_1}+c_2\partial_{\xi_2}\right)\frac{1}{4\pi\|\xi\|}, \tag{9.71}$$

and after multiplication by an appropriate cut-off function the main asymptotic term (9.71) of the boundary layer produces lower order discrepancies in equation (9.63a) and in the Neumann conditions (9.63b).

- The expression (9.71) can be rewritten in the original coordinates (d,s,ν) and becomes

$$h^3\left(c_1\partial_s+c_2\partial_\nu\right)\left(4\pi(d^2+s^2+\nu^2)^{1/2}\right)^{-1}. \tag{9.72}$$

The function (9.72) is not singular far from the point $\mathscr{O}$ where the discrepancies are mainly located due to the cut-off function. These discrepancies are compensated by a lower order regular corrector (in the variable x) determined by a boundary value problem whose compatibility conditions depend on a smooth function. In addition, such a regular term represents the main asymptotic correction of the eigenvalue λ_j^0.
- The coefficients of differential operators written in the curvilinear coordinates depends on curvilinear variables, which influences the construction of asymptotic expansions and the estimates derivation for the asymptotic remainders. For example, the discrepancies of the expression (9.71) appears in the problem in Ξ for the next boundary layer corrector as well as in the problem for the next regular corrector within the procedure of *rearrangement of discrepancies* [143]. This procedure is in common use in this section without any indication, and it has been explained in Section 9.2 for a simpler problem.
- The general structure of singularities of the regular and boundary layer correctors for $x\to\mathscr{O}$ and $\xi\to\infty$, respectively, is predicted by the Kondratiev theory [117] (see also monographs [121, 170]) but exact formulas for the decompositions of the solutions should be evaluated.
- The method of compound asymptotic expansions [143] is applied to identify different terms of ansätze (9.69)-(9.70). In Sections 9.3.1 and 9.3.2 the first and second boundary layers w_m^1 and w_m^2 in (9.69) are determined, respectively. The functions w_m^1 and w_m^2 decay for $\|\xi\|\to\infty$, with order $\|\xi\|^{-2}$ and $\|\xi\|^{-1}$, respectively. The regular corrector v_m^3 in (9.70) is determined in Section 9.3.3. With this correction, the term λ_m' of ansätz (9.69) is obtained. It is given by (9.157) in the case of a simple eigenvalue λ_m^0 and by (9.167) in the case of multiple eigenvalues.
- The justification of asymptotic expansions is given in Appendix B. It uses the *weighted Poincaré inequality* of Lemma B.2. The derivation of estimates for the remainders in ansätze (9.69)-(9.70) is performed for an abstract equation in the Hilbert space and it uses Lemma A.1 on *almost eigenvalues and eigenvectors*. The simple and multiple eigenvalues are considered.

9.3.1 First Boundary Layer Corrector

The projection of a point $P = P(d,s,\nu) \in \mathfrak{N}$ in a neighborhood of the origin $\mathscr{O} \in \Gamma$ onto Γ is denoted by $P_\Gamma = P_\Gamma(s,\nu) \in \Gamma$,

$$P(d,s,\nu) = d\,e_d + P_\Gamma(s,\nu). \tag{9.73}$$

Let us recall, that the components of the metric tensor are given by (see e.g., [51, pp. 83]):

$$\begin{aligned}
g_{dd} = \|\partial_d P\|^2 &= \|e_d\|^2 = 1, && (9.74)\\
g_{ss} = \|\partial_s P\|^2 &= \|d\partial_s e_d + \partial_s P_\Gamma(s,\nu)\|^2 \\
&= \|d\varkappa_s(s,\nu)e_s + d\tau_s(s,\nu)e_\nu + e_s\|^2 \\
&= (1 + d\varkappa_s(s,\nu))^2 + (d\tau_s(s,\nu))^2, && (9.75)\\
g_{\nu\nu} = \|\partial_\nu P\|^2 &= \|\nu\partial_\nu e_d + \partial_\nu P_\Gamma(s,\nu)\|^2 \\
&= \|\nu\varkappa_\nu(s,\nu)e_\nu + d\tau_\nu(s,\nu)e_s + e_\nu\|^2 \\
&= (1 + d\varkappa_\nu(s,\nu))^2 + (d\tau_\nu(s,\nu))^2, && (9.76)
\end{aligned}$$

where $\varkappa_s$ and $\varkappa_\nu$ stand for the two curvatures corresponding to the curves $\nu = const$ and $s = const$ containing the surface point (s,ν), respectively, while τ_s and τ_ν are the torsions of these curves, respectively. Since the coordinates system corresponding to (d,s,ν) is orthogonal, we have $g_{ds} = g_{d\nu} = g_{s\nu} = 0$. We can always assume, shrinking the neighborhood $\mathfrak{N}$, that $1 + d\varkappa_s > 0$ and $1 + d\varkappa_\nu > 0$ in $\mathfrak{N}$. Thus, the Jacobian is equal

$$\mathfrak{g}(d,s,\nu) = \left[(1 + d\varkappa_s)^2 + (d\tau_s)^2\right]^{1/2} \left[(1 + d\varkappa_s) + (d\tau_\nu)^2\right]^{1/2}. \tag{9.77}$$

The Laplace operator Δ_x in the curvilinear coordinates (d,s,ν) admits the representation

$$\begin{aligned}
\Delta_x &= \mathfrak{g}^{-1}\left[\partial_d(\mathfrak{g}\partial_d) + \partial_s\left(\frac{\mathfrak{g}}{g_{ss}}\partial_s\right) + \partial_\nu\left(\frac{\mathfrak{g}}{g_{\nu\nu}}\partial_\nu\right)\right] \\
&= \partial_d^2 + g_{ss}^{-1}\partial_s^2 + g_{\nu\nu}^{-1}\partial_\nu^2 + \mathfrak{g}^{-1}\partial_d\mathfrak{g}\partial_d \\
&+ \mathfrak{g}^{-1}\left(\left[\frac{\partial_s\mathfrak{g}}{g_{ss}} - \frac{\mathfrak{g}\partial_s g_{ss}}{g_{ss}^2}\right]\partial_s + \left[\frac{\partial_\nu\mathfrak{g}}{g_{\nu\nu}} - \frac{\mathfrak{g}\partial_\nu g_{\nu\nu}}{g_{\nu\nu}^2}\right]\partial_\nu\right).
\end{aligned} \tag{9.78}$$

If the transformation defined in (9.62) with $\xi = (\xi_1, \xi_2, \xi_3)$ is performed, the terms depending on the torsion in $\mathfrak{g}(d,s,\nu)$ are of order $O(h^2)$. Hence in the expression of the Laplace operator the terms of orders $O(h^{-2})$ and $O(h^{-1})$ are independent of the torsion,

$$\Delta_x \sim h^{-2}\Delta_\xi + h^{-1}\left(\varkappa_s(\mathscr{O})(\partial_{\xi_1} - 2\xi_1\partial_{\xi_2}^2) + \varkappa_\nu(\mathscr{O})(\partial_{\xi_1} - 2\xi_1\partial_{\xi_3}^2)\right). \tag{9.79}$$

In the coordinates (d,s,ν) the gradient takes the form

$$\begin{aligned}\nabla_x &= \left(g_{dd}{}^{-1/2}\partial_d, g_{ss}{}^{-1/2}\partial_s, g_{\nu\nu}{}^{-1/2}\partial_\nu\right)\\ &= \left(\partial_d, (1+d\varkappa_s)^{-1}\partial_s, (1+d\varkappa_\nu)^{-1}\partial_\nu\right). \end{aligned} \tag{9.80}$$

The decomposition of the unit normal vector $\mathfrak{n}$ to Ω_h in the basis (e_d, e_s, e_ν) is

$$\mathfrak{n} = \mathfrak{d}^{-1/2}\left[N_1\mathfrak{g}e_d + N_2(1+d\varkappa_\nu)e_s + N_3(1+d\varkappa_s)e_\nu\right], \tag{9.81}$$

with

$$\mathfrak{d} = [N_1\mathfrak{g}]^2 + [N_2(1+d\varkappa_\nu)]^2 + [N_3(1+d\varkappa_s)]^2, \tag{9.82}$$

where $N = (N_1, N_2, N_3)$ is the outward unit normal vector on the boundary $\partial\Xi \subset \mathbb{R}^3$. Therefore, denoting by ∂_N the directional derivative along N, we obtain

$$\begin{aligned}\partial_\mathfrak{n} &= d^{-1/2}\left(N_1\mathfrak{g}\partial_d + N_2\frac{1+d\varkappa_\nu}{1+d\varkappa_s}\partial_s + N_3\frac{1+d\varkappa_s}{1+d\varkappa_\nu}\partial_\nu\right)\\ &\sim h^{-1}\partial_N + \xi_1(N_2^2\varkappa_s(\mathcal{O}) + N_3^2\varkappa_\nu(\mathcal{O}))\partial_N\\ &- 2\xi_1(N_2\varkappa_s(\mathcal{O})\partial_{\xi_2} + N_3\varkappa_\nu(\mathcal{O})\partial_{\xi_3}). \end{aligned} \tag{9.83}$$

In view of the homogeneous Neumann boundary condition (9.67b), the function v^0 in the ℓ-neighborhood of the origin $\mathcal{O}$, with $\ell := Ch$, admits the expansion

$$\begin{aligned}v^0(x) &= v^0(\mathcal{O}) + s\partial_s v^0(\mathcal{O}) + \nu\partial_\nu v^0(\mathcal{O}) + \frac{1}{2}(d^2\partial_d^2 v^0(\mathcal{O}) + s^2\partial_s^2 v^0(\mathcal{O})\\ &+ \nu^2\partial_\nu^2 v^0(\mathcal{O}) + 2s\nu\partial_{s\nu}^2 v^0(\mathcal{O})) + O((d^2+s^2+\nu^2)^{3/2})\\ &= v^0(\mathcal{O}) + h(\xi_2\partial_s v^0(\mathcal{O}) + \xi_3\partial_\nu v^0(\mathcal{O})) + \frac{1}{2}h^2(\xi_1^2\partial_d^2 v^0(\mathcal{O})\\ &+ \xi_2^2\partial_s^2 v^0(\mathcal{O}) + \xi_3^2\partial_\nu^2 v^0(\mathcal{O}) + 2\xi_2\xi_3\partial_{\xi_2\xi_3}^2 v^0(\mathcal{O})) + O(h^3). \end{aligned} \tag{9.84}$$

Under the coordinate dilation by factor h^{-1} and setting $h=0$, the domain Ω_h becomes $\Xi = \mathbb{R}^3_- \setminus \overline{\omega}$, thus the boundary layer w^1 is defined in Ξ. Let us replace u^h, Δ and $\partial_\mathfrak{n}$ by their expansions in (9.70), (9.79) and (9.83), respectively. Then, after collecting the terms of order $O(h^{-1})$ in the equation and of order $O(h^0)$ in the boundary conditions, we arrive at the following boundary value problem, obtained formally for $h=0$,

$$-\Delta_\xi w^1(\xi) = 0, \quad \xi \in \Xi, \tag{9.85a}$$

$$\partial_N w^1(\xi) = -N_2(\xi)\partial_s v^0(\mathcal{O}) - N_3(\xi)\partial_\nu v^0(\mathcal{O}), \quad \xi \in \partial\Xi. \tag{9.85b}$$

Now we make use of the evident formulae

$$\int_{\partial\Xi\cap\partial\omega} N_k(\xi)\,ds_\xi = 0, \int_{\partial\Xi\cap\partial\omega} \xi_j N_k(\xi)\,ds_\xi = -\delta_{jk}|\omega|, \text{ for } j,k = 1,2,3. \tag{9.86}$$

The first formula in (9.86) shows that the right hand side of the boundary condition in (9.85b) is of the null mean value over the surface $\partial\Xi$. Note that $N_2 = N_3 = 0$ on the plane surface $\partial\Xi \setminus \partial\omega$ of the boundary $\partial\Xi$ therefore the right hand side in (9.85b) is compactly supported. Thus, there exists a unique generalized solution $w^1 \in H^1_{\rm loc}(\overline{\Xi})$ of problem (9.85), decaying at infinity. The solution is represented in the form

$$w^1(\xi) = \partial_s v^0(\mathscr{O})W_2(\xi) + \partial_v v^0(\mathscr{O})W_3(\xi), \tag{9.87}$$

where W_2 and W_3 are canonical solutions of the Neumann problem

$$-\Delta_\xi W_k(\xi) = 0, \quad \xi \in \Xi, \tag{9.88a}$$

$$\partial_n W_k(\xi) = -N_k(\xi), \quad \xi \in \partial\Xi. \tag{9.88b}$$

They admit the representation

$$W_k(\xi) = -\sum_{j=2}^{3} \frac{m_{kj}}{2\pi}\frac{\xi_j}{\rho^3} + O(\|\xi\|^{-3}), \quad \|\xi\| > R, \tag{9.89}$$

where R is sufficiently large and the coefficients m_{kj} of the *virtual mass matrix* are introduced in [198, Note G], a generalization of this tensor is described in details in Appendix D. The notation used in (9.89) requires some explanation.

Condition 9.1. We say that

$$z(\xi) = z_0(\xi) + O(\rho^{-p}) \qquad \text{for } \rho = \|\xi\| \to \infty, \tag{9.90}$$

holds in an infinite set $\{\xi \,:\, \rho = \|\xi\| > R\}$, with R sufficiently large, provided that the following conditions are verified:

$$z(\xi) = z_0(\xi) + \widetilde{z}(\xi), \quad \text{with} \quad \|\nabla^q_\xi \widetilde{z}(\xi)\| \leqslant c_q \rho^{-p-q}, \quad q \in \mathbb{N}_0, \tag{9.91}$$

where $\nabla^q_\xi \widetilde{z}$ is used to denote the collection of derivatives of order $q \in \mathbb{N}$ of the remainder $\widetilde{z}$.

Remark 9.6. For a solution w^1 of problem (9.85), an estimate of the form (9.91) is obtained for the remainder $\widetilde{w}^1$, since the remainder verifies the Laplace equation in $\{\xi \in \mathbb{R}^3_- : \rho > R\}$. The Fourier method applied to the Laplace equation can produces a convergent series with harmonic functions decaying at infinity for the representation of a solution. In Condition 9.1, the required pointwise estimates for the remainder in the representation (9.107) follow from the general theory (see [152] and [170, Chapter 3]).

In the spherical coordinate system (ρ, θ, ϕ) we have $\xi_1 = \rho\cos\phi$, $\xi_2 = \rho\cos\theta\sin\phi$, $\xi_3 = \rho\sin\theta\sin\phi$ and

$$W_2(\xi) = -\frac{m_{22}}{2\pi}\rho^{-2}\cos\theta\sin\phi - \frac{m_{23}}{2\pi}\rho^{-2}\sin\theta\sin\phi + O(\rho^{-3}), \tag{9.92}$$

$$W_3(\xi) = -\frac{m_{33}}{2\pi}\rho^{-2}\sin\theta\sin\phi - \frac{m_{32}}{2\pi}\rho^{-2}\sin\theta\sin\phi + O(\rho^{-3}). \tag{9.93}$$

In order to establish general properties of m_{kj}, we apply Green's formula on the set $\Xi_R = \{\xi \in \Xi : \rho < R\}$ with the functions W_k and $Y_k = \xi_k + W_k$, $k = 2,3$,

$$\begin{aligned}\int_{\partial\Xi} Y_2 \partial_N W_2 ds_\xi &= \int_{\{\xi\in\mathbb{R}^3_- : \rho = R\}} W_2 \partial_\rho Y_2 - Y_2 \partial_\rho W_2 \, ds_\xi \\ &= \int_{\{\xi\in\mathbb{R}^3_- : \rho = R\}} W_2 \partial_\rho \xi_2 - \xi_2 \partial_\rho W_2 \, ds_\xi \end{aligned} \tag{9.94}$$

and taking into account the representation in spherical coordinate system

$$\begin{aligned}&\int_{\partial\Xi} Y_2 \partial_N W_2 ds_\xi = -\int_0^{2\pi}\int_{\pi/2}^{\pi} \left(\frac{3m_{22}}{2\pi} R^{-2} (\cos\theta \sin\phi)^2\right) R^2 \sin\phi \, d\phi \, d\theta - \\ &\int_0^{2\pi}\int_{\pi/2}^{\pi} \left(\frac{3m_{23}}{2\pi} R^{-2} \cos\theta \sin\theta \sin^2\phi\right) R^2 \sin\phi \, d\phi \, d\theta + O(R^{-1}) = \\ &-\frac{3m_{22}}{2\pi}\int_0^{2\pi}\int_{\pi/2}^{\pi} \cos^2\theta \sin^3\phi \, d\phi \, d\theta + O(R^{-1}) = -m_{22} + O(R^{-1}).\end{aligned} \tag{9.95}$$

On the other hand, applying Green's formula in ω and changing the direction of the normal, we have

$$\begin{aligned}\int_{\partial\Xi} Y_j \partial_N W_k ds_\xi &= \int_{\partial\Xi} W_j \partial_N W_k ds_\xi - \int_{\partial\Xi} \xi_j N_k ds_\xi \\ &= \int_\Xi \nabla_\xi W_k \cdot \nabla_\xi W_j \, d\xi + \delta_{kj}|\omega|.\end{aligned} \tag{9.96}$$

Therefore as $R \to \infty$, and in a similar way for m_{33} and $m_{23} = m_{32}$ we get

$$m_{kj} = -\int_\Xi \nabla_\xi W_k \cdot \nabla_\xi W_j \, d\xi - \delta_{kj}|\omega|, \quad \text{for} \quad k, j = 1,2. \tag{9.97}$$

In other words, the 2×2-matrix

$$m(\Xi) = \begin{pmatrix} m_{22} & m_{23} \\ m_{32} & m_{33} \end{pmatrix} \tag{9.98}$$

is symmetric and negative definite because it is the sum of two Gram matrices.

Example 9.1. For a semi-ball of radius R, $m(\Xi)$ is a multiple of the identity matrix with the coefficient $-\pi R^3$.

Example 9.2. If $\overline{\varpi}$ is a plain crack (cf. fig. 9.3a) then $|\overline{\varpi}| = 0$ and the matrix (9.98) becomes singular. For example, if $\overline{\varpi}$ belongs to the plane $\{\xi_2 = 0\}$, then $m_{33} = m_{23} = 0$ while obviously $W_3 = 0$. However, for a curved or broken crack (cf. fig. 9.3b) the solutions W_2 and W_3 are linearly independent and $m(\Xi)$ is non-degenerate although $|\overline{\varpi}| = 0$.

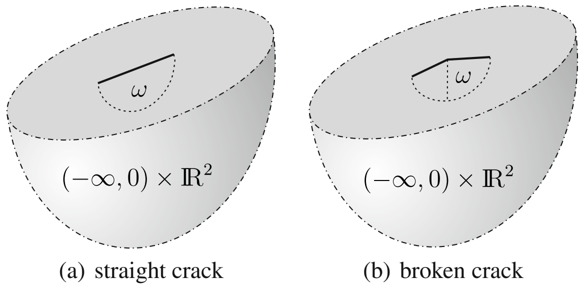


Fig. 9.3 The domain $\mathbb{R}^3_-$ with a crack ω

9.3.2 Second Boundary Layer Corrector

The right hand sides in the problem

$$-\Delta_\xi w^2(\xi) = F^2(\xi), \quad \xi \in \Xi, \tag{9.99a}$$

$$\partial_N w^2(\xi) = G^2(\xi), \quad \xi \in \partial\Xi, \tag{9.99b}$$

are to be determined using (9.70), (9.79) and (9.83), and collecting terms of order $O(h^0)$ in the equation, and of order $O(h^1)$ in the boundary conditions. As a result, we arrive at the following functions of fast variables

$$F^2(\xi) = [\varkappa_s(\mathscr{O})(\partial_{\xi_1} - 2\xi_1\partial^2_{\xi_2}) + \varkappa_v(\mathscr{O})(\partial_{\xi_1} - 2\xi_1\partial^2_{\xi_3})]w^1(\xi) \tag{9.100}$$

and

$$\begin{aligned} G^2(\xi) \;=\; & -N_1\xi_1\partial^2_n v^0(\mathscr{O}) - N_2\xi_2\partial^2_s v^0(\mathscr{O}) \\ & -N_3\xi_3\partial^2_v v^0(\mathscr{O}) - (N_2\xi_3 + N_3\xi_2)\partial^2_{sv} v^0(\mathscr{O}) \\ & -\xi_1(N_2^2\varkappa_s(\mathscr{O}) + N_3^2\varkappa_v(\mathscr{O}))(N_2\partial_s v^0(\mathscr{O}) + N_3\partial_v v^0(\mathscr{O})) \\ & +2N_2\xi_1\varkappa_s(\mathscr{O})\partial_s v^0(\mathscr{O}) + 2N_3\xi_1\varkappa_v(\mathscr{O})\partial_v v^0(\mathscr{O}) \\ & -\xi_1(N_2^2\varkappa_s(\mathscr{O}) + N_3^2\varkappa_v(\mathscr{O}))\partial_N w^1(\xi) \\ & +2N_2\xi_1\varkappa_s(\mathscr{O})\partial_{\xi_2} w^1(\xi) + 2N_3\xi_1\varkappa_v(\mathscr{O})\partial_{\xi_3} w^1(\xi) \\ =: & \; G^2_1(\xi) + G^2_2(\xi) + G^2_3(\xi) + G^2_4(\xi) + G^2_5(\xi). \end{aligned} \tag{9.101}$$

We notice that $G^2_2(\xi) + G^2_4(\xi) = 0$ according to the boundary conditions (9.85b). Now we denote

$$\begin{aligned} \eta_1(\xi) &:= \varkappa_s(\mathscr{O})(\partial_{\xi_1} - 2\xi\partial^2_{\xi_2}) + \varkappa_v(\mathscr{O})(\partial_{\xi_1} - 2\xi\partial^2_{\xi_3}), \\ \eta_2(\xi) &:= \partial_s v^0(\mathscr{O})W_2(\xi) + \partial_v v^0(\mathscr{O})W_3(\xi). \end{aligned} \tag{9.102}$$

In view of (9.89) and (9.100), the following expansion holds true:

$$\begin{aligned} F^2(\xi) &= \eta_1(\xi)\eta_2(\xi) \\ &= \varkappa_s(\mathscr{O})\partial_s v^0(\mathscr{O})\frac{m_2}{\pi}\left(15\frac{\xi_1\xi_2}{\rho^5} - 30\frac{\xi_1\xi_2^3}{\rho^7}\right) \\ &+ \varkappa_v(\mathscr{O})\partial_v v^0(\mathscr{O})\frac{m_3}{\pi}\left(15\frac{\xi_1\xi_3}{\rho^5} - 30\frac{\xi_1\xi_3^3}{\rho^7}\right) \\ &+ \varkappa_s(\mathscr{O})\partial_v v^0(\mathscr{O})\frac{m_3}{\pi}\left(-27\frac{\xi_1\xi_3}{\rho^5} + 30\frac{\xi_1^3\xi_3 + \xi_1\xi_3^3}{\rho^7}\right) \\ &+ \varkappa_v(\mathscr{O})\partial_s v^0(\mathscr{O})\frac{m_2}{\pi}\left(-27\frac{\xi_1\xi_2}{\rho^5} + 30\frac{\xi_1^3\xi_2 + \xi_1\xi_2^3}{\rho^7}\right) + O(\rho^{-2}), \end{aligned} \tag{9.103}$$

where $\rho \to \infty$. We denote

$$\eta_3(\xi) = \varkappa_s(\mathscr{O})(\partial_{\xi_1} - 2\xi\partial_{\xi_2}^2) + \varkappa_v(\mathscr{O})(\partial_{\xi_1} - 2\xi\partial_{\xi_3}^2), \tag{9.104}$$

$$\eta_4(\xi) = \partial_s v^0(\mathscr{O})W_2(\xi) + \partial_v v^0(\mathscr{O})W_3(\xi). \tag{9.105}$$

The function

$$\begin{aligned} U^2(\xi) &= \eta_3(\xi)\eta_4(\xi) \\ &= \varkappa_s(\mathscr{O})\partial_s v^0(\mathscr{O})\frac{m_2}{\pi}\left(15\frac{\xi_1\xi_2}{6\rho^3} - 30\frac{\xi_1^3\xi_2 + \xi_1\xi_3^2\xi_2 + \xi_1\xi_2^3}{20\rho^5}\right) \\ &+ \varkappa_v(\mathscr{O})\partial_v v^0(\mathscr{O})\frac{m_3}{\pi}\left(15\frac{\xi_1\xi_3}{6\rho^3} - 30\frac{\xi_1^3\xi_3 + \xi_1\xi_2^2\xi_3 + \xi_1\xi_3^3}{20\rho^5}\right) \\ &+ \varkappa_s(\mathscr{O})\partial_v v^0(\mathscr{O})\frac{m_3}{\pi}\left(-27\frac{\xi_1\xi_3}{6\rho^3} - 30\frac{3\xi_1^3\xi_3 + 2\xi_1\xi_2^2\xi_3 + 3\xi_1\xi_3^3}{20\rho^5}\right) \\ &+ \varkappa_v(\mathscr{O})\partial_s v^0(\mathscr{O})\frac{m_2}{\pi}\left(-27\frac{\xi_1\xi_2}{6\rho^3} - 30\frac{3\xi_1^3\xi_2 + 2\xi_1\xi_3^2\xi_2 + 3\xi_1\xi_2^3}{20\rho^5}\right) \end{aligned} \tag{9.106}$$

is homogeneous of order $O(\rho^{-1})$, i.e., of the same order as the *fundamental solutions*, and it compensates the leading term of $F^2(\xi)$. Therefore, the expansion of $w^2(\xi)$ at infinity can be written as follows:

$$w^2(\xi) = a\rho^{-1} + U^2(\xi) + O(\rho^{-2}). \tag{9.107}$$

To evaluate the coefficient a, we compute the following integrals on the semi-sphere of radius R taking into account the expansion (9.107):

$$\begin{aligned} \int_{\Xi_R} F^2(\xi)d\xi + \int_{\partial\omega\cap\partial\Xi} G^2(\xi)ds_\xi &= -\int_{\partial\Xi_R} \partial_N w^2(\xi)ds_\xi + \int_{\partial\omega\cap\partial\Xi} G^2(\xi)ds_\xi \\ &= -\int_{\{\xi\in\mathbb{R}^3_-:\rho=R\}} \partial_\rho w^2(\xi)ds_\xi, \end{aligned} \tag{9.108}$$

where we have used the fact that $G^2(\xi) = 0$ on $\partial \Xi_R \setminus \partial \omega$ due to the relations $\xi_1 = 0$ and $N_2 = N_3 = 0$ on $\partial \Xi_R \setminus \partial \omega$. In view of expansion (9.107) we obtain

$$\partial_\rho w^2(\xi) = -a\rho^{-2} + \partial_\rho U^2(\xi) + O(\rho^{-3}) = -a\rho^{-2} - \rho^{-1} U^2(\xi) + O(\rho^{-3}) \quad (9.109)$$

and thus

$$\begin{aligned} -\int_{\{\xi \in \mathbb{R}^3_- : \rho = R\}} \partial_\rho w^2(\xi) ds_\xi &= \int_{\{\xi \in \mathbb{R}^3_- : \rho = R\}} [a\rho^{-2} - \partial_\rho U^2(\xi)] ds_\xi + O(R^{-1}) \\ &= 2\pi a + O(R^{-1}). \end{aligned} \quad (9.110)$$

Note that all terms in $U^2(\xi)$ are odd in either ξ_2 or ξ_3, thus it is also true for $\partial_\rho U^2(\xi)$ so that

$$\int_{\{\xi \in \mathbb{R}^3_- : \rho = R\}} \partial_\rho U^2(\xi) = 0. \quad (9.111)$$

By using (9.101), let us consider the integral

$$\int_{\partial \omega \cap \partial \Xi} G^2(\xi) ds_\xi. \quad (9.112)$$

If we denote by ω^+ the domain obtained by adding to ω its mirror image with respect to the plane $\xi_1 = 0$, in view of (9.86), we have

$$\begin{aligned} \int_{\partial \omega \cap \partial \Xi} G_1^2(\xi) ds_\xi &= \frac{1}{2} \int_{\partial \omega^+} G_1^2(\xi) ds_\xi \\ &= -\frac{1}{2} \sum_{k=1}^{3} \partial_k^2 v^0(\mathscr{O}) \int_{\partial \omega^+} N_k \xi_k ds_\xi \\ &\quad -\frac{1}{2} \partial_{sv}^2 v^0(\mathscr{O}) \int_{\partial \omega^+} (N_2 \xi_3 + N_3 \xi_2) ds_\xi \\ &= -\frac{1}{2} \lambda^0 v^0(\mathscr{O}) |\omega^+| = -\lambda^0 v^0(\mathscr{O}) |\omega|. \end{aligned} \quad (9.113)$$

According to (9.86),

$$\int_{\partial \omega \cap \partial \Xi} G_3^2(\xi) ds_\xi = 0. \quad (9.114)$$

Let us consider the integral

$$\int_{\Xi_R} F^2(\xi) d\xi. \quad (9.115)$$

Owing to (9.100), we first compute

$$\int_{\Xi_R} \partial_{\xi_1}(\xi) ds_\xi = \int_{\partial \omega \cap \partial \Xi} N_1(\xi) w^1(\xi) ds_\xi + \int_{\{\xi \in \mathbb{R}^3_- : \rho = R\}} \rho^{-1} \xi_1 w^1(\xi) ds_\xi. \quad (9.116)$$

The last integral on the right hand side of (9.116) is of order $O(R^{-1})$. Indeed, the main terms of $w^1(\xi)$ are of order $O(R^{-2})$. However, according to (9.89), they are odd functions in either the variable ξ_2 or ξ_3. Therefore, the terms of order $O(1)$ vanish in the last integral on the right hand side of (9.116) due to the full symmetry of the semi-sphere $\{\xi \in \mathbb{R}^3_- : \rho = R\}$. The first integral on the right hand side of (9.116) is equal to

$$\begin{aligned}\int_{\partial\omega\cap\partial\Xi} N_1(\xi) w^1(\xi) ds_\xi &= \int_{\partial\omega\cap\partial\Xi} w^1(\xi)\partial_N \xi_1 ds_\xi \\ &= \int_{\partial\omega\cap\partial\Xi} \xi_1 \partial_N w^1(\xi) ds_\xi \\ &+ \int_{\{\xi\in\mathbb{R}^3_-:\rho=R\}} (\xi\partial_\rho w^1(\xi) - w^1(\xi)\partial_\rho \xi_1) ds_\xi . \quad (9.117)\end{aligned}$$

The integral

$$\int_{\{\xi\in\mathbb{R}^3_-:\rho=R\}} (\xi_1\partial_\rho w^1(\xi) - w^1(\xi)\partial_\rho \xi_1) ds_\xi \quad (9.118)$$

is also of order $O(R^{-1})$ by the same argument as above, since $\partial_\rho w^1(\xi)$ has the same symmetry in ξ_2 and ξ_3 as $w^1(\xi)$. We also have

$$\int_{\partial\omega\cap\partial\Xi} \xi_1 \partial_N w^1(\xi) ds_\xi = 0 \quad (9.119)$$

due to the boundary conditions (9.88b) and the second equality in (9.86). We compute now

$$\begin{aligned}\varkappa_s(\mathscr{O}) \int_{\Xi_R} \xi_1 \partial^2_{\xi_2} w^1(\xi) d\xi &= \varkappa_s(\mathscr{O}) \int_{\partial\omega\cap\partial\Xi} \xi_1 N_2(\xi) \partial_{\xi_2} w^1(\xi) ds_\xi \\ &+ \varkappa_s(\mathscr{O}) \int_{\{\xi\in\mathbb{R}^3_-:\rho=R\}} \rho^{-1} \xi_1 \xi_2 \partial_{\xi_2} w^1(\xi) ds_\xi . \quad (9.120)\end{aligned}$$

The latter integral is of order $O(R^{-1})$, hence the leading asymptotic term of order $O(\rho^{-2})$ coming from the expression $\xi_2\partial_{\xi_2}$ is still odd with respect to the variable ξ_2 or ξ_3, therefore it is annihilated by integration. The first integrand on the right hand side in (9.120) is the opposite of the first term in $G^2_5(\xi)$, and, hence, they cancel each other. Finally, recalling that $G^2_2(\xi) + G^2_4(\xi) = 0$, collecting the aforementioned integrals and taking (9.113) into account, we pass to the limit $R \to \infty$ and get the equality

$$a = -\frac{1}{2\pi} \lambda^0 v^0(\mathscr{O}) |\omega|. \quad (9.121)$$

Remark 9.7. The coefficient a is independent of the curvatures $\varkappa_s(\mathscr{O})$ and $\varkappa_v(\mathscr{O})$, in contrast with the original expressions (9.101) and (9.103).

9.3.3 Correction Term of Regular Type

We start by writing the boundary layers for $\rho \to \infty$ in the following condensed form

$$w^q(\xi) = t^q(\xi) + O(\rho^{q-4}), \; q = 1, 2, \tag{9.122}$$

where t^1 and t^2 denote the sum of homogeneous functions for $\rho \to \infty$ of orders $O(\rho^{-2})$ and $O(\rho^{-1})$ in (9.87), (9.89) and (9.107), respectively. In other words, $t^1(\xi) = h^2 t^1(d,s,\nu)$ and $t^2(\xi) = ht^2(d,s,\nu)$. Outside a small neighborhood of the point $\mathscr{O}$ we have,

$$\begin{aligned} hw^1(\xi) + h^2 w^2(\xi) &= h^3(t^1(d,s,\nu) + t^2(d,s,\nu)) + O(h^4) \\ &=: h^3 T(x) + O(h^4). \end{aligned} \tag{9.123}$$

In view of the multiplier h^3, the expression for $T(x)$ should be present in the following problem for the regular corrector v^3 in the asymptotic ansätz (9.70)

$$-\Delta_x v^3(x) = \lambda^0 v^3(x) + \lambda' v^0(x) + f^3(x), \quad x \in \Omega, \tag{9.124a}$$

$$\partial_n v^3(x) = g^3(x), \quad x \in \Gamma. \tag{9.124b}$$

The first two terms on the right hand side of (9.124a) are obtained if we replace the eigenvalues and eigenfunctions in (9.63a) by the ansätze (9.69)-(9.70) and collect terms of order $O(h^3)$ written in the slow variable x. The right hand side g^3 of the boundary condition (9.124b) is the discrepancy which results from the multiplication of the boundary layers with the cut-off function χ. If we assume that in the vicinity of the boundary the cut-off function χ depends only on the tangential variables s and ν, and it is independent of the normal variable d, then $g^3 = 0$, since the boundary conditions (9.85b) and (9.99b) on $\partial \Xi \setminus \partial \omega$ are homogeneous. It is clear that such a requirement can be readily satisfied, and thus we further assume $g^3 = 0$. The correction f^3 in (9.124a) is given by

$$f^3(x) = \lambda^0 \chi(x) T(x) + \Delta_x(\chi(x) T(x)). \tag{9.125}$$

We will verify that the function f^3, smooth outside a neighborhood of the origin $\mathscr{O}$, is of the growth $O(\|x\|^{-2})$ as $x \to \mathscr{O}$ which means that f^3 belongs to $H^{-1}(\Omega)$, since a function of order $\|x\|^{-5/2+\iota}$ is in $H^{-1}(\Omega)$ for all $\iota > 0$. This ensures that f^3 is admissible for the right hand side of equation (9.124a). The observation is obvious for the first term of f^3, since $t^1(d,s) = O(\|x\|^{-2})$ and $t^2(d,s) = O(\|x\|^{-1})$. Let us consider the second term $\Delta_x(\chi(x)T(x))$. According to (9.78), the representation of the Laplacian in curvilinear coordinates can be rewritten in the form

$$\Delta_x = \mathscr{L}^0(\partial_d, \partial_s, \partial_\nu) + \mathscr{L}^1(d, \partial_d, \partial_s, \partial_\nu) + \mathscr{L}^2(d, s, \nu, \partial_d, \partial_s, \partial_\nu), \tag{9.126}$$

with the ingredients

$$\mathscr{L}^0(\partial_d,\partial_s,\partial_\nu) = (\partial_d^2+\partial_s^2+\partial_\nu^2), \tag{9.127}$$

$$\mathscr{L}^1(d,\partial_d,\partial_s,\partial_\nu) = \varkappa_s(\mathscr{O})(\partial_d-2d\partial_s^2)+\varkappa_\nu(\mathscr{O})(\partial_d-2d\partial_\nu^2), \tag{9.128}$$

$$\mathscr{L}^2(d,s,\nu,\partial_d,\partial_s,\partial_\nu) = a_{11}\partial_d^2+a_{22}\partial_s^2+a_{33}\partial_\nu^2+a_1\partial_d+a_2\partial_s+a_3\partial_\nu, \tag{9.129}$$

while the functions a_{jj} and a_j are smooth in a neighborhood of $\mathscr{O}$, in variables d and s, and in addition they have the properties

$$a_{jj}(0,0)=0, \quad \partial_k a_{jj}(0,0)=0, \quad a_j(0,0)=0, \quad j=1,2,3. \tag{9.130}$$

Therefore, we can write

$$\Delta_x T = \mathscr{L}^0 t^1 + (\mathscr{L}^0 t^2 + \mathscr{L}^1 t^1) + \mathscr{L}^1 t^2 + \mathscr{L}^2(t^1+t^2). \tag{9.131}$$

We readily check that $\mathscr{L}^0 t^1 = 0$ and $\mathscr{L}^0 t^2 + \mathscr{L}^1 t^1 = 0$ due to the definition of w^1 and w^2 (see (9.85a) and (9.99a)). Function t^2 is of order $O(\|x\|^{-1})$ thus $\mathscr{L}^1 t^2$ is of order $O(\|x\|^{-2})$, and $\mathscr{L}^2(t^1+t^2)$ is also of order $O(\|x\|^{-2})$ due to (9.130). Thus, we have concluded that $g^3=0$ and $f^3 \in H^{-1}(\Omega)$.

According to the Fredholm theorem, and under the assumption that λ^0 is a simple eigenvalue, the problem (9.124) with the described right hand sides admits a solution v^3 in the Sobolev space $H^1(\Omega)$ if and only if the following orthogonality condition is satisfied by the right hand side of (9.124):

$$\lambda'(v^0,v^0)_\Omega + (f^3,v^0)_\Omega + (g^3,v^0)_{\partial\Omega} = 0. \tag{9.132}$$

Owing to the normalization condition and since $g^3=0$, relation (9.132) becomes

$$\lambda' = -(f^3,v^0)_\Omega. \tag{9.133}$$

Integral of the product $f^3 v^0$ is convergent, which means that

$$(f^3,v^0)_\Omega = \lim_{\iota\to+0}\int_{\Omega_\iota}(\lambda^0\chi T + \Delta_x(\chi T))v^0\,dx, \tag{9.134}$$

where $\Omega_\iota = \Omega \setminus \{x : d^2+s^2+\nu^2 \leqslant \iota^2\}$. The *surface patch* $S_\iota = \partial\Omega_\iota \setminus \partial\Omega$ turns out to be a semi-sphere in the curvilinear coordinate system. We imitate the spherical coordinate system in the curvilinear coordinates by setting $d = r\sin\theta\cos\varphi$, $s = r\sin\theta\sin\varphi$ and $\nu = r\cos\theta$ while denoting (r,φ,θ) the spherical coordinate system, with $r = h\rho \geqslant 0$, $\varphi \in (-\pi/2,\pi/2)$, $\theta \in (0,\pi)$. Using Green's formula for the smooth functions T and v^0 in the domain Ω_ι yields

$$\int_{\Omega_\iota} f^3 v^0\,dx = \int_{S_\iota}(v^0\partial_N T - T\partial_N v^0)\,ds_x. \tag{9.135}$$

Let us observe that $ds_x = \mathfrak{d}(d,s)^{1/2}\mathfrak{g}(d,s)\, r^2 \sin\theta d\theta d\varphi$ on S_ι, and according to formulae (9.81) the derivative ∂_{N_S} along the normal to the patch S_ι satisfies the relation

$$\partial_{N_S} T = \mathfrak{d}(d,s)^{1/2}(N_d\partial_d T + N_s\partial_s T + N_\nu\partial_\nu T), \tag{9.136}$$

where

$$N_d = \mathfrak{g}\sin\theta\cos\varphi,\ N_s = (1+d\varkappa_\nu)\sin\theta\sin\varphi,\ N_\nu = \cos\theta(1+d\varkappa_s), \tag{9.137}$$

and

$$\begin{aligned}\mathfrak{d} := \mathfrak{d}(d,s) &= \mathfrak{d}(r\sin\theta\cos\varphi, r\sin\theta\sin\varphi)\\ &= \mathfrak{g}^2\sin^2\theta\cos^2\varphi + (1+d\varkappa_\nu)^2\sin^2\theta\sin^2\varphi + (1+d\varkappa_s)\cos^2\theta.\end{aligned} \tag{9.138}$$

We can split the integral (9.135) into several pieces

$$\int_{\Omega_\iota} f^3 v^0\, dx = \mathscr{I}_1 + \mathscr{I}_2 + \mathscr{I}_3 + \mathscr{I}_4 + o(1), \tag{9.139}$$

with

$$\mathscr{I}_1 = \int_{-\pi/2}^{\pi/2}\int_0^\pi v^0(\mathscr{O})\partial_{N_S} T\iota^2 \sin\theta d\theta d\varphi, \tag{9.140}$$

$$\mathscr{I}_2 = \int_{-\pi/2}^{\pi/2}\int_0^\pi v^0(\mathscr{O})\partial_{N_S} T d\eta\iota^2 \sin\theta d\theta d\varphi, \tag{9.141}$$

$$\mathscr{I}_3 = \int_{-\pi/2}^{\pi/2}\int_0^\pi (\partial_s v^0(\mathscr{O}) s\partial_{N_S} T + \partial_\nu v^0(\mathscr{O})\nu\partial_{N_S} T)\iota^2 \sin\theta d\theta d\varphi, \tag{9.142}$$

$$\mathscr{I}_4 = -\int_{-\pi/2}^{\pi/2}\int_0^\pi T\partial_{N_S} v^0 d^{1/2}\mathfrak{g}\,\iota^2 \sin\theta d\theta d\varphi, \tag{9.143}$$

where $\eta := \varkappa_s(\mathscr{O})(1+\sin^2\theta\cos^2\varphi+\cos^2\theta) + \varkappa_\nu(\mathscr{O})(1+\sin^2\theta)$. In view of formulae (9.137) and (9.138), we get the following expansion for $\partial_{N_S} T$:

$$\begin{aligned}\partial_{N_S} T &= \partial_r T + d[\partial_d T(\varkappa_\nu(\mathscr{O})\cos^2\theta + \varkappa_s(\mathscr{O})(\sin^2\theta\sin^2\varphi))\sin\theta\cos\varphi\\ &+ \partial_s T(\varkappa_\nu(\mathscr{O})\cos^2\theta + \varkappa_s(\mathscr{O})(\sin^2\theta\sin^2\varphi - 1))\sin\theta\sin\varphi\\ &+ \partial_\nu T(-\varkappa_\nu(\mathscr{O})\cos^2\theta + \varkappa_s(\mathscr{O})(\sin^2\theta\sin^2\varphi))\cos\theta] + o(\iota).\end{aligned} \tag{9.144}$$

The asymptotic expansions of integrands in $\mathscr{I}_1$ and $\mathscr{I}_2$ already derived, lead to

$$\begin{aligned}\mathscr{I}_1 + \mathscr{I}_2 &= v^0(\mathscr{O})\iota^2\int_{-\pi/2}^{\pi/2}\int_0^\pi \partial_r T\sin\theta d\theta d\varphi\\ &+ v^0(\mathscr{O})\iota\int_{-\pi/2}^{\pi/2}\int_0^\pi d[d\partial_d T(\varkappa_\nu(\mathscr{O})\cos^2\theta + \varkappa_s(\mathscr{O})(\sin^2\theta\sin^2\varphi))\\ &+ s\partial_s T(\varkappa_\nu(\mathscr{O})\cos^2\theta + \varkappa_s(\mathscr{O})(\sin^2\theta\sin^2\varphi - 1))\\ &+ \nu\partial_\nu T(-\varkappa_\nu(\mathscr{O})\cos^2\theta + \varkappa_s(\mathscr{O})(\sin^2\theta\sin^2\varphi))]d\theta d\varphi + o(1).\end{aligned} \tag{9.145}$$

After simplification of the expression in brackets we get

$$\mathscr{I}_1+\mathscr{I}_2 = v^0(\mathscr{O})\iota^2\int_{-\pi/2}^{\pi/2}\int_0^{\pi}\partial_r T\sin\theta d\theta d\varphi \tag{9.146}$$
$$+ v^0(\mathscr{O})\varkappa_s(\mathscr{O})\iota\int_{-\pi/2}^{\pi/2}\int_0^{\pi} d(2d\partial_d T+s\partial_s T+2\nu\partial_\nu T)d\theta d\varphi$$
$$+ v^0(\mathscr{O})\varkappa_\nu(\mathscr{O})\iota\int_{-\pi/2}^{\pi/2}\int_0^{\pi} d(2d\partial_d T+2s\partial_s T+\nu\partial_\nu T)d\theta d\varphi+o(1).$$

We note that the expressions $2d\partial_d T+s\partial_s T+2\nu\partial_\nu T$ and $2d\partial_d T+2s\partial_s T+\nu\partial_\nu T$ are odd in either s or ν. Therefore, the corresponding integrals over the patch S_ι vanish and we obtain

$$\mathscr{I}_1+\mathscr{I}_2 = v^0(\mathscr{O})\iota^2\int_{-\pi/2}^{\pi/2}\int_0^{\pi}\partial_r T\sin\theta d\theta d\varphi+o(1). \tag{9.147}$$

For integrals $\mathscr{I}_3$ and $\mathscr{I}_4$, we have

$$\mathscr{I}_3+\mathscr{I}_4 = \partial_s v^0(\mathscr{O})\iota^2\int_{-\pi/2}^{\pi/2}\int_0^{\pi}(s\partial_{N_S}T-T\partial_{N_S}s)\sin\theta d\theta d\varphi$$
$$+ \partial_\nu v^0(\mathscr{O})\iota^2\int_{-\pi/2}^{\pi/2}\int_0^{\pi}(\nu\partial_{N_S}T-T\partial_{N_S}\nu)\sin\theta d\theta d\varphi+o(1)$$
$$= \partial_s v^0(\mathscr{O})\iota^2\int_{-\pi/2}^{\pi/2}\int_0^{\pi}(s\partial_r t^1-t^1\partial_r s)_{|r=\iota}\sin\theta d\theta d\varphi$$
$$+ \partial_\nu v^0(\mathscr{O})\iota^2\int_{-\pi/2}^{\pi/2}\int_0^{\pi}(\nu\partial_r t^1-t^1\partial_r \nu)_{|r=\iota}\sin\theta d\theta d\varphi+o(1). \tag{9.148}$$

Gathering all the integrals in (9.139), we obtain

$$\int_{\Omega_\iota} f^3 v^0\,dx = v^0(\mathscr{O})\iota^2\int_{-\pi/2}^{\pi/2}\int_0^{\pi}\partial_r T_{|r=\iota}\sin\theta d\theta d\varphi$$
$$+ \partial_s v^0(\mathscr{O})\iota^2\int_{-\pi/2}^{\pi/2}\int_0^{\pi}(s\partial_r t^1-t^1\partial_r s)_{|r=\iota}\sin\theta d\theta d\varphi$$
$$+ \partial_\nu v^0(\mathscr{O})\iota^2\int_{-\pi/2}^{\pi/2}\int_0^{\pi}(\nu\partial_r t^1-t^1\partial_r \nu)_{|r=\iota}\sin\theta d\theta d\varphi+o(1). \tag{9.149}$$

The first integral in (9.149) is equal to

$$\int_{-\pi/2}^{\pi/2}\int_0^{\pi}\partial_r T_{|r=\iota}\sin\theta d\theta d\varphi = \int_{-\pi/2}^{\pi/2}\int_0^{\pi}\partial_r t^1{}_{|r=\iota}\sin\theta d\theta d\varphi$$
$$+\int_{-\pi/2}^{\pi/2}\int_0^{\pi}\partial_r t^2{}_{|r=\iota}\sin\theta d\theta d\varphi, \tag{9.150}$$

and according to (9.86) we get

$$\int_{-\pi/2}^{\pi/2}\int_0^{\pi} \partial_r t^1{}_{|_{r=\iota}} \sin\theta d\theta d\varphi = 0. \tag{9.151}$$

In view of (9.110) we also obtain

$$\int_{-\pi/2}^{\pi/2}\int_0^{\pi} \partial_r t^2{}_{|_{r=\iota}} \sin\theta d\theta d\varphi = -\frac{2\pi a}{\iota^2}. \tag{9.152}$$

The last two integrals in (9.149) are evaluated with the help of (9.96) and (9.97), and we obtain in a similar way that

$$\begin{aligned}\partial_s v^0(\mathscr{O})\iota^2 \int_{-\pi/2}^{\pi/2}\int_0^{\pi} (s\partial_r t^1 - t^1\partial_r s)_{|_{r=\iota}} \sin\theta d\theta d\varphi + \\ \partial_\nu v^0(\mathscr{O})\iota^2 \int_{-\pi/2}^{\pi/2}\int_0^{\pi} (\nu\partial_r t^1 - t^1\partial_r \nu)_{|_{r=\iota}} \sin\theta d\theta d\varphi = \\ (\nabla_{s,\nu} v^0(\mathscr{O}))^\top m(\Xi)\nabla_{s,\nu} v^0(\mathscr{O}),\end{aligned} \tag{9.153}$$

where $m(\Xi)$ is the virtual mass matrix of the cavity ω in the half-space given by

$$m(\Xi) = \begin{pmatrix} m_{22} & m_{23} \\ m_{32} & m_{33} \end{pmatrix}, \tag{9.154}$$

which depends on the shape of Ξ. Furthermore,

$$\nabla_{s,\nu} v^0(\mathscr{O}) = (\partial_s v^0(\mathscr{O}), \partial_\nu v^0(\mathscr{O}))^T. \tag{9.155}$$

The previous results show that

$$(f^3, v^0)_\Omega = (\nabla v^0(\mathscr{O}))^\top m(\Xi)\nabla v^0(\mathscr{O}) - 2\pi a, \tag{9.156}$$

and finally the perturbation term in the asymptotic ansätz (9.69) of the simple eigenvalue λ_m^0 takes the form

$$\lambda_m' = (\nabla_{s,\nu} v_m^0(\mathscr{O}))^T m(\Xi)\nabla_{s,\nu} v_m^0(\mathscr{O}) + |\omega|\lambda_m^0|v_m^0(\mathscr{O})|^2. \tag{9.157}$$

Remark 9.8. The max-min principle of Proposition A.1 reads:

$$\lambda_j^h = \max_{\mathscr{E}_j^h \subset H^1(\Omega_h)} \inf_{u^h \in \mathscr{E}_j^h \setminus \{0\}} \left\{ \frac{\|\nabla_x u^h\|^2_{L^2(\Omega_h)}}{\|u^h\|^2_{L^2(\Omega_h)}} \right\}, \tag{9.158}$$

$$\lambda_j^0 = \max_{\mathscr{E}_j^0 \subset H^1(\Omega)} \inf_{v \in \mathscr{E}_j^0 \setminus \{0\}} \left\{ \frac{\|\nabla_x v\|^2_{L^2(\Omega)}}{\|v\|^2_{L^2(\Omega)}} \right\}, \tag{9.159}$$

where $\mathscr{E}_j^h$ and $\mathscr{E}_j^0$ stand for any subspaces of codimension $j-1$, i.e.

$$\dim(H^1(\Omega_h) \ominus \mathscr{E}_j^h) = j-1 \quad \text{and} \quad \dim(H^1(\Omega) \ominus \mathscr{E}_j^0) = j-1. \tag{9.160}$$

For the cavity ω_h of a general shape, there is no obvious relation between $H^1(\Omega_h)$ and $H^1(\Omega)$ so that (9.158) and (9.159) do not allow to establish directly a connection between λ_j^h and λ_j^0. Notice that in case $|\omega| > 0$, λ_m' in (9.157) can be made both, negative or positive. Indeed, assume that the eigenfunction v_m changes sign on the boundary Γ and put the coordinate origin $\mathscr{O}$ at a point where v_m vanishes. Then the last term in (9.157) becomes null and $\lambda_m' \leqslant 0$ due to the above-mentioned properties of the matrix $m(\Xi)$. On the contrary, if the point $\mathscr{O}$ constitutes an extremum of the function $\Gamma \ni x \mapsto v_m(x)$, then $\nabla_{s,v} v_m(\mathscr{O}) = 0$ and $\lambda_m' > 0$ provided $v_m(\mathscr{O}) \neq 0$ and $|\omega| > 0$. In the limiting case of a crack $\overline{\omega}$, i.e. a domain flattens into a two-dimensional surface (see fig. 9.3), one easily observes that $H^1(\Omega) \subset H^1(\Omega_h)$ since a function in $H^1(\Omega_h)$ can have a nontrivial jump over $\overline{\omega_h}$ but $v \in H^1(\Omega)$ cannot. As a consequence of (9.158) and (9.159), we conclude the general relationship

$$\lambda_j^h \leqslant \lambda_j^0. \tag{9.161}$$

This formula is in agreement with (9.157) for the correction term in (9.69) because $|\omega| = 0$ for a crack and, therefore,

$$\lambda_m' = (\nabla_{s,v} v_m^0(\mathscr{O}))^T m(\Xi) \nabla_{s,v} v_m^0(\mathscr{O}) \leqslant 0, \tag{9.162}$$

since the matrix $m(\Xi)$ in the case of a crack is negative or negative definite (see Example 9.2).

9.3.4 Multiple Eigenvalues

Assume now, that λ_m^0 is an eigenvalue of the multiplicity $\varkappa_m > 1$, i.e.,

$$\lambda_{m-1}^0 < \lambda_m^0 = \cdots = \lambda_{m+\varkappa_m-1}^0 < \lambda_{m+\varkappa_m}^0. \tag{9.163}$$

In such a case ansätze (9.69) and (9.70) are valid for $p = m, \ldots, m+\varkappa_m - 1$. However, the principal terms in the expansions of the eigenfunctions $u_m^h, \ldots, u_{m+\varkappa_m-1}^h$ of Problem 9.6 are predicted in the form of linear combinations

$$v^{p0} = a_1^p v_m^0 + \cdots + a_{\varkappa_m}^p v_{m+\varkappa_m-1}^0 \tag{9.164}$$

of eigenfunctions of problem (9.67) corresponding to the eigenvalue λ_m^0, and subject to the orthogonality and normalization conditions (9.68). The coefficients of the columns $a^p = (a_1^p, \ldots, a_{\varkappa_m}^p)^\top$ in (9.164) are to be determined. We use the name column for a column vector for short. If the columns $a^m, \ldots, a^{m+\varkappa_m-1}$ are unit vectors and

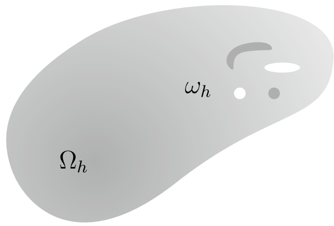


Fig. 9.4 Domain Ω_h with singular perturbations ω_h close to the boundary

$$a^p \cdot a^q = \delta_{pq}, \quad p,q = m,\dots,m+\varkappa_m - 1, \tag{9.165}$$

then the linear combinations (9.164), with $p = m,\dots,m+\varkappa_m-1$, are simply a new orthonormal basis in the eigenspace of the eigenvalue λ_m.

The construction of boundary layers is performed in the same way as in the previous section. When solving problem (9.124) for the regular corrector v^{p3}, there appear $\varkappa_m$ compatibility conditions

$$\varsigma_p(v^{p0}, v^0_{m+k})_\Omega + (f^{p3}, v^0_{m+k})_\Omega = 0, \quad k = 0,\dots,\varkappa_m - 1, \tag{9.166}$$

which can be written in the form of the linear system of $\varkappa_m$ algebraic equations

$$\mathsf{Q}a^p = \varsigma_p a^p \tag{9.167}$$

with the matrix $\mathsf{Q} = (\mathsf{Q}_{ik})^{\varkappa_m-1}_{j,k=0}$ of the size $\varkappa_m \times \varkappa_m$,

$$\mathsf{Q}_{jk} = (\nabla_{s,v} v^0_{m+k}(\mathscr{O}))^T m(\Xi) \nabla_{s,v} v^0_{m+j}(\mathscr{O}) + |\omega| \lambda^0_m v^0_{m+k}(\mathscr{O}) v^0_{m+j}(\mathscr{O}). \tag{9.168}$$

Formula (9.168) is derived in exactly the same way as it is for formula (9.157). The matrix Q is symmetric, and its real eigenvalues $\varsigma_m,\dots,\varsigma_{m+\varkappa_m-1}$ correspond to eigenvectors $a^m,\dots,a^{m+\varkappa_m-1}$, which satisfy conditions (9.165). Actually, just these attributes of the matrix Q with elements (9.168) are included in ansätze (9.69), (9.70) and (9.164) for eigenvalues λ^h_p and eigenfunctions u^h_p of Problem 9.6 for $p = m,\dots,m+\varkappa_m-1$ in the case (9.163).

9.4 Configurational Perturbations of Spectral Problems in Elasticity

Spectral problems for linearized elasticity in the case of low frequencies are considered in this section. The asymptotic analysis of eigenvalues and eigenfunctions is performed for *elasticity systems* with respect to singular perturbations of geometrical domains close to the boundary [179]. The singular perturbation takes the form e.g., of the creation of new parts of the boundary due to the nucleation of small voids (cf. fig. 9.4).

The related results in the literature are given for singular perturbations of isolated points of the boundary (small holes in the domain, see for instance [41, 105, 145, 147, 143, 192]) and perturbations of straight boundaries including changes in the type of boundary conditions (cf. [65, 68]). The scalar spectral problems in general geometrical domains and the specific question on the dependence of the asymptotics of eigenvalues on the curvature of the boundaries is addressed in [131, 177, 178].

In the proposed approach to asymptotic analysis the anisotropy of physical properties, and the variable coefficients of differential operators, i.e., inhomogeneity of elastic materials, are taken into account. Some of the existing results on elasticity problems with singular perturbations of boundaries (see, for instance, monographs [143], [200] and [201]) concern homogeneous and isotropic elastic bodies.

9.4.1 Anisotropic and Inhomogeneous Elastic Body

Problem 9.8. Let us consider the elasticity problem for an elastic body Ω in three spatial dimensions, written in the matrix/column notation which we call for simplicity of writing *Voigt notation* as in [180],

$$\mathscr{D}(-\nabla_x)^\top \mathscr{A}(x)\mathscr{D}(\nabla_x)u(x) = 0, \quad x \in \Omega, \tag{9.169a}$$

$$\mathscr{D}(n)^\top \mathscr{A}(x)\mathscr{D}(\nabla_x)u(x) = g(x), \quad x \in \partial\Omega. \tag{9.169b}$$

Here $\mathscr{A}$ is a symmetric positive definite matrix function in $\overline{\Omega}$ of size 6×6, with measurable or smooth elements, consisting of the *elastic material moduli* (the *Hooke's* or *stiffness matrix*) and $\mathscr{D}(\nabla_x)$ is (6×3)-matrix of the first order differential operators,

$$\mathscr{D}(\xi)^\top = \begin{bmatrix} \xi_1 & 0 & 0 & 0 & 2^{-1/2}\xi_3 & 2^{-1/2}\xi_2 \\ 0 & \xi_2 & 0 & 2^{-1/2}\xi_3 & 0 & 2^{-1/2}\xi_1 \\ 0 & 0 & \xi_3 & 2^{-1/2}\xi_2 & 2^{-1/2}\xi_1 & 0 \end{bmatrix}, \tag{9.170}$$

$u = (u_1, u_2, u_3)^\top$ is displacement column, $n = (n_1, n_2, n_3)^\top$ is the unit outward normal vector on $\partial\Omega$ and $(\cdot)^\top$ stands for transposition of $(\cdot)$. In this notation the strain $\vartheta(u(x))$ and stress $\sigma(u(x)) = \mathscr{A}(x)\mathscr{D}(\nabla_x)u(x)$ columns are given respectively by

$$\mathscr{D}(\nabla_x)u = \vartheta(u) = \left(\varepsilon_{11}, \varepsilon_{22}, \varepsilon_{33}, \sqrt{2}\varepsilon_{23}, \sqrt{2}\varepsilon_{31}, \sqrt{2}\varepsilon_{12}\right)^\top, \tag{9.171}$$

$$\mathscr{A}\mathscr{D}(\nabla_x)u = \sigma(u) = \left(\sigma_{11}, \sigma_{22}, \sigma_{33}, \sqrt{2}\sigma_{23}, \sqrt{2}\sigma_{31}, \sqrt{2}\sigma_{12}\right)^\top. \tag{9.172}$$

The factors $2^{-1/2}$ and $\sqrt{2}$ imply that the norms of strain and stress tensors coincide with the norms of columns (9.171) and (9.172), respectively. From the latter property in the matrix/column notation, any orthogonal transformation of coordinates in $\mathbb{R}^3$ gives rise to orthogonal transformations of columns (9.171) and (9.172) in $\mathbb{R}^6$ (cf. [166, Chapter 2]).

Remark 9.9. The strains (9.171) and the stresses (9.172) degenerate on the space of *rigid body motions*,

$$\mathscr{R} = \{p(x) := \mathbb{D}(x)c : c \in \mathbb{R}^6\}\,, \quad \dim \mathscr{R} = 6\,, \tag{9.173}$$

where

$$\mathbb{D}(x) = \begin{bmatrix} 1\,0\,0 & 0 & -2^{-1/2}x_3 & 2^{-1/2}x_2 \\ 0\,1\,0 & 2^{-1/2}x_3 & 0 & -2^{-1/2}x_1 \\ 0\,0\,1 & -2^{-1/2}x_2 & 2^{-1/2}x_1 & 0 \end{bmatrix}. \tag{9.174}$$

This subspace plays a crucial role in many questions in the elasticity theory, it appears also in the so-called polynomial property [162, 164] (see also [172]). The following equalities can be verified by a direct computation,

$$\begin{aligned} \mathbb{D}(\nabla)\mathbb{D}(x)^\top\Big|_{x=0} &= \mathrm{I}_6\,, \qquad \mathbb{D}(\nabla)\mathscr{D}(x)^\top\Big|_{x=0} = \mathrm{O}_6\,, \\ \mathscr{D}(\nabla)\mathbb{D}(x)^\top &= \mathrm{O}_6\,, \qquad \mathscr{D}(\nabla)\mathscr{D}(x)^\top = \mathrm{I}_6\,, \end{aligned} \tag{9.175}$$

where I_N and O_N are the unit and null $(N \times N)$-matrices, respectively.

In order to assure the existence of a solution to the elasticity system, the boundary load g is supposed to be self equilibrated, namely

$$\int_{\partial\Omega} \mathbb{D}(x)^\top g(x) ds_x = 0 \in \mathbb{R}^6. \tag{9.176}$$

9.4.2 Vibrations of Elastic Bodies

Consider inhomogeneous anisotropic elastic body $\Omega \subset \mathbb{R}^3$ with the Lipschitz boundary $\partial\Omega$. Spectral problems for the body are formulated in a fixed cartesian coordinate system $x = (x_1, x_2, x_3)^\top$, and in the matrix notation. We assume that the matrix $\mathscr{A}$ of elastic moduli is a matrix function of the spatial variable $x \in \mathbb{R}^3$, symmetric and positive definite for $x \in \Omega \cup \partial\Omega$. We denote

$$\mathscr{L}(x, \nabla_x)u(x) := \mathscr{D}(-\nabla_x)^\top \mathscr{A}(x)\mathscr{D}(\nabla_x)u(x), \tag{9.177a}$$

$$\mathscr{N}^\Omega(x, \nabla_x)u(x) := \mathscr{D}(n)^\top \mathscr{A}(x)\mathscr{D}(\nabla_x)u(x). \tag{9.177b}$$

Problem 9.9. The problem on eigenvibrations of the body Ω takes the form

$$\mathscr{L}(x, \nabla_x)u(x) = \lambda\gamma(x)u(x), \quad x \in \Omega, \tag{9.178a}$$

$$\mathscr{N}^\Omega(x, \nabla_x)u(x) = 0, \quad x \in \Sigma, \tag{9.178b}$$

$$u(x) = 0, \quad x \in \Gamma, \tag{9.178c}$$

where $\gamma > 0$ is the material density, λ is an eigenvalue, the square of eigenfreguency. The part Γ of the surface $\partial\Omega$ is clamped, and the first boundary condition is prescribed on the traction free remaining part $\Sigma = \partial\Omega \setminus \overline{\Gamma}$ of the surface.

Remark 9.10. The analysis of boundary value problems with the collision line $\overline{\Sigma}\cap\overline{\Gamma}$ should be performed in the weighted Sobolev and Hölder spaces (cf. [166, Chapter 2, pp. 94–113]) taking into account the singularities caused by the change of boundary conditions over the collision line.

We denote by $H^1_\Gamma(\Omega;\mathbb{R}^3)$ the energy space, i.e., the subspace of the Sobolev space $H^1(\Omega;\mathbb{R}^3)$ with null traces on the subset Γ. The variational formulation of problem (9.178) reads:

Problem 9.10. Find a non trivial function $u \in H^1_\Gamma(\Omega;\mathbb{R}^3)$ and a number λ such that for all test functions $v \in H^1_\Gamma(\Omega;\mathbb{R}^3)$ the following integral identity is verified

$$(\mathscr{A}\mathscr{D}u, \mathscr{D}v)_\Omega = \lambda(\gamma u, v)_\Omega \ , \tag{9.179}$$

where $(\cdot,\cdot)_\Omega$ is the scalar product in the Lebesgue space $L^2(\Omega;\mathbb{R}^3)$.

If the stiffness matrix $\mathscr{A}$ and the density γ are measurable functions of the spatial variables x, and in addition uniformly positive definite and bounded, then the variational problem (9.179) admits normal positive eigenvalues λ_p, which form the sequence

$$0 < \lambda_1 \leqslant \lambda_2 \leqslant \cdots \leqslant \lambda_p \leqslant \cdots \to \infty \tag{9.180}$$

taking into account its multiplicities, and the *elastic vibration modes*: for an eigenvalue λ_p the corresponding orthonormalized eigenfunction is denoted by $u_{(p)}$.

Remark 9.11. In the case of multiple eigenvalues the notation is slightly changed. For an multiple eigenvalue $\lambda_p = \cdots = \lambda_{p+\varkappa_p-1}$ of the multiplicity $\varkappa_p$ the orthonormalized eigenfunctions are denoted by $u^{(q)}_{(p)} \in L^2(\Omega;\mathbb{R}^3)$ for $q = p,\ldots,p+\varkappa_p-1$.

The elastic vibration modes are subject to the orthogonality and normalization conditions

$$(\gamma u_{(p)}, u_{(q)})_\Omega = \delta_{pq} \ , \quad p,q \in \mathbb{N} := \{1,2,\ldots\} \ , \tag{9.181}$$

where δ_{pq} is the Kronecker symbol.

In the sequel it is assumed that elements of the matrix $\mathscr{A}$ and the density γ are smooth functions in Ω, continuous up to the boundary. In such the case Ω is called a *smooth* inhomogeneous body. For such a body the elastic modes $u_{(p)}$ are smooth functions in the interior of Ω, and up to the boundary in the case of the smooth surface $\partial\Omega$. We have also the equivalence between the variational form and the differential form (9.178) of the spectral problem. We require only the *interior* regularity of elastic modes in the sequel. In any case the elastic modes have singularities on the collision line $\overline{\Sigma}\cap\overline{\Gamma}$ and therefore, are excluded from the Sobolev space $H^2(\Omega;\mathbb{R}^3)$.

Along with the smooth inhomogeneous body Ω, let us consider a body Ω_h with inclusions or defects; here $h > 0$ stands for a small dimensionless geometrical parameter, which describes the relative size of inclusions or defects. Actually, we select in the interior of Ω the *points* $p^1,\ldots,p^{(J)}$ and denote by $\omega_1,\ldots,\omega_J$ elastic bodies bounded by the Lipschitz surfaces $\partial\omega_1,\ldots,\partial\omega_J$. Furthermore, for the sake of simplicity we assume that the origin $\mathscr{O}$ belongs to ω_j, $j=1,\ldots,J$. The body with inclusions or defects is defined by

$$\Xi(h) = \Omega_h \cup \omega_1^h \cup \cdots \cup \omega_J^h, \qquad (9.182)$$

where

$$\omega_j^h = \left\{x \in \mathbb{R}^3 : \xi^j := h^{-1}(x-p^j) \in \omega_j\right\}, \quad \Omega_h = \Omega \setminus \bigcup_{j=1}^{J} \overline{\omega_j^h}. \qquad (9.183)$$

In the limit case of $h \to 0$, the open domain $\Omega \setminus \{p^1,\ldots,p^J\}$ is called the *punctured domain*. The stiffness matrix and the density of the *composite* body (9.182) take the form

$$\mathscr{A}^h(x) = \begin{cases} \mathscr{A}(x), & x \in \Omega_h, \\ \mathscr{A}_{(j)}(\xi^j), & x \in \omega_j^h, \end{cases} \qquad \gamma^h(x) = \begin{cases} \gamma(x), & x \in \Omega_h, \\ \gamma_j(\xi^j), & x \in \omega_j^h, \end{cases} \qquad (9.184)$$

where $\xi^j := h^{-1}(x-p^j)$.

The matrices $\mathscr{A}$ and $\mathscr{A}_{(j)}$ as well as the scalars γ and $\gamma_{(j)}$ are different from each other, i.e., ω_j^h are inhomogeneous inclusions of small diameters. We assume that $\mathscr{A}_{(j)}$ and $\gamma_{(j)}$ are measurable, bounded and positive definite uniformly on ω_j. In particular, for almost all $\xi \in \omega_j$ the eigenvalues of the matrix $\mathscr{A}_{(j)}(\xi)$ are bounded from below by a constant $c_j > 0$. There is no special assumption on the relation between the properties of the inclusions and of the matrix (body without inclusions), we assume only that the densities γ, $\gamma_{(j)}$, and entries of the matrices $\mathscr{A}$, $\mathscr{A}_{(j)}$ are of similar orders, respectively.

In the fracture mechanics, the most interesting case is the weakening of elastic material due to the crack formation. The cracks are modeled by two-sided, two dimensional surfaces, with the first boundary conditions (9.178b) prescribed on both crack lips, i.e. the surface is traction free from both sides. The case of a microcrack is not formally included in our problem statement, since we assume that the inclusion or defect ω_j is of positive volume and with the Lipschitz boundary $\partial\omega_j$. However, the asymptotic procedure works also for the cracks. Small changes which are required in the justification part, are given separately (see the proof of Proposition C.1 and Remark C.2). The *polarization matrices* for the cracks can be found in [180, 220].

The exchange of γ and $\mathscr{A}$ by γ^h and $\mathscr{A}^h$ from (9.184), respectively, transforms (9.179) in the integral identity for the body weakened by the inclusions or defects $\omega_1^h,\ldots,\omega_J^h$, this integral identity is further denoted by (9.185).

Problem 9.11. Find a non trivial function $u^h \in H^1_\Gamma(\Xi(h);\mathbb{R}^3)$ and a number λ^h such that for all test functions $v \in H^1_\Gamma(\Xi(h);\mathbb{R}^3)$ the following integral identity is verified

$$(\mathscr{A}^h \mathscr{D} u^h, \mathscr{D} v)_{\Xi(h)} = \lambda^h (\gamma^h u^h, v)_{\Xi(h)} , \tag{9.185}$$

where $(\cdot,\cdot)_{\Xi(h)}$ is the scalar product in the Lebesgue space $L^2(\Xi(h);\mathbb{R}^3)$.

We denote

$$\mathscr{L}_h(x,\nabla_x)u^h(x) := \mathscr{D}(-\nabla_x)^\top \mathscr{A}^h(x)\mathscr{D}(\nabla_x)u^h(x), \tag{9.186a}$$
$$\mathscr{N}_h(x,\nabla_x)u^h(x) := \mathscr{D}(n)^\top \mathscr{A}^h(x)\mathscr{D}(\nabla_x)u^h(x). \tag{9.186b}$$

We observe also, that for the stiffness matrix $\mathscr{A}^h$ and the density γ^h the differential problem for vibrations of a composite body does not consist only of the system of equations, but also of the *transmission conditions* on the surface $\partial\omega_j^h$ where the *ideal contact* is assumed. The problem on eigenvibrations of the composite body $\Xi(h)$ takes the form:

Problem 9.12. Let us now consider the *strong system* associated to Problem 9.11, namely

$$\mathscr{L}_h(x,\nabla_x)u^h(x) = \lambda\gamma^h(x)u^h(x), \quad x \in \Xi(h), \tag{9.187a}$$
$$\mathscr{N}_h(x,\nabla_x)u^h(x) = 0, \quad x \in \Sigma, \tag{9.187b}$$
$$u^h(x) = 0, \quad x \in \Gamma, \tag{9.187c}$$
$$[\![u^h]\!](x) = 0, \quad x \in \partial\omega_j^h, \ j = 1,\dots,J, \tag{9.187d}$$
$$[\![\mathscr{N}_h(x,\nabla_x)u^h]\!](x) = 0, \quad x \in \partial\omega_j^h, \ j = 1,\dots,J, \tag{9.187e}$$

where $[\![\cdot]\!]$ stands for the jumps over the interfaces $\partial\omega_j^h$, $j = 1,\dots,J$.

In a similar way as for problem (9.180) the general theory is applied, hence there is the sequence of eigenvalues for the problem (9.185)

$$0 < \lambda_1^h \leqslant \lambda_2^h \leqslant \cdots \leqslant \lambda_p^h \leqslant \cdots \to +\infty, \tag{9.188}$$

and the corresponding eigenfunctions $u^h_{(j)}$ meet the orthogonality and normalization conditions

$$(\gamma^h u^h_{(p)}, u^h_{(q)})_\Omega = \delta_{pq}, \quad p,q \in \mathbb{N}. \tag{9.189}$$

9.4.3 Formal Construction of Asymptotic Expansions

We introduce the following asymptotic *ansätze* for eigenvalues and eigenfunctions in problem (9.185)

$$\lambda_p^h \sim \lambda_p + h^3 \varsigma_p, \tag{9.190}$$

and

$$u^h_{(p)}(x) \sim u_{(p)}(x) + h \sum_{j=1}^{J} \chi_j(x) \left(w^{1j}_{(p)} \left(h^{-1}\left(x - p^j\right)\right) + \right.$$
$$\left. h w^{2j}_{(p)} \left(h^{-1}\left(x - p^j\right)\right)\right) + h^3 v_{(p)}, \tag{9.191}$$

where $\chi_j \in C^\infty_c(\Omega), j = 1,\dots,J$, are cut-off functions, with non overlapping supports in Ω, and for each j, $\chi_j(x) = 1$ for $x \in \omega_j$ and $\chi_i(p^j) = \delta_{ij}$.

First, we assume that the eigenvalue $\lambda = \lambda_p$ in problem (9.179) is simple, and for brevity the subscript p is omitted. The corresponding eigenfunction $u = u_{(p)} \in H^1_\Gamma(\Omega;\mathbb{R}^3)$, normalized by condition (9.181), is smooth in the interior of the domain Ω. The columns $\mathbb{M}^j(x), j = 1,\dots,12$ of the matrix $\mathbb{M}(x) := \left[\mathbb{D}(x), \mathscr{D}(x)^\top\right]$

$$\mathbb{P}(x) = \begin{bmatrix} 1\,0\,0 & 0 & -2^{-1/2}x_3 & 2^{-1/2}x_2 & x_1 & 0 & 0 & 0 & 2^{-1/2}x_3 & 2^{-1/2}x_2 \\ 0\,1\,0 & 2^{-1/2}x_3 & 0 & -2^{-1/2}x_1 & 0 & x_2 & 0 & 2^{-1/2}x_3 & 0 & 2^{-1/2}x_1 \\ 0\,0\,1 & -2^{-1/2}x_2 & 2^{-1/2}x_1 & 0 & 0 & 0 & x_3 & 2^{-1/2}x_2 & 2^{-1/2}x_1 & 0 \end{bmatrix}$$

form a basis in the twelve dimensional space of the first order polynomial vector functions in $\mathbb{R}^3$. In this way, the Taylor formula takes the form

$$u(x) = \mathbb{D}(x - p^j)a^j + \mathscr{D}(x - p^j)^\top \vartheta^j + O(\|x - p^j\|^2)\,, \tag{9.192}$$

where $a^j := a^{(j)}$ and $\vartheta^j := \vartheta^{(j)}$. The summation convention is used as usually for the repeated indices $j = 1,\dots,6$. By equalities (9.171), (9.172) and (9.175), the columns

$$a^j = \mathbb{D}(\nabla_x)^\top u(p^j)\,, \quad \vartheta^j = \mathscr{D}(\nabla_x) u(p^j)\,, \tag{9.193}$$

represent the column of rigid motions, and of strains, at the point p^j, respectively.

By the Taylor formula (9.192) we obtain an expansion of the strains in the vicinity of each inclusion ω^h_j

$$\vartheta(u(x)) = \vartheta^j + O(x) = \vartheta^j + O(h)\,. \tag{9.194}$$

If the displacement field u, which as usually is the first term of the approximate solution, is inserted in the problem (9.185) for the composite body Ω^h, it gives rise to discrepancies. The main terms of the discrepancies, left by the field u in the problem (9.185) for the composite body Ω^h, appear in the system of equations in ω^h_j and in the transmission conditions on $\partial\omega^h_j$.

For the compensation of the discrepancies we use the special solutions of the elasticity problem in a homogeneous space with the inclusion ω_j of unit size

$$\begin{aligned}\mathscr{L}^{0j}(\nabla_\xi)\mathsf{W}^{jk}(\xi) &:= \mathscr{D}(-\nabla_\xi)^\top \mathscr{A}(p^j)\mathscr{D}(\nabla_\xi)\mathsf{W}^{jk}(\xi) \\ &= 0, \quad \xi \in \Theta_j = \mathbb{R}^3 \setminus \overline{\omega_j},\end{aligned} \tag{9.195a}$$

$$\begin{aligned}\mathscr{L}^{j}(\xi,\nabla_\xi)\mathsf{W}^{jk}(\xi) &:= \mathscr{D}(-\nabla_\xi)^\top \mathscr{A}_{(j)}(\xi)\mathscr{D}(\nabla_\xi)\mathsf{W}^{jk}(\xi) \\ &= \mathscr{D}(\nabla_\xi)\mathscr{A}_{(j)}(\xi) e_k, \quad \xi \in \omega_j,\end{aligned} \tag{9.195b}$$

with jump conditions of the form

$$\mathsf{W}^{jk}_{+}(\xi) = \mathsf{W}^{jk}_{-}(\xi), \quad \xi \in \partial\omega_j, \tag{9.195c}$$

$$\mathscr{D}(\nu(\xi))^{\top}(\mathscr{A}_{(j)}(\xi)\mathscr{D}(\nabla_{\xi})\mathsf{W}^{jk}_{-}(\xi) - \mathscr{A}(p^j)\mathscr{D}(\nabla_{\xi})\mathsf{W}^{jk}_{+}(\xi)) = \\ \mathscr{D}(\nu(\xi))^{\top}(\mathscr{A}(p^j) - \mathscr{A}_{(j)}(\xi))e_k, \quad \xi \in \partial\omega_j. \tag{9.195d}$$

Here ν is the unit vector of the exterior normal on the boundary $\partial\omega_j$ of the inclusion ω_j, $e_k = (\delta_{1k}, \dots, \delta_{6k})^{\top}$ is an orthant in the space $\mathbb{R}^6$, W_+ and W_- are limit values of the function W on the surface $\partial\omega_j$ evaluated from outside and from inside of the inclusion ω_j, respectively.

We denote by $\boldsymbol{\Phi}^j$ the *fundamental* (3×3)*-matrix* of the operator $\mathscr{L}^{0j}(\nabla_{\xi})$ in $\mathbb{R}^3$. This matrix is infinitely differentiable in $\mathbb{R}^3 \setminus \{\mathscr{O}\}$ and enjoys the following positive homogeneity property

$$\boldsymbol{\Phi}^j(t\xi) = t^{-1}\boldsymbol{\Phi}^j(\xi), \quad t > 0. \tag{9.196}$$

It is known (see [170, Chapter 6]), that the solutions W^{jk} of problem (9.195a)-(9.195d) admit the expansion

$$\mathsf{W}^{jk}(\xi) = \sum_{p=1}^{6} \mathsf{P}^{(j)}_{kp} \sum_{q=1}^{3} \mathscr{D}^q_p(\nabla_x)\boldsymbol{\Phi}^{jq}(\xi) + O(\|\xi\|^{-3}), \quad \xi \in \mathbb{R}^3 \setminus B_R, \tag{9.197}$$

where $\mathscr{D}_p = (\mathscr{D}^1_p, \mathscr{D}^2_p, \mathscr{D}^3_p)$ is a line of the matrix $\mathscr{D}$ (see (9.170)), $\boldsymbol{\Phi}^{j1}, \boldsymbol{\Phi}^{j2}, \boldsymbol{\Phi}^{j3}$ are columns of the matrix $\boldsymbol{\Phi}^j$, and the radius R of the ball $B_R = \{\xi : \|\xi\| < R\}$ is chosen such that $\overline{\omega}_j \subset B_R$. If the radius $R = 1$ then the unit ball $B := \{\xi : \|\xi\| < 1\}$ as well as $B := \{x : \|x\| < 1\}$. The coefficients $\mathsf{P}^{(j)}_{kp}$ in (9.197) form the (6×6)-matrix $\mathsf{P}^{(j)}$, $j = 1, \dots, J$, which is called the *polarization matrix* of the elastic inclusion ω_j (see [165, 220] and also [105], [170, Chapter 6], [172]). Some properties of the polarization matrix, and some comments on the solvability of problem (9.195a)-(9.195d) are given in Section 9.4.4 as well as in Appendix D.

The columns $\mathsf{W}^{j1}, \dots, \mathsf{W}^{j6}$ compose the (3×6)-matrix W^j and we set

$$w^{1j}(\xi) = \mathsf{W}^j(\xi)\vartheta^j. \tag{9.198}$$

In Appendix C, Section C.1, it is verified that the right choice of boundary layer is given by formula (9.198), since it compensates the main terms of discrepancies. From (9.197) and (9.198) it follows that

$$w^{1j}(\xi) = (\mathsf{P}^{(j)}\mathscr{D}(\nabla_{\xi})\boldsymbol{\Phi}^j(\xi)^{\top})^{\top}\vartheta^j + O(\|\xi\|^{-3}), \quad \xi \in \mathbb{R}^3 \setminus B_R. \tag{9.199}$$

Relation (9.199) can be *differentiated term by term* on the set $\mathbb{R}^3 \setminus B_R$ under the rule $\nabla_{\xi} O(\|\xi\|^{-p}) = O(\|\xi\|^{-p-1})$ for the remainder.

In view of (9.196) the detached asymptotic expansion term equals

$$h^2(\mathsf{P}^{(j)}\mathscr{D}(\nabla_x)\Phi^j(x-p^j)^\top)^\top\vartheta^j. \tag{9.200}$$

It produces discrepancies of order $O(h^3)$, which should be taken into account when constructing the regular type term h^3v (we point out that there is the factor h on w^{1j} in (9.191)). On the other hand, discrepancies of the same order $O(h^3)$ are left in the problem for v by the subsequent term $h^2w(h^{-1}(x-p^j))$, which solves the transmission problem analogous to (9.195a)-(9.195d), that is

$$\mathscr{L}^{0j}(\nabla_\xi)w^{2j}(\xi) = F^{0j}(\xi), \quad \xi\in\Theta_j, \tag{9.201}$$
$$\mathscr{L}^{j}(\xi,\nabla_\xi)w^{2j}(\xi) = F^{j}(\xi), \quad \xi\in\omega_j, \tag{9.202}$$

with jump conditions of the form

$$w_+^{2j}(\xi) = w_-^{2j}(\xi), \quad \xi\in\partial\omega_j, \tag{9.203}$$

$$\begin{aligned}\mathscr{D}(\nu(\xi))^\top(\mathscr{A}_{(j)}(\xi)\mathscr{D}(\nabla_\xi)w_-^{2j}(\xi)-&\\ \mathscr{A}(p^j)\mathscr{D}(\nabla_\xi)w_+^{2j}(\xi)) = G^j(\xi), &\quad \xi\in\partial\omega_j,\end{aligned} \tag{9.204}$$

and with the decay rate $O(\|\xi\|^{-1})$ at $\|\xi\|\to\infty$, smaller compared to the decay rate of w^{1j}.

Now, we evaluate the right hand sides of the problems (9.201)-(9.204). First, by the representation of the stiffness matrix

$$\mathscr{A}(x) = \mathscr{A}(p^j) + (x-p^j)^\top\nabla_x\mathscr{A}(p^j) + O(\|x-p^j\|^2) \tag{9.205}$$

and the corresponding splitting of differential operator with the variable coefficients $\mathscr{L}^0(x,\nabla_x)$ from (9.178a), we find that the right hand side of system (9.201)-(9.202) is the main term of the expression

$$\begin{aligned}-\mathscr{L}^0(x,\nabla_x)w^{1j}(h^{-1}(x-p^j)) &\sim h^{-1}\mathscr{D}(\nabla_\xi)^\top(\xi^\top\nabla_x\mathscr{A}(p^j))\mathscr{D}(\nabla_\xi)w^{1j}(\xi)\\ &=: h^{-1}F^{0j}(\xi).\end{aligned} \tag{9.206}$$

We note that $\mathscr{L}^{0j}(\nabla_x)w^{1j}(h^{-1}(x-p^j)) = 0$ in (9.206). The following discrepancy appears in the second transmission condition (9.204):

$$\begin{aligned}G^j(\xi) &= \mathscr{D}(\nu(\xi))^\top(\xi^\top\nabla_x\mathscr{A}(p^j))(\mathscr{D}(\nabla_\xi)w^{1j}(\xi)+\vartheta^j)\\ &+ \mathscr{D}(\nu(\xi))^\top(\mathscr{A}(p^j)-\mathscr{A}_{(j)}(\xi))\mathscr{D}(\nabla_\xi)\mathsf{U}^j(\xi).\end{aligned} \tag{9.207}$$

The second term comes out from the second order elaborated Taylor formula (9.205)

$$u(x) = \mathbb{D}(x-p^j)a^j + \mathscr{D}(x-p^j)^\top\vartheta^j + \mathsf{U}^j(x-p^j) + O(\|x-p^j\|^3) \tag{9.208}$$

and involves the quadratic vector functions $\xi \to \mathsf{U}^j(\xi)$, $j = 1,\dots,J$,

$$\mathsf{U}^j(x-p^j) := \frac{1}{2}(x-p^j)^\top U^j(x-p^j) = \frac{1}{2}\sum_{p,q=1}^{3}(x_p - p^j_p)U^j_{pq}(x_q - p^j_q), \quad (9.209)$$

where U^j stands for the second order differential of the vector function u evaluated at p^j, i.e., U^j is the symmetric matrix with entries

$$U^j_{pq} := \frac{\partial^2 u}{\partial x_p \partial x_q}(p^j).$$

Finally, the right hand side of system (9.201)-(9.202) takes the form

$$F^j(\xi) = -\lambda\gamma_j(\xi)u(p^j) + \mathscr{D}(\nabla_\xi)^\top \mathscr{A}_{(j)}(\xi)\mathscr{D}(\nabla_\xi)\mathsf{U}^j(\xi). \quad (9.210)$$

Besides the term obtained from the quadratic vector function (9.209) in the Taylor formula (9.208), the expression (9.210) contains the discrepancy $\lambda\gamma_j u(p^j)$ which originates from the inertial term $\lambda^h\gamma_j u^h$ in accordance to the asymptotic ansätze (9.209).

In order to establish properties of solutions to the problem (9.201)-(9.204), we need some complementary results.

Lemma 9.1. *Assume that* $\mathsf{Z}(\xi) = \mathscr{D}(\nabla_\xi)^\top \mathsf{Y}(\xi)$ *and*

$$\mathsf{Y}(\xi) = \rho^{-2}\mathfrak{Y}(\theta), \quad \mathsf{Z}(\xi) = \rho^{-3}\mathfrak{Z}(\theta), \quad (9.211)$$

where (ρ,θ) *are spherical coordinates and* $\mathfrak{Y} \in C^\infty(\partial B;\mathbb{R}^6)$, $\mathfrak{Z} \in C^\infty(\partial B;\mathbb{R}^3)$ *are smooth vector functions on the unit sphere* $\partial B := \{\xi : \|\xi\| = 1\}$. *The model problem*

$$\mathscr{L}^{0j}(\nabla_\xi)\mathsf{X}(\xi) = \mathsf{Z}(\xi), \quad \xi \in \mathbb{R}^3 \setminus \{0\}, \quad (9.212a)$$

admits a solution $\mathsf{X}(\xi) = \rho^{-1}\mathfrak{X}(\theta)$, *which is defined up to the term* $\Phi^j(\xi)c$ *with* $c \in \mathbb{R}^3$, *and becomes unique under the orthogonality condition*

$$\int_{\partial B} \mathscr{D}(\xi)^\top \mathscr{A}^0(p^j)\mathscr{D}(\nabla_\xi)\mathsf{X}(\xi)\,ds_\xi = 0 \in \mathbb{R}^3. \quad (9.212b)$$

Proof. After separating variables and rewriting the operator $\mathscr{L}^{0j}(\nabla_\xi)$ in the spherical coordinates ($\mathscr{L}^{0j}(\nabla_\xi) = r^{-2}\mathfrak{L}(\theta,\nabla_\theta, r\partial/\partial r)$), the system (9.212a) takes the form

$$\mathfrak{L}^j(\theta,\nabla_\theta,-1)\mathfrak{X}(\theta) = \mathfrak{Z}(\theta), \quad \theta \in \partial B. \quad (9.213)$$

Since $\mathfrak{L}(\theta,\nabla_\theta,0)$ is the formally adjoint operator for $\mathfrak{L}^j(\theta,\nabla_\theta,-1)$ (see, for example, [170, Lemma 3.5.9]), the compatibility condition for the system of differential equations (9.213) implies the equality

$$\int_{\partial B} \mathfrak{Z}(\theta)\,ds_\theta = 0 \in \mathbb{R}^3. \quad (9.214)$$

The equality represents the orthogonality condition in the space $L^2(\partial B;\mathbb{R}^3)$ of the right hand side $\mathfrak{Z}$ of system (9.213) to the solutions of the system

$$\mathfrak{L}^j(\theta,\nabla_\theta,0)\mathfrak{V}(\theta)=0, \quad \theta\in\partial B\,, \tag{9.215}$$

which are nothing but constant columns. Indeed, after transformation to the cartesian coordinate system ξ, equations (9.215) take the form

$$\mathscr{L}^{0j}(\nabla_\xi)V(\xi)=0, \quad \xi\in\mathbb{R}^3\setminus\{\mathscr{O}\}, \tag{9.216}$$

and any solution $V(\xi)=\rho^0\mathfrak{V}(\theta)$ is constant. Let $b>a>0$ be some numbers, and let Ξ be the annulus $\{\xi : a<\rho<b\}$. We have

$$\begin{aligned}\ln\frac{b}{a}\int_{\partial B}\mathfrak{Z}(\theta)ds_\theta &= \int_a^b\rho^{-1}d\rho\int_{\partial B}\mathfrak{Z}(\theta)ds_\theta=\int_\Xi\rho^{-3}\mathfrak{Z}(\theta)d\xi\\ &=\int_\Xi\mathscr{D}(\nabla_\xi)^\top\mathsf{Y}(\xi)d\xi=\int_{\partial B_b}\mathscr{D}(\rho^{-1}\xi)^\top\mathsf{Y}(\xi)ds_\xi\\ &-\int_{\partial B_a}\mathscr{D}(\rho^{-1}\xi)^\top\mathsf{Y}(\xi)ds_\xi=0.\end{aligned} \tag{9.217}$$

We have used here the Green formula and the fact that the integrands on the spheres of radii a and b are equal to $b^{-2}\mathscr{D}(\theta)^\top\mathfrak{Y}$ and $a^{-2}\mathscr{D}(\theta)^\top\mathfrak{Y}$, respectively, i.e., the integrals cancel one another. Therefore, the compatibility condition (9.214) is verified and the system (9.213) has a solution $\mathfrak{X}\in C^\infty(\partial B;\mathbb{R}^3)$. The solution is determined up to a linear combination of traces on ∂B of columns of the *fundamental matrix* $\Phi(\xi)$. Recall that the columns Φ^q of matrix $\Phi(\xi)$ are the only homogeneous solutions of degree -1 of the homogeneous model problem (9.212a) and verify the relations

$$\begin{aligned}-\int_{\partial B}\mathscr{D}(\xi)^\top\mathscr{A}(p^j)\mathscr{D}(\nabla_\xi)\Phi^q(\xi)ds_\xi &= \int_B\mathscr{L}^{0j}(\nabla_\xi)\Phi^q(\xi)d\xi\\ &=\int_B\delta(\xi)e_q d\xi=e_q,\end{aligned} \tag{9.218}$$

where we take into account that $\xi\in\partial B$ is the unit outer normal to the sphere $\partial B=\{\xi : \rho=1\}$, the boundary of the unit ball $B=\{\xi : \rho<1\}$, $\delta\in\mathscr{D}'(\mathbb{R}^3)$ is the Dirac measure, $e_q=(\delta_{1q},\delta_{2q},\delta_{3q})^\top\in\mathbb{R}^3, q=1,2,3$, is the basis vector of the axis x_q, where δ_{ij} stands for the Kronecker symbol, and the last integral over B is understood in the sense of the theory of distributions. Thus, owing to (9.218), the orthogonality condition (9.212b) can be satisfied that implies the uniqueness of the solution $\mathfrak{X}$ to the problem (9.212a)-(9.212b). □

In view of (9.199), (9.200) and (9.206), the right hand side of (9.212a) takes the form

$$\mathsf{Z}(\xi)=\mathscr{D}(\nabla_\xi)^\top(\xi^\top\nabla_\xi\mathscr{A}(p^j))\mathscr{D}(\nabla_\xi)(\mathsf{P}^{(j)}\mathscr{D}(\nabla_\xi)\Phi^j(\xi)^\top)^\top\vartheta^j. \tag{9.219}$$

General results of [117] (see also [170, §3.5, §6.1, §6.4]) show that there exists a unique decaying solution of problem (9.201)-(9.204), which admits the expansion

$$w^{2j}(\xi) = \mathsf{X}^j(\xi) + \Phi^j(\xi)C^j + O(\rho^{-2}(1+|\ln\rho|)), \quad \xi \in \mathbb{R}^3 \setminus B_R. \tag{9.220}$$

In the same way as in relation (9.199), the relation (9.220) can be *differentiated term by term* under the rule $\nabla_\xi O(|\rho|^{-p}(1+|\ln\rho|)) = O(|\rho|^{-p-1}(1+|\ln\rho|))$. The method [149] is applied in order to evaluate the column C^j.

Lemma 9.2. *The equality is valid*

$$C^j = -\lambda(\overline{\gamma_j} - \gamma(p^j))|\omega_j|u(p^j) - \mathscr{I}^j, \tag{9.221}$$

where $|\omega_j|$ *is the volume, and*

$$\overline{\gamma_j} = \frac{1}{|\omega_j|}\int_{\omega_j}\gamma_j(\xi)d\xi \tag{9.222}$$

the mean scaled density of the inclusion ω_j*, i.e., its mass is* $\overline{\gamma_j}|\omega_j|$*, and*

$$\mathscr{I}^j = \int_{\partial B}\mathscr{D}(\xi)^\top(\xi^\top\nabla_\xi\mathscr{A}(p^j))\mathscr{D}(\nabla_\xi)(\mathsf{P}^{(j)}\mathscr{D}(\nabla_\xi)\Phi^j(\xi)^\top)^\top ds_\xi\,\vartheta^j. \tag{9.223}$$

Proof. In the ball B_R we apply the Gauss formula and obtain, that for $R \to \infty$,

$$\begin{aligned}
&\int_{B_R\setminus\omega_j}F^{0j}d\xi + \int_{\omega_j}F^jd\xi + \int_{\partial\omega_j}G^jds_\xi = \qquad (9.224)\\
&\int_{B_R\setminus\omega_j}\mathscr{L}^{j0}w^{2j}d\xi\int_{\omega_j}\mathscr{L}^jw^{2j}d\xi +\\
&\int_{\partial\omega_j}\mathscr{D}(\nu)^\top(\mathscr{A}_{(j)}(\xi)\mathscr{D}(\nabla_\xi)w_-^{2j} - \mathscr{A}(p^j)\mathscr{D}(\nabla_\xi)w_+^{2j})ds_\xi =\\
&-\int_{\partial B_R}\mathscr{D}(\rho^{-1}\xi)^\top\mathscr{A}(p^j)\mathscr{D}(\nabla_\xi)w^{2j}(\xi)ds_\xi =\\
&-\int_{\partial B_R}\mathscr{D}(R^{-1}\xi)^\top\mathscr{A}(p^j)\mathscr{D}(\nabla_\xi)(\mathsf{X}^j(\xi)+\Phi^j(\xi)C^j)d\xi + o(1) = C^j + o(1).
\end{aligned}$$

We have also taken into account equalities (9.212b) and (9.218). On the other hand, in view of formulae (9.206) and (9.210) it follows that

$$\begin{aligned}
\int_{\omega_j}F^j(\xi)d\xi &= -\lambda\int_{\omega_j}\gamma_j(\xi)d\xi u(p^j) + \int_{\omega_j}\mathscr{D}(\nabla_\xi)^\top\mathscr{A}_{(j)}(\xi)\mathscr{D}(\nabla_\xi)\mathsf{U}^j(\xi)d\xi\\
&= -\lambda\overline{\gamma_j}|\omega_j|u(p^j) + \int_{\partial\omega_j}\mathscr{D}(\nu(\xi))^\top\mathscr{A}_{(j)}(\xi)\mathscr{D}(\nabla_\xi)\mathsf{U}^j(\xi)d\xi, \qquad (9.225)
\end{aligned}$$

and

$$\int_{B_R\setminus\omega_j} F^{0j}(\xi)d\xi = -\int_{\partial\omega_j} \mathscr{D}(\nu(\xi))^\top(\xi^\top\nabla_\xi\mathscr{A}(p^j))\mathscr{D}(\nabla_\xi)w^{1j}(\xi)ds_\xi + \int_{\partial B_R} \mathscr{D}(R^{-1}\xi)^\top(\xi^\top\nabla_x\mathscr{A}(p^j))\mathscr{D}(\nabla_\xi)w^{1j}(\xi)ds_\xi. \quad (9.226)$$

We turn back to the decomposition (9.199). Then, by taking into account the homogeneity degree of the integrand, we can see that the integral over the sphere ∂B_R equals

$$\int_{\partial B} \mathscr{D}(\xi)^\top(\xi^\top\nabla_x\mathscr{A}(p^j))\mathscr{D}(\nabla_\xi)(\mathsf{P}^{(j)}\mathscr{D}(\nabla_\xi)\Phi^j(\xi)^\top)^\top ds_\xi\,\vartheta^j + O(R^{-1}). \quad (9.227)$$

The integrals over the surfaces $\partial\omega_j$ in the right hand sides of (9.225)-(9.226) cancel with two integrals, which according to (9.207) appear in the formula

$$\begin{aligned}\int_{\partial\omega_j} G^j(\xi)ds_\xi = &\int_{\partial\omega_j} \mathscr{D}(\nu(\xi))^\top(\xi^\top\nabla_x\mathscr{A}(p^j))\mathscr{D}(\nabla_\xi)w^{1j}(\xi)ds_\xi\\ &-\int_{\partial\omega_j} \mathscr{D}(\nu(\xi))^\top\mathscr{A}_{(j)}(\xi)\mathscr{D}(\nabla_\xi)\mathsf{U}^j(\xi)d\xi\\ &+\int_{\partial\omega_j} \mathscr{D}(\nu(\xi))^\top(\xi^\top\nabla_x\mathscr{A}(p^j))ds_\xi\,\vartheta^j\\ &+\int_{\partial\omega_j} \mathscr{D}(\nu(\xi))^\top\mathscr{A}(p^j)\mathscr{D}(\nabla_\xi)\mathsf{U}^j(\xi)ds_\xi. \end{aligned} \quad (9.228)$$

Finally, by the equality

$$\mathscr{D}(-\nabla_x)^\top\mathscr{A}^0(p^j)\mathscr{D}(-\nabla_x)\mathsf{U}^j(\xi) + \mathscr{D}(-\nabla_x)^\top(x^\top\nabla_x\mathscr{A}^0(p^j))\vartheta^j = \lambda\gamma^0(p^j)u(p^j)\,, \quad (9.229)$$

resulting from equation (9.207) at the point $x = p^j$, the sum of the pair of two last integrals in (9.228) takes the form

$$\int_{\omega_j}\Big(\mathscr{D}(-\nabla_\xi)^\top\mathscr{A}^0(p^j)\mathscr{D}(\nabla_\xi)\mathsf{U}^j(\xi) + \mathscr{D}(-\nabla_\xi)^\top(\xi^\top\nabla_x\mathscr{A}^0(p^j))\vartheta^j\Big)d\xi = \lambda\gamma^0(p^j)|\omega_j|u(p^j). \quad (9.230)$$

It remains to pass to the limit $R\to+\infty$. □

Now, we are in position to determine the first regular corrector $v := v_{(p)}$ of the eigenfunction $u := u_{(p)}$ and the first corrector $\varsigma := \varsigma_p$ of the eigenvalue λ_p in the ansätze (9.191) and (9.190), which are given by solutions of

Problem 9.13. Find v and ς such that

$$\mathscr{L}(x,\nabla_x)v(x) = \lambda\gamma(x)v(x) + \varsigma\gamma(x)u(x) + f(x), \quad x \in \Omega \setminus \{p^1,\dots,p^J\}, \tag{9.231a}$$

$$\mathscr{D}(n(x))^\top \mathscr{A}(x)\mathscr{D}(\nabla_x)v(x) = 0, \quad x \in \Sigma, \quad v(x) = 0, \quad x \in \Gamma, \tag{9.231b}$$

where $n(x) := \nu(x)$ stands for the unit normal vector on Γ.

The weak formulation of Problem 9.13 is given below by (9.241) in the subspace $H^1_\Gamma(\Omega;\mathbb{R}^3)$ of the Sobolev space $H^1(\Omega;\mathbb{R}^3)$. The right hand side f includes the discrepancies, which results from the boundary layer correctors of order h^3. By decompositions (9.199) and (9.220) we obtain

$$\begin{aligned} f(x) = &\sum_{j=1}^{J} (\mathscr{L}(x,\nabla_x) - \lambda\gamma(x)\mathrm{I}_3)\chi_j(x)(\mathsf{P}^{(j)}\mathscr{D}(\nabla_x)\Phi^j(x-p^j)^\top)^\top \vartheta^j \\ &+ \sum_{j=1}^{J} \{\mathsf{X}^j(x) + \Phi^j(x-p^j)C^j\}. \end{aligned} \tag{9.232}$$

The terms $\mathscr{D}(\nabla_x)\Phi^j(x-p^j)$ and $\Phi^j(x-p^j)$ in (9.232) enjoy the singularities of orders $O(\|x-p^j\|^{-2})$ and $O(\|x-p^j\|^{-1})$, respectively. Therefore, it should be clarified in what sense the differential Problem 9.13 is solvable. Equation (9.231a) is not considered in Ω, but it is posed in the *punctured domain* $\Omega \setminus \{p^1,\dots,p^J\}$. Thus the Dirac measure and its derivatives, which are obtained by the action of the operator $\mathscr{L}$ on the *fundamental matrix*, are not taken into account. Besides that, by virtue of the definition of the term X^j implying a solution to the model problem (9.212a) with the right hand side (9.219), and according to the estimates of remainders in the expansions (9.199) and (9.220), the following relations are valid

$$f(x) = O(r_j^{-2}(1+\ln r_j)), \quad r_j := \|x-p^j\| \to 0, \quad j = 1,\dots,J, \tag{9.233}$$

which can be *differentiated term by term* according to the rule

$$\nabla_x O(r_j^{-p}(1+|\ln r_j|)) = O(r_j^{-p-1}(1+|\ln r_j|)). \tag{9.234}$$

In other words, expression (9.232) should be rewritten

$$\begin{aligned} f(x) = &\sum_{j=1}^{J} ([\mathscr{L},\chi_j] - \lambda\gamma\chi_j\mathrm{I}_3)(S^{j1}+S^{j2}) + \sum_{j=1}^{J} (\mathscr{A} - \mathscr{A}(p^j))\mathscr{D}(\nabla_x)S^{j2} \\ &+ \sum_{j=1}^{J} \chi_j \mathscr{D}(\nabla_x)^\top((\mathscr{A} - \mathscr{A}(p^j) - (x-p^j)^\top\nabla_x\mathscr{A}(p^j))\mathscr{D}(\nabla_x)S^{j1}. \end{aligned} \tag{9.235}$$

Here, $[\mathscr{L}_1,\mathscr{L}_2] = \mathscr{L}_1\mathscr{L}_2 - \mathscr{L}_2\mathscr{L}_1$ is the commutator of operators $\mathscr{L}_1$ and $\mathscr{L}_2$, and

$$S^{j1}(x) = (\mathsf{P}^{(j)}\mathscr{D}(\nabla_x)\Phi^j(x-p^j)^\top)^\top\vartheta^j, \tag{9.236}$$

$$S^{j2}(x) = S^{j1}(x) + \mathsf{X}^j(x) + \Phi^j(x-p^j)C^j. \tag{9.237}$$

Lemma 9.3. *Let* λ *be a simple eigenvalue in the problem* (9.178a)-(9.178c)*, and* u *the corresponding vector eigenfunction normalized by the condition* (9.181)*. Then, Problem 9.13 admits a solution* $v \in H^1(\Omega;\mathbb{R}^3)$ *if and only if*

$$\varsigma = -\lim_{\iota\to 0}\int_{\Omega_\iota} u(x)^\top f(x)dx\,, \tag{9.238}$$

where $\Omega_\iota := \Omega \setminus (B^1_\iota \cup \cdots \cup B^J_\iota)$ *and* $B^j_\iota = \{x : r_j = \|x - p^j\| < \iota\}$.

Proof. The variant of the one dimensional *Hardy's inequality*

$$\int_0^1 |z(r)|^2 dr \leqslant c\left(\int_0^1 r^2|\partial_r z(r)|^2 dr + \int_{1/2}^1 |z(r)|^2 dr\right) \tag{9.239}$$

provides the estimate

$$\|r_j^{-1}\upsilon\|_{L^2(\Omega;\mathbb{R}^3)} \leqslant c\|\upsilon\|_{H^1(\Omega;\mathbb{R}^3)}. \tag{9.240}$$

In this way, the last term in the integral identity serving for Problem 9.13

$$(\mathscr{A}\nabla_x v, \nabla_x \upsilon)_\Omega - \lambda(\gamma v, \upsilon)_\Omega = \varsigma(\rho u, \upsilon)_\Omega + (f, \upsilon)_\Omega\ \forall\, \upsilon \in H^1_\Gamma(\Omega;\mathbb{R}^3), \tag{9.241}$$

is a continuous functional over the Sobolev space $H^1(\Omega;\mathbb{R}^3)$, owing to the inequalities

$$\begin{aligned}|(f,\upsilon)_\Omega| &\leqslant c\left(\|\upsilon\|_{L^2(\Omega;\mathbb{R}^3)} + \sum_{j=1}^J \left(\int_{B^j_\iota} r_j^2\|f(x)\|^2 dx\right)^{\frac12}\left(\int_{B^j_\iota} r_j^{-2}\|\upsilon(x)\|^2 dx\right)^{\frac12}\right)\\ &\leqslant c\|\upsilon\|_{H^1(\Omega;\mathbb{R}^3)},\end{aligned} \tag{9.242}$$

and

$$\int_{B^j_\iota} r_j^2\|f(x)\|^2 dx \leqslant c\int_0^\iota r_j^2 r_j^{-2}(1+|\ln r_j|)^2 dr_j < +\infty. \tag{9.243}$$

Thus, the result follows by the Riesz representation theorem and the Fredholm alternative. In addition, formula (9.238) holds true since the integrand is a smooth function in $\Omega \setminus \{p^1,\dots,p^J\}$, with absolutely integrable singularities at the points $p^1,\dots,p^J$. □

Remark 9.12. If the points p^j are considered as tips of the complete cones $\mathbb{R}^3 \setminus \{p^j\}$, the *elliptic theory in domains with conical points* (see the fundamental contributions [117, 149, 152] and also monograph [170]) provides estimates in weighted norms of the solution v to Problem 9.13. Indeed, owing to relation (9.233) for any $\tau > 1/2$ the inclusions $r_j^\tau f \in L^2(\mathfrak{N}^j;\mathbb{R}^3)$ are valid, where $\mathfrak{N}^j$ stands for a neighborhood of the point p^j, in addition $\mathfrak{N}^j \cap \mathfrak{N}^k = \varnothing$ for $j \neq k$, therefore, the terms $r_j^{\tau-2}v$, $r_j^{\tau-1}\nabla_x v$ and $r_j^\tau \nabla_x^2 v$ are square integrable in $\mathfrak{N}^j$.

We evaluate the limit in the right hand side of (9.238) for $\iota \to +0$. By the Green formula and representation (9.232), the limit is equal to the sum of the surface integrals

$$\lim_{\iota\to 0}\int_{\Omega_\iota} u(x)^\top f(x)dx = -\int_{\partial B_\iota^j}\Big(S^j(x)^\top \mathscr{D}(\iota^{-1}(x-p^j))^\top \mathscr{A}(x)\mathscr{D}(\nabla_x)u(x)\Big)\,ds_x$$
$$+\int_{\partial B_\iota^j}\Big(u(x)^\top \mathscr{D}(\iota^{-1}(x-p^j))^\top \mathscr{A}(x)\mathscr{D}(\nabla_x)S^{j1}(x)+S^{j2}\Big)\,ds_x\,. \quad (9.244)$$

We apply the Taylor formulae (9.192) and (9.205) to the matrix $\mathscr{A}$ and to the vector u, and take into account relations (9.175) for the matrices $\mathbb{D}$ and $\mathscr{D}$. We also introduce the stretched coordinates $\xi = \iota^{-1}(x-p^j)$. As a result, up to an infinitesimal term as $\iota \to +0$, integral (9.244) equals to

$$\begin{aligned}
&-\iota^{-1}\mathscr{I}_0+\mathscr{I}_1+\mathscr{I}_2+\mathscr{I}_3+\mathscr{I}_4+o(1)=\\
&-\iota^{-1}\int_{\partial B} u(p^j)^\top \mathscr{D}(\xi)^\top \mathscr{A}(p^{(i)})\mathscr{D}(\nabla_\xi)S^{j1}(\xi)ds_\xi\\
&-\int_{\partial B}(\mathbb{D}(\xi)a^j-u(p^j))^\top \mathscr{D}(\xi)^\top \mathscr{A}(p^j)\mathscr{D}(\nabla_\xi)S^{j1}(\xi)ds_\xi\\
&-\int_{\partial B} u(p^j)^\top \mathscr{D}(\xi)^\top(\xi^\top\nabla_x\mathscr{A}(p^j))\mathscr{D}(\nabla_\xi)S^{j1}(\xi)ds_\xi\\
&-\int_{\partial B} u(p^j)^\top \mathscr{D}(\xi)^\top \mathscr{A}(p^j)\mathscr{D}(\nabla_\xi)(\mathsf{X}^j(\xi)+\Phi^j(\xi)C^j)ds_\xi\\
&+\int_{\partial B}(S^{j0}(\xi)^\top \mathscr{D}(\xi)^\top \mathscr{A}(p^j)\mathscr{D}(\nabla_\xi)\mathscr{D}(\xi)^\top\vartheta^j\\
&-(\mathscr{D}(\xi)^\top\vartheta^j)^\top \mathscr{D}(\xi)^\top \mathscr{A}(p^j)\mathscr{D}(\nabla_\xi)S^{j1}(\xi))ds_\xi+o(1).
\end{aligned} \quad (9.245)$$

The integrals $\mathscr{I}_0$ and $\mathscr{I}_1$ vanish. Indeed, due to the identity $\mathscr{D}(\nabla_x)\mathbb{D}(x) = \mathrm{O}_6$ we have

$$\begin{aligned}
&\int_{\partial B}\mathbb{D}(\xi)^\top \mathscr{D}(\xi)^\top \mathscr{A}(p^j)\mathscr{D}(\nabla_\xi)S^{j1}(\xi)ds_\xi=\\
&-\int_B \mathbb{D}(\xi)^\top \mathscr{D}(\xi)^\top \mathscr{A}(p^j)\mathscr{D}(\nabla_\xi)(\mathsf{P}^{(j)}\mathscr{D}(\nabla_\xi)\Phi^j(\xi)^\top)^\top\vartheta^j d\xi=\\
&-\int_B \mathbb{D}(\xi)^\top \mathscr{D}(\xi)^\top\delta(\xi)d\xi\,\mathsf{P}^{(j)}\vartheta^j=\\
&-(\mathscr{D}(\nabla_\xi)\mathbb{D}(\xi))^\top|_{\xi=0}\mathsf{P}^{(j)}\vartheta^j=0\in\mathbb{R}^6,
\end{aligned} \quad (9.246)$$

where $\delta(\xi)$ is the Dirac measure, hence these equalities are understood in the sense of the theory of distributions. By formula (9.223), we obtain

$$\mathscr{I}_2 = -u(p^j)^\top \mathscr{I}^j. \quad (9.247)$$

Relations (9.212b) and (9.218) yield

$$\mathscr{I}_3 = u(p^j)^\top C^j. \quad (9.248)$$

Finally, in the same way as in (9.246), we obtain

$$\begin{aligned}\mathscr{I}_4 &= \int_B (\mathscr{D}(\xi)^\top \vartheta^j)^\top \mathscr{D}(\nabla_\xi)^\top \mathscr{A}(p^j)\mathscr{D}(\nabla_\xi)S^{j1}(\xi)d\xi \\ &= -(\vartheta^j)^\top \int_B \mathscr{D}(\xi)\mathscr{D}(\nabla_\xi)^\top \mathsf{P}^{(j)}\vartheta^j \delta(\xi)d\xi = (\vartheta^j)^\top \mathsf{P}^{(j)}\vartheta^j. \quad (9.249)\end{aligned}$$

Now, we could apply the derived formulae. We insert the obtained expressions for $\mathscr{I}_q$ into (9.245) $\to$ (9.244) $\to$ (9.238) and in view of equation (9.221) for the column C^j, we conclude that

$$\varsigma = \sum_{j=1}^{J} \Big((\vartheta^j)^\top \mathsf{P}^{(j)}\vartheta^j + |\omega_j|\lambda(\gamma(p^j) - \overline{\gamma_j})\|u(p^j)\|^2 \Big). \quad (9.250)$$

If equality (9.250) holds, then Problem 9.13 admits a solution $v \in H^1(\Omega;\mathbb{R}^3)$. The construction of the detached terms in the asymptotic ansätze (9.190) and (9.191) is completed.

In Appendix C the formal asymptotic analysis is confirmed and generalized into the following result obtained for multiple eigenvalues [180].

Theorem 9.2. *Let λ_p be a multiple eigenvalue in problem* (9.179) *with multiplicity $\varkappa_p$, this means that in the sequence* (9.180)

$$\lambda_{p-1} < \lambda_p = \cdots = \lambda_{p+\varkappa_p-1} < \lambda_{p+\varkappa_p}. \quad (9.251)$$

Then there exist $h_p > 0$ and $c_p > 0$ such that for $h \in (0, h_p]$ the only eigenvalues $\lambda^h_p, \ldots, \lambda^h_{p+\varkappa_p-1}$ of the singularly perturbed problem (C.14) *verify the estimates*

$$\left|\lambda^h_{p+q-1} - \lambda_p - h^3\varsigma^{(q)}_p\right| \leqslant c_p(\alpha)h^{3+\alpha}\ , \quad q = 1, \ldots, \varkappa_p\ , \quad (9.252)$$

where $c_p(\alpha)$ depends on p and the exponent $\alpha \in (0, 1/2)$ but it is independent of $h \in (0, h_p]$, with the eigenvalues $\varsigma^{(1)}_p, \ldots, \varsigma^{(\varkappa_p)}_p$ of the symmetric matrix $\mathsf{Q}^{(p)} = \{\mathsf{Q}^{(p)}_{km}\}_{1\leqslant k,m\leqslant \varkappa_p}$, the entries are given

$$\begin{aligned}\mathsf{Q}^{(p)}_{km} &= \sum_{j=1}^{J} \vartheta(u_{(p+k-1)}(p^j))^\top \mathsf{P}^{(j)}\vartheta(u_{(p+m-1)}(p^j)) \\ &\quad - \sum_{j=1}^{J} \lambda_p(\overline{\gamma_j} - \gamma(p^j))|\omega_j| u_{(p+k-1)}(p^j)^\top u_{(p+m-1)}(p^j)\ , \quad (9.253)\end{aligned}$$

where $\mathsf{P}^{(j)}$ is the polarization matrix *of the scaled inclusion given in* (9.197) *and* (9.199)*, $u_{(p)}, \ldots, u_{(p+\varkappa_p-1)}$ are the vector eigenfunctions of the problem* (9.179) *for the eigenvalue λ_p and orthonormalized by condition* (9.181). *Finally, the quantities $\overline{\gamma_j}$ and $|\omega_j|$ are defined in Lemma 9.2.*

Remark 9.13. The formal asymptotic procedure is described only in the case of a simple eigenvalue. Now, we explain briefly changes in the asymptotic ansätze (9.190), (9.191) and in the asymptotic procedure in order to perform the asymptotic analysis in the case of a multiple eigenvalue λ_p. It is the framework for the proof of Theorem 9.2 in Appendix C.

1. A single number ς_p and a single vector eigenfunction $u_{(p)}$ in (9.190) and (9.191) are replaced by the numbers $\varsigma_p^{(q)}$, $q = 1,\ldots,\varkappa_p$, and the linear combinations

$$u_{(p)}^{(q)} = b_1^{(q)} u_{(p)} + \cdots + b_{\varkappa_p}^{(q)} u_{(p+\varkappa_p-1)} \tag{9.254}$$

   of vector eigenfunctions, respectively. The columns $b^{(q)} = (b_1^{(q)},\ldots,b_{\varkappa_p}^{(q)})^\top$ belong to $\mathbb{R}^{\varkappa_p}$, $q = 1,\ldots,\varkappa_p$, are the unit vectors.
2. With the changes, the formulae for the boundary layers w^{1jq} and w^{2jq} remain of the same form.
3. Problem 9.13 for the regular correctors $v_{(p)}^{(q)}$, $q = 1,\ldots,\varkappa_p$, requires the modification of the compatibility conditions which turn into the $\varkappa_p$ relations

$$\varsigma_p^{(q)} (\gamma u_{(p)}^{(q)}, u_{p+m-1})_\Omega = - \lim_{\iota\to+0} \int_{\Omega_\iota} u_{p+m-1}(x)^\top f(x) dx\ , \ m = 1,\ldots,\varkappa_p. \tag{9.255}$$

4. The left hand side of (9.255) equals $\varsigma_p^{(q)} b_m^{(q)}$ by (9.181) and (9.254). It is evaluated by the same method as used to evaluate (9.238), that (9.255) becomes the system of algebraic equations

$$\varsigma_p^{(q)} b_m^{(q)} = \sum_{k=1}^{\varkappa_p} \mathsf{Q}_{mk}^{(p)} b_k^{(q)}\ , \quad m = 1,\ldots,\varkappa_p, \tag{9.256}$$

   with coefficients from (9.253). In this way, the eigenvalues of the matrix $\mathsf{Q}^{(p)}$ and its eigenvectors $b^{(q)} \in \mathbb{R}^{\varkappa_p}$ furnish the explicit values for the terms of the asymptotic ansätze (9.190) and (9.191). We emphasize that by the orthogonality and normalization conditions $(b^{(q)})^\top b^{(k)} = \delta_{qk}$ for the eigenvectors of the symmetric matrix $\mathsf{Q}^{(p)}$, it follows that the vector eigenfunctions $u_{(p)} = (u_{(p)}^{(1)},\ldots,u_{(p)}^{(\varkappa_p)})$, with $p = 1,\ldots,\varkappa_p$, in problem (9.179), which are given by formulae (9.254), are as well orthonormalized by the conditions (9.181).

9.4.4 Polarization Matrices

The results on *polarization matrices* for inclusions in elasticity are presented in this section and also in Appendix D. These integral attributes of inclusions in elastic bodies can be useful in *configurational mechanics* theory.

Variational formulation of problem (9.195) for the special fields W^{jk}, which define the elements of the polarization matrix $\mathsf{P}^{(j)}$ in decomposition (9.197), are of the form

$$\begin{aligned} 2E^j(\mathsf{W}^{jk},\zeta) &:= (\mathscr{A}(p^j)\mathscr{D}(\nabla_\xi)\mathsf{W}^{jk},\mathscr{D}(\nabla_\xi)\zeta)_{\Theta_j} \\ &+ (\mathscr{A}_{(j)}\mathscr{D}(\nabla_\xi)\mathsf{W}^{jk},\mathscr{D}(\nabla_\xi)\zeta)_{\omega_j} \\ &= (\mathscr{R}_{(j)}e_k,\mathscr{D}(\nabla_\xi)\zeta)_{\omega_j}, \quad \zeta\in V_0^1(\mathbb{R}^3;\mathbb{R}^3). \end{aligned} \tag{9.257}$$

The following result is established in Appendix D.

Proposition 9.4. *The equalities hold true*

$$\mathsf{P}^{(j)}_{km} = -2E^j(\mathsf{W}^{jk},\mathsf{W}^{jm}) - \int_{\omega_j}(\mathscr{A}_{km}(p^j) - (\mathscr{A}_{(j)})_{km}(\xi))d\xi\,. \tag{9.258}$$

From the above representation it is clear that the matrix $\mathsf{P}^{(j)}$, $j=1,\dots,J$, is symmetric, the property follows by the symmetry of the stiffness matrices $\mathscr{A}^0$, $\mathscr{A}_{(j)}$ and of the energy quadratic form E^j. In addition, the representation allows us to deduce if the matrix $\mathsf{P}^{(j)}$ is negative or positive definite. We write $\mathsf{P}^1 < \mathsf{P}^2$ for the symmetric matrices P^1 and P^2 provided all eigenvalues of $\mathsf{P}^2 - \mathsf{P}^1$ are positive.

Proposition 9.5. *The matrix* $\mathsf{P}^{(j)}$ *has the following properties:*

1. *If* $\mathscr{A}_{(j)}(\xi) < \mathscr{A}(p^j)$ *for* $\xi\in\omega_j$ *(the inclusion is* softer *compared to the bulk phase), then* $\mathsf{P}^{(j)}$ *is a negative definite matrix.*
2. *If the matrix* $\mathscr{A}_{(j)}$ *is constant and* $\mathscr{A}_{(j)}^{-1} < \mathscr{A}(p^j)^{-1}$ *(the homogeneous inclusion is* rigid *compared to the bulk phase), then* $\mathsf{P}^{(j)}$ *is a positive definite matrix.*

It is also possible to consider the limit cases [140, 201], either of a cavity with $\mathscr{A}_{(j)}=0$, or of an absolutely stiff (rigid) inclusion with $\mathscr{A}_{(j)}=\infty$.

- For a cavity the differential problem takes the form

$$\mathscr{L}^{0j}(\nabla_\xi)\mathsf{W}^{jk}(\xi) = 0, \quad \xi\in\Theta_j := \mathbb{R}^3\setminus\overline{\omega_j}, \tag{9.259a}$$
$$\mathscr{D}(\nu(\xi))^\top\mathscr{A}(p^j)\mathscr{D}(\nabla_\xi)\mathsf{W}^{jk}(\xi) = -\mathscr{D}(\nu(\xi))^\top\mathscr{A}(p^j)e_k, \quad \xi\in\partial\omega_j. \tag{9.259b}$$

- For an absolutely rigid inclusion the integral-differential equations occur as follows

$$\mathscr{L}^{0j}(\nabla_\xi)\mathsf{W}^{jk}(\xi) = 0, \quad \xi\in\Theta_j, \tag{9.260a}$$
$$\mathsf{W}^{jk}(\xi) = \mathbb{D}(\xi)c^{jk} - \mathscr{D}(\xi)^\top e_k, \quad \xi\in\partial\omega_j, \tag{9.260b}$$

together with the additional condition

$$\int_{\partial\omega_j}\mathbb{D}(\xi)^\top\mathscr{D}(\nu(\xi))^\top\mathscr{A}(p^j)(\mathscr{D}(\nabla_\xi)\mathsf{W}^{jk}(\xi) - e_k)ds_\xi = 0\in\mathbb{R}^6, \tag{9.260c}$$

where the matrices $\mathscr{D}$ and $\mathbb{D}$ are introduced in (9.170) and (9.174), respectively.

Remark 9.14. The Dirichlet conditions in (9.260b) contains an arbitrary column $c^{jk} \in \mathbb{R}^6$, which permits for rigid motion of ω_j and it is determined from the momentum balance laws (9.260c) applied to the body ω_j.

Remark 9.15. The variational formulation of problems (9.259) and (9.260) is established in the *Kondratiev spaces* $V_0^1(\Theta_j;\mathbb{R}^3)$ (see [117], and e.g., [170]) normed by the weighted norm (C.44) (cf. the right hand side of (C.1)) and in its linear subspace $\{\zeta \in V_0^1(\Theta_j;\mathbb{R}^3) : \zeta_{|\partial\omega_j} \in \mathscr{R}\}$, respectively, where $\mathscr{R}$ is the linear space of rigid motions (9.173).

Remark 9.16. In accordance with Proposition 9.5 the polarization matrix for a cavity is always negative definite, and that for an absolutely rigid inclusion, it is always positive definite. Theorem 9.2 gives an asymptotic formula, which can be combined with the indicated facts and the information from Proposition 9.5, and it makes possible to deduce the sign of the variation of a given eigenvalue in terms of the defect properties. For example, in the case of a crack, with the null volume and negative polarization matrix, the eigenvalues of the weakened body are smaller compared to the initial body.

Chapter 10
Topological Asymptotic Analysis for Semilinear Elliptic Boundary Value Problems

There are very few mathematical results on the shape and topology optimization for nonlinear boundary value problems. We refer the reader to [196] for the mathematical theory of shape optimization in aerodynamics. The new results obtained for compressible Navier-Stokes equations can be summarized as follows:

- The compressible Navier-Stokes equations with the weak renormalized global solutions are well-posed from the point of view of shape optimization which means that for the typical shape functionals of aerodynamics there is the existence of optimal shapes under realistic assumptions on the family of admissible domains.
- The shape differentiability of the drag functional requires the regularity of solutions to the stationary boundary value problems and it is obtained for the strong, local approximate solutions of the stationary problem which means that the numerical methods for shape optimization problems is a vast field of research in progress.

The shape sensitivity analysis results obtained for compressible Navier-Stokes could be completed by shape-topological perturbation theory, but it is out of the scope of this monograph. We refer to [12] for some results in this direction for the incompressible case.

In this chapter the classical solutions of a nonlinear elliptic problem are considered. The nonlinear problem admits the linearization with classical solutions of the linear problem. Asymptotics of solutions to *semilinear elliptic equations* in singularly perturbed domains are investigated in this chapter following the ideas developed in [99]. The equations are considered in two and three spatial dimensions. The singular domain perturbations takes the form of small holes or cavities far from the boundary of the reference (unperturbed) domain. In two spatial dimensions, homogeneous Neumann boundary conditions are prescribed on the boundaries of holes. In three spatial dimensions, we consider homogeneous Dirichlet boundary conditions on the boundaries of cavities. The proof of asymptotic approximation of solutions by the method of compound asymptotic expansions is presented in Appendix E in three spatial dimensions. In the proof, the Banach fixed point theorem in weighted

Hölder spaces provides the estimate for the remainder in asymptotic approximation of the solution. Besides that, an example of shape optimization problem is given for the equation with cubic nonlinearity. It is shown that the example fits in our framework.

The asymptotic analysis of solutions to the semilinear problems is performed by technical reasons only for the classical solutions which belong to the *Hölder space* $C^{2,\alpha}(\Omega)$, with the exponent $\alpha > 0$. It means that for the purposes of asymptotic analysis the existence of a unique classical solution $u \in C^{2,\alpha}(\Omega)$ is required for a semilinear elliptic problem in the C^3 domain $\Omega \subset \mathbb{R}^d$, $d = 2,3$,

$$\begin{cases} -\Delta u(x) = F(x,u(x)), \; x \in \Omega \subset \mathbb{R}^d, \\ \quad u(x) = 0, \qquad\qquad x \in \partial\Omega, \end{cases} \tag{10.1}$$

where $F \in C^{0,\alpha}(\overline{\Omega} \times \mathbb{R})$ is a given function, with $\alpha \in (0,1)$. The results on the existence of classical solutions to the semilinear problems with subcritical nonlinearity can be found e.g., in the textbook [58]. We are interested in the topological asymptotic expansion of a class of shape functionals of the form

$$\mathscr{J}_\Omega(u) = \int_\Omega J(x,u(x)) \,, \qquad \Omega \subset \mathbb{R}^d \,, \tag{10.2}$$

where we assume that the function J, which defines the shape functional, is of class $C^{0,\alpha}(\overline{\Omega} \times \mathbb{R})$, with $\alpha \in (0,1)$.

Condition 10.1. The following regularity is assumed throughout this chapter for the semilinear equation (10.1) and the integral shape functional (10.2) with a given $\alpha \in (0,1)$:

Assumption 10.1. The nonlinear term in (10.1) is given by the function $F \in C^{0,\alpha}(\overline{\Omega} \times \mathbb{R})$, which admits the partial derivative $0 \leqslant F'_u \in C^{0,\alpha}(\overline{\Omega} \times \mathbb{R})$.

Assumption 10.2. The function $J \in C^{0,\alpha}(\overline{\Omega} \times \mathbb{R})$ in (10.2), admits the partial derivative $J'_u \in C^{0,\alpha}(\overline{\Omega} \times \mathbb{R})$.

Assumption 10.3. Given $v \in C^{2,\alpha}(\overline{\Omega})$ and $\eta \in C(\Omega)$, then for all $\sigma \in (0,1)$ and a positive constant C

$$| J(x,v(x)+\eta(x)) - J(x,v(x)) - \eta(x)J'_v(x,v(x)) | \leqslant C \mid \eta(x) \mid^{1+\sigma} . \tag{10.3}$$

Remark 10.1. Assumption 10.3 is required to justify estimate (10.91) in Ω_ε, where v is the solution of semilinear boundary value problem in the reference (unperturbed) domain Ω and η is a given function.

Remark 10.2. If Assumption 10.1 holds, then Assumption E.2 is also satisfied.

Let Ω, ω be bounded domains in $\mathbb{R}^d$ with $C^{2,\alpha}$ boundaries $\partial\Omega$, $\partial\omega$, for some $\alpha \in (0,1)$, and the compact closures $\overline{\Omega}$, $\overline{\omega}$, respectively. We are dealing with singular domain perturbations of $\Omega \subset \mathbb{R}^d$, for $d = 2,3$, far from the boundary $\partial\Omega$. We assume that the center $\widehat{x}$ of singular perturbation is an arbitrary point of the reference

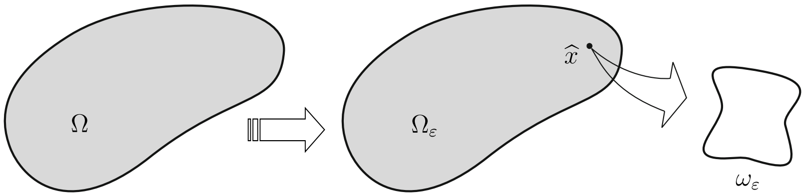


Fig. 10.1 Original (unperturbed) domain Ω and topologically perturbed domain $\Omega_\varepsilon = \Omega \setminus \overline{\omega_\varepsilon}$

domain Ω far from the boundary $\partial\Omega$, and the origin $\mathscr{O}$ belongs to ω. Without loss of generality, we perform the asymptotic analysis for $\widehat{x} := \mathscr{O}$, where $\mathscr{O}$ is the origin of the coordinate system. The following sets are introduced:

$$\omega_\varepsilon = \left\{ x \in \mathbb{R}^d : \xi := \varepsilon^{-1} x \in \omega \right\} \qquad \text{and} \qquad \Omega_\varepsilon = \Omega \setminus \overline{\omega_\varepsilon}, \tag{10.4}$$

where $\varepsilon > 0$ is a small parameter. The upper bound $\varepsilon_0 > 0$ is chosen in such a way that for $\varepsilon \in (0, \varepsilon_0]$ the set ω_ε belongs to the domain Ω, that is $\overline{\omega_\varepsilon} \Subset \Omega$. The set ω_ε is called a cavity, a hole, a void, or an opening, included into the domain Ω_ε. Therefore, Ω represents the original (unperturbed) reference domain and Ω_ε is used to denote the topologically perturbed domain, as shown in fig. 10.1.

Remark 10.3. The regularity of the domains is supposed for the simplicity of the presentation. We require the regularity of the reference domain and the classical solutions of elliptic PDE's because in the approximation procedure of asymptotic analysis we use the Taylor's formula for the solution in the reference domain. In fact we need only the local regularity of solutions to this end. On the other hand, the assumption on the regularity of ω can be weakened.

10.1 Topological Derivatives in $\mathbb{R}^2$

Let us consider two bounded domains Ω and ω in two spatial dimensions $\mathbb{R}^2$. We assume that the closed sets $\overline{\Omega}$ and $\overline{\omega}$ are simply connected and with the smooth boundaries $\partial\Omega$ and $\partial\omega$. The center $\mathscr{O}$ belongs at the same time to Ω and ω. The topological perturbation is defined through (10.4) for $d = 2$. In such a case ω_ε is called a hole in the domain Ω_ε. Let us consider the mixed elliptic *boundary value problem*:

$$\begin{cases} -\Delta u_\varepsilon(x) = F(x, u_\varepsilon(x)), & x \in \Omega_\varepsilon \subset \mathbb{R}^2, \\ u_\varepsilon(x) = 0, & x \in \partial\Omega, \\ \partial_n u_\varepsilon(x) = 0, & x \in \partial\omega_\varepsilon. \end{cases} \tag{10.5}$$

The topological derivative of a shape functional is obtained by formal asymptotic analysis. It means that the construction of an asymptotic approximation for the solutions to problem (10.5) is performed formally. This result is used to obtain directly the topological derivative of the shape functional (10.2).

10.1.1 Formal Asymptotic Analysis

By $\mathfrak{r}_\varepsilon(x)$ we denote a remainder which is different in different places. We suppose that a solution to problem (10.5) admits an asymptotic approximation for $\varepsilon \to 0$ in the form of the *ansätz*

$$u_\varepsilon(x) = v(x) + \varepsilon w_1(\varepsilon^{-1}x) + \varepsilon^2 w_2(\varepsilon^{-1}x) + \varepsilon^2 v'(x) + \mathfrak{r}_\varepsilon(x) \,. \tag{10.6}$$

Some terms in the above expansion require explanation:

- v is a solution of the original semilinear boundary value problem;
- since there is no singularity at the origin in the semilinear boundary value problem, its classical solution coincides with the solution of the semilinear problem in the punctured domain $\Omega \setminus \{\mathscr{O}\}$;
- v' is a regular corrector defined by a solution of a linearized equation in the punctured domain;
- w_1, w_2 are boundary layer correctors given by solutions to exterior problems for the principal part of the elliptic operator in $\mathbb{R}^2 \setminus \overline{\omega}$.

Now, we specify the boundary value problems for all terms in (10.6).

Remark 10.4. In asymptotic analysis of linear elliptic equations in singularly perturbed domains [172] with respect to small parameter $\varepsilon \to 0$, there are involved two sorts of boundary value problems associated with the perturbed boundary value problem: the inner problems in the punctured domain, and the outer problems in the exterior domains. We proceed now with the construction of subsequent inner and outer problems for semilinear equation (10.5). It turns out that as a result all obtained boundary value problems are linear except of the first, which is the unperturbed semilinear boundary value problem. However, for the purposes of the asymptotic analysis it is required that the classical solution to the semilinear problem is locally sufficiently smooth, since the Taylor formula for the classical solution is used in a neighborhood of the origin where the singular perturbation is localised.

In asymptotic analysis of equation (10.5) for $\varepsilon \to 0$, the first boundary value problem is:

$$\begin{cases} -\Delta v(x) = F(x, v(x)), & x \in \Omega \subset \mathbb{R}^2, \\ \quad v(x) = 0, & x \in \partial\Omega. \end{cases} \tag{10.7}$$

It is assumed that the above problem has a solution v defined in Ω, which can be developed at the point $\mathscr{O}$ as follows

$$v(x) = v(\mathscr{O}) + \nabla v(\mathscr{O}) \cdot x + \frac{1}{2} \nabla\nabla v(\mathscr{O}) x \cdot x + O(\|x\|^3) \,. \tag{10.8}$$

The second boundary value problem, which is an exterior problem, is obtained when (10.6) is introduced in (10.5), taking into account that $\Delta = \varepsilon^{-2}\Delta_\xi$, where $\xi = \varepsilon^{-1}x$. Therefore,

$$\begin{aligned} &-\Delta v(x) - \varepsilon^{-1}\Delta_\xi w_1(\xi) - \Delta_\xi w_2(\xi) - \varepsilon^2 \Delta v'(x) + \mathfrak{r}_\varepsilon(x) \\ &= F(x, v(x) + \varepsilon w_1(\xi) + \varepsilon^2 w_2(\xi) + \varepsilon^2 v'(x) + \mathfrak{r}_\varepsilon(x)) \\ &= F(x, v(x)) + (\varepsilon w_1(\xi) + \varepsilon^2 w_2(\xi) + \varepsilon^2 v'(x)) F'_v(x, v(x)) + \mathfrak{r}_\varepsilon(x) \,. \end{aligned} \tag{10.9}$$

In view of (10.7) the leading terms cancel and we have

$$\begin{aligned} &-\varepsilon^{-1}\Delta_\xi w_1(\xi) - \Delta_\xi w_2(\xi) - \varepsilon^2 \Delta v'(x) \\ &= (\varepsilon w_1(\xi) + \varepsilon^2 w_2(\xi) + \varepsilon^2 v'(x)) F'_v(x, v(x)) + \mathfrak{r}_\varepsilon(x) \,. \end{aligned} \tag{10.10}$$

Multiplication of both sides by ε followed by the limit passage $\varepsilon \to 0$ leads to the exterior problem

$$\begin{cases} -\Delta_\xi w_1(\xi) = 0, & \xi \in \mathbb{R}^2 \setminus \overline{\omega}, \\ \partial_{n(\xi)} w_1(\xi) = -\nabla v(\mathscr{O}) \cdot n(\xi), & \xi \in \partial\omega, \end{cases} \tag{10.11}$$

where the condition for the normal derivative of w_1 on the boundary of ω follows from the relations

$$\begin{aligned} 0 &= \partial_{n(x)} u_\varepsilon(x) \\ &= \partial_{n(x)} v(x) + \varepsilon \partial_{n(x)} w_1(\varepsilon^{-1}x) + \varepsilon^2 \partial_{n(x)} w_2(\varepsilon^{-1}x) + \varepsilon^2 \partial_{n(x)} v'(x) + \mathfrak{r}_\varepsilon(x) \\ &= \nabla v(\mathscr{O}) \cdot n(x) + \varepsilon \partial_{n(x)} w_1(\varepsilon^{-1}x) + \varepsilon^2 (\partial_{n(x)} w_2(\varepsilon^{-1}x) + \partial_{n(x)} v'(x)) + \mathfrak{r}_\varepsilon(x) \,. \end{aligned} \tag{10.12}$$

Since $\partial_{n(\xi)}(\cdot) = \varepsilon^{-1}\partial_{n(x)}(\cdot)$, we have

$$\begin{aligned} 0 \;&=\; \nabla v(\mathscr{O}) \cdot n(\xi) + \partial_{n(\xi)} w_1(\xi) + \varepsilon^2 (\partial_{n(x)} w_2(\varepsilon^{-1}x) + \partial_{n(x)} v'(\varepsilon^{-1}x)) + \mathfrak{r}_\varepsilon(x) \\ &\xrightarrow{\varepsilon \to 0} \nabla v(\mathscr{O}) \cdot n(\xi) + \partial_{n(\xi)} w_1(\xi), \; \xi \in \partial\omega \,. \end{aligned} \tag{10.13}$$

In the same way as in (10.9) and (10.10) the second exterior problem is obtained:

$$\begin{cases} -\Delta_\xi w_2(\xi) = 0, & \xi \in \mathbb{R}^2 \setminus \overline{\omega}, \\ \partial_{n(\xi)} w_2(\xi) = -\nabla\nabla v(\mathscr{O}) \xi \cdot n(\xi), & \xi \in \partial\omega, \end{cases} \tag{10.14}$$

with the boundary condition derived as follows:

$$\begin{aligned} 0 &= \partial_{n(x)} u_\varepsilon(x) \\ &= \nabla v(\mathscr{O}) \cdot n(x) + \nabla\nabla v(\mathscr{O}) x \cdot n(x) \\ &+ \varepsilon \partial_{n(x)} w_1(\varepsilon^{-1} x) + \varepsilon^2 \partial_{n(x)} w_2(\varepsilon^{-1} x) + \varepsilon^2 \partial_{n(x)} v'(x) + \mathfrak{r}_\varepsilon(x) \\ &= \nabla v(\mathscr{O}) \cdot n(\xi) + \partial_{n(\xi)} w_1(\xi) \\ &+ \varepsilon(\nabla\nabla v(\mathscr{O}) \xi \cdot n(\xi) + \partial_{n(\xi)} w_2(\xi)) + \varepsilon^2 \partial_{n(x)} v'(x) + \mathfrak{r}_\varepsilon(x) \\ &\xrightarrow{\varepsilon \to 0} \nabla\nabla v(\mathscr{O}) \xi \cdot n(\xi) + \partial_{n(\xi)} w_2(\xi), \ \xi \in \partial\omega \,, \end{aligned} \tag{10.15}$$

by taking into account (10.11) and after division by $\varepsilon > 0$.

Following [198, Appendix 6], we have

$$\nabla v(\mathscr{O}) \cdot n(\xi) = \partial_{n(\xi)} (\nabla v(\mathscr{O}) \cdot \xi) = \partial_{x_i} v(\mathscr{O})\, \partial_{n(\xi)} \xi_i \,, \tag{10.16}$$

where Einstein's summation convention is used for $i = 1,2$. We introduce two functions $W = (W_1, W_2)$ given by solutions of the canonical set of equations:

$$\begin{cases} -\Delta_\xi W_i(\xi) = 0, & \xi \in \mathbb{R}^2 \setminus \overline{\omega}, \\ \partial_{n(\xi)} W_i(\xi) = -\partial_{n(\xi)} \xi_i, & \xi \in \partial\omega, \end{cases} \tag{10.17}$$

for $i = 1,2$. The solution of the above exterior problem is a vector function $W(\xi)$ with the asymptotic behavior [198] for $\|\xi\| \to \infty$:

$$W(\xi) = -\frac{1}{2\pi} \frac{\xi^\top}{\|\xi\|^2} m(\omega) + O(\|\xi\|^{-2}) \,, \tag{10.18}$$

where $m(\omega)$ is the symmetric *virtual mass matrix*. Therefore, we can conclude [198] that the solution of (10.11) admits the asymptotic representation

$$w_1(\xi) := W_i(\xi)\, \partial_{x_i} v(\mathscr{O}) = -\frac{1}{2\pi} \frac{\xi^\top}{\|\xi\|^2} m(\omega) \nabla v(\mathscr{O}) + O(\|\xi\|^{-2}) \,. \tag{10.19}$$

Remark 10.5. For the particular case of a circular hole, $m(\omega)$ is proportional to the identity matrix [198].

Note 10.1. Recall that the solution in the sense of distributions to

$$-\Delta_\xi \phi(\xi) = \delta(\xi), \quad \xi \in \mathbb{R}^2, \tag{10.20}$$

where $\delta(\xi)$ is the Dirac measure concentrated at the origin, is named the *fundamental solution* of Laplacian in two spatial dimensions. This solution is given by

$$\phi(\xi) = -\frac{1}{2\pi} \ln \|\xi\| \,. \tag{10.21}$$

Thus, the asymptotic representation of the solution to (10.14) is written as:

$$w_2(\xi) = -\frac{c}{2\pi}\ln\|\xi\| + c_0 + O(\|\xi\|^{-1}) , \tag{10.22}$$

with the constants c, c_0 to be determined.

Integration by parts in (10.14) over $B_R \setminus \overline{\omega}$ leads to

$$\int_{B_R\setminus\overline{\omega}} \Delta w_2(\xi) = \int_{\partial B_R} \partial_{n(\xi)} w_2(\xi) + \int_{\partial\omega} \partial_{n(\xi)} w_2(\xi) = 0 , \tag{10.23}$$

where B_R is a ball of radius $R > 1$ and center at the origin. Let us consider a polar coordinate system (r,θ) with center at the origin. Therefore, the normal derivative of $w_2(\xi)$ on ∂B_R is given by

$$\begin{aligned} \partial_{n(\xi)} w_2(\xi)_{|\partial B_R} &= -\frac{c}{2\pi}\frac{\partial}{\partial r}\ln(r)_{|r=R} + O(\|\xi\|^{-2}) \\ &= -\frac{c}{2\pi R} + O(\|\xi\|^{-2}) , \end{aligned} \tag{10.24}$$

and the constant c can be determined from the boundary condition

$$\int_{\partial\omega} \partial_{n(\xi)} w_2(\xi) = -\int_{\partial B_R} \partial_{n(\xi)} w_2(\xi) = \frac{c}{2\pi R}\int_0^{2\pi} R d\theta = c , \tag{10.25}$$

where the integral of the term $O(\|\xi\|^{-2})$ on ∂B_R vanishes when R tends to ∞. On the other hand, by taking into account the divergence theorem (G.35), we have:

$$\begin{aligned} \int_{\partial\omega} \partial_{n(\xi)} w_2(\xi) &= -\int_{\partial\omega} \nabla\nabla v(\mathscr{O})\xi \cdot n(\xi) = -\int_{\omega} \operatorname{div}_\xi(\nabla\nabla v(\mathscr{O})\xi) \\ &= -\int_{\omega} \nabla\nabla v(\mathscr{O}) \cdot \mathrm{I} = -|\omega|\Delta v(\mathscr{O}) = |\omega| F(\mathscr{O}, v(\mathscr{O})) . \end{aligned} \tag{10.26}$$

Therefore, $c = |\omega| F(\mathscr{O}, v(\mathscr{O}))$, where $|\omega|$ is the Lebesgue measure of the set ω, and the solution $w_2(\varepsilon^{-1}x)$ is given by:

$$w_2(\varepsilon^{-1}x) = -\frac{1}{2\pi}|\omega| F(\mathscr{O}, v(\mathscr{O}))\ln\|x\| + O(\varepsilon\|x\|^{-1}), \tag{10.27}$$

where the arbitrary constant c_0 has been fixed as

$$c_0 = -\frac{1}{2\pi}|\omega| F(\mathscr{O}, v(\mathscr{O}))\ln\varepsilon . \tag{10.28}$$

Finally, let us consider the last component of the solution (10.6) and note that in view of (10.10) we have:

$$-\varepsilon^2 \Delta v'(x) = \left(\varepsilon w_1(\varepsilon^{-1}x) + \varepsilon^2 w_2(\varepsilon^{-1}x) + \varepsilon^2 v'(x)\right) F'_v(x, v(x)) + \mathfrak{r}_\varepsilon(x) . \tag{10.29}$$

Whence, the problem for v' can be written:

$$\begin{cases} -\Delta v'(x) - v'(x)F_v'(x,v(x)) = g(x)F_v'(x,v(x)), & x \in \Omega, \\ v'(x) = -g(x), & x \in \partial\Omega, \end{cases} \tag{10.30}$$

where function $g(x)$ is defined as

$$g(x) = -\frac{1}{2\pi}\frac{x^\top}{\|x\|^2}m(\omega)\nabla v(\mathscr{O}) + \frac{1}{2\pi}|\omega|F(\mathscr{O},v(\mathscr{O}))\ln\|x\| \,. \tag{10.31}$$

10.1.2 Formal Asymptotics of Shape Functional

In this section the formal asymptotic analysis is applied to the energy functional in two spatial dimensions. In this way, the form of topological derivative of the shape functional can be identified.

The function F being monotone, hence by the Lax-Milgram Lemma and Condition 10.1 it follows that the adjoint state equation

$$\begin{cases} -\Delta p(x) - F_v'(x,v(x))p(x) = J_v'(x,v(x)), & x \in \Omega \subset \mathbb{R}^2, \\ p(x) = 0, & x \in \partial\Omega, \end{cases} \tag{10.32}$$

admits a unique solution $p \in C^{2,\alpha}(\Omega)$. Now, the solution u_ε in the perturbed domain is replaced by its asymptotic approximation (10.6). In this way the first term of the asymptotics of order ε^2 is obtained for the functional

$$\mathscr{J}_{\Omega_\varepsilon}(u_\varepsilon) = \int_{\Omega_\varepsilon} J(x,u_\varepsilon(x))\,, \qquad \Omega_\varepsilon \subset \mathbb{R}^2\,, \tag{10.33}$$

with respect to the small parameter ε. The functional (10.33) is written as follows:

$$\begin{aligned} \mathscr{J}_{\Omega_\varepsilon}(u_\varepsilon) &= \int_{\Omega_\varepsilon} J(x,v(x)) + \int_{\Omega_\varepsilon} (J(x,u_\varepsilon(x)) - J(x,v(x))) \\ &= \mathscr{J}_\Omega(v) - \varepsilon^2|\omega|J(\mathscr{O},v(\mathscr{O})) + \int_{\Omega_\varepsilon} (u_\varepsilon(x) - v(x))J_v'(x,v(x)) + \mathfrak{r}(\varepsilon) \\ &= \mathscr{J}_\Omega(v) - \varepsilon^2|\omega|J(\mathscr{O},v(\mathscr{O})) \\ &\quad + \int_\Omega J_v'(x,v(x))(\varepsilon w_1(\varepsilon^{-1}x) + \varepsilon^2 w_2(\varepsilon^{-1}x) + \varepsilon^2 v'(x)) + \mathfrak{r}(\varepsilon) \\ &= \mathscr{J}_\Omega(v) - \varepsilon^2|\omega|J(\mathscr{O},v(\mathscr{O})) + \varepsilon^2\int_\Omega J_v'(x,v(x))G(x) + \mathfrak{r}(\varepsilon)\,, \end{aligned} \tag{10.34}$$

where $\mathfrak{r}(\varepsilon)$ is a remainder and we denote $G(x) = g(x) + v'(x)$, that is

$$G(x) = -\frac{1}{2\pi}\frac{x^\top}{\|x\|^2}m(\omega)\nabla v(\mathscr{O}) + \frac{1}{2\pi}|\omega|F(\mathscr{O},v(\mathscr{O}))\ln\|x\| + v'(x)\,. \tag{10.35}$$

We introduce the notation and evaluate the integral obtained in (10.34)

$$
\begin{aligned}
\mathscr{I} &:= \int_\Omega J'_v(x,v(x))G(x) \\
&= \int_\Omega (-\Delta p(x) - F'_v(x,v(x))p(x))G(x) \\
&= \lim_{\rho\to 0} \int_{\Omega\setminus\overline{B_\rho}} (-\Delta p(x) - F'_v(x,v(x))p(x))G(x) \,, \qquad (10.36)
\end{aligned}
$$

where B_ρ is a ball of radius ρ and center at the origin. From the Green's formula, we have

$$
\begin{aligned}
\mathscr{I} = \lim_{\rho\to 0} \Bigg(&\int_{\Omega\setminus\overline{B_\rho}} (-\Delta G(x) - F'_v(x,v(x))G(x))p(x) \\
&+ \int_{\partial\Omega} (\partial_n G(x)p(x) - \partial_n p(x)G(x)) \\
&+ \int_{\partial B_\rho} (\partial_n G(x)p(x) - \partial_n p(x)G(x)) \Bigg) . \qquad (10.37)
\end{aligned}
$$

From (10.11), (10.14), (10.30), we conclude that the first term vanishes. Furthermore, by (10.30) and (10.32), the second term equals zero on $\partial\Omega$. Finally, we obtain:

$$
\mathscr{I} = \lim_{\rho\to 0} \left[\int_{\partial B_\rho} \partial_n G(x)p(x) - \int_{\partial B_\rho} \partial_n p(x)G(x) \right] . \qquad (10.38)
$$

The above integral can be evaluated explicitly. We start by expanding $p(x)$ and $v'(x)$ in Taylor's series around the origin $\mathscr{O}$ to obtain

$$
p(x) = p(\mathscr{O}) + \nabla p(\mathscr{O})\cdot x + \mathfrak{r}_\varepsilon(x) \,, \qquad (10.39)
$$

$$
v'(x) = v'(\mathscr{O}) + \nabla v'(\mathscr{O})\cdot x + \mathfrak{r}_\varepsilon(x) \,. \qquad (10.40)
$$

The gradient of the function $G(x)$ can be expressed as follows

$$
\begin{aligned}
\nabla G(x) = &-\frac{1}{2\pi\|x\|^2}\left(\mathrm{I} - \frac{2}{\|x\|^2}(x\otimes x)\right) m(\omega)\nabla v(\mathscr{O}) \\
&+ \frac{x}{2\pi\|x\|^2}|\omega| F(\mathscr{O}, v(\mathscr{O})) + \nabla v'(\mathscr{O}) + \mathfrak{r}_\varepsilon(x) \,. \qquad (10.41)
\end{aligned}
$$

Since on the boundary of the ball B_ρ we have $x = -\rho n$, then the normal derivative of $G(x)$ on ∂B_ρ is given by

$$
\begin{aligned}
\partial_n G(x)_{|\partial B_\rho} = &-\frac{1}{2\pi\rho^2}(\mathrm{I} - 2(n\otimes n))m(\omega)\nabla v(\mathscr{O})\cdot n \\
&- \frac{1}{2\pi\rho}|\omega| F(\mathscr{O}, v(\mathscr{O})) + \nabla v'(\mathscr{O})\cdot n + O(\rho) \,. \qquad (10.42)
\end{aligned}
$$

Therefore, the first integral in (10.38) becomes

$$\int_{\partial B_\rho} \partial_n G(x) p(x) = -\frac{1}{2\pi\rho}\int_{\partial B_\rho} |\omega| F(\mathscr{O}, v(\mathscr{O}))p(\mathscr{O}) \qquad (10.43)$$
$$-\frac{1}{2\pi\rho}(m(\omega)\nabla v(\mathscr{O})\otimes\nabla p(\mathscr{O}))\cdot\int_{\partial B_\rho} n\otimes n + O(\rho)$$
$$= -|\omega|F(\mathscr{O}, v(\mathscr{O})p(\mathscr{O}) - \frac{1}{2}m(\omega)\nabla v(\mathscr{O})\cdot\nabla p(\mathscr{O}) + O(\rho)\,,$$

while the second integral can be written as

$$-\int_{\partial B_\rho} \partial_n p(x) G(x) = -\frac{1}{2\pi\rho}(m(\omega)\nabla v(\mathscr{O})\otimes\nabla p(\mathscr{O}))\cdot\int_{\partial B_\rho} n\otimes n + O(\rho)$$
$$= -\frac{1}{2}m(\omega)\nabla v(\mathscr{O})\cdot\nabla p(\mathscr{O}) + O(\rho)\,, \qquad (10.44)$$

where we have used

$$\int_{\partial B_\rho} n = 0 \qquad \text{and} \qquad \int_{\partial B_\rho} n\otimes n = \pi\rho \mathrm{I}\,. \qquad (10.45)$$

Finally, the limit passage $\rho \to 0$ in (10.38) leads to

$$\mathscr{I} = -m(\omega)\nabla v(\mathscr{O})\cdot\nabla p(\mathscr{O}) - |\omega|F(\mathscr{O}, v(\mathscr{O})p(\mathscr{O})\,. \qquad (10.46)$$

After comparing (10.34) and (10.36) together with (10.46), we can state the following result:

Theorem 10.1. *Under Assumptions 10.1 and 10.2, the (topological) asymptotic expansion of the shape functional* (10.33) *is given by*

$$\mathscr{J}_{\Omega_\varepsilon}(u_\varepsilon) = \mathscr{J}_\Omega(v) - \varepsilon^2\,[|\omega|J(\mathscr{O}, v(\mathscr{O})) +$$
$$m(\omega)\nabla v(\mathscr{O})\cdot\nabla p(\mathscr{O}) + |\omega|F(\mathscr{O}, v(\mathscr{O}))p(\mathscr{O})] + \mathfrak{r}(\varepsilon)\,. \qquad (10.47)$$

Corollary 10.1. *The* topological derivative $\mathscr{T}(\widehat{x})$ *at* $\widehat{x}\in\Omega\subset\mathbb{R}^2$ *far from the boundary* $\partial\Omega$ *of the shape functional* (10.2) *for problem* (10.5) *with homogeneous Neumann boundary condition on the boundary of the hole is given by:*

$$\mathscr{T}(\widehat{x}) = -|\omega|J(\widehat{x}, v(\widehat{x})) - m(\omega)\nabla v(\widehat{x})\cdot\nabla p(\widehat{x}) - |\omega|F(\widehat{x}, v(\widehat{x}))p(\widehat{x})\,, \qquad (10.48)$$

where $v(x)$ *and* $p(x)$ *are solutions to the direct* (10.7) *and adjoint* (10.32) *problems in the unperturbed domain* Ω.

Remark 10.6. The results of analysis for perturbations close to the boundary are given in Chapters 9 for linear spectral problems with the complete proofs in Appendices B and C.

10.2 Topological Derivatives in $\mathbb{R}^3$

Let us consider two bounded domains Ω and ω in three spatial dimensions $\mathbb{R}^3$. We assume again that the closed sets $\overline{\Omega}$ and $\overline{\omega}$ are simply connected and with the smooth boundaries $\partial\Omega$ and $\partial\omega$. The origin $\mathscr{O}$ belongs to Ω and ω. The topological perturbation far from the boundary is defined through (10.4) in three spatial dimensions ($d = 3$). In such a case ω_ε is called a cavity in the domain Ω_ε. Let us consider the Dirichlet elliptic *boundary value problem*:

$$\begin{cases} -\Delta u_\varepsilon(x) = F(x, u_\varepsilon(x)), & x \in \Omega_\varepsilon \subset \mathbb{R}^3, \\ u_\varepsilon(x) = 0, & x \in \partial\Omega, \\ u_\varepsilon(x) = 0, & x \in \partial\omega_\varepsilon. \end{cases} \tag{10.49}$$

In this section, the construction of an asymptotic approximation for the solutions to problem (10.49) is performed. In this way, the topological derivative of the shape functional (10.2) is obtained directly. In Appendix E the proofs are given in the framework of compound asymptotics expansions.

Remark 10.7. The asymptotic approximations of solutions to nonlinear PDE's can be found in [146], (cf. [148, Chapter 5.7]) but without derivation of the form of topological derivatives. We refer also to [14] for topological derivatives of shape functional for nonlinear elliptic problems obtained from the one term exterior approximation of the solutions. In Chapter 11 the asymptotic analysis of the energy functional is performed for the frictionless contact problems.

10.2.1 Asymptotic Approximation of Solutions

We need an *ansätz* for asymptotic behavior of the solutions to nonlinear problems in singularly perturbed domains as $\varepsilon \to 0$. Therefore, the formal analysis serves to devise an asymptotic approximation of the solutions and to determine the boundary value problems for regular as well as boundary layer correctors in asymptotic approximation. The method of compound asymptotics expansions [148] proposes an ansätz for the solution to (10.49) of the for

$$u_\varepsilon(x) = v(x) + w(\varepsilon^{-1}x) + \varepsilon v'(x) + \mathscr{R}_\varepsilon(x)\,, \tag{10.50}$$

where v is the solution of unperturbed problem and $x \mapsto v'(x)$ is regular corrector defined in Ω. The boundary layer corrector $\xi \mapsto w(\xi)$ depends on the fast variable $\xi := \varepsilon^{-1}x$, and it is given by a solution to an exterior boundary value problem. The remainder $\mathscr{R}_\varepsilon(x)$ of (10.50) is in the space $\Lambda^{2,\alpha}_\beta(\Omega_\varepsilon)$ introduced in Appendix E.

We want to simplify the notation, so the subsequent remainders are denoted by the same symbol $\mathscr{R}_\varepsilon(x)$. The remainders are analyzed within the proof of the asymptotic precision of our approximation.

As in [146] (see also [148]; §5.7), the first term in (10.50) is given by the solution of nonlinear problem

$$\begin{cases} -\Delta v(x) = F(x, v(x)), & x \in \Omega \subset \mathbb{R}^3, \\ v(x) = 0, & x \in \partial\Omega . \end{cases} \tag{10.51}$$

The asymptotic approximation is constructed by using the solution to problem (10.51) in unperturbed domain Ω and the solutions to auxiliary linear boundary value problems. The first boundary value problem which defines the regular corrector in (10.50) includes the linearized equation in the *punctured domain* $\Omega \setminus \{\mathscr{O}\}$, with the origin $\mathscr{O}$ as the center of the cavity. The second family of such boundary problems for the boundary layer correctors in (10.50) includes linear exterior problems in $\mathbb{R}^3 \setminus \overline{\omega}$ for the Laplacian which is the principal part of the differential operator in semilinear equation. The proposed asymptotic approximation of the solution to (10.49) uses the *fundamental solution* for the Laplacian and its derivatives, and therefore it enjoys the singularities at the origin, that is why the punctured domain is considered for the regular correctors in the approximation.

Let us consider now the terms v, w and v' in (10.50) and determine the boundary value problems for each of the terms. We assume that the first term v is given by a solution to the first boundary value problem of the form (10.49). Indeed, let us recall that for all $x \in \mathbb{R}^3$ we have $\xi := \varepsilon^{-1}x$, thus $\Delta = \varepsilon^{-2}\Delta_\xi$, and by introducing (10.50) into (10.49) it follows that

$$\begin{aligned} &-\Delta v(x) - \varepsilon^{-2}\Delta_\xi w(\xi) - \varepsilon\Delta v'(x) + \mathscr{R}_\varepsilon(x) \\ &= F(x, v(x) + w(\varepsilon^{-1}x) + \varepsilon v'(x) + \mathscr{R}_\varepsilon(x)) , \end{aligned} \tag{10.52}$$

where $\mathscr{R}_\varepsilon(x)$ represents the higher order terms with respect to ε, which are included in the remainder $\Delta\mathscr{R}_\varepsilon(x)$. Now, by the Taylor's formula for F with respect to the second argument in the neighborhood of $v(x)$ with fixed $x \in \mathbb{R}^3$, we obtain (taking into account that $w(\varepsilon^{-1}x) = w(\xi) \to 0$ with $\varepsilon \to 0$ or, equivalently with $\|\xi\| \to \infty$):

$$\begin{aligned} &F(x, v(x) + w(\varepsilon^{-1}x) + \varepsilon v'(x) + \mathscr{R}_\varepsilon(x)) \\ &= F(x, v(x)) + (w(\varepsilon^{-1}x) + \varepsilon v'(x))F'_v(x, v(x)) + \mathscr{R}_\varepsilon(x) . \end{aligned} \tag{10.53}$$

Therefore, from (10.52) and (10.53) we have:

$$\begin{aligned} &-\Delta v(x) - \varepsilon^{-2}\Delta_\xi w(\xi) - \varepsilon\Delta v'(x) \\ &= F(x, v(x)) + (w(\varepsilon^{-1}x) + \varepsilon v'(x))F'_v(x, v(x)) + \mathscr{R}_\varepsilon(x) . \end{aligned} \tag{10.54}$$

From (10.51) the first terms in (10.54) cancel each other and we obtain

$$-\varepsilon^{-2}\Delta_\xi w(\xi) - \varepsilon\Delta v'(x) = (w(\varepsilon^{-1}x) + \varepsilon v'(x))F'_v(x, v(x)) + \mathscr{R}_\varepsilon(x) , \tag{10.55}$$

hence, multiplying by ε^2 we get:

$$-\Delta_\xi w(\xi) = \varepsilon^3\Delta v'(x) + \varepsilon^2(w(\varepsilon^{-1}x) + \varepsilon v'(x))F'_v(x, v(x)) + \mathscr{R}_\varepsilon(x) . \tag{10.56}$$

As already mentioned, w is given by a solution of an exterior problem, i.e. boundary value problem defined for all $\xi \in \mathbb{R}^3 \setminus \overline{\omega}$. Thus, by the limit passage $\varepsilon \to 0$, and from the condition $w(\varepsilon^{-1}x) = w(\xi) \to 0$ with $\varepsilon \to 0$, or equivalently $\|\xi\| \to \infty$, the following exterior boundary value problem is obtained:

$$\begin{cases} -\Delta_\xi w(\xi) = 0, & \xi \in \mathbb{R}^3 \setminus \overline{\omega}, \\ w(\xi) = -v(\mathscr{O}), & \xi \in \partial\omega, \end{cases} \tag{10.57}$$

whence $w(\xi)$ is a harmonic function in an unbounded domain. The boundary conditions for $w(\xi)$ follows by the boundary condition for $u_\varepsilon(x)$ which vanishes on $\partial\omega_\varepsilon$. Therefore, for all $x \in \partial\omega_\varepsilon$, with $\varepsilon \to 0$, we have:

$$\begin{aligned} 0 &= u_\varepsilon(x) \\ &= v(\mathscr{O}) + w(\varepsilon^{-1}x) + O(\varepsilon) \\ &\xrightarrow{\varepsilon \to 0} v(\mathscr{O}) + w(\xi),\ \xi \in \partial\omega\,. \end{aligned} \tag{10.58}$$

Note 10.2. Recall that the solution in the sense of distributions to

$$-\Delta_\xi \phi(\xi) = \delta(\xi), \quad \xi \in \mathbb{R}^3\,, \tag{10.59}$$

where $\delta(\xi)$ is the Dirac measure concentrated at the origin, is named the *fundamental solution* of Laplacian in three spatial dimensions. This solution is given by

$$\phi(\xi) = \frac{1}{4\pi\|\xi\|}\,. \tag{10.60}$$

Arbitrary solution of (10.57) is of the form

$$w(\xi) = c\phi(\xi) + g(\xi)\,. \tag{10.61}$$

The coefficient c and the function $g(\xi)$ are determined from the condition $w(\xi) = -v(\mathscr{O}), \xi \in \partial\omega$, and by taking into account that the solution (10.61) vanishes at infinity. Therefore, a potential denoted by $\wp$ is introduced here, since the function w enjoys the properties of a potential, i.e. it is a harmonic function with the constant value on the boundary $\partial\omega$. Such potentials are known in the literature [128, 198]. In particular, the potential $\wp$ is a harmonic function in $\mathbb{R}^3 \setminus \overline{\omega}$ such that $\wp(\xi) = 1$, for $\xi \in \partial\omega$, and it admits the asymptotic representation for $\|\xi\| \to \infty$:

$$\wp(\xi) = \frac{\operatorname{cap}(\omega)}{\|\xi\|} + O(\|\xi\|^{-2})\,, \tag{10.62}$$

where $\operatorname{cap}(\omega)$ stands for the *capacity* of $\overline{\omega}$. See Note 9.2 for the definition of Bessel capacity.

Note 10.3. The capacity potential $\wp$ of ω is a minimizer of the energy functional

$$\mathrm{cap}(\omega) := \int_\omega \|\nabla \wp\|^2 = \inf\left\{ \int_\omega \|\nabla \varphi\|^2 : \varphi_{|\omega} \geqslant 1, \varphi \in C_0^\infty(\mathbb{R}^3) \right\}$$

for a compact $\overline{\varpi} \subset \mathbb{R}^3$.

Thus, we can write the following equality for $\|\xi\| \to \infty$

$$\begin{aligned} w(\xi) &= -v(\mathscr{O})\wp(\xi) \\ &= -v(\mathscr{O})\frac{\mathrm{cap}(\omega)}{\|\xi\|} + O(\|\xi\|^{-2}) \\ &= -\frac{4\pi v(\mathscr{O})\mathrm{cap}(\omega)}{4\pi\|\xi\|} + O(\|\xi\|^{-2}) \,. \end{aligned} \tag{10.63}$$

It turns out, that for the following choice

$$c = 4\pi v(\mathscr{O})\mathrm{cap}(\omega) \qquad \text{and} \qquad g(\xi) = O(\|\xi\|^{-2}) \,, \tag{10.64}$$

the function w is given by:

$$w(\varepsilon^{-1}x) = -\varepsilon\frac{\mathrm{cap}(\omega)}{\|x\|}v(\mathscr{O}) + O(\varepsilon^2\|x\|^{-2}) \,, \tag{10.65}$$

hence for $\xi = \varepsilon^{-1}x$, and for $\|\xi\| \to \infty$ we have

$$w(\xi) = -\frac{\mathrm{cap}(\omega)}{\|\xi\|}v(\mathscr{O}) + O(\|\xi\|^{-2}) \,. \tag{10.66}$$

The boundary value problem for the regular corrector $v'(x)$ is now introduced. First, the boundary conditions on $\partial\Omega$ are determined. From (10.49) and (10.50), we have for all $x \in \partial\Omega$

$$0 = u_\varepsilon(x) = v(x) + w(\varepsilon^{-1}x) + \varepsilon v'(x) + \mathscr{R}_\varepsilon(x) \,. \tag{10.67}$$

In view of (10.51), the function $v(x) = 0$ on $\partial\Omega$. Taking into account (10.65), we have $w(\varepsilon^{-1}x) = -\varepsilon c\phi(x) + \mathscr{R}_\varepsilon(x)$ for all $x \in \Omega \setminus \overline{\omega_\varepsilon}$, hence on the boundary $\partial\Omega$ it holds:

$$0 = -\varepsilon c\phi(x) + \varepsilon v'(x) + \mathscr{R}_\varepsilon(x) \,, \tag{10.68}$$

which gives the boundary condition

$$v'(x) = c\phi(x), \quad x \in \partial\Omega \,. \tag{10.69}$$

In order to obtain the equation for $v'(x)$, we can comeback to (10.55), namely

$$-\varepsilon\Delta v'(x) = \varepsilon(-c\phi(x) + v'(x))F_v'(x, v(x)) + \mathscr{R}_\varepsilon(x) \,, \tag{10.70}$$

since $-\Delta_\xi w(\xi) = 0$ for all $\xi \in \mathbb{R}^3 \setminus \overline{\omega}$. Thus we divide both sides of (10.70) by ε and pass to the limit $\varepsilon \to 0$. As a result we obtain

$$\begin{cases} -\Delta v'(x) - v'(x)F_v'(x,v(x)) = -c\phi(x)F_v'(x,v(x)), & x \in \Omega, \\ v'(x) = c\phi(x), & x \in \partial\Omega, \end{cases} \tag{10.71}$$

where $c = 4\pi v(\mathscr{O})\mathrm{cap}(\omega)$.

Remark 10.8. In Appendix E the analysis of the boundary value problem for the regular corrector is presented in the scale of the weighted Hölder spaces. In particular, it can be shown that $F_v'(\cdot,v)\phi \in \Lambda_\gamma^{0,\alpha}(\Omega)$ for all $\gamma > 1+\alpha$ and the solution $v' \in \Lambda_\beta^{2,\alpha}(\Omega)$ of problem (10.71) is such that $v' - v'(\mathscr{O}) \in \Lambda_\gamma^{2,\alpha}(\Omega)$, where $\beta - \alpha \in (2,3)$ and $\gamma - \alpha \in (1,2)$ are arbitrary.

Finally, the following form of the solution to (10.49) is postulated:

$$u_\varepsilon(x) = v(x) + w(\varepsilon^{-1}x) + \varepsilon v'(x) + \widetilde{u}_\varepsilon(x)\ , \tag{10.72}$$

with $v(x)$ given by a solution to (10.51), $w(\varepsilon^{-1}x)$ given by a solution to (10.57) and $v'(x)$ given by a solution of the linearized problem (10.71). The remainder in (10.72), denoted by $\widetilde{u}_\varepsilon(x) := \mathscr{R}_\varepsilon(x)$, is given by the relation:

$$\widetilde{u}_\varepsilon(x) = u_\varepsilon(x) - v(x) - w(\varepsilon^{-1}x) - \varepsilon v'(x)\ . \tag{10.73}$$

Now, our goal is to show that the remainder $\widetilde{u}_\varepsilon(x)$ can be neglected as it is *small* or of higher order with respect to the parameter ε, which means that the expression

$$u_\varepsilon(x) \approx v(x) + w(\varepsilon^{-1}x) + \varepsilon v'(x) \tag{10.74}$$

can be used as an approximation of the solution $u_\varepsilon(x)$ for $\varepsilon \to 0$. Thus, for $x \in \Omega \setminus \overline{\omega_\varepsilon}$

$$-\Delta\widetilde{u}_\varepsilon(x) = -\Delta u_\varepsilon(x) + \Delta v(x) + \Delta w(\varepsilon^{-1}x) + \varepsilon\Delta v'(x)\ , \tag{10.75}$$

since $\Delta w(\varepsilon^{-1}x) = \varepsilon^{-2}\Delta_\xi w(\xi) = 0$, $\xi \in \mathbb{R}^3 \setminus \overline{\omega}$, and in view of (10.71), for $x \in \Omega \setminus \overline{\omega_\varepsilon}$,

$$\varepsilon\Delta v'(x) = -\varepsilon v'(x)F_v'(x,v(x)) + \varepsilon c\phi(x)F_v'(x,v(x))\ , \tag{10.76}$$

then, from (10.49) and (10.51), it follows that

$$\begin{aligned} -\Delta\widetilde{u}_\varepsilon(x) &= F(x,u_\varepsilon(x)) - F(x,v(x)) - \varepsilon F_v'(x,v(x))v' + \varepsilon c\phi(x)F_v'(x,v(x)) \\ &= F(x,v(x) + w(\varepsilon^{-1}x) + \varepsilon v'(x) + \widetilde{u}_\varepsilon(x)) - F(x,v(x)) \\ &- \varepsilon(v'(x) - c\phi(x))F_v'(x,v(x)) \\ &:= F^\varepsilon(x,\widetilde{u}_\varepsilon)\ . \end{aligned} \tag{10.77}$$

On the exterior boundary of Ω we have $u_\varepsilon(x) = 0$ and $v(x) = 0$, hence

$$\widetilde{u}_\varepsilon(x) = -w(\varepsilon^{-1}x) - \varepsilon c\phi(x) := g_\Omega^\varepsilon(x), \quad x \in \partial\Omega\ . \tag{10.78}$$

In addition, on $\partial\omega_\varepsilon$ we have $u_\varepsilon(x)=0$ and $w(\varepsilon^{-1}x)=-v(\mathscr{O})$, whence

$$\widetilde{u}_\varepsilon(x)=-v(x)+v(\mathscr{O})-\varepsilon v'(x):=g^\varepsilon_\omega(x),\quad x\in\partial\omega_\varepsilon\,. \tag{10.79}$$

With the notation we have introduced, the nonlinear problem associated to the remainder $\widetilde{u}_\varepsilon(x)$ takes the form:

$$\begin{cases} -\Delta\widetilde{u}_\varepsilon(x) = F^\varepsilon(x,\widetilde{u}_\varepsilon),\ x\in\Omega_\varepsilon, \\ \widetilde{u}_\varepsilon(x) = g^\varepsilon_\Omega(x),\qquad x\in\partial\Omega, \\ \widetilde{u}_\varepsilon(x) = g^\varepsilon_\omega(x),\qquad x\in\partial\omega_\varepsilon, \end{cases} \tag{10.80}$$

where

$$\begin{aligned} F^\varepsilon(x,\widetilde{u}_\varepsilon) &= F(x,v(x)+w(\varepsilon^{-1}x)+\varepsilon v'(x)+\widetilde{u}_\varepsilon(x))-F(x,v(x)) \\ &\quad -\varepsilon(v'(x)-c\phi(x))F'_v(x,v(x))\,, \end{aligned} \tag{10.81}$$

$$g^\varepsilon_\Omega(x) = -w(\varepsilon^{-1}x)-c\varepsilon\phi(x)\,, \tag{10.82}$$

$$g^\varepsilon_\omega(x) = -v(x)+v(\mathscr{O})-\varepsilon v'(x)\,, \tag{10.83}$$

with the solution defined by the formula (10.73). In the Appendix E we show that the remainder $\widetilde{u}_\varepsilon$, solution to the nonlinear boundary value problem (10.80), is *small* with respect to the parameter ε. The argument used in the proof is based on the Banach fixed point theorem.

10.2.2 Asymptotics of Shape Functional

In this section the asymptotic analysis of (10.2) is performed in three spatial dimensions. In this way the first term of order ε is identified for the asymptotic expansion of the functional

$$\mathscr{J}_{\Omega_\varepsilon}(u_\varepsilon)=\int_{\Omega_\varepsilon}J(x,u_\varepsilon(x)),\qquad \Omega_\varepsilon\subset\mathbb{R}^3\,, \tag{10.84}$$

which is clearly the topological derivative.

We obtain by the Taylor's formula for the function J, which holds in view of Assumption 10.2,

$$\begin{aligned} \mathscr{J}_{\Omega_\varepsilon}(u_\varepsilon) &= \int_{\Omega_\varepsilon}J(x,v(x))+\int_{\Omega_\varepsilon}(w(\varepsilon^{-1}x)+\varepsilon v'(x))J'_v(x,v(x))+\mathscr{R}(\varepsilon) \\ &= \int_\Omega J(x,v(x))+\varepsilon\int_\Omega(v'(x)-c\phi(x))J'_v(x,v(x))+\mathscr{R}(\varepsilon) \\ &= \int_\Omega J(x,v(x))+\varepsilon\int_\Omega G(x)J'_v(x,v(x))+\mathscr{R}(\varepsilon)\,, \end{aligned} \tag{10.85}$$

where $\mathscr{R}(\varepsilon)$ stands for the terms of higher order with respect to the small parameter ε and function $G(x)$ is now defined as

$$G(x) = v'(x) - c\phi(x)\,. \tag{10.86}$$

Let $p \in C^{2,\alpha}(\Omega)$ be a solution of the boundary value problem

$$\begin{cases} -\Delta p(x) - F_v'(x, v(x))p(x) = J_v'(x, v(x)), & x \in \Omega, \\ \qquad\qquad\qquad\qquad p(x) = 0, & x \in \partial\Omega. \end{cases} \tag{10.87}$$

Integration by parts in $\Omega \setminus \overline{B_\rho}$, where B_ρ is a ball of radius ρ and center at the origin, leads to

$$\begin{aligned} \mathscr{I} &= \int_\Omega G(x) J_v'(x, v(x)) \\ &= \lim_{\rho\to 0} \int_{\Omega\setminus\overline{B_\rho}} (-\Delta p(x) - F_v'(x, v(x))p(x))G(x) \\ &= \lim_{\rho\to 0} \int_{\Omega\setminus\overline{B_\rho}} (-\Delta G(x) - F_v'(x, v(x))G(x))p(x) \\ &+ \int_{\partial\Omega} (\partial_n G(x)p(x) - \partial_n p(x)G(x)) \\ &+ \lim_{\rho\to 0} \int_{\partial B_\rho} (\partial_n G(x)p(x) - \partial_n p(x)G(x))\,. \end{aligned} \tag{10.88}$$

From (10.57) and (10.71) we have that the first term vanishes. In addition, by (10.71) and (10.87) the second term is equal to zero, since $p(x) = 0$ and $G(x) = v'(x) - c\phi(x) = 0$ for $x \in \partial\Omega$. Therefore

$$\begin{aligned} \mathscr{I} &= \lim_{\rho\to 0} \int_{\partial B_\rho} (\partial_n (v'(x) - c\phi(x))p(x) - \partial_n p(x)(v'(x) - c\phi(x))) \\ &= -\frac{c}{4\pi} \lim_{\rho\to 0} \frac{1}{\rho^2} \int_{\partial B_\rho} (p(\mathscr{O}) + O(\rho)) \\ &= -c\, p(\mathscr{O}) = -4\pi v(\mathscr{O})p(\mathscr{O})\mathrm{cap}(\omega)\,, \end{aligned} \tag{10.89}$$

hence, the topological asymptotic expansion of the shape functional leads to

$$\mathscr{J}_{\Omega_\varepsilon}(u_\varepsilon) = \mathscr{J}_\Omega(v) - 4\pi\varepsilon\, v(\mathscr{O})p(\mathscr{O})\mathrm{cap}(\omega) + \mathscr{R}(\varepsilon)\,. \tag{10.90}$$

We assume that the function $J \in C^{0,\alpha}(\overline{\Omega} \times \mathbb{R})$, $\alpha \in (0,1)$, verifies Assumptions 10.2, 10.3. Thus,

$$
\begin{aligned}
&| \mathscr{J}_{\Omega_\varepsilon}(u_\varepsilon) - \mathscr{J}_\Omega(v) - \int_{\Omega_\varepsilon} (w(\varepsilon^{-1}x) + \varepsilon v'(x) + \widetilde{u}_\varepsilon(x)) J'_v(x, v(x)) \, | \\
&\leqslant C \int_{\Omega_\varepsilon} | \, w(\varepsilon^{-1}x) + \varepsilon v'(x) + \widetilde{u}_\varepsilon(x) \, |^{1+\sigma} \\
&\leqslant C \int_{\Omega_\varepsilon} \left(\|\varepsilon^{-1}x\|^{-1-\sigma} + \|x\|^{-(1+\sigma)(\beta-2-\alpha)} \left(\varepsilon^{1+\sigma} \|v'\|^{1+\sigma}_{\Lambda^{2,\alpha}_\beta(\Omega)} + \|\widetilde{u}_\varepsilon(x)\|^{1+\sigma}_{\Lambda^{2,\alpha}_\beta(\Omega)} \right) \right) \\
&\leqslant C\varepsilon^{1+\sigma} \left(\int_\varepsilon^1 \tau^{-1-\sigma} \tau^2 d\tau + \int_\varepsilon^1 \tau^{-(1+\sigma)(\beta-2-\alpha)} \tau^2 d\tau \left(\varepsilon^{1+\sigma} + \varepsilon^{(1+\kappa)(1+\sigma)} \right) \right) \\
&\leqslant C\varepsilon^{1+\sigma} \, ,
\end{aligned} \tag{10.91}
$$

since $1+\sigma \leqslant 2$ and $(1+\sigma)(\beta-2-\alpha) \leqslant 2$, it is sufficient to recall the following estimates

$$
|\mathscr{J}_{\Omega_\varepsilon}(u_\varepsilon) - \mathscr{J}_\Omega(v)| \leqslant C\varepsilon \, , \tag{10.92}
$$

$$
\int_{\Omega_\varepsilon} |w(\varepsilon^{-1}x) + c\varepsilon\phi(x)| \times |J'_v(x, v(x))| \leqslant C \int_\varepsilon^1 \left(\frac{\tau}{\varepsilon}\right)^{-2} \tau d\tau \leqslant C\varepsilon^2 \, , \tag{10.93}
$$

$$
\int_{\Omega_\varepsilon} |\widetilde{u}_\varepsilon| \times |J'_v(x, v(x))| \leqslant C\varepsilon^{1+\kappa} \int_{\Omega_\varepsilon} \|x\|^{-(\beta-2-\alpha)} \tau \leqslant C\varepsilon^{1+\kappa} \, , \tag{10.94}
$$

to complete the proof of the result:

Theorem 10.2. *Under Assumptions 10.1, 10.2 and 10.3, it follows that*

$$
\mathscr{J}_{\Omega_\varepsilon}(u_\varepsilon) = \mathscr{J}_\Omega(v) - 4\pi\varepsilon \, v(\mathscr{O}) p(\mathscr{O}) \mathrm{cap}(\omega) + O(\varepsilon^{1+\min(\sigma,\kappa)}) \, . \tag{10.95}
$$

Corollary 10.2. *The* topological derivative *of the shape functional* (10.2) *in the space* $\mathbb{R}^3$ *for problem* (10.49) *with the Dirichlet boundary condition on the boundary of the hole is given, for all* $\widehat{x} \in \Omega$ far from the boundary $\partial\Omega$, *by*

$$
\mathscr{T}(\widehat{x}) = -4\pi v(\widehat{x}) p(\widehat{x}) \mathrm{cap}(\omega) \, , \tag{10.96}
$$

where $v(x)$ *and* $p(x)$ *are solutions to the direct* (10.51) *and adjoint* (10.87) *problems, both associated to the unperturbed domain* Ω.

Remark 10.9. The case of singular perturbations *close to the boundary* is considered in Chapter 9.

10.3 Exercises

1. Consider the semilinear problem in two spatial dimensions as described in Section 10.1:

   a. Show that (10.21) is solution to (10.20).
   b. Derive formulas (10.41)-(10.44).
   c. Proof the identities (10.45).
   d. Consider a shape functional of the form

   $$\mathscr{J}_\Omega(u) = \frac{1}{2}\int_\Omega \|\nabla u\|^2 - \int_\Omega bu\,,$$

   where u is solution to (10.1) for $d=2$ and $F(x,u(x)) = b(x)$, with the function $b(x)$ used to denote a given source term. By taking into account that the perturbation $\omega_\varepsilon(\widehat{x}) = B_\varepsilon(\widehat{x})$, where $B_\varepsilon(\widehat{x})$ is a ball of radius ε and center at $\widehat{x}\in\Omega$, show that the topological asymptotic expansion in Theorem 10.1 leads to

   $$\mathscr{J}_{\Omega_\varepsilon}(u_\varepsilon) = \mathscr{J}_\Omega(u) - \pi\varepsilon^2(\|\nabla u(\widehat{x})\|^2 - b(\widehat{x})u(\widehat{x})) + \mathfrak{r}(\varepsilon)\,,$$

   where in the particular case of circular holes the virtual mass matrix is given by $m(\omega) = -2\pi\mathrm{I}$. Compare this result with the one given in Section 4.1 through expression (4.55), with $\psi(\chi) := \mathscr{J}_\Omega(u)$.

2. Consider the semilinear problem in three spatial dimensions as described in Section 10.2:

   a. Show that the solution to (10.59) is given by (10.60).
   b. Derive formula (10.89).
   c. Repeat the formal derivation presented in this section by taking $F(x,u(x)) = b(x)$ in (10.1) for $d=3$, where the function $b(x)$ is a given source term. The asymptotic analysis in the linear case is well known (see monographs [100, 148]). According to the method of compound asymptotic expansions, the solution u_ε to the perturbed problem can be decomposed as follows

   $$u_\varepsilon(x) = u(x) + w(\varepsilon^{-1}x) + \widetilde{u}_\varepsilon(x)\,,$$

   where the first term is obtained by formally taking $\varepsilon = 0$ and the second one is the boundary value problem which furnishes the leading boundary layers term:

   $$\begin{cases} -\Delta_\xi w(\xi) = 0, & \xi\in\mathbb{R}^3\setminus\overline{\omega},\\ \quad w(\xi) = -u(\widehat{x}), & \xi\in\partial\omega, \end{cases}$$

   where $u(\widehat{x})$ is the value of u at the center $\widehat{x}\in\Omega$ of the perturbation ω_ε. The last term in the expansion is the remainder, which is of order $o(\varepsilon)$.

3. Let us consider a shape optimization problem for a semilinear elliptic equation. For the specific problem the shape and topological derivatives can be obtained

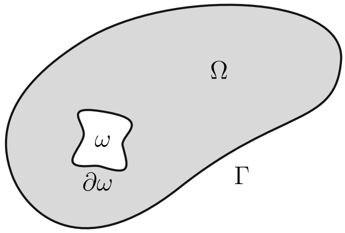


Fig. 10.2 Example of an admissible domain $\Omega = \mathfrak{D} \setminus \overline{\omega}$ with one hole inside

for a general class of shape functionals. Let $\mathfrak{B}$ and $\mathfrak{D}$ be two bounded open sets in $\mathbb{R}^2$ such that $\mathfrak{B} \Subset \mathfrak{D}$. Given a set ω in $\mathbb{R}^2$, we denote by $\#\omega$ the number of connected components of $\overline{\omega}$, and $\#\omega \leqslant k$ means that there are at most k holes in an admissible domain Ω, where k is an integer, as shown in fig. 10.2. In general, the set ω can be represented in the form $\omega = \cup_{i=1}^N \omega^i$, $N \leqslant k$, with simply connected, mutually disjoint sets $\omega^i, i = 1, \ldots, N$. The boundary is of the form $\partial\omega = \cup_{i=1}^N \partial\omega^i$. We introduce the following family of admissible domains

$$\mathscr{U}_{ad} = \left\{\Omega = \mathfrak{D} \setminus \overline{\omega} : \omega \text{ open}, \omega \subset \mathfrak{B}, \#\omega \leqslant k, \mathscr{H}^1(\partial\omega) \leqslant p_0\right\},$$

where p_0 is given and $\mathscr{H}^1(\partial\omega)$ is the *Hausdorff* 1-dimensional measure of $\partial\omega$, i.e., the perimeter of $\partial\omega$. We assume that the boundary $\partial\mathfrak{D} = \Gamma$ of the hold-all domain $\mathfrak{D}$ is $C^{2,\alpha}$, and denote $\partial\Omega = \Gamma \cup \partial\omega$. The semilinear elliptic state equation includes the polynomial nonlinearity, and admits a unique classical solution,

$$\begin{cases} -\Delta u(x) + u(x)^3 = b(x), & x \in \Omega, \\ u(x) = 0, & x \in \Gamma, \\ \partial_n u(x) = 0 & x \in \partial\omega, \end{cases}$$

here n is the unit normal vector on $\partial\Omega$ directed to the exterior of Ω. We denote by

$$H^1_\Gamma(\Omega) = \left\{\varphi \in H^1(\Omega) : \varphi_{|_\Gamma} = 0\right\}$$

the linear subspace of the Sobolev space $H^1(\Omega)$. We recall here the classical result on the existence of solutions for the state equation.

Lemma 10.1. *For any given $b \in L^2(\mathfrak{D})$ there exists a unique solution $u \in H^1_\Gamma(\Omega) \cap L^4(\Omega)$ to the above boundary value problem. The solution minimizes the energy functional*

$$\mathscr{I}_\Omega(\varphi) = \frac{1}{2}\int_\Omega \|\nabla\varphi\|^2 + \frac{1}{4}\int_\Omega |\varphi|^4 - \int_\Omega b\varphi$$

over the space $H^1_\Gamma(\Omega) \cap L^4(\Omega)$.

Given a function z_d defined on $\mathfrak{D}$, the following tracking type shape functional is introduced

$$\mathscr{J}_\Omega(u) := \frac{1}{2}\int_\Omega (u - z_d)^2 .$$

The existence of an optimal domain for the above shape optimization problem can be assured by an appropriate regularization [63, 64] of the shape functional. In our case the regularized version of the shape functional can be taken e.g., in the form

$$\Psi_\Omega(u) := \mathscr{J}_\Omega(u) + \alpha|\Omega| - \beta \max(0, \mathscr{H}^1(\partial\Omega) - p_0)^2 ,$$

where the constants α and β are strictly positive and define the constraints on the surface and the perimeter of the domain Ω. The constant p_0 is strictly positive and defines the threshold for the perimeter. The perimeter constraints become active for domains with the perimeter greater then the constant. Therefore:

a. Show the existence of an optimal domain $\Omega^\star$ for the regularized shape optimization problem.
b. Compute the topological derivative of the regularized shape functional by using the general result given by (10.48). Make some comments on the topological derivative associated to the perimeter constraint.

Chapter 11
Topological Derivatives for Unilateral Problems

In this chapter variational inequalities are considered from the point of view of topological sensitivity analysis. We concentrate on the specific class of problems with the unilateral boundary conditions. This class of variational inequalities includes the frictionless contact problems in linearized elasticity. For the contact problems in two and three spatial dimensions the linearized nonpenetration condition is imposed for the normal displacements in the *potential contact zone* including crack problems [52, 103, 108, 109, 110, 111, 112, 113]. Topological derivatives for unilateral problems are obtained in [208, 209].

The specific method of topological sensitivity analysis which is adapted to the energy functionals associated with the unilateral problems is proposed in this chapter. The complete mathematical justification is presented in this chapter and in Appendix F for the obtained topological derivatives. The proposed framework is based on two important mathematical concepts. The first one is the domain decomposition technique and the associated Steklov-Poincaré pseudodifferential operators. The second concept is the so-called Hadamard directional derivative of the metric projection onto a positive cone with respect to the natural order in a Dirichlet-Sobolev space.

In the proposed framework we can determine one term approximate solution for the unilateral problem with respect to the hole size $\varepsilon \to 0$ created in the geometrical domain Ω far from the boundary hence far from the contact zone. The proposed method is constructive for unilateral problems including the frictionless contact problem in elasticity. As a result, the closed form of the topological derivative for the energy shape functional is obtained for such problems. We present an example of the topological derivative for the elastic body with a rigid inclusion, the boundary of the inclusion is an interface in the domain Ω. The crack is located at the inclusion interface, and the unilateral conditions are prescribed on the crack lips (faces).

11.1 Preliminaries

The properties of solutions to the variational inequalities used in this chapter are obtained in Section 11.3.2 and in Appendix F in the framework of nonsmooth analysis.

Note 11.1. In an abstract setting, the unilateral problem can be reduced to the constrained optimization of the quadratic energy functional

$$\varphi \mapsto \mathscr{E}(\varphi) := \frac{1}{2}a(\varphi,\varphi) - L(\varphi) \tag{11.1}$$

over a convex cone K of the Hilbert space H. Here $H \ni \varphi, \psi \mapsto a(\varphi,\psi) \in \mathbb{R}$ is a continuous bilinear form, and $H \ni \varphi \mapsto L(\varphi) \in \mathbb{R}$ is a continuous linear form on H. A minimizer, if any, satisfies the variational inequality:

Problem 11.1. Find $u \in K$ such that

$$a(u,\varphi - u) \geqslant L(\varphi - u) \quad \forall \varphi \in K. \tag{11.2}$$

We can describe briefly the results obtained for the contact problems. In the presence of constraints due to the convex set K the elliptic regularity of the solutions to variational inequalities is lost. However, the local regularity of solutions is still available. In particular, the topological derivatives of the energy functionals, evaluated far from the boundary, are of the same form as in the case of the energy functional associated to the linear problem:

Problem 11.2. Find $u \in H$ such that

$$a(u,\varphi) = L(\varphi) \quad \forall \varphi \in H. \tag{11.3}$$

Therefore, the derivation of topological derivatives for contact problems can be performed within the following framework:

- The method of derivation combines the domain decomposition technique together with the conical differentiability [62] of the metric projection onto a polyhedric cone in a Dirichlet space.
- The Steklov-Poincaré pseudodifferential boundary operators are employed within the domain decomposition technique.

As a result, the original variational inequality is decomposed into two subproblems, which are:

1. The first subproblem is defined in the subdomain which includes the topological perturbation and can be solved explicitly for the *Dirichlet to Neumann map* or equivalently for the *Steklov-Poincaré operator*.
2. The second subproblem is defined in the subdomain far from the singularity caused by topological perturbation and takes the form of a variational inequality with the nonlocal pseudodifferential operator in the boundary conditions.

In this way the *asymptotic analysis* is separated from the *nonsmooth analysis* which makes the derivation of topological derivatives for the energy functionals of *contact problems* somehow simpler.

Let us point out that such a method of sensitivity analysis was already exploited, however with a different decomposition technique, in [210] for the shape sensitivity analysis of frictionless contact problems.

The direct asymptotic analysis of variational inequalities seems to be possible [22, 23, 24, 25, 26, 27, 28], however, under the restrictive hypothesis of *strict complementarity* for unilateral constraints. The method proposed here [62, 208, 209, 210] allows for the derivation of topological derivatives for the energy functionals without any regularity assumptions on the unknown solutions to the variational inequality under considerations.

Let us describe the properties of subproblems resulting from the domain decomposition applied to the variational inequality. It turns out that the asymptotic expansions of the energy shape functional with respect to singular domain perturbations for the linear elliptic boundary value problems imply the expansions of the related nonlocal Steklov-Poincaré boundary operators. In other words, the knowledge of the asymptotic expansion of the energy is sufficient to determine the regular expansion of the boundary operators. In the proof of asymptotic expansions of the energy functionals are employed the local representation formulae for pointwise values of the first order derivatives of the solutions to the linear elliptic boundary value problems obtained by decomposition. For harmonic functions in two spatial dimensions it is a line integral given by Proposition 11.2. The obtained results are applied for the topological sensitivity analysis of unilateral contact problems in Section 11.4 for the crack modeling with the nonpenetration condition on the crack's lips for $d = 2$.

Note 11.2. We need also some explanation, why the compound asymptotics method should be adapted to the variational inequalities. The *compound asymptotics method* can be applied to *linear elliptic problems* with a postulated ansätz for solutions in singularly perturbed domain. Such an ansätz defines an approximate solution depending on the small parameter ε. Now, we want to replace the exact solution by its approximation. The discrepancies left by the approximate solution in the linear boundary value problem are estimated in such a way, which implies that the remainder can be neglected in the first order expansion of the energy functional, i.e., the remainder leads to the terms of higher order with respect to ε in the first order expansion of the energy shape functional. Thus, the solution of a linear boundary value problem in singularly perturbed domain can be represented by a sum of an approximate solution of specific form and a discrepancy bounded in an appropriate norm. This representation includes few regular and boundary layer correctors (terms), and a small remainder estimated usually in the weighted function space. The method is applied to the semilinear boundary value problems in Chapter 10 since the semilinear boundary value problem admits a linearization at the classical solution. Unfortunately, for the variational inequalities it is in general impossible to linearize boundary value problem with unilateral conditions without the strict complementarity hypothesis. We refer to [28] for the asymptotic analysis with the

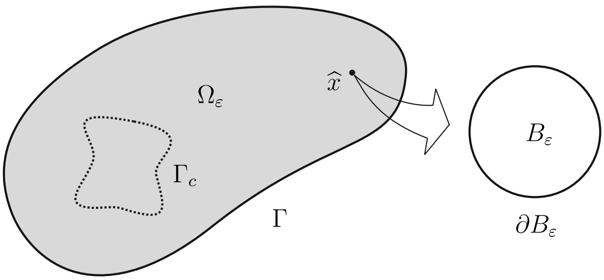


Fig. 11.1 Topologically perturbed domain Ω_ε by the nucleation of a small circular hole B_ε

hypothesis (for asymptotic analysis of related boundary value problems see also [22, 23, 24, 25, 26, 27]). Therefore, the compound asymptotics method seems to be inapplicable in its genuine form for derivation of topological derivatives for variational inequalities.

11.2 Domain Decomposition and the Steklov-Poincaré Operator

Let us consider the linear elliptic boundary value problems, and describe the domain decomposition technique for the energy functional. The method is presented for simplicity for circular holes and for the Laplacian with Neumann conditions on the hole, and the Dirichlet condition on the outer boundary. In such a case the function $f(\varepsilon)=\varepsilon^2$ is used in asymptotic analysis. The shape functional is defined by the associated energy functional to the boundary value problem.

The domain decomposition technique and the Steklov-Poincaré nonlocal boundary operators are used in the topological sensitivity analysis of nonlinear variational problems. We start with a scalar linear boundary value problem in order to present the outline of the method. Therefore, given domains Ω and $\Omega_\varepsilon(\widehat{x})=\Omega\setminus\overline{B_\varepsilon(\widehat{x})}\subset\mathbb{R}^2$ as shown in fig 11.1, where $B_\varepsilon(\widehat{x})$ is a ball of radius $\varepsilon\to 0$ and center at a point $\widehat{x}\in\Omega$ far from the boundary $\Gamma=\partial\Omega$, with $\overline{B_\varepsilon}\Subset\Omega$. By u_ε we denote a unique classical solution of the Poisson equation in singularly perturbed domain:

$$\begin{cases}\text{Find } u_\varepsilon \text{ such that}\\ -\Delta u_\varepsilon = b \text{ in } \Omega_\varepsilon\ ,\\ \quad u_\varepsilon = 0 \text{ on } \partial\Omega\ ,\\ \partial_n u_\varepsilon = 0 \text{ on } \partial B_\varepsilon\ ,\end{cases}\tag{11.4}$$

where $b\in C^{0,\alpha}(\overline{\Omega})$, with $\alpha\in(0,1)$, is a given element which vanishes in the vicinity of the point $\widehat{x}\in\Omega$. The solution u_ε of the boundary value problem (11.4) is variational, since $u_\varepsilon\in\mathscr{V}_\varepsilon\subset H^1(\Omega_\varepsilon)$ minimizes the quadratic functional

$$\mathscr{I}_\varepsilon(\varphi) = \frac{1}{2}\int_{\Omega_\varepsilon} \|\nabla\varphi\|^2 - \int_{\Omega_\varepsilon} b\varphi \tag{11.5}$$

over the linear subspace $\mathscr{V}_\varepsilon \subset H^1(\Omega_\varepsilon)$, where $\mathscr{V}_\varepsilon$ is defined as

$$\mathscr{V}_\varepsilon := \{\varphi \in H^1(\Omega_\varepsilon) : \varphi_{|\Gamma} = 0\}\ . \tag{11.6}$$

The shape functional

$$\mathscr{J}_{\Omega_\varepsilon}(u_\varepsilon) := \frac{1}{2}\int_{\Omega_\varepsilon} \|\nabla u_\varepsilon\|^2 - \int_{\Omega_\varepsilon} bu_\varepsilon = -\frac{1}{2}\int_{\Omega_\varepsilon} bu_\varepsilon \tag{11.7}$$

defined by the equality

$$\mathscr{J}_{\Omega_\varepsilon}(u_\varepsilon) = \mathscr{I}_\varepsilon(u_\varepsilon) \tag{11.8}$$

is the energy functional evaluated for the solution of the boundary value problem (11.4) posed in the singularly perturbed domain Ω_ε.

Proposition 11.1. *We know already that the energy admits the expansion with respect to the small parameter* $\varepsilon \to 0$ *of the following form:*

$$\mathscr{J}_{\Omega_\varepsilon}(u_\varepsilon) = \mathscr{J}_\Omega(u) - \pi\varepsilon^2\|\nabla u(\widehat{x})\|^2 + o(\varepsilon^2)\ , \tag{11.9}$$

where $\|\nabla u(\widehat{x})\|^2$ *is the bulk energy density at the point* $\widehat{x} \in \Omega$ *and* u *is a solution to* (11.4) *for* $\varepsilon = 0$.

Proof. See Section 4.1, expansion (4.55) for $b = 0$ in the neighborhood of $\widehat{x} \in \Omega$. □

Remark 11.1. The bulk energy density functional $H^1(\Omega) \ni \varphi \mapsto \|\nabla\varphi(\widehat{x})\|^2 \in \mathbb{R}$ in general is not continuous at a point $\widehat{x} \in \Omega$. Therefore, the bulk energy density is replaced by a continuous bilinear form $H^1(\Omega) \ni \varphi \mapsto \langle \mathscr{B}(\varphi), \varphi\rangle_{\Gamma_R} \in \mathbb{R}$. For the Laplacian in two spatial dimensions, and the solution of unperturbed problem u which is harmonic in a neighborhood of $\widehat{x}$, the appropriate continuous bilinear form with respect to $H^1(\Omega)$ norm, such that there is equality for u,

$$\|\nabla u(\widehat{x})\|^2 = \langle \mathscr{B}(u), u\rangle_{\Gamma_R}$$

is given by (11.13) or (11.15). This replacement of $\|\nabla\varphi(\widehat{x})\|^2$ by $\langle \mathscr{B}(\varphi), \varphi\rangle_{\Gamma_R}$ in the energy functional for problem (11.4) has been introduced in [208, 209] for the purposes of topological derivatives evaluation in the framework of domain decomposition method.

Note 11.3. If we combine (11.5) with (11.9), we arrive at the conclusion that the modified energy functional

$$H^1(\Omega) \ni \varphi \to \frac{1}{2}\int_\Omega \|\nabla\varphi\|^2 - \int_\Omega b\varphi - \pi\varepsilon^2\langle \mathscr{B}(\varphi), \varphi\rangle_{\Gamma_R} \in \mathbb{R}$$

is an approximation of (11.5) which furnishes the topological derivative (11.9) but with the minimization over unperturbed space $H^1(\Omega)$. This observation is in fact used in the domain decomposition method for unilateral problems.

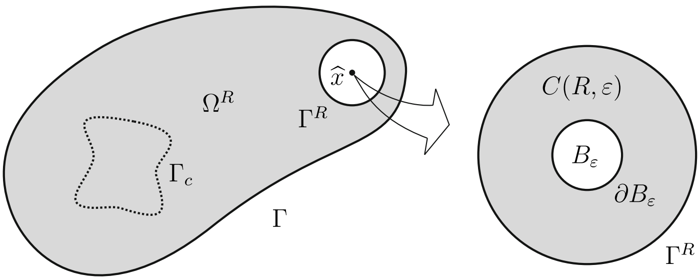


Fig. 11.2 Truncated domain Ω^R and the ring $C(R,\varepsilon)$

11.2.1 Domain Decomposition Technique

Now, we are going to decompose the linear elliptic problem (11.4) into two parts, defined in two disjoint domains Ω_R and $C(R,\varepsilon) := B_R \setminus \overline{B_\varepsilon} \subset \Omega$, $R > \varepsilon > 0$ as shown in fig. 11.1. Two non-overlapping subdomains $\Omega_R, C(R,\varepsilon)$ of Ω_ε are selected $\Omega_\varepsilon = \Omega_R \cup \Gamma_R \cup C(R,\varepsilon)$, where we assume that $R > \varepsilon_0$, $\varepsilon \in (0,\varepsilon_0]$ and Γ_R stands for the exterior boundary ∂B_R of $C(R,\varepsilon)$. Since the gradient of Sobolev functions is not continuous for test functions in $H^1(\Omega)$, but it is the case for harmonic functions, we replace the pointwise values of the gradient of test functions by a representation formula valid only for the pointwise values of the gradient of a harmonic function.

Proposition 11.2. *If the function u is harmonic in a ball $B_R \subset \mathbb{R}^2$, of radius $R > 0$ and center at $\widehat{x} \in \Omega$, then the gradient of u evaluated at $\widehat{x}$ is given by*

$$\nabla u(\widehat{x}) = \frac{1}{\pi R^3} \int_{\Gamma_R} (x - \widehat{x}) u(x) \, . \tag{11.10}$$

Proof. The proof of this result we leave as an exercise. □

In view of (11.10), since $b \equiv 0$ in B_R for sufficiently small $R > \varepsilon_0$, expansion (11.9) can be rewritten in the equivalent form

$$\mathscr{J}_{\Omega_\varepsilon}(u_\varepsilon) = \mathscr{J}_\Omega(u) - \frac{\varepsilon^2}{\pi R^6} \left[\left(\int_{\Gamma_R} u x_1 \right)^2 + \left(\int_{\Gamma_R} u x_2 \right)^2 \right] + o(\varepsilon^2) \, , \tag{11.11}$$

where $x - \widehat{x} = (x_1, x_2)$. As observed in [208, 209], it is interesting to note that (11.11) can be rewritten as follows

$$\mathscr{J}_{\Omega_\varepsilon}(u_\varepsilon) = \mathscr{J}_\Omega(u) - \varepsilon^2 \langle \mathscr{B}(u), u \rangle_{\Gamma_R} + o(\varepsilon^2) \, , \tag{11.12}$$

with the nonlocal, positive and selfadjoint boundary operator $\mathscr{B}$ uniquely determined by its bilinear form

$$\langle \mathscr{B}(u), u\rangle_{\Gamma_R} = \frac{1}{\pi R^6}\left[\left(\int_{\Gamma_R} u x_1\right)^2 + \left(\int_{\Gamma_R} u x_2\right)^2\right] . \tag{11.13}$$

From the above representation, since the line integrals on Γ_R are well defined for functions in $L^1(\Gamma_R)$, it follows that the operator $\mathscr{B}$ can be extended e.g., to a bounded operator on $L^2(\Gamma_R)$, namely

$$\mathscr{B} \in \mathscr{L}(L^2(\Gamma_R); L^2(\Gamma_R)) , \tag{11.14}$$

with the same symmetric bilinear form

$$\langle \mathscr{B}(\varphi), \phi\rangle_{\Gamma_R} = \frac{1}{\pi R^6}\left[\int_{\Gamma_R} \varphi x_1 \int_{\Gamma_R} \phi x_1 + \int_{\Gamma_R} \varphi x_2 \int_{\Gamma_R} \phi x_2\right] , \tag{11.15}$$

which is continuous for all $\varphi, \phi \in L^2(\Gamma_R)$. We observe that the bilinear form

$$L^2(\Gamma_R) \times L^2(\Gamma_R) \ni (\varphi, \phi) \mapsto \langle \mathscr{B}(\varphi), \phi\rangle_{\Gamma_R} \in \mathbb{R} \tag{11.16}$$

is continuous with respect to the weak convergence since it has the simple structure

$$\langle \mathscr{B}(\varphi), \phi\rangle_{\Gamma_R} = L_1(\varphi)L_1(\phi) + L_2(\varphi)L_2(\phi) \quad \varphi, \phi \in L^1(\Gamma_R) \tag{11.17}$$

with two linear forms $\varphi \mapsto L_1(\varphi)$ and $\phi \mapsto L_2(\phi)$, given by the line integrals on Γ_R.

11.2.2 Steklov-Poincaré Pseudodifferential Boundary Operators

Note 11.4. We determine the family Steklov-Poincaré boundary operators on the *outer boundary* Γ_R of the domain $C(R,\varepsilon)$, if there is a hole B_ε inside of $C(R,\varepsilon)$.

We select $R > 0$ such that the circle (or the ball for $d = 3$) B_R contains the hole B_ε and introduce the truncated domain Ω_R. For the boundary value problem defined in Ω_ε, we introduce its approximation in Ω_R. The singular perturbation Ω_ε of the geometrical domain Ω is replaced by a regular perturbation of the Steklov-Poincaré boundary operator living on the interface, which coincides with the interior boundary Γ_R of Ω_R.

Definition 11.1. The Steklov-Poincaré boundary operator

$$\mathscr{A}_\varepsilon : H^{1/2}(\Gamma_R) \to H^{-1/2}(\Gamma_R) \tag{11.18}$$

is defined for the Poisson's equation in the domain $C(R,\varepsilon)$. For a fixed parameter $\varepsilon > 0$ and a given element $v \in H^{1/2}(\Gamma_R)$ the corresponding element in the range of the operator $\mathscr{A}_\varepsilon$ is given by the Neumann trace of a unique solution to the boundary value problem

$$\begin{cases} \text{Find } w_\varepsilon \text{ such that} \\ -\Delta w_\varepsilon = 0 \text{ in } C(R,\varepsilon) , \\ w_\varepsilon = v \text{ on } \Gamma_R , \\ \partial_n w_\varepsilon = 0 \text{ on } \partial B_\varepsilon . \end{cases} \tag{11.19}$$

Then we set

$$\mathscr{A}_\varepsilon(v) = \partial_n w_\varepsilon \quad \text{on} \quad \Gamma_R , \tag{11.20}$$

here n is the unit exterior normal vector on $\partial C(R,\varepsilon)$.

Remark 11.2. Let us note that, in absence of the source term b, the energy shape functional in $C(R,\varepsilon)$ evaluated for the harmonic function w_ε coincides with the boundary energy of the Steklov-Poincaré operator on Γ_R evaluated for the Dirichlet trace of the solution w_ε, namely

$$\int_{C(R,\varepsilon)} \|\nabla w_\varepsilon\|^2 = \langle \mathscr{A}_\varepsilon(v), v\rangle_{\Gamma_R} . \tag{11.21}$$

Therefore, the asymptotics of the energy shape functional in $C(R,\varepsilon)$ for $\varepsilon \to 0$, gives rise to the regular expansion of the Steklov-Poincaré operator (see Appendix F, Theorem F.2):

$$\mathscr{A}_\varepsilon = \mathscr{A} - 2\varepsilon^2 \mathscr{B} + \mathscr{R}_\varepsilon , \tag{11.22}$$

where the remainder denoted by $\mathscr{R}_\varepsilon$ in the above expansion is of order $o(\varepsilon^2)$ in the operator norm $\mathscr{L}(H^{1/2}(\Gamma_R); H^{-1/2}(\Gamma_R))$.

By Remark 11.2 we obtain the strong convergence of solutions in the truncated domain. In fact, let us state the following important result:

Proposition 11.3. *The sequence of solutions u_ε converges as $\varepsilon \to 0$ in the following sense. For any $R > 0$,*

$$u_\varepsilon^R \to u^R \quad \textit{strongly in} \quad H^1(\Omega_R) , \tag{11.23}$$

where $\Omega_R := \Omega \setminus \overline{B_R}$, $\varepsilon \in (0,\varepsilon_0]$, and $R > \varepsilon_0 > 0$, where B_R is a ball of radius R and center at $\widehat{x} \in \Omega$.

Proof. Let u_ε^R be the restriction to Ω_R of the solution u_ε to (11.4), namely

$$u_\varepsilon^R \in H^1_\Gamma(\Omega_R) : \int_{\Omega_R} \nabla u_\varepsilon^R \cdot \nabla \eta + \int_{\Gamma_R} \mathscr{A}_\varepsilon(u_\varepsilon^R)\eta = \int_{\Omega_R} b\eta \quad \forall \eta \in H^1_\Gamma(\Omega_R) . \tag{11.24}$$

In the same way, for $\varepsilon = 0$ we have

$$u^R \in H^1_\Gamma(\Omega_R) : \int_{\Omega_R} \nabla u^R \cdot \nabla \eta + \int_{\Gamma_R} \mathscr{A}(u^R)\eta = \int_{\Omega_R} b\eta \quad \forall \eta \in H^1_\Gamma(\Omega_R) , \tag{11.25}$$

where u^R is the restriction to Ω_R of the solution to (11.4) for $\varepsilon = 0$. In addition, $H^1_\Gamma(\Omega_R)$ is a subset of $H^1(\Omega_R)$, which is defined as

$$H^1_\Gamma(\Omega_R) := \{\varphi \in H^1(\Omega_R) : \varphi_{|_\Gamma} = 0\} . \tag{11.26}$$

By taking $\eta = u_\varepsilon^R - u^R$ and after subtracting the second equation from the first one we get

$$\int_{\Omega_R} \|\nabla(u_\varepsilon^R - u^R)\|^2 + \int_{\Gamma_R} (\mathscr{A}_\varepsilon(u_\varepsilon^R) - \mathscr{A}(u^R))(u_\varepsilon^R - u^R) = 0\,. \tag{11.27}$$

By taking into account the expansion (11.22) we observe that

$$\int_{\Omega_R} \|\nabla(u_\varepsilon^R - u^R)\|^2 = \int_{\Gamma_R} (2\varepsilon^2 \mathscr{B}(u^R) - \mathscr{R}_\varepsilon(u^R))(u_\varepsilon^R - u^R)\,. \tag{11.28}$$

From the *Cauchy-Schwarz inequality* we obtain

$$\begin{aligned}\int_{\Omega_R} \|\nabla(u_\varepsilon^R - u^R)\|^2 \leqslant{} & 2\varepsilon^2 \|\mathscr{B}(u^R)\|_{H^{-1/2}(\Gamma_R)} \|u_\varepsilon^R - u^R\|_{H^{1/2}(\Gamma_R)} \\ & + \|\mathscr{R}_\varepsilon(u^R)\|_{H^{-1/2}(\Gamma_R)} \|u_\varepsilon^R - u^R\|_{H^{1/2}(\Gamma_R)}\,. \end{aligned} \tag{11.29}$$

Taking into account the *trace theorem* and the compactness of the remainder $\mathscr{R}_\varepsilon$ given by Theorem F.2, we have

$$\int_{\Omega_R} \|\nabla(u_\varepsilon^R - u^R)\|^2 \leqslant \varepsilon^2 C_1 \|u_\varepsilon^R - u^R\|_{H^1(\Omega_R)}\,. \tag{11.30}$$

Finally, from the *coercivity* of the bilinear form on the left hand side of the above inequality, namely,

$$c\|u_\varepsilon^R - u^R\|_{H^1(\Omega_R)}^2 \leqslant \int_{\Omega_R} \|\nabla(u_\varepsilon^R - u^R)\|^2\,, \tag{11.31}$$

we obtain

$$\|u_\varepsilon^R - u^R\|_{H^1(\Omega_R)} \leqslant C\varepsilon^2\,, \tag{11.32}$$

which leads to the result, with $C = C_1/c$. □

Now, we make use of the Steklov-Poincaré operator defined above for the annulus $C(R,\varepsilon)$ in order to rewrite the energy shape functional in Ω_ε as a sum of integrals over Ω_R and of the boundary bilinear form on Γ_R,

$$\mathscr{J}_{\Omega_\varepsilon}(u_\varepsilon) = \frac{1}{2}\int_{\Omega_R} \|\nabla u_\varepsilon\|^2 - \int_{\Omega_R} b u_\varepsilon + \frac{1}{2}\langle \mathscr{A}_\varepsilon(u_\varepsilon), u_\varepsilon\rangle_{\Gamma_R}\,, \tag{11.33}$$

which is possible since the source term b vanishes in the small ball B_R around the point $\widehat{x} \in \Omega$.

In conclusion, another method of evaluation of the topological derivative for the energy shape functional is now available. We have the energy shape functional in the form

$$\mathscr{J}_{\Omega_\varepsilon}(u_\varepsilon) = \inf_{\varphi \in H^1_\Gamma(\Omega_R)} \left\{ \frac{1}{2}\int_{\Omega_R} \|\nabla \varphi\|^2 - \int_{\Omega_R} b\varphi + \frac{1}{2}\langle \mathscr{A}_\varepsilon(\varphi), \varphi\rangle_{\Gamma_R} \right\}\,, \tag{11.34}$$

where $H^1_\Gamma(\Omega_R)$ is defined trough (11.26). Taking into account expansion (11.22), from (11.34) it follows by an elementary argument that

$$\mathscr{J}_{\Omega_\varepsilon}(u_\varepsilon) = \inf_{\varphi \in H^1_\Gamma(\Omega_R)} \left\{ \frac{1}{2}\int_{\Omega_R} \|\nabla\varphi\|^2 - \int_{\Omega_R} b\varphi + \frac{1}{2}\langle \mathscr{A}(\varphi), \varphi\rangle_{\Gamma_R} \right\} - \varepsilon^2 \langle \mathscr{B}(u), u\rangle_{\Gamma_R} + o(\varepsilon^2)\,, \quad (11.35)$$

where (11.35) coincides with (11.12). The range of applications of the presented method is not limited to linear problems only. In fact, this is the only available method without any strict complementarity type assumptions on the unknown solution of the variational inequality, for evaluation of topological derivatives of the energy shape functional for unilateral problems.

11.3 Domain Decomposition Method for Variational Inequalities

The topological derivative of the energy shape functional is obtained for a class of variational inequalities. To this end the domain decomposition technique is applied. The method introduced in Section 11.2 is adapted to a class of unilateral problems. The specific class of variational inequalities is equivalent to constrained optimization problems over a positive cone in the Dirichlet-Sobolev space. We recall that the Sobolev space $H^1(\Omega)$ is the Dirichlet space for the natural order, we refer the reader e.g. to [62] for further details in the case of contact problems in linear elasticity. By the Dirichlet-Sobolev space we mean the ordered Sobolev spaces e.g., $H^1(\Omega)$ or $H^{1/2}(\partial\Omega)$ with the following property for the natural order. If the function $x \mapsto u(x)$ is in the Sobolev space, then the function $x \mapsto u^+(x) := \max\{u(x), 0\}$ belongs to the Sobolev space.

11.3.1 Problem Formulation

Let us consider the new boundary value problem, with nonlinear boundary conditions on $\Gamma_c \subset \Omega$. For the domain with a hole $B_\varepsilon(\widehat{x})$, where $\widehat{x} \in \Omega$, the *boundary value problem* takes the following form:

$$\left\{ \begin{array}{l} \text{Find } u_\varepsilon \text{ such that} \\ \begin{array}{rcll} -\Delta u_\varepsilon &=& b & \text{in } \Omega_\varepsilon\,, \\ u_\varepsilon &=& 0 & \text{on } \Gamma\,, \\ \partial_n u_\varepsilon &=& 0 & \text{on } \partial B_\varepsilon\,, \\ \left.\begin{array}{rcl} u_\varepsilon &\geqslant& 0 \\ \partial_n u_\varepsilon &\leqslant& 0 \\ u_\varepsilon\,\partial_n u_\varepsilon &=& 0 \end{array}\right\} & & & \text{on } \Gamma_c\,, \end{array} \end{array} \right. \quad (11.36)$$

where the source term $b \in C^{0,\alpha}(\overline{\Omega})$ vanishes in the neighborhood of the point $\widehat{x} \in \Omega$. See sketch in fig. 11.1. A weak solution u_ε of problem (11.36) minimizes the energy functional (11.5) over a cone in the Sobolev space, and the shape energy functional takes the form

$$\mathscr{J}_{\Omega_\varepsilon}(u_\varepsilon) = \inf_{\varphi \in \{\mathscr{V}_\varepsilon : \varphi_{|\Gamma_c} \geqslant 0\}} \left\{ \frac{1}{2}\int_{\Omega_\varepsilon} \|\nabla\varphi\|^2 - \int_{\Omega_\varepsilon} b\varphi \right\} , \tag{11.37}$$

where the liner space $\mathscr{V}_\varepsilon$ is defined by (11.6).

Now, let us consider the domain decomposition method for (11.36), assuming that $\Gamma_c \subset \Omega_R$, as shown in fig. 11.2. In particular it means that the linear space $H^1_\Gamma(\Omega_R)$ defined through (11.26) is replaced in (11.34) by the *convex and closed subset*

$$\mathscr{K} := \{\varphi \in H^1_\Gamma(\Omega_R) : \varphi_{|\Gamma_c} \geqslant 0\} , \tag{11.38}$$

and the functional including the Steklov-Poincaré operator is as follows

$$\mathscr{I}^R_\varepsilon(u^R_\varepsilon) = \inf_{\varphi \in \mathscr{K}} \left\{ \frac{1}{2}\int_{\Omega_R} \|\nabla\varphi\|^2 - \int_{\Omega_R} b\varphi + \frac{1}{2}\langle \mathscr{A}_\varepsilon(\varphi), \varphi\rangle_{\Gamma_R} \right\} . \tag{11.39}$$

In order to establish the equality

$$\mathscr{I}^R_\varepsilon(u^R_\varepsilon) \equiv \mathscr{J}_{\Omega_\varepsilon}(u_\varepsilon) , \tag{11.40}$$

it is sufficient to show that the minimizer u^R_ε in (11.39) coincides with the restriction to Ω_R of the minimizer u_ε of the corresponding quadratic functional defined in the whole singularly perturbed domain Ω_ε, which is left as an exercise. In this way we obtain

$$\begin{aligned}
\mathscr{J}_{\Omega_\varepsilon}(u_\varepsilon) &= \frac{1}{2}\int_{\Omega_\varepsilon} \|\nabla u_\varepsilon\|^2 - \int_{\Omega_\varepsilon} b u_\varepsilon \\
&= \frac{1}{2}\int_{\Omega_R} \|\nabla u_\varepsilon\|^2 - \int_{\Omega_R} b u_\varepsilon + \frac{1}{2}\langle \mathscr{A}_\varepsilon(u_\varepsilon), u_\varepsilon\rangle_{\Gamma_R} \\
&= \mathscr{I}^R_\varepsilon(u^R_\varepsilon) \\
&= \inf_{\varphi \in \mathscr{K}} \left\{ \frac{1}{2}\int_{\Omega_R} \|\nabla\varphi\|^2 - \int_{\Omega_R} b\varphi + \frac{1}{2}\langle \mathscr{A}_\varepsilon(\varphi), \varphi\rangle_{\Gamma_R} \right\} ,
\end{aligned} \tag{11.41}$$

thus the topological derivative of $\mathscr{J}_\Omega(u)$ can be evaluated by using the expansion of $\mathscr{I}^R_\varepsilon(u^R_\varepsilon)$. The assumption required for the derivation of $\mathscr{I}^R_\varepsilon(u^R_\varepsilon)$ with respect to the parameter ε at $\varepsilon = 0^+$ is only the strong convergence as $\varepsilon \to 0$ for fixed $R > 0$, namely $u^R_\varepsilon \to u^R$ strongly in $H^1(\Omega_R)$, i.e., there is no need for differentiability properties of the minimizer $u^R_\varepsilon \in H^1(\Omega_R)$ with respect to ε (see the proof of Proposition 11.3).

11.3.2 Hadamard Differentiability of Minimizer

The existence of the conical differential for the mapping

$$[0,\varepsilon_0) \ni \varepsilon \mapsto u^R_\varepsilon \in H^1(\Omega_R) \tag{11.42}$$

is established.

We introduce:

- The quadratic functional

$$\mathscr{G}^R(\varphi) := \frac{1}{2}a^R(\varphi,\varphi) - l^R(\varphi) + \frac{1}{2}\langle \mathscr{A}(\varphi),\varphi\rangle_{\Gamma_R} - \varepsilon^2\langle \mathscr{B}(\varphi),\varphi\rangle_{\Gamma_R}\ , \tag{11.43}$$

  where

$$a^R(\varphi,\varphi) = \int_{\Omega_R} \|\nabla\varphi\|^2 \quad \text{and} \quad l^R(\varphi) = \int_{\Omega_R} b\varphi\ . \tag{11.44}$$

- The coincidence set

$$\Xi := \{x \in \Gamma_c : u^R = 0\}\ . \tag{11.45}$$

- The linear form (nonegative measure)

$$\langle \mu_c,\varphi\rangle := a^R(u^R,\varphi) - l^R(\varphi) + \langle \mathscr{A}(u^R),\varphi\rangle_{\Gamma_R}\ . \tag{11.46}$$

- The convex cone

$$\mathscr{S}_K(u^R) = \{\varphi \in H^1_\Gamma(\Omega_R) : \varphi \geqslant 0 \quad \text{q.e. on} \quad \Xi, \quad \langle \mu_c,\varphi\rangle = 0\}\ . \tag{11.47}$$

We recall that the symbol q.e. reads ”quasi everywhere” and it means, everywhere, with possible exception on a set of *null capacity*. For the notion of the Bessel capacity in two or three spatial dimensions (cf. Definitions 2.2.1, 2.2.2, 2.2.4 in [1]) see Note 9.2.

Theorem 11.1. *For fixed $R > 0$ we have*

$$\|u^R_\varepsilon - u^R\|_{H^1_\Gamma(\Omega_R)} \leqslant C_R\varepsilon^2\ . \tag{11.48}$$

Furthermore, there is an expansion with respect to $\varepsilon \to 0^+$,

$$u^R_\varepsilon = u^R + \varepsilon^2 v^R + o^R(\varepsilon^2) \quad in \quad H^1(\Omega_R)\ . \tag{11.49}$$

The element $v^R \in H^1(\Omega_R)$ is uniquely determined by a solution to the following quadratic minimization problem

$$\mathscr{G}^R(v^R) = \inf_{\varphi \in \mathscr{S}_K(u^R)} \mathscr{G}^R(\varphi)\ . \tag{11.50}$$

Proof. The proof follows from the general result in Appendix F given by Theorem F.1 and it is left as an exercise. □

Remark 11.3. The result established in Theorem 11.1 can be obtained as well for a class of contact problems by an application of general results given in [62, 210].

11.3.3 Topological Derivative Evaluation

Now the outline of the domain decomposition method for variational inequalities is given. The topological derivative can be evaluated for the energy shape functional. The scalar elliptic equation as well as the linear elasticity system in two spatial dimensions with the unilateral conditions far from the hole are considered. The case of three spatial dimensions can be described in the same manner. The unilateral conditions are imposed for the weak solutions of elliptic boundary value problems by a cone constraint for the minimization of the quadratic energy functional. We recall that the cone of admissible displacements in contact problems of linear elasticity is defined by the nonpenetration condition. The unilateral condition is only an approximation of the real condition and it is prescribed for normal displacements in the contact zone. Thus the normal displacements in the contact zone belong to a positive cone in the space of traces. We refer to Section 11.4 for more details associated to the particular case of cracks.

In this part we restrict ourselves to the circular holes. Let us recall the notation for the domain decomposition technique. Given a domain $\Omega_\varepsilon = \Omega \setminus \overline{B_\varepsilon} \subset \mathbb{R}^2$, with a small hole $B_\varepsilon \subset B_R$ of radius $\varepsilon \to 0$ and center at $\widehat{x} \in \Omega$, we denote by $\Omega_R = \Omega \setminus \overline{B_R}$ the domain without the hole B_ε, and by $C(R,\varepsilon) = B_R \setminus \overline{B_\varepsilon}$ the ring with the small hole B_ε inside. It means that the domain Ω_ε is decomposed into two subdomains, the truncated one Ω_R and the ring $C(R,\varepsilon)$. The main idea which is employed here is to perform the asymptotic analysis for a linear problem and then apply the result to the nonlinear problem in a smaller domain called truncated domain. This is possible for unilateral conditions prescribed on $\Gamma_c \subset \Omega_R$, where the set Γ_c is far from the hole B_ε, and therefore far from the ball B_R.

Under this geometrical assumption it is possible to restrict the asymptotic analysis to the ring $C(R,\varepsilon)$. Then the obtained result on the asymptotic behavior of the associated solution to the boundary value problem defined in the ring is applied to the variational inequality considered in the truncated domain Ω_R. In this way the singular domain perturbation in the ring influences, by a regular perturbation, the boundary conditions on the interface for variational inequality. The regular perturbation is governed by a nonlocal, pseudodifferential, selfadjoint boundary operator of Steklov-Poincaré type. The nonlocal Steklov-Poincaré operator is introduced on the interface between two subdomains, it is the exterior boundary Γ_R of the ring, which is exactly the interior boundary of the truncated domain Ω_R. The subproblem to be solved in the truncated domain is a variational inequality associated to the constrained minimization problem over a closed convex cone $\mathscr{K} \subset H^1(\Omega_R)$:

Find a unique minimizer $u_\varepsilon \in \mathscr{K}$ of the quadratic energy functional

$$\mathscr{I}_\varepsilon^R(\varphi) = \frac{1}{2} a^R(\varphi,\varphi) - l^R(\varphi) + \frac{1}{2}\langle \mathscr{A}_\varepsilon(\varphi), \varphi \rangle_{\Gamma_R} , \tag{11.51}$$

where $\mathscr{A}_\varepsilon$ stands for the Steklov-Poincaré operator for the ring $C(R,\varepsilon)$ and $\langle\cdot,\cdot\rangle_{\Gamma_R}$ is the duality pairing defined for the fractional Sobolev spaces $H^{-1/2}(\Gamma_R)\times H^{1/2}(\Gamma_R)$ on the interface Γ_R, associated with the corresponding Steklov-Poincaré operator $\mathscr{A}_\varepsilon : H^{1/2}(\Gamma_R)\mapsto H^{-1/2}(\Gamma_R)$. We need an assumption on its asymptotic behavior, which is:

Condition 11.1. The Steklov-Poincaré operator for the ring $C(R,\varepsilon)$ admits the expansion for $\varepsilon>0$, ε small enough,

$$\mathscr{A}_\varepsilon=\mathscr{A}-2f(\varepsilon)\mathscr{B}+\mathscr{R}_\varepsilon\,, \tag{11.52}$$

with an appropriate function $f(\varepsilon)\to 0$, when $\varepsilon\to 0$, depending on the boundary conditions on the hole, where the remainder $\mathscr{R}_\varepsilon$ is of order $o(f(\varepsilon))$ in the operator norm $\mathscr{L}(H^{1/2}(\Gamma_R);H^{-1/2}(\Gamma_R))$.

Remark 11.4. In the scalar case the operator $\mathscr{B}$ is defined by the bilinear form (11.15). From (11.22) it follows that $f(\varepsilon)=\varepsilon^2$ for the Neumann boundary conditions on the hole B_ε. For our specific applications, expansion (11.52) results from the asymptotics of the shape energy functional in the ring $C(R,\varepsilon)$, as it is for the scalar problem. If the form of operator $\mathscr{B}$ in (11.52) is known, in order to apply the general scheme the only assumption to check is the compactness condition for the remainder in the operator norm $\mathscr{L}(H^{1/2}(\Gamma_R);H^{-1/2}(\Gamma_R))$.

Therefore, the original variational inequality defined in the domain Ω_ε is replaced by the variational inequality defined in the truncated domain Ω_R. In this way, for the purposes of asymptotic analysis the original quadratic functional defined in the domain of integration Ω_ε, namely $\mathscr{J}_{\Omega_\varepsilon}(\varphi)$, is replaced by the functional $\mathscr{I}_\varepsilon^R(\varphi)$ defined in the truncated domain without any hole. Two problems are equivalent under the following assumption on the minimizers u_ε and u_ε^R of $\mathscr{J}_{\Omega_\varepsilon}(\varphi)$ and $\mathscr{I}_\varepsilon^R(\varphi)$, respectively.

Condition 11.2. For $\varepsilon>0$, with ε small enough, the minimizer u_ε^R in the truncated domain coincides with the restriction to the truncated domain Ω_R of the minimizer u_ε in the singularly perturbed domain Ω_ε.

If Conditions 11.1 and 11.2 are fulfilled, then the topological asymptotic expansion of the energy functional

$$\mathscr{J}_{\Omega_\varepsilon}(u_\varepsilon)=\frac{1}{2}\int_{\Omega_\varepsilon}\|\nabla u_\varepsilon\|^2-\int_{\Omega_\varepsilon}bu_\varepsilon \tag{11.53}$$

can be determined from the expansion of the energy functional in the truncated domain, namely

$$\mathscr{I}_\varepsilon^R(u_\varepsilon^R)=\frac{1}{2}a^R(u_\varepsilon^R,u_\varepsilon^R)-l^R(u_\varepsilon^R)+\frac{1}{2}\langle\mathscr{A}_\varepsilon(u_\varepsilon^R),u_\varepsilon^R\rangle_{\Gamma_R}\,, \tag{11.54}$$

where u_ε^R is the restriction to the truncated domain Ω_R of the solution u_ε to the variational inequality in the perturbed domain Ω_ε. Under our assumptions, the solution u_ε coincides with the solution obtained by the domain decomposition method.

The evaluation of the topological asymptotics expansion for the energy functional (11.53) is based on the equality (11.40), so we have $\mathscr{J}_{\Omega_\varepsilon}(u_\varepsilon) = \mathscr{I}^R_\varepsilon(u^R_\varepsilon)$, combined with the following characterization of the energy functional

$$\mathscr{I}^R_\varepsilon(u^R_\varepsilon) = \inf_{\varphi\in\mathscr{K}} \left\{ \frac{1}{2} a^R(\varphi,\varphi) - l^R(\varphi) + \frac{1}{2}\langle \mathscr{A}_\varepsilon(\varphi), \varphi\rangle_{\Gamma_R} \right\} . \tag{11.55}$$

The quadratic term $\varphi \mapsto \frac{1}{2}\langle \mathscr{A}_\varepsilon(\varphi), \varphi\rangle_{\Gamma_R}$ of the functional $\mathscr{I}^R_\varepsilon(\varphi)$ is, in view of assumption (11.52) or of Condition 11.1, the regular perturbation of the bilinear form in the quadratic functional $\mathscr{I}^R_\varepsilon(\varphi)$. Therefore, we obtain the result on the differentiability of the optimal value in (11.54) with respect to the parameter ε.

Proposition 11.4. *Assume that:*

- *The Condition 11.1 given by* (11.52) *holds in the operator norm.*
- *The strong convergence takes place $u^R_\varepsilon \to u^R$ in the norm of the space $H^1(\Omega_R)$, which also defines the energy norm for the functional* (11.55).

Then, the energy in the truncated domain Ω^R has the following topological asymptotic expansion

$$\mathscr{I}^R_\varepsilon(u^R_\varepsilon) = \mathscr{I}^R(u^R) - f(\varepsilon)\langle \mathscr{B}(u^R), u^R\rangle_{\Gamma_R} + o(f(\varepsilon)) , \tag{11.56}$$

where u^R is the restriction to the truncated domain Ω_R of the solution u to the original variational inequality in the unperturbed domain Ω. Therefore, the topological derivative of the energy shape functional is obtained from the asymptotic expansion

$$\mathscr{J}_{\Omega_\varepsilon}(u_\varepsilon) = \mathscr{J}_\Omega(u) - f(\varepsilon)\langle \mathscr{B}(u), u\rangle_{\Gamma_R} + o(f(\varepsilon)) . \tag{11.57}$$

Proof. There are inequalities

$$\frac{\mathscr{I}^R_\varepsilon(u^R_\varepsilon) - \mathscr{I}^R(u^R_\varepsilon)}{f(\varepsilon)} \leqslant \frac{\mathscr{I}^R_\varepsilon(u^R_\varepsilon) - \mathscr{I}^R(u^R)}{f(\varepsilon)} \leqslant \frac{\mathscr{I}^R_\varepsilon(u^R) - \mathscr{I}^R(u^R)}{f(\varepsilon)} , \tag{11.58}$$

which imply the existence of the limit

$$\begin{aligned} &\limsup_{f(\varepsilon)\to 0} \frac{\mathscr{I}^R_\varepsilon(u^R_\varepsilon) - \mathscr{I}^R(u^R_\varepsilon)}{f(\varepsilon)} = \\ &\lim_{f(\varepsilon)\to 0} \frac{\mathscr{I}^R_\varepsilon(u^R_\varepsilon) - \mathscr{I}^R(u^R)}{f(\varepsilon)} = \\ &\liminf_{f(\varepsilon)\to 0} \frac{\mathscr{I}^R_\varepsilon(u^R) - \mathscr{I}^R(u^R)}{f(\varepsilon)} = \langle \mathscr{B}(u^R), u^R\rangle_{\Gamma_R} . \end{aligned} \tag{11.59}$$

From (11.56), in view of (11.40), it follows (11.57). □

Remark 11.5. From the above results, we highlight the following important issues:

- It is clear, that expansion (11.52) in evaluation of the topological derivatives for contact problems is a technical result required in the proof of Theorem 11.1.

- The expansion (11.52) leads to one term expansion of solutions (11.49). In principle (11.49) can be used for evaluation of topological derivatives for a general class of shape functionals for contact problems. However, the general class of shape functionals requires the framework of non-smooth and nonconvex analysis for necessary conditions of optimality.
- If for u^R there is the condition

$$\mathscr{S}_K(u^R) \neq \{\mathscr{S}_K(u^R) - \mathscr{S}_K(u^R)\} , \tag{11.60}$$

i.e. the cone $\mathscr{S}_K(u^R)$ is not a linear subspace, then there is no classical adjoint state equation defined for the problem and only the subgradient theory in nonconvex analysis can be employed for derivation of necessary optimality conditions.

We can conclude the analysis for the Signorini problem, and confirm that the topological derivative of the energy shape functional is given by the same formula as it is in the linear case.

Theorem 11.2. *The energy functional for the Signorini problem admits the expansion*

$$\mathscr{J}_{\Omega_\varepsilon}(u_\varepsilon) = \mathscr{J}_\Omega(u) - \pi\varepsilon^2\|\nabla u\|^2 + o(\varepsilon^2) , \tag{11.61}$$

where the topological derivative $\mathscr{T}(\widehat{x}) = -\|\nabla u(\widehat{x})\|^2$ is the negative bulk energy density at the point $\widehat{x} \in \Omega$. Since the solution of the Signorini problem is harmonic in a vicinity of $\widehat{x}$, the expansion is well defined. Therefore, the topological derivative of the energy shape functional is given by the same expression as it is in the case of linear problem.

11.4 Cracks on Boundaries of Rigid Inclusions

The problem associated to cracks on boundaries of rigid inclusions embedded in elastic bodies appears in a vast number of applications in civil, mechanical, aerospace, biomedical and nuclear industries. In particular, some classes of materials are composed by a bulk phase with inclusions inside. When the inclusions are much stiffer than the bulk material, we can treat them as rigid inclusions. In addition, it is quite common to have cracks within an interface between two different materials. Thus, in this section we deal with the mechanical modeling as well as the shape and topology sensitivity analysis associated to the limit case of rigid inclusions in elastic bodies with a crack at the interface [109].

The mechanical modeling is based on the assumption of nonpenetration conditions at the crack faces between the elastic material and the rigid inclusion, which do not allow the opposite crack faces to penetrate each other, leading to a new class of variational inequalities.

For the shape sensitivity analysis, the result on the Hadamard directional differentiability of the solutions to the variational inequality is given. This result leads to the existence of standard shape derivatives of solutions in the case of moving boundaries which are far from the crack. However, it seems that the shape perturbations of the crack tip is a more complicated issue if the shape of the rigid inclusion remains invariant for the perturbations. In [109] we attempt to define the new shape derivative of the elastic energy with respect to the perturbations of the crack tip at the interface between the rigid inclusion and the elastic material.

The topological derivatives of the energy shape functional associated to the nucleation of a smooth imperfection in the bulk elastic material are also considered. In order to apply the domain decomposition method it is assumed that the imperfections in the bulk phase are far from the crack, so the body is splitted into one part with the rigid inclusion and the crack inside and the other part within the bulk phase with the singular geometrical perturbations. Two subdomains are coupled by the Steklov-Poincaré operator. The asymptotic analysis is performed in the subdomain which is located far from the crack. The topological derivatives can be used in design procedures of elastic structures and in numerical solution of inverse problems. The shape and topology optimization for problems with rigid inclusions seem to be a new field. The obtained results are useful from the mathematical and the mechanical point of views as well.

The elasticity boundary value problem associated with the cracks in elastic bodies on the boundaries of rigid inclusions is formulated in Section 11.4.1. The limit passage from elastic to rigid inclusions is presented in Section 11.4.2. Some results concerning shape sensitivity analysis with respect to the perturbations of the crack tip are given in Section 11.4.3. The topological derivatives of the energy shape functional are evaluated in Section 11.4.4. The formulae for such derivatives are given in the case of nucleation of circular holes in two spatial dimensions.

11.4.1 Problem Formulation

Let $\Omega \subset \mathbb{R}^2$ be a bounded domain with smooth boundary Γ, and $\omega \subset \Omega$ be a subdomain with smooth boundary $\partial\omega$ such that $\overline{\omega} \cap \Gamma = \varnothing$. We assume that $\partial\omega$ consists of two parts Υ and $\partial\omega \setminus \Upsilon$, such that $|\partial\omega \setminus \Upsilon| > 0$. Denote by n a unit outward normal vector to $\partial\omega$. The subdomain ω is a rigid inclusion, the curve Υ is a crack located within the interface $\partial\omega$, while the domain $\Omega \setminus \overline{\omega}$ is the elastic part of the body. The crack Υ is split into two curves $\Upsilon^{\pm}$, where $\pm$ fit positive Υ^+ and negative Υ^- crack lips Υ with respect to the normal n. All the details can be seen in fig. 11.3.

We denote by $\mathscr{R}(\omega)$ the set of infinitesimal *rigid displacements*. Let us consider a second order tensor A decomposed in its symmetric S and skew W parts, namely

$$S = \frac{1}{2}(A + A^\top) \qquad \text{and} \qquad W = \frac{1}{2}(A - A^\top)\,. \tag{11.62}$$

Therefore, the set $\mathscr{R}(\omega)$ is defined as

$$\mathscr{R}(\omega) := \{\rho : \rho(x) = Wx + a,\, x \in \omega,\, a \in \mathbb{R}^2\}\,. \tag{11.63}$$

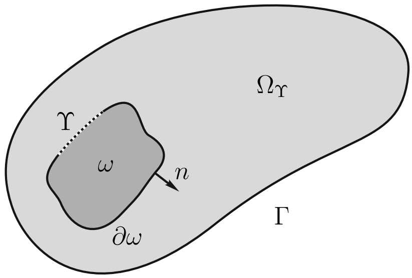


Fig. 11.3 Cracked domain Ω_Υ with rigid inclusion ω inside

The body with the rigid inclusion and the crack is denoted by $\Omega_\Upsilon = \Omega \setminus \overline{\Upsilon}$. The equilibrium of an elastic body with a rigid inclusion ω and the crack Υ is governed by a boundary value problem written in the domain Ω_Υ, namely:

$$\left\{\begin{array}{l} \text{Find a function } u \text{ and a rigid displacement } \rho_0 := u_{|\omega} \text{ such that} \\ \begin{array}{rcll} -\mathrm{div}\sigma(u) &=& b & \text{in } \Omega\setminus\overline{\omega}\,, \\ \sigma(u) &=& \mathbb{C}\nabla u^s\,, & \\ u &=& 0 & \text{on } \Gamma\,, \\ \left.\begin{array}{r} (u-\rho_0)\cdot n \geqslant 0 \\ \sigma^\tau(u) = 0 \\ \sigma^{nn}(u) \leqslant 0 \\ \sigma^{nn}(u)(u-\rho_0)\cdot n = 0 \end{array}\right\} & & & \text{on } \Upsilon^+\,, \\ -\displaystyle\int_{\partial\omega}\sigma(u)n\cdot\rho &=& \displaystyle\int_\omega b\cdot\rho \;\; \forall\;\rho\in\mathscr{R}(\omega)\,, & \end{array} \end{array}\right. \tag{11.64}$$

where the source term $b \in C^{0,\alpha}(\overline{\Omega};\mathbb{R}^2)$, with $\alpha \in (0,1)$ and

$$\sigma^{nn}(u) = n\cdot\sigma(u)n \quad \text{and} \quad \sigma^\tau(u) = \sigma(u)n - \sigma^{nn}n\,. \tag{11.65}$$

The elasticity tensor $\mathbb{C}$ satisfies usual symmetry and positive definiteness properties. The isotropic case is considered, namely

$$\mathbb{C} = 2\mu\mathbb{I} + \lambda(\mathrm{I}\otimes\mathrm{I})\,, \tag{11.66}$$

where I and $\mathbb{I}$ are the second and fourth order identity tensors, respectively, and μ and λ are the Lamé's coefficients. In (11.64), the conditions $(u-\rho_0)\cdot n \geqslant 0$ and $\sigma^\tau(u) = 0$ on Υ^+ describe the frictionless contact between the crack lips with mutual nonpenetration. Note that external forces b are applied to $\Omega\setminus\overline{\omega}$ as well as to ω, however there are no equilibrium equations inside of the rigid inclusion ω. Influence of these forces on the rigid inclusion is taken into account through the last nonlocal condition in (11.64). If there is no crack Υ on $\partial\omega$, the conditions on Υ^+ should be omitted. This particular problem formulation for the case $b = 0$ in ω can be found in [157].

First of all we provide a variational formulation of the problem (11.64). To this end, let us introduce the Sobolev space

$$H_{\Gamma}^{1,\omega}(\Omega_{\Upsilon}) = \{\varphi \in H^1(\Omega_{\Upsilon};\mathbb{R}^2) : \nabla\varphi^s = 0 \text{ in } \omega,\ \varphi_{|_\Gamma} = 0\} \tag{11.67}$$

and define for all functions in the Sobolev space two traces φ^+, φ^- on $\Upsilon^{\pm}$, respectively, and denote by $[\![\varphi]\!] = \varphi^+ - \varphi^-$ the jump of φ across the crack Υ. Recall that $\varphi^- \in \mathscr{R}(\omega)$ by definition of the space $H_{\Gamma}^{1,\omega}(\Omega_{\Upsilon})$. The *set of admissible displacements* takes into account the unilateral nonpenetration condition

$$\mathscr{K}_{\omega} = \{\varphi \in H_{\Gamma}^{1,\omega}(\Omega_{\Upsilon}) : [\![\varphi]\!] \cdot n \geqslant 0 \text{ on } \Upsilon^+\}\ . \tag{11.68}$$

Let us consider the energy functional

$$\mathscr{I}(\varphi) = \frac{1}{2}\int_{\Omega\setminus\overline{\omega}} \sigma(\varphi)\cdot\nabla\varphi^s - \int_{\Omega_{\Upsilon}} b\cdot\varphi\ . \tag{11.69}$$

The weak solution u is a unique minimizer for the minimization problem,

$$\mathscr{I}(u) = \inf_{\varphi\in\mathscr{K}_{\omega}} \mathscr{I}(\varphi)\ . \tag{11.70}$$

Proposition 11.5. *Problem* (11.70) *admits a unique solution given by the variational inequality*

$$u \in \mathscr{K}_{\omega} : \int_{\Omega\setminus\overline{\omega}} \sigma(u)\cdot\nabla(\eta-u)^s \geqslant \int_{\Omega_{\Upsilon}} b\cdot(\eta-u) \quad \forall\eta\in\mathscr{K}_{\omega}\ . \tag{11.71}$$

Proof. The set $\mathscr{K}_{\omega}$ is weakly closed in the Hilbert space $H_{\Gamma}^{1,\omega}(\Omega_{\Upsilon})$, and the functional $\mathscr{I}$ is coercive and weakly lower semicontinuous on this space. Therefore, there is a solution to the minimization problem (11.70). □

Remark 11.6. If a solution of (11.71) is sufficiently smooth then it satisfies (11.64). Conversely, any smooth solution of (11.64) satisfies (11.71). On the other hand, for a solution of (11.71), the complementarity conditions on Υ^+ in (11.64) are satisfied only in a weak sense. This issue requires more explanations, which can be found in [109].

11.4.2 Approximation of a Rigid Inclusion with Contrast Parameter

The nonlinear system (11.64) with the rigid inclusion ω is obtained as a limit for a family of elasticity boundary value problems formulated in the domain Ω_{Υ} with an elastic inclusion ω inside and a crack Υ on the interface. Through this limit passage, the stiffness of the elastic inclusion tends to infinity and the inclusion ω becomes rigid.

This means that a family of elasticity boundary value problems depending on a positive parameter γ is introduced in such a way that for any fixed $\gamma > 0$ the problem describes an equilibrium state for an elastic body occupying the domain Ω_Υ with an elastic inclusion ω and the crack Υ on $\partial\omega$. For the limit passage $\gamma \to 0$ we obtain a rigid inclusion ω. Thus, in the limit, any point $x \in \omega$ admits a displacement given by a unique rigid displacement $\rho_0(x)$ with $\rho_0 \in \mathscr{R}(\omega)$.

Let us introduce the tensor $\mathbb{C}_\gamma$ such that

$$\mathbb{C}_\gamma = \begin{cases} \mathbb{C} \text{ in } \Omega \setminus \overline{\omega} , \\ \gamma^{-1}\mathbb{C} \text{ in } \omega , \end{cases} \tag{11.72}$$

and consider the following problem in the domain Ω_Υ:

$$\begin{cases} \text{Find } u_\gamma \text{ such that} & & \\ -\operatorname{div}\sigma_\gamma(u_\gamma) = b & \text{in } \Omega_\Upsilon , \\ \sigma_\gamma(u_\gamma) = \mathbb{C}_\gamma \nabla u_\gamma^s , & \\ u_\gamma = 0 & \text{on } \Gamma , \\ \left.\begin{array}{r} [\![u_\gamma]\!] \cdot n \geqslant 0 \\ [\![\sigma_\gamma^{nn}(u_\gamma)]\!] = 0 \\ \sigma_\gamma^{nn}(u_\gamma)[\![u_\gamma]\!] \cdot n = 0 \end{array}\right\} & \text{on } \Upsilon , \\ \left.\begin{array}{r} \sigma_\gamma^\tau(u_\gamma) = 0 \\ \sigma_\gamma^{nn}(u_\gamma) \leqslant 0 \end{array}\right\} & \text{on } \Upsilon^\pm , \end{cases} \tag{11.73}$$

where $[\![\varphi]\!] = \varphi^+ - \varphi^-$ is a jump of φ across Υ, and $\pm$ fit positive and negative crack lips $\Upsilon^\pm$ with respect to n.

For any fixed $\gamma > 0$ problem (11.73) is well known [107, 112, 113]. It admits a variational formulation. Indeed, let us introduce the set of admissible displacements

$$\mathscr{K} = \{\varphi \in H^1_\Gamma(\Omega_\Upsilon) : [\![\varphi]\!] \cdot n \geqslant 0 \text{ on } \Upsilon\} , \tag{11.74}$$

where

$$H^1_\Gamma(\Omega_\Upsilon) = \{\varphi \in H^1(\Omega_\Upsilon; \mathbb{R}^2) : \varphi_{|_\Gamma} = 0\} . \tag{11.75}$$

Proposition 11.6. *There exists a unique solution u_γ to the minimization problem*

$$\inf_{\varphi \in \mathscr{K}} \left\{ \frac{1}{2} \int_{\Omega_\Upsilon} \sigma_\gamma(\varphi) \cdot \nabla\varphi^s - \int_{\Omega_\Upsilon} b \cdot \varphi \right\} , \tag{11.76}$$

which satisfies the variational inequality

$$u_\gamma \in \mathscr{K} : \int_{\Omega_\Upsilon} \sigma_\gamma(u_\gamma) \cdot \nabla(\eta - u_\gamma)^s \geqslant \int_{\Omega_\Upsilon} b \cdot (\eta - u_\gamma) \quad \forall \eta \in \mathscr{K} . \tag{11.77}$$

Proof. Proof is left as an exercise. □

Problems (11.76) and (11.77) are equivalent by convexity of the quadratic functional in (11.76). Moreover, the system (11.73) follows from (11.77), and conversely, from (11.73) it follows (11.77).

Theorem 11.3. *The solution u_γ of problem* (11.77) *weakly converges in $H^1_\Gamma(\Omega_\Upsilon)$ to the solution u of problem* (11.71) *as $\gamma \to 0$.*

Proof. We justify the limit passage as $\gamma \to 0$ in (11.77). Substituting $\eta = 0$, $\eta = 2u_\gamma$ as test functions in (11.77), and summing up the obtained equalities leads to

$$\int_{\Omega_\Upsilon} \sigma_\gamma(u_\gamma) \cdot \nabla u^s_\gamma = \int_{\Omega_\Upsilon} b \cdot u_\gamma \,. \tag{11.78}$$

Assuming that $\gamma \in (0, \gamma_0)$, from (11.78) we obtain

$$\|u_\gamma\|_{H^1_\Gamma(\Omega_\Upsilon)} \leqslant C_1 \,, \tag{11.79}$$

$$\frac{1}{\gamma} \int_\omega \sigma(u_\gamma) \cdot \nabla u^s_\gamma \leqslant C_2 \,, \tag{11.80}$$

with $\sigma(u_\gamma) = \mathbb{C} \nabla u^s_\gamma$ and the constants C_1, C_2 uniformly bounded on the interval $\gamma \in (0, \gamma_0)$. Choosing a subsequence, if necessary, it follows that for $\gamma \to 0$

$$u_\gamma \to u \text{ weakly in } H^1_\Gamma(\Omega_\Upsilon) \,. \tag{11.81}$$

Then by (11.80)

$$\nabla u^s = 0 \text{ in } \omega \,. \tag{11.82}$$

Therefore there is a function $\rho_0 \in \mathscr{R}(\omega)$ such that

$$u_{|\omega} = \rho_0 \text{ in } \omega \,. \tag{11.83}$$

Since u_γ converges to u weakly in $H^1_\Gamma(\Omega_\Upsilon)$, the jump of traces across the crack $[\![u]\!]_\gamma \geqslant 0$ converges weakly in the space of traces on Υ to the jump of traces $u_{|\omega}$ on both crack's lips $\Upsilon^\pm$, thus the inequality

$$[\![u]\!] = u^+ - u^- := (u - \rho_0) \cdot n \geqslant 0 \text{ on } \Upsilon^+ \tag{11.84}$$

is satisfied in the limit, and $u \in \mathscr{K}_\omega$. Let us take any fixed element $\eta \in \mathscr{K}_\omega$. Then, there exists $\rho \in \mathscr{R}(\omega)$ such that $\eta = \rho$ in ω, and η can be taken as a test function in (11.77). In such a case, inequality (11.77) implies

$$\int_{\Omega_\Upsilon} \sigma_\gamma(u_\gamma) \cdot \nabla(\eta - u_\gamma)^s \geqslant \int_{\Omega_\Upsilon} b \cdot (\eta - u_\gamma) \,. \tag{11.85}$$

By accounting $\mathbb{C}_\gamma = \mathbb{C}$ in $\Omega \setminus \overline{\omega}$, we can pass to the limit in (11.85) as $\gamma \to 0$ which implies

$$u \in \mathscr{K}_\omega : \int_{\Omega \setminus \overline{\omega}} \sigma(u) \cdot \nabla(\eta - u) \geqslant \int_{\Omega_\Upsilon} b \cdot (\eta - u) \quad \forall \eta \in \mathscr{K}_\omega \,, \tag{11.86}$$

what is precisely (11.71). □

Observe that there is no limit for the stress tensor σ_γ in ω as $\gamma \to 0$. It is interesting to compare the above passage to the limit with the fictitious domain approach in contact problems [98].

11.4.3 Hadamard Differentiability of Solutions to Variational Inequalities

We use the result on the Hadamard differentiability of the metric projection on polyhedric convex sets in Hilbert spaces due to Mignot 1976 [156] and Haraux 1977 [85] given in Appendix F. Let us introduce the description of the convex cone $\mathscr{S}_K(u)$,

$$\mathscr{S}_K(u) = \left\{ \varphi \in H^{1,\omega}_\Gamma(\Omega_\Upsilon) : [\![\varphi]\!] \cdot n \geqslant 0 \text{ on } \Upsilon_0 ; \int_{\Omega\setminus\overline{\omega}} \sigma(u) \cdot \nabla \varphi^s = \int_{\Omega_\Upsilon} b \cdot \varphi \right\} \tag{11.87}$$

where $\Upsilon_0 = \{x \in \Upsilon : (u - \rho_0) \cdot n = 0\}$, where $\rho_0 := u_{|\omega}$. We have the following result:

Theorem 11.4. *Let there be given the right hand side $b_t = b + th$ of variational inequality* (11.71)*, then the unique solution $u_t \in \mathscr{K}_\omega$ is Lipschitz continuous*

$$\|u_t - u\|_{H^1(\Omega_\Upsilon;\mathbb{R}^2)} \leqslant Ct \tag{11.88}$$

and conically differentiable in $H^1(\Omega_\Upsilon;\mathbb{R}^2)$, that is, for $t > 0$, t small enough,

$$u_t = u + tv + o(t)\,, \tag{11.89}$$

where the conical differential solves the variational inequality

$$v \in \mathscr{S}_K(u) : \int_{\Omega\setminus\overline{\omega}} \sigma(v) \cdot \nabla(\eta - v)^s \geqslant \int_{\Omega_\Upsilon} h \cdot (\eta - v) \quad \forall \eta \in \mathscr{S}_K(u)\,. \tag{11.90}$$

The remainder converges to zero

$$\frac{1}{t}\|o(t)\|_{H^1(\Omega_\Upsilon;\mathbb{R}^2)} \underset{t\to 0}{\to} 0 \tag{11.91}$$

uniformly with respect to the direction h on the compact sets of the dual space $(H^{1,\omega}_\Gamma(\Omega_\Upsilon))'$. Thus v is the Hadamard directional derivative of the solution to the variational inequality with respect to the right hand side.

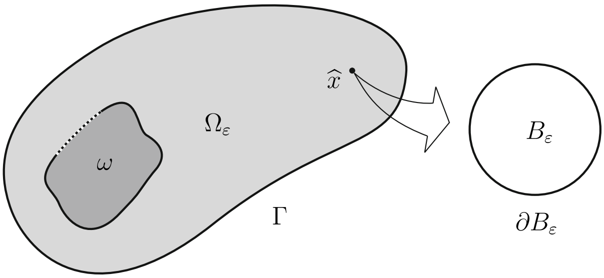


Fig. 11.4 Perforated domain Ω_ε with a rigid inclusion ω inside

11.4.4 Topological Derivative Evaluation

Let us now consider a singularly perturbed domain $\Omega_\varepsilon(\widehat{x}) = \Omega \setminus \overline{B_\varepsilon(\widehat{x})}$, where $B_\varepsilon(\widehat{x})$ is a ball of radius $\varepsilon > 0$, $\varepsilon \to 0$, and center at $\widehat{x} \in \Omega \setminus \overline{\omega}$. We assume that the hole B_ε do not touch the rigid inclusion ω, namely $\overline{B_\varepsilon} \Subset \Omega \setminus \overline{\omega}$. See the details in fig. 11.4.

We are interested in the topological asymptotic expansion of the energy shape functional of the form

$$\mathscr{J}_{\Omega_\varepsilon}(\varphi) = \frac{1}{2}\int_{\Omega_\varepsilon \setminus \overline{\omega}} \sigma(\varphi) \cdot \nabla \varphi^s - \int_{\Omega_\Upsilon} b \cdot \varphi \,, \tag{11.92}$$

with $\varphi = u_\varepsilon$ solution to the following *nonlinear system*:

$$\begin{cases} \text{Find } u_\varepsilon \text{ such that} \\ \quad -\mathrm{div}\,\sigma(u_\varepsilon) = b \quad \text{in } \Omega_\varepsilon \setminus \overline{\omega} \,, \\ \quad \sigma(u_\varepsilon) = \mathbb{C}\nabla u_\varepsilon^s \,, \\ \quad u_\varepsilon = 0 \quad \text{on } \Gamma \,, \\ \quad \sigma(u_\varepsilon)n = 0 \quad \text{on } \partial B_\varepsilon \,, \\ \left.\begin{aligned} (u_\varepsilon - \rho_0)\cdot n &\geqslant 0 \\ \sigma^\tau(u_\varepsilon) &= 0 \\ \sigma^{nn}(u_\varepsilon) &\leqslant 0 \\ \sigma^{nn}(u_\varepsilon)(u_\varepsilon - \rho_0)\cdot n &= 0 \end{aligned}\right\} \quad \text{on } \Upsilon^+ \,, \\ \quad -\displaystyle\int_{\partial\omega} \sigma(u_\varepsilon)n \cdot \rho = \int_\omega b \cdot \rho \quad \forall\ \rho \in \mathscr{R}(\omega) \,. \end{cases} \tag{11.93}$$

Since the problem is nonlinear, let us introduce two disjoint domains Ω_R and $C(R,\varepsilon)$, with $\Omega_R = \Omega \setminus \overline{B_R(\widehat{x})}$ and $C(R,\varepsilon) = B_R \setminus \overline{B_\varepsilon} \Subset \Omega \setminus \overline{\omega}$, where $B_R(\widehat{x})$ is a ball of radius $R > \varepsilon$ and center at $\widehat{x} \in \Omega \setminus \overline{\omega}$, as shown in fig. 11.5. For the sake of simplicity, we assume that $b = 0$ in $B_R(\widehat{x})$, that is, the source term b vanishes in the neighborhood of the point $\widehat{x} \in \Omega \setminus \overline{\omega}$. Thus, we have the following linear elasticity system defined in the ring $C(R,\varepsilon)$:

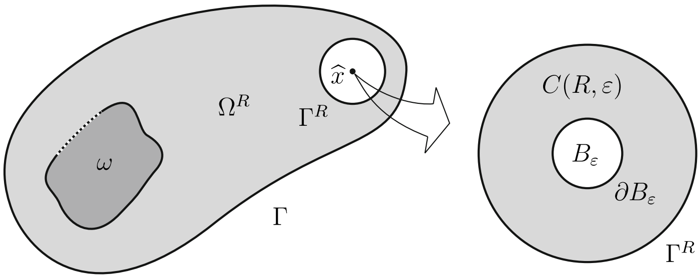


Fig. 11.5 Truncated domain Ω^R and the ring $C(R,\varepsilon)$

$$\begin{cases} \text{Find } w_\varepsilon \text{ such that} \\ -\operatorname{div}\sigma(w_\varepsilon) = 0 & \text{in } C(R,\varepsilon)\,, \\ \sigma(w_\varepsilon) = \mathbb{C}\nabla w_\varepsilon^s\,, \\ w_\varepsilon = v & \text{on } \Gamma_R\,, \\ \sigma(u_\varepsilon)n = 0 & \text{on } \partial B_\varepsilon\,, \end{cases} \tag{11.94}$$

where Γ_R is used to denote the exterior boundary ∂B_R of the ring $C(R,\varepsilon)$. We are interested in the Steklov-Poincaré operator on Γ_R, that is

$$\mathscr{A}_\varepsilon : v \in H^{1/2}(\Gamma_R;\mathbb{R}^2) \to \sigma(w_\varepsilon)n \in H^{-1/2}(\Gamma_R;\mathbb{R}^2)\,. \tag{11.95}$$

Then we have $\sigma(u_\varepsilon^R)n = \mathscr{A}_\varepsilon(u_\varepsilon^R)$ on Γ_R, where u_ε^R is solution of the variational inequality in Ω_R, that is

$$u_\varepsilon^R \in \mathscr{K}_\omega : \int_{\Omega_R} \sigma(u_\varepsilon^R)\cdot\nabla(\eta - u_\varepsilon^R) + \int_{\Gamma_R} \mathscr{A}_\varepsilon(u_\varepsilon^R)\cdot(\eta - u_\varepsilon^R) \geqslant \int_{\Omega_\Upsilon\setminus\overline{B_R}} b\cdot(\eta - u_\varepsilon^R) \quad \forall \eta \in \mathscr{K}_\omega\,. \tag{11.96}$$

Finally, in the ring $C(R,\varepsilon)$ we have

$$\int_{C(R,\varepsilon)} \sigma(w_\varepsilon)\cdot\nabla w_\varepsilon^s = \int_{\Gamma_R} \mathscr{A}_\varepsilon(w_\varepsilon)\cdot w_\varepsilon\,, \tag{11.97}$$

where w_ε is the solution of the elasticity system in the ring (11.94). Therefore the solutions u_ε^R and w_ε are defined as restriction of u_ε to the truncated domain Ω_R and to the ring $C(R,\varepsilon)$, respectively.

In particular, according to Section 4.2, expansion (4.175) for $b = 0$ in the neighborhood of $\widehat{x} \in \Omega\setminus\overline{\omega}$, the energy in the ring $C(R,\varepsilon)$ admits the following topological asymptotic expansion

$$\int_{C(R,\varepsilon)} \sigma(w_\varepsilon)\cdot\nabla w_\varepsilon^s = \int_{B_R} \sigma(w)\cdot\nabla w^s - 2\pi\varepsilon^2\mathbb{P}\sigma(w(\widehat{x}))\cdot\nabla w^s(\widehat{x}) + o(\varepsilon^2)\,. \tag{11.98}$$

where w is solution to (11.94) for $\varepsilon = 0$ and $\mathbb{P}$ is the polarization tensor given by (4.174). It means that w is the restriction to the disk B_R of the solution u to the non-linear system (11.64) defined in the unperturbed domain Ω_Υ. Therefore, following the same steps as presented in the beginning of this chapter for the scalar case, we have that the Steklov-Poincaré operator defined by (11.95) admits the expansion for $\varepsilon > 0$, with ε small enough,

$$\mathscr{A}_\varepsilon = \mathscr{A} - 2\varepsilon^2 \mathscr{B} + o(\varepsilon^2) , \tag{11.99}$$

where the operator $\mathscr{B}$ is determined by its bilinear form

$$\langle \mathscr{B}(w), w \rangle_{\Gamma_R} = \pi \mathbb{P} \sigma(w(\widehat{x})) \cdot \nabla w^s(\widehat{x}) . \tag{11.100}$$

From the above results, we have that the energy shape functional associated to the cracks on boundaries of rigid inclusions embedded in elastic bodies has the following topological asymptotic expansion

$$\mathscr{J}_{\Omega_\varepsilon}(u_\varepsilon) = \mathscr{J}_\Omega(u) - \pi \varepsilon^2 \mathbb{P} \sigma(u(\widehat{x})) \cdot \nabla u^s(\widehat{x}) + o(\varepsilon^2) , \tag{11.101}$$

with the *topological derivative* $\mathscr{T}(\widehat{x})$ given by

$$\mathscr{T}(\widehat{x}) = -\mathbb{P} \sigma(u(\widehat{x})) \cdot \nabla u^s(\widehat{x}) , \tag{11.102}$$

where u is solution of the variational inequality (11.71) in the unperturbed domain Ω_Υ and $\mathbb{P}$ is the Pólya-Szegö polarization tensor given by (4.174).

Remark 11.7. From equality (11.97) we observe that the bilinear form (11.100) represents the topological derivative of the Steklov-Poincaré operator (11.95). In addition, since solution $u \in \mathscr{K}_\omega$ of the variational inequality (11.71) is a $H^1(\Omega_\Upsilon; \mathbb{R}^2)$ function, then it is convenient to compute the topological derivative from quantities evaluated on the boundary Γ_R in similar way as presented in the beginning of this chapter for the scalar case. This task we leave as an exercise.

11.5 Exercises

1. Proof Proposition 11.2.
2. Show equality (11.78).
3. Consider Remark 11.7.
4. Extend the result in Proposition 11.3 to the elasticity system and write the proof.
5. Extend the result in Theorem F.2 to the elasticity system and write the proof.

Appendix A
Auxiliary Results for Spectral Problems

In this appendix we provide some auxiliary results for spectral problems. In particular, we recall some classical results on spectral problems including a *lemma on almost eigenvalues and eigenvectors*. The possible sources are [37, 106, 166, 200], for instance.

A.1 Preliminaries Results

Let $\mathfrak{K} : \mathfrak{H} \to \mathfrak{H}$ be a compact, symmetric and positive, linear operator in the Hilbert space $\mathfrak{H}$:

$$(\mathfrak{K}u, v)_{\mathfrak{H}} = (u, \mathfrak{K}v)_{\mathfrak{H}} \quad \forall u, v \in \mathfrak{H}, \tag{A.1a}$$

$$(\mathfrak{K}v, v)_{\mathfrak{H}} > 0 \quad \forall v \in \mathfrak{H} \setminus \{0\}, \tag{A.1b}$$

$$\|\mathfrak{K}(u_n - u)\|_{\mathfrak{H}} \to 0 \quad \text{whenever} \quad (u_n - u, v)_{\mathfrak{H}} \to 0 \quad \forall v \in \mathfrak{H}. \tag{A.1c}$$

The following result can be found in [37, 200]:

Proposition A.1. *The abstract spectral problem* (A.1) *enjoys the following properties:*

- *The spectrum $\mathfrak{Sp}(\mathfrak{K})$ contains real eigenvalues μ^k, algebraic simple with the finite multiplicity, ordered taking into account the multiplicity*

$$\|\mathfrak{K}\|_{\mathscr{L}(\mathfrak{H}\to\mathfrak{H})} \geqslant \mu^1 \geqslant \mu^2 \geqslant \cdots \geqslant \mu^n \to 0^+. \tag{A.2}$$

  The associated eigenvectors

$$\mathfrak{K}\mathfrak{v}^n = \mu^n \mathfrak{v}^n. \tag{A.3}$$

  The family of eigenvectors is an orthonormal basis in $\mathfrak{H}$, normalized by the conditions

$$(\mathfrak{v}^n, \mathfrak{v}^k)_{\mathfrak{H}} = \delta_{nk}, \tag{A.4}$$

where δ_{nk} *is the Kronecker symbol.*

- *Rayleigh's principle*

$$\mu^n = \max\{\mathfrak{Q}(v) \,:\, v \in \mathfrak{H}, \quad (v, \mathfrak{v}^k)_{\mathfrak{H}} = 0, \quad k = 1, \cdots, n-1\}, \tag{A.5}$$

where

$$\mathfrak{Q}(v) := \frac{(\mathfrak{K}v, v)_{\mathfrak{H}}}{(v, v)_{\mathfrak{H}}}, \quad \textit{for} \quad v \neq 0. \tag{A.6}$$

- *Poincaré max-min principle*

$$\mu^n = \max_{\{\mathfrak{V}\subset\mathfrak{H},\ \dim\mathfrak{V}=n\}} \min_{\{v\in\mathfrak{V}, v\neq 0\}} \mathfrak{Q}(v). \tag{A.7}$$

Each element $\mathfrak{h}$ of $\mathfrak{H}$ admits the decomposition in the basis

$$\mathfrak{h} = \sum_{k=1}^{\infty} (\mathfrak{h}, \mathfrak{v}^k)_{\mathfrak{H}} \mathfrak{v}^k. \tag{A.8}$$

Remark A.1. For the inverses $\lambda^n := (\mu^n)^{-1}$ obviously we have

$$0 < \frac{1}{\|\mathfrak{K}\|_{\mathscr{L}(\mathfrak{H}\to\mathfrak{H})}} \leqslant \lambda^1 \leqslant \lambda^2 \leqslant \cdots \leqslant \lambda^n \to \infty. \tag{A.9}$$

The family $\{\lambda^n\}$ serves as eigenvalues for the unbounded inverse operator $\mathfrak{K}^{-1}$: $\mathscr{D}(\mathfrak{K}^{-1}) \subset \mathfrak{H} \to \mathfrak{H}$, where by $\mathscr{D}(\mathfrak{K}^{-1})$ we denote the domain of $\mathfrak{K}^{-1}$ in $\mathfrak{H}$.

We recall also two results useful for the asymptotic analysis of spectral problems [166]. The norm $\|A\|$ of a matrix A with the real entries a_k^j and the columns a^j is defined as the norm of the associated linear mapping $A : \mathbb{R}^n \to \mathbb{R}^n$. Such a matrix norm is invariant for the transposition and for the multiplication by an orthogonal matrix.

Proposition A.2. *If the matrix A satisfies*

$$\|A^\top A - \mathrm{I}\| =: \beta \in [0, 1), \tag{A.10}$$

then there exists an orthogonal matrix B such that

$$\|AB - \mathrm{I}\| \leqslant \beta. \tag{A.11}$$

Proof. The matrix $A^\top A$ is nonnegative, symmetric, therefore there is an orthogonal matrix S such that $S^\top A^\top A S = \mathrm{diag}[1+s_1, \cdots, 1+s_n] =: D$. Matrix B takes the form $B = SD^{-1/2}S^\top A^\top$, where $D^{-1/2} := \mathrm{diag}[(1+s_1)^{-1/2}, \cdots, (1+s_n)^{-1/2}]$. First of all

$$BB^\top = SD^{-1/2}S^\top A^\top ASD^{-1/2}S^\top = SD^{-1/2}DD^{-1/2}S^\top = \mathrm{I}. \tag{A.12}$$

In addition,

$$\begin{aligned}\|AB-\mathrm{I}\| &= \|(A-B^\top)B\| = \|S^\top B(A-B^\top)BB^\top S\| \\ &= \|S^\top BAS-\mathrm{I}\| = \|D^{-1/2}D-\mathrm{I}\| \\ &= \max_j\{(1+s_j)^2-1\} \leqslant s_j=\beta, \end{aligned} \tag{A.13}$$

which completes the proof. □

Proposition A.3. *Let the family* $\{\mathfrak{h}^1,\cdots,\mathfrak{h}^n\}\subset\mathfrak{H}$ *be orthonormal, i.e.,* $(\mathfrak{h}^l,\mathfrak{h}^k)_{\mathfrak{H}}=\delta_{lk}$*, for all admissible* l,k*, and let the family* $\{\mathfrak{U}^1,\cdots,\mathfrak{U}^N\}\subset\mathfrak{H}$ *verifies the following conditions*

$$\left\|\mathfrak{U}^j\right\|_{\mathfrak{H}}=1, \quad |(\mathfrak{U}^j,\mathfrak{U}^i)_{\mathfrak{H}}-\delta_{ji}|\leqslant\tau, \quad \left\|\mathfrak{U}^j-\sum_{l=1}^n a_l^j\mathfrak{h}^l\right\|_{\mathfrak{H}}\leqslant\sigma \tag{A.14}$$

for all admissible indices, where $a_l^j, l=1,\cdots,n, j=1,\cdots,N$ *are given constants. Then:*

- *The following inequality*

$$(\min\{n,N\}+1)(\tau+(2+\sigma)\sigma)<1 \tag{A.15}$$

  implies $N\leqslant n$*;*
- *for* $N=n$ *and* $(\tau+(2+\sigma)\sigma)<1$*, there exist orthonormal family of vectors* $\mathfrak{g}^k=(\mathfrak{g}_1^k,\cdots,\mathfrak{g}_n^k)^\top$*,* $k=1,\cdots,n$*, such that*

$$\left\|\mathfrak{h}^k-\sum_{l=1}^n\mathfrak{g}_l^k\mathfrak{U}^l\right\|_{\mathfrak{H}}\leqslant n(\tau+(3+\sigma)\sigma). \tag{A.16}$$

Proof. First, we prove (A.15). From relations (A.14) it follows that

$$\begin{aligned}\left|(\mathfrak{U}^j,\mathfrak{U}^k)_{\mathfrak{H}}-a^k\cdot a^j\right| &= \Bigg|(\mathfrak{U}^j,\mathfrak{U}^k-\sum_{m=1}^n a_m^k\mathfrak{h}^m)_{\mathfrak{H}}+(\mathfrak{U}^j-\sum_{m=1}^n a_m^j\mathfrak{h}^m,\mathfrak{U}^k)_{\mathfrak{H}}- \\ &(\mathfrak{U}^j-\sum_{m=1}^n a_m^j\mathfrak{h}^m,\mathfrak{U}^k-\sum_{m=1}^n a_m^k\mathfrak{h}^m)_{\mathfrak{H}}\Bigg|\leqslant\sigma+\sigma+\sigma^2=(2+\sigma)\sigma, \end{aligned} \tag{A.17}$$

hence the vectors $a^j=(a_j^1,\cdots,a_n^j)^\top$ satisfy

$$\left|a^k\cdot a^j-\delta_{kj}\right|\leqslant\tau+(2+\sigma)\sigma. \tag{A.18}$$

If $N>n$ then there are only n linearly independent vectors within the family $a^1,\cdots,a^N$. Therefore, in the linear combination $\alpha_1 a^1+\cdots+\alpha_N a^N=0$ there are at most $n+1$ coefficients $\alpha_j \neq 0$, for $j \in I(N)$ here $I(N) \subset \{1, \cdots, N\}$ and $\#I(N) \leqslant n+1$. We select $k \in I(N)$ such that $|\alpha_k| \geqslant |\alpha_j| > 0$ for all $j \in I(N)$. Taking into account (A.17) it follows that

$$1 - \tau - (2+\sigma)\sigma \leqslant a^k \cdot a^k = - \sum_{j \in I(N)\setminus\{k\}} \frac{\alpha_j}{\alpha_k} a^k \cdot a^j \leqslant n(\tau + (2+\sigma)\sigma), \tag{A.19}$$

hence $(n+1)(\tau + (2+\sigma)\sigma) \geqslant 1$. Thus (A.15) follows for $N \leqslant n$. Now we turn to the proof of (A.16). By Proposition A.2 there is an orthonormal family of vectors $\mathfrak{g}^j$, $j = 1, \cdots, n$ which form an orthogonal $n \times n$-matrix denoted by $\mathfrak{g} := \left[\mathfrak{g}^1, \ldots, \mathfrak{g}^n\right] = (\mathfrak{g}_i^j)$ such that

$$\sum_{k=1}^{n} \left(\sum_{l=1}^{n} (a_l^k - \mathfrak{g}_k^l) \mathfrak{g}^k \right)^2 \leqslant n^2 (\tau + (2+\sigma)\sigma)^2. \tag{A.20}$$

By the triangle inequality we have

$$\begin{aligned} \left\| \mathfrak{h}^k - \sum_{l=1}^{n} \mathfrak{g}_l^k \mathfrak{U}^l \right\|_{\mathfrak{H}} &\leqslant \left\| \mathfrak{h}^k - \sum_{l,m=1}^{n} \mathfrak{g}_l^k \mathfrak{g}_l^m \mathfrak{h}^m \right\|_{\mathfrak{H}} \\ &\quad + \left\| \sum_{l=1}^{n} \mathfrak{g}_l^k \left(\mathfrak{U}^l - \sum_{m=1}^{n} a_m^l \mathfrak{h}^m \right) \right\|_{\mathfrak{H}} \\ &\quad + \left\| \sum_{l,m=1}^{n} \left(a_m^l - \mathfrak{g}_l^m \right) \mathfrak{g}_l^k \mathfrak{h}^m \right\|_{\mathfrak{H}}. \end{aligned} \tag{A.21}$$

Since $\mathfrak{g}^l \cdot \mathfrak{g}^m = \delta_{lm}$ we have

$$\left\| \mathfrak{h}^k - \sum_{l,m=1}^{n} \mathfrak{g}_l^k \mathfrak{g}_l^m \mathfrak{h}^m \right\|_{\mathfrak{H}} = 0. \tag{A.22}$$

In addition $|\mathfrak{g}_l^k| \leqslant \|\mathfrak{g}^k\| = 1$, hence

$$\sum_{l=1}^{n} |\mathfrak{g}_l^k| \leqslant n, \tag{A.23}$$

and by $(\mathfrak{h}^k, \mathfrak{h}^m)_{\mathfrak{H}} = \delta_{km}$ we have

$$\left\| \sum_{l,m=1}^{n} \left(a_m^l - \mathfrak{g}_l^m \right) \mathfrak{g}_l^k \mathfrak{h}^m \right\|_{\mathfrak{H}}^2 = \sum_{k=1}^{n} \left(\sum_{l=1}^{n} (a_l^k - \mathfrak{g}_k^l) \mathfrak{g}^k \right)^2 \tag{A.24}$$

which completes the proof in view of (A.20). □

A.2 Lemma on Almost Eigenvalues and Eigenvectors

Now, we recall a lemma on *almost eigenvalues and eigenvectors* [122], which is a standard tool, [131, 166, 177, 178, 179] in the asymptotic analysis of spectral problems.

Lemma A.1. *Let there be given* $\mathfrak{h} \in \mathfrak{H}$ *with* $\|\mathfrak{h}\|_{\mathfrak{H}} = 1$, *and* $\mathfrak{m} \in \mathbb{R}_+$ *such that*

$$\|\mathfrak{K}\mathfrak{h} - \mathfrak{m}\mathfrak{h}\|_{\mathfrak{H}} = \delta. \tag{A.25}$$

Then:

- *The distance* $d := dist\ \{\mathfrak{m}, \mathfrak{Sp}(\mathfrak{K})\} \leqslant \delta$, *i.e., the interval* $[\mathfrak{m} - \delta, \mathfrak{m} + \delta]$ *contains at least one eigenvalue of the operator* $\mathfrak{K}$.
- *If there are eigenvalues* $\mathfrak{Sp}(\mathfrak{K}) \ni \mu^k, \ldots, \mu^{n-1} \in [\mathfrak{m} - \varepsilon, \mathfrak{m} + \varepsilon]$ *for a given* $\varepsilon \in (0, \mathfrak{m})$, *and* $\mathfrak{v}^k, \cdots, \mathfrak{v}^{n-1}$ *denote the associated eigenvectors, then we can find the coefficients* $a_k, \ldots, a_{n-1} \in \mathbb{R}$ *such that*

$$\left\| \mathfrak{h} - \sum_{l=k}^{n-1} a_l \mathfrak{v}^l \right\|_{\mathfrak{H}} \leqslant \frac{\delta}{\varepsilon}. \tag{A.26}$$

Proof. We have

$$\mathfrak{h} = \sum_{l=1}^{\infty} (\mathfrak{h}, \mathfrak{v}^l)_{\mathfrak{H}} \mathfrak{v}^l := \sum_{l=1}^{\infty} a_l \mathfrak{v}^l. \tag{A.27}$$

Since $\mathfrak{K}\mathfrak{v}^l = \mu^l \mathfrak{v}^l$ and $(\mathfrak{v}^m, \mathfrak{v}^l)_{\mathfrak{H}} = \delta_{ml}$, it follows that

$$\begin{aligned} \delta^2 &= \|\mathfrak{K}\mathfrak{h} - \mathfrak{m}\mathfrak{h}\|_{\mathfrak{H}}^2 = \left\| \sum_{l=1}^{\infty} a_l (\mu^l - \mathfrak{m}) \mathfrak{v}^l \right\|_{\mathfrak{H}}^2 = \sum_{l=1}^{\infty} a_l^2 (\mu^l - \mathfrak{m})^2 \\ &\geqslant \min_{l \in \mathbb{N}} \{(\mu^l - \mathfrak{m})^2\} \sum_{l=1}^{\infty} a_l^2 = d^2 \, \|\mathfrak{h}\|_{\mathfrak{H}}^2 = d^2, \end{aligned} \tag{A.28}$$

and the first claim of lemma is proved. For the second claim, we have

$$\begin{aligned} \left\| \mathfrak{h} - \sum_{l=k}^{n-1} a_l \mathfrak{v}^l \right\|_{\mathfrak{H}}^2 &= \sum_{l \in \mathbb{N} \setminus \{k, n-1\}}^{\infty} a_l^2 \leqslant \frac{1}{\varepsilon^2} \sum_{l \in \mathbb{N} \setminus \{k, n-1\}}^{\infty} a_l^2 (\mu^l - \mathfrak{m})^2 \\ &\leqslant \frac{1}{\varepsilon^2} \sum_{l \in \mathbb{N}}^{\infty} a_l^2 (\mu^l - \mathfrak{m})^2 = \frac{1}{\varepsilon^2} \, \|\mathfrak{K}\mathfrak{h} - \mathfrak{m}\mathfrak{h}\|_{\mathfrak{H}}^2 = \frac{d^2}{\varepsilon^2}. \end{aligned} \tag{A.29}$$

Thus the results are established. □

Appendix B
Spectral Problem for the Neumann Laplacian

In this appendix the justification of the asymptotic expansions is established in few steps, which are:

- The justification of asymptotic expansions is based upon the *weighted Poincaré inequality* in Lemma B.2.
- The analysis of perturbed spectral problem is reduced itself to the analysis of an abstract equation in the Hilbert space combined with Lemma A.1 in Appendix A on *almost eigenvalues and eigenvectors*. In such a way the necessary estimates for the remainders in ansätze (9.69)-(9.70), for the simple and multiple eigenvalues are derived.
- First, the remainder which is a combination of the terms appearing in ansätze (9.69)-(9.70) need to be estimated.
- After, the remainder is decomposed in such a way that an estimate of order $O(h^{7/2})$ is obtained.
- The estimates for different terms of this decomposition are obtained by analysis of the boundary layers behavior as $x \to \mathcal{O}$ and $\|\xi\| \to \infty$.
- The estimates for the remainders in ansätze (9.69)-(9.70) are determined in Theorem B.1.
- In the proof of Theorem B.1, first the existence of a certain number of eigenvalues close to the eigenvalue λ_m^0 with the multiplicity $\varkappa_m$ is assured by Lemma A.1. Then it is shown that these eigenvalues are small perturbations of the eigenvalue λ_m^0 of the multiplicity $\varkappa_m$.

B.1 The Weighted Poincaré Inequality

Let $H^1_{\mathrm{m}}(\Omega_h)$ denote a subspace of the Sobolev space $H^1(\Omega_h)$ which contains functions of zero mean over the set Ω_h. First, we need the following auxiliary assertions:

Lemma B.1. *Let $\Omega_1 \subset \Omega_2$ be two smooth domains, with $|\Omega_1| \neq 0$, then for any $w \in H^1(\Omega_2)$ we have*

$$\|w\|_{L^2(\Omega_2)} \leqslant c\left(\|\nabla_x w\|_{L^2(\Omega_2)} + \|w\|_{L^2(\Omega_1)}\right), \tag{B.1}$$

where the constant c depends on Ω_1 and Ω_2.

Proof. Assume that (B.1) is not true and take a sequence w_n such that $\|w_n\|_{L^2(\Omega_2)} = 1$ and the right hand side of (B.1) tends to zero. From the boundedness of w and $\nabla_x w$ in $L^2(\Omega_2)$ we get the boundedness of w in $H^1(\Omega_2)$. Thus, up to a subsequence, w_n converges to some $\overline{w} \in H^1(\Omega_2)$ and since $\|\nabla_x w_n\|_{L^2(\Omega_2)} \to 0$ we get $\nabla_x \overline{w} = 0$ and $\overline{w}$ is constant. Since $\|w_n\|_{L^2(\Omega_1)} \to 0$, this constant is zero and thus $\overline{w} \equiv 0$. This implies

$$\|w_n\|_{L^2(\Omega_2)} \to 0, \tag{B.2}$$

in contradiction with $\|w_n\|_{L^2(\Omega_2)} = 1$. Thus, (B.1) holds true. □

Lemma B.2. *The following* weighted Poincaré inequality *is valid*

$$\|u\|_{L^2(\Omega_h)} \leqslant c\|r_h^{-1}u\|_{L^2(\Omega_h)} \leqslant C\|\nabla_x u\|_{L^2(\Omega_h)}, \tag{B.3}$$

where $r_h = r + h$ with $r(x) = \operatorname{dist}(x, \mathscr{O}) = \|x\|$, the constants c, C are independent of $h \in (0, h_0]$ and of $u \in H^1_{\mathfrak{m}}(\Omega_h)$.

Proof. We use the representation

$$u(x) = u_{\mathsf{T}}(x) + b_{\mathsf{T}}, \tag{B.4}$$

where the constant b_{T} is chosen such that

$$\int_{\Omega_{\mathsf{T}}} u_{\mathsf{T}}(x)\,dx = 0, \quad b_{\mathsf{T}} = \frac{1}{|\Omega_{\mathsf{T}}|}\int_{\Omega_{\mathsf{T}}} u(x)\,dx. \tag{B.5}$$

In (B.5), the domain $\Omega_{\mathsf{T}} \subset \Omega$ satisfies $\Omega_{\mathsf{T}} \neq \varnothing$ and $\Omega_{\mathsf{T}} \cap \omega_h = \varnothing$ for $h \in (0, h_0]$. Let us construct an extension $\hat{u}_{\mathsf{T}}$ of u_{T} in the class H^1, from the set $\Omega_\ell := \Omega \setminus B_\ell$ onto Ω, in such a way that the following estimate is valid

$$\|\nabla_x \hat{u}_{\mathsf{T}}\|_{L^2(\Omega)} \leqslant c\|\nabla_x u_{\mathsf{T}}\|_{L^2(\Omega_\ell)} = c\|\nabla_x u\|_{L^2(\Omega_\ell)} \leqslant c\|\nabla_x u_{\mathsf{T}}\|_{L^2(\Omega_h)}. \tag{B.6}$$

Here $B_\ell = \{x : \|x - \mathscr{O}\| < \ell\}$, with $\ell = \ell(h) := Rh$ and the constant R chosen such that $\omega_h \subset B_\ell$. The reason for such procedure is that a direct extension of Ω_h onto Ω may not exist in the class H^1, for example in the case of a crack (cf. Remark 9.8). Stretching coordinates $x \mapsto \xi = h^{-1}x$ transforms the set $\Sigma_\ell = \{x \in \Omega : \ell > r > \ell/2\}$ into the three-dimensional half-annulus Υ_h with fixed radii and gently sloped ends, due to the smoothness of the boundary $\partial\Omega$. In stretched coordinates, we write $\mathfrak{u}_{\mathsf{T}}(\xi) = u_{\mathsf{T}}(x)$. Then, we proceed to the decomposition

$$\mathfrak{u}_{\mathsf{T}}(\xi) = \mathfrak{u}_{\mathfrak{m}}(\xi) + b_{\mathfrak{m}}, \tag{B.7}$$

where the constant $b_{\mathfrak{m}}$ is chosen such that

$$\int_{\Upsilon_h} \mathfrak{u}_{\mathfrak{m}}(\xi)d\xi = 0, \quad b_{\mathfrak{m}} = \frac{1}{|\Upsilon_h|}\int_{\Upsilon_h} \mathfrak{u}_{\mathsf{T}}(\xi)d\xi. \tag{B.8}$$

The extension ought to be made in the stretched variables. Due to the orthogonality condition in (B.8), the *Poincaré inequality* holds true for $\mathfrak{u}_{\mathfrak{m}}$ in Υ_h

$$\|\mathfrak{u}_{\mathfrak{m}}\|_{L^2(\Upsilon_h)} \leqslant c\|\nabla_\xi \mathfrak{u}_{\mathfrak{m}}\|_{L^2(\Upsilon_h)} = c\|\nabla_\xi \mathfrak{u}_{\mathsf{T}}\|_{L^2(\Upsilon_h)}, \tag{B.9}$$

where the constant c does not depend on h because Υ_h has gently sloped ends. Therefore, there exists an extension $\hat{\mathfrak{u}}_{\mathfrak{m}}$ of $\mathfrak{u}_{\mathfrak{m}}$ from Υ_h onto $\hat{\Upsilon}_h = \{\xi : x \in \Omega, r < \ell\}$, such that

$$\|\hat{\mathfrak{u}}_{\mathfrak{m}}\|_{H^1(\hat{\Upsilon}_h)} \leqslant c\|\mathfrak{u}_{\mathfrak{m}}\|_{H^1(\Upsilon_h)} \leqslant c\|\nabla_\xi \mathfrak{u}_{\mathfrak{m}}\|_{L^2(\Upsilon_h)}, \tag{B.10}$$

where c is independent of $h \in (0, h_0]$ and $\mathfrak{u}_{\mathfrak{m}}$. Choosing $\Omega_{\mathsf{T}} = \Omega \setminus B_\ell$, the required extension $\hat{u}_{\mathsf{T}}$ is thus defined as follows:

$$\hat{u}_{\mathsf{T}}(x) = \begin{cases} u_{\mathsf{T}}(x), & x \in \Omega \setminus B_\ell, \\ \hat{\mathfrak{u}}_{\mathfrak{m}}(\xi) + b_{\mathfrak{m}}, & \Omega \cap B_\ell. \end{cases} \tag{B.11}$$

Now we give estimates for the extension $\hat{u}_{\mathsf{T}}$

$$\|\nabla_x \hat{u}_{\mathsf{T}}\|_{L^2(\Omega)} = \|\nabla_x u_{\mathsf{T}}\|_{L^2(\Omega\setminus B_\ell)} + \|\nabla_x \hat{\mathfrak{u}}_{\mathfrak{m}}\|_{L^2(\Omega\cap B_\ell)}, \tag{B.12}$$

and further, using the previous estimates, we obtain

$$\begin{aligned} \|\nabla_x \hat{\mathfrak{u}}_{\mathfrak{m}}\|_{L^2(\Omega\cap B_\ell)} &= h^{1/2}\|\nabla_\xi \hat{\mathfrak{u}}_{\mathfrak{m}}\|_{L^2(\hat{\Upsilon}_h)} \\ &\leqslant h^{1/2}\|\hat{\mathfrak{u}}_{\mathfrak{m}}\|_{H^1(\hat{\Upsilon}_h)} \leqslant ch^{1/2}\|\nabla_\xi \mathfrak{u}_{\mathfrak{m}}\|_{L^2(\Upsilon_h)} \\ &\leqslant ch^{1/2}\|\nabla_\xi \mathfrak{u}_{\mathsf{T}}\|_{L^2(\Upsilon_h)} = c\|\nabla_x u_{\mathsf{T}}\|_{L^2(\Sigma_\ell))}. \end{aligned} \tag{B.13}$$

Gathering the two previous estimates for $\nabla_x \hat{u}_{\mathsf{T}}$ we obtain due to the definition of Σ_ℓ that

$$\|\nabla_x \hat{u}_{\mathsf{T}}\|_{L^2(\Omega)} \leqslant c\|\nabla_x u_{\mathsf{T}}\|_{L^2(\Omega\setminus B_{\ell/2})} \leqslant c\|\nabla_x u\|_{L^2(\Omega_h)}. \tag{B.14}$$

The last inequality is true if $\Omega \setminus B_{\ell/2} \subset \Omega_h$, which is certainly verified for an appropriate choice of R and h small enough. The constant c in the previous inequality is independent of h. We show using the *Poincaré inequality* that

$$\|\hat{u}_{\mathsf{T}}\|_{L^2(\Omega)} \leqslant c\|\nabla_x \hat{u}_{\mathsf{T}}\|_{L^2(\Omega)} \leqslant c\|\nabla_x u\|_{L^2(\Omega_h)}. \tag{B.15}$$

Applying Lemma B.1 to our problem, we get

$$\begin{aligned} \|\hat{u}_{\mathsf{T}}\|_{L^2(\Omega)} &\leqslant c\left(\|\nabla_x \hat{u}_{\mathsf{T}}\|_{L^2(\Omega)} + \|\hat{u}_{\mathsf{T}}\|_{L^2(\Omega_{\mathsf{T}})}\right) \\ &\leqslant c\left(\|\nabla_x \hat{u}_{\mathsf{T}}\|_{L^2(\Omega)} + \|\nabla_x \hat{u}_{\mathsf{T}}\|_{L^2(\Omega_{\mathsf{T}})}\right) \\ &\leqslant c\|\nabla_x \hat{u}_{\mathsf{T}}\|_{L^2(\Omega)}, \end{aligned} \tag{B.16}$$

where we have also used the Poincaré inequality in Ω_T, since $\hat{u}_\mathsf{T}$ coincides with u_T and has zero mean value on this set. Then with (B.14) and the previous inequality we obtain the desired estimate (B.15). Next we invoke the one-dimensional *Hardy's inequality*

$$\int_0^1 |z(r)|^2\,dr \leqslant 4\int_0^1 r^2|\partial_r z(r)|^2\,dr, \qquad z\in C_c^1([0,1)), \tag{B.17}$$

which, after the integration in the angular variables θ and ϕ, leads to

$$\|r^{-1}\hat{u}_\mathsf{T}\|_{L^2(\Omega)} \leqslant \|\nabla_x \hat{u}_\mathsf{T}\|_{L^2(\Omega)} \leqslant c\|\nabla_x u\|_{L^2(\Omega_h)}. \tag{B.18}$$

For the constant $b_\mathfrak{m}$ in decomposition (B.7) we now obtain

$$\begin{aligned}|b_\mathfrak{m}| &= \left|\frac{1}{|\Upsilon_h|}\int_{\Upsilon_h}\mathfrak{u}_\mathsf{T}(\xi)d\xi\right| \\ &\leqslant c\|\mathfrak{u}_\mathsf{T}\|_{L^2(\Upsilon_h)} = c\|\hat{\mathfrak{u}}_\mathsf{T}\|_{L^2(\Upsilon_h)} = ch^{-3/2}\|\hat{u}_\mathsf{T}\|_{L^2(\Sigma_\ell)} \\ &\leqslant ch^{-1/2}\|r^{-1}\hat{u}_\mathsf{T}\|_{L^2(\Sigma_\ell)}.\end{aligned} \tag{B.19}$$

Further, the image $\Sigma_\omega(h)$ of the set $\Omega_h \cap B_\ell$ under stretching of coordinates, possesses a gently sloped boundary, hence, applying Lemma B.1 we obtain

$$\|\mathfrak{u}_\mathsf{T}\|_{L^2(\Sigma_\omega(h))} \leqslant c\left(\|\nabla_\xi \mathfrak{u}_\mathsf{T}\|_{L^2(\Sigma_\omega(h))} + \|\mathfrak{u}_\mathsf{T}\|_{L^2(\Upsilon_h)}\right). \tag{B.20}$$

Recall that $r_h = r+h > h$. In this way we have

$$\begin{aligned}\|r_h^{-1}u_\mathsf{T}\|_{L^2(\Omega_h\cap B_\ell)} &\leqslant h^{-1}\|u_\mathsf{T}\|_{L^2(\Omega_h\cap B_\ell)} = h^{1/2}\|\mathfrak{u}_\mathsf{T}\|_{L^2(\Sigma_\omega(h))} \\ &\leqslant ch^{1/2}\left(\|\nabla_\xi \mathfrak{u}_\mathsf{T}\|_{L^2(\Sigma_\omega(h))} + \|\mathfrak{u}_\mathsf{T}\|_{L^2(\Upsilon_h)}\right) \\ &\leqslant ch^{1/2}\left(\|\nabla_\xi \mathfrak{u}_\mathsf{T}\|_{L^2(\Sigma_\omega(h))} + \|\mathfrak{u}_\mathfrak{m}\|_{L^2(\Upsilon_h)} + |b_\mathfrak{m}|\right).\end{aligned} \tag{B.21}$$

Using the *Poincaré inequality* for $\mathfrak{u}_\mathfrak{m}$ in Υ_h and the estimate for $b_\mathfrak{m}$, we get from the previous inequality

$$\|r_h^{-1}u_\mathsf{T}\|_{L^2(\Omega_h\cap B_\ell)} \leqslant c\left(h\|\nabla_x u_\mathsf{T}\|_{L^2(\Omega_h\cap B_\ell)} + \|r^{-1}\hat{u}_\mathsf{T}\|_{L^2(\Sigma_\ell)}\right). \tag{B.22}$$

We can now, after applying (B.18) and (B.22), write

$$\begin{aligned}\|r_h^{-1}u_\mathsf{T}\|_{L^2(\Omega_h)} &= \|r_h^{-1}u_\mathsf{T}\|_{L^2(\Omega\setminus B_\ell)} + \|r_h^{-1}u_\mathsf{T}\|_{L^2(\Omega_h\cap B_\ell)} \\ &\leqslant c\|r_h^{-1}\hat{u}_\mathsf{T}\|_{L^2(\Omega)} + c\left(h\|\nabla_x u_\mathsf{T}\|_{L^2(\Omega_h\cap B_\ell)} + \|r^{-1}\hat{u}_\mathsf{T}\|_{L^2(\Sigma_\ell)}\right) \\ &\leqslant c\|\nabla_x u_\mathsf{T}\|_{L^2(\Omega_h)}.\end{aligned} \tag{B.23}$$

We give an estimate for the constant b_{T} as follows:

$$|b_{\mathsf{T}}| = \left| \frac{1}{|\Omega_h|} \int_{\Omega_h} (u(x) - u_{\mathsf{T}}(x))\, dx \right| = \left| \int_{\Omega_h} u_{\mathsf{T}}(x)\, dx \right|$$
$$\leqslant c\|u_{\mathsf{T}}\|_{L^2(\Omega_h)} \leqslant c\|r^{-1}u_{\mathsf{T}}\|_{L^2(\Omega_h)} \leqslant c\|\nabla_x u\|_{L^2(\Omega_h)}. \tag{B.24}$$

Finally we have

$$\|r_h^{-1}u\|_{L^2(\Omega_h)} \leqslant c\left(\|r_h^{-1}u_{\mathsf{T}}\|_{L^2(\Omega_h)} + \|r_h^{-1}b_{\mathsf{T}}\|_{L^2(\Omega_h)}\right) \leqslant c\|\nabla_x u\|_{L^2(\Omega_h)}, \tag{B.25}$$

which completes the proof. □

B.2 Asymptotics for Spectral Problem

In the proof of Lemma B.2, an extension $\hat{u} := \hat{u}_{\mathsf{T}} + b_{\mathsf{T}}$ of the function $u \in H^1_{\mathfrak{m}}(\Omega_h)$ onto the domain Ω is constructed such that

$$\|r_h^{-1}u\|_{L^2(\Omega_h)} + \|\nabla_x \hat{u}\|_{L^2(\Omega)} \leqslant c\|\nabla_x u\|_{L^2(\Omega_h)}. \tag{B.26}$$

Assume that $m \geqslant 1$ and $\hat{u}_m^h$ is the extension described above of the eigenfunction u_m^h. In view of (9.65) and the integral identity [123], namely

$$(\nabla_x u_m^h, \nabla_x z)_{\Omega_h} = \lambda_m^h (u_m^h, z)_{\Omega_h},\ z \in H^1_{\mathfrak{m}}(\Omega_h), \tag{B.27}$$

which serves for the problem (9.63), the following relation is valid:

$$\|\hat{u}_m^h\|^2_{H^1(\Omega)} \leqslant c\|\nabla_x u_m^h\|^2_{L^2(\Omega_h)} = c\lambda_m^h. \tag{B.28}$$

The max-min principle of Proposition A.1 with the test functions from the space $C_c^\infty(\Omega_{\mathsf{T}})$ show that for an integer m there exist positive numbers h_m and c_m, such that

$$\lambda_m^h \leqslant c_m \qquad \text{for } h \in (0, h_m]. \tag{B.29}$$

Therefore the norms $\|\hat{u}_m^h\|_{H^1(\Omega)}$ are uniformly bounded with respect to the parameter $h \in (0, h_m]$ for a fixed m, i.e. the pairs $\{\lambda_m^h, \hat{u}_m^h\}$ admit the weak limit $\{\lambda_m^0, \hat{u}_0^h\} \in \mathbb{R} \times H^1(\Omega)$ for $h \to +0$ and the strong limit in $\mathbb{R} \times L^2(\Omega)$. In the integral identity (B.27) we choose a test function $z \in C_c^\infty(\overline{\Omega} \setminus \{\mathscr{O}\})$ with null mean value. For sufficiently small h, $\hat{u}_m^h = u_m^h$ on the support of the function z, thus passing to the limit in (B.27) leads to the equality

$$(\nabla_x \hat{v}_m^0, \nabla_x z)_\Omega = \hat{\lambda}_m^0 (\hat{v}_m^0, z)_\Omega, \tag{B.30}$$

where $(\cdot,\cdot)_\Omega$ stands for the scalar product in $L^2(\Omega)$. Since $C_c^\infty(\overline{\Omega} \setminus \{\mathscr{O})\}$ is dense in $H^1(\Omega)$ (elements of the Sobolev space $H^1(\Omega)$ have no traces at a single point), then by a density argument, we can assume that in (B.30), the test function z belongs to $H^1_{\mathfrak{m}}(\Omega)$. In view of (B.26), (B.27) and (B.28), it follows that

$$\left|\int_{\Omega} \hat{u}_m^h dx - \int_{\Omega_h} u_m^h dx\right| \leqslant \left|\int_{\Omega\cap B_\ell} |\hat{u}_m^h| dx - \int_{\Omega_h\cap B_\ell} |u_m^h| dx\right|$$
$$\leqslant ch^{5/2}\left(\|r_h^{-1}\hat{u}_m^h\|_{L^2(\Omega)} + \|r_h^{-1}u_m^h\|_{L^2(\Omega_h)}\right) \leqslant ch^{5/2} \quad \text{(B.31)}$$

and

$$\left|\int_{\Omega} |\hat{u}_m^h|^2 dx - \int_{\Omega_h} |u_m^h|^2 dx\right| \leqslant ch^2. \quad \text{(B.32)}$$

Since $\|\hat{u}_m^h\|_{L^2(\Omega)} \to \|\hat{v}_m^0\|_{L^2(\Omega)}$ and $\|\hat{u}_m^h\|_{L^2(\Omega)} = 1$, the previous inequality provides

$$\hat{v}_m^0 \in H^1(\Omega) \quad \text{and} \quad \|\hat{v}_m^0\|_{L^2(\Omega)} = 1, \quad \text{(B.33)}$$

i.e. in view of (B.30), $\hat{\lambda}_m^0$ is an eigenvalue and $\hat{v}_m^0$ is a normalized eigenfunction of problem (9.67).

Proposition B.1. *Entries of sequences* (9.64) *and* (9.66) *are related by passing to the limit*

$$\lambda_m^h \to \lambda_m^0 \quad \text{as} \quad h \to +0. \quad \text{(B.34)}$$

Proof of Proposition B.1 is completed in fact within the proof of Theorem B.1. We only observe that it has been already shown that $\lambda_m^h \to \lambda_p^0$, thus it suffices to prove that $p = m$.

From Lemma B.2 it follows that the left hand side of identity (B.27) can be chosen as the scalar product $\langle u, z\rangle_{\Omega_h} := (\nabla_x u, \nabla_x z)_{\Omega_h}$ in the space $H^1_{\mathfrak{m}}(\Omega_h)$. We define the operator K^h in the space $H^1_{\mathfrak{m}}(\Omega_h)$ by the formula

$$\langle K^h u, z\rangle_{\Omega_h} = (u, z)_{\Omega_h}, \quad u, z \in H^1_{\mathfrak{m}}(\Omega_h). \quad \text{(B.35)}$$

It is easy to check that K^h is symmetric, positive, compact and, therefore, self-adjoint. Hence, the general theory applies to the spectral problem with the operator K^h. For $m \geqslant 1$ we set $\mu_m^h = (\lambda_m^h)^{-1}$. The positive eigenvalues and the corresponding eigenfunction of problem (9.63) can be considered in an abstract framework, so we deal with the spectral equation in the Hilbert space $H = H^1_{\mathfrak{m}}(\Omega_h)$:

$$K^h u^h = \mu^h u^h. \quad \text{(B.36)}$$

The norm, defined by the scalar product $\langle\cdot,\cdot\rangle_{\Omega_h}$ is denoted by $\|\cdot\|_H$. We are going to apply Lemma A.1 on *almost eigenvalues and eigenvectors* for the compact operator K^h. Thus, for given $\mu > 0$ and $\mathfrak{u} \in H$, $\|\mathfrak{u}\|_H = 1$, such that $\|K^h\mathfrak{u} - \mu\mathfrak{u}\|_H = \alpha$, there exists an eigenvalue μ_m^h of the operator K^h, which satisfies the inequality

$$|\mu - \mu_m^h| \leqslant \alpha. \quad \text{(B.37)}$$

Moreover, for any $\alpha_{\Bbbk} > \alpha$ the following inequality holds

$$\|\mathfrak{u} - \mathfrak{u}_{\Bbbk}\|_H \leqslant 2\alpha/\alpha_{\Bbbk}, \tag{B.38}$$

where $\mathfrak{u}_{\Bbbk}$ is a linear combination of eigenfunctions of the operator K^h, corresponding to the eigenvalues from the segment $[\mu - \alpha_{\Bbbk}, \mu + \alpha_{\Bbbk}]$ and $\|\mathfrak{u}_{\Bbbk}\|_H = 1$. The asymptotic approximations μ and $\mathfrak{u}$ of a solution to equation (B.35) are defined by the number $(\lambda_m^0 + h^3\lambda_m')^{-1}$ and by the function $\|\upsilon_m^h\|_H^{-1}\upsilon_m^h$, respectively, where $m \geqslant 1$ and λ_m' with υ_m^h are, respectively, the correction given by (9.157) and the sum of the first four terms in the ansätz (9.70). In the case of multiple eigenvalue λ_p^0, we consider the specification provided at the end of section 9.3.4. We estimate the quantity α in (B.38), such an estimate is used in Lemma A.1. Since $\|\upsilon_m^h\|_H \geqslant \|v_m^0\|_H - c_m h$ and $\lambda_m^0 + h^3\lambda_m' \geqslant \lambda_m^0 - c_m h^3$, for h sufficiently small it follows that

$$\begin{aligned}
\alpha &= \|K^h\mathfrak{u} - \mu\mathfrak{u}\|_H \\
&= (\lambda_m^0 + h^3\lambda_m')^{-1}\|\upsilon_m^h\|_H^{-1}\|(\lambda_m^0 + h^3\lambda_m')(K^h - \mu)\upsilon_m^h\|_H \\
&= (\lambda_m^0 + h^3\lambda_m')^{-1}\|\upsilon_m^h\|_H^{-1}\sup\left|\langle(\lambda_m^0 + h^3\lambda_m')(K^h - \mu)\upsilon_m^h, z\rangle_{\Omega_h}\right| \\
&\leqslant c_m \sup\left|(\lambda_m^0 + h^3\lambda_m')(\upsilon_m^h, z)_{\Omega_h} - \langle\upsilon_m^h, z\rangle_{\Omega_h}\right|,
\end{aligned} \tag{B.39}$$

where the supremum is taken over the set $\{z \in H^1_{\mathfrak{m}}(\Omega_h) : \|z\|_H = 1\}$ and, hence, the L^2-norms of the test function z indicated in inequality (B.3), both standard and weighted, are bounded by a constant $\mathfrak{C}$. Besides that, the standard proof of the trace theorem [123, pp. 30] implies

$$h^{-1/2}\|z\|_{L^2(\partial\omega_h\cap\Gamma_h)} \leqslant c\left(\|r_h^{-1}z\|_{L^2(\Omega_h)} + \|\nabla z\|_{L^2(\Omega_h)}\right) \leqslant c\mathfrak{C}. \tag{B.40}$$

The expression in the sup in (B.39) can be processed as follows:

$$\begin{aligned}
\mathscr{I} \;&=\; (\lambda_m^0 + h^3\lambda_m')(\upsilon_m^h, z)_{\Omega_h} - \langle\upsilon_m^h, z\rangle_{\Omega_h} \\
&=\; \mathscr{I}^1 + h^3\mathscr{I}^2 - h^6\mathscr{I}^3 + \mathscr{I}^4 - \mathscr{I}^5 - h^3\mathscr{I}^6 \\
&:= (\nabla_x v_m^0, \nabla_x z)_{\Omega_h} - \lambda_m^0(v_m^0, z)_{\Omega_h} \\
&+\; h^3\left((\nabla_x v_m^3, \nabla_x z)_{\Omega_h} - (\lambda_m^0 v_m^3 + \lambda_m' v_m^0, z)_{\Omega_h}\right) - h^6\lambda_m'(v_m^3, z)_{\Omega_h} \\
&+\; (\nabla_x\chi(hw_m^1 + h^2w_m^2), \nabla_x z)_{\Omega_h} - \lambda_m^0(\chi(hw_m^1 + h^2w_m^2), z)_{\Omega_h} \\
&-\; h^3\lambda_m'(\chi(hw_m^1 + h^2w_m^2), z)_{\Omega_h}.
\end{aligned} \tag{B.41}$$

The estimates of $\mathscr{I}^3$ and $\mathscr{I}^6$ are straightforward, that is

$$|\mathscr{I}^3| \leqslant c_m\|v_m^3\|_{L^2(\Omega)}\mathfrak{C} \leqslant c_m\mathfrak{C}, \tag{B.42}$$

$$
\begin{aligned}
|\mathscr{I}^6| &\leqslant c_m \left| \int_{\Omega_h} \chi r_h (h w_m^1 + h^2 w_m^2)(r_h^{-1} z)\, dx \right| \\
&\leqslant c_m \|r_h^{-1} z\|_{L^2(\Omega_h)} \left(\int_{\Omega_h} (\chi r_h (h w_m^1 + h^2 w_m^2))^2\, dx \right)^{1/2} \\
&\leqslant c_m \mathfrak{C} h^{3/2} \left(\int_{\Xi \cap B_R} h^2 (1+\rho)^2 (h w_m^1 + h^2 w_m^2)^2\, d\xi \right. \\
&\quad \left. + \int_{\Xi \setminus B_R} \chi^2 h^2 (1+\rho)^2 (h\rho^{-2} + h^2 \rho^{-1})^2\, d\xi \right)^{1/2} \leqslant c_m \mathfrak{C} h^{5/2}. \quad \text{(B.43)}
\end{aligned}
$$

Here, expressions (9.87) and (9.107) of the boundary layers are taken into account. The remaining integrals require additional work. In view of relations (9.67) and (9.123)-(9.125) we have

$$
\mathscr{I}^1 = (\partial_{\mathfrak{n}} v_m^0, z)_{\partial\omega_h \cap \Gamma_h}, \quad \text{(B.44)}
$$

$$
\begin{aligned}
\mathscr{I}^2 &= \mathscr{I}_1^2 + \mathscr{I}_2^2 + \mathscr{I}_3^2 := (\partial_{\mathfrak{n}} v_m^3, z)_{\partial\omega_h \cap \Gamma_h} + (f^3, z)_{\Omega_h} \\
&= (\partial_{\mathfrak{n}} v_m^3, z)_{\partial\omega_h \cap \Gamma_h} + (\Delta_x \chi (t_m^1 + t_m^2), z)_{\Omega_h} + \lambda_m^0 (\chi (t_m^1 + t_m^2), z)_{\Omega_h}, \quad \text{(B.45)}
\end{aligned}
$$

where $\mathfrak{n}$ is the unit normal vector on $\partial\Omega_h$.

To get the estimate for $\mathscr{I}_1^2$, first of all, we need to prove

$$
\|r^{-1/2} z\|_{L^2(\Gamma_h)} + \|r^{-1} z\|_{L^2(\Omega_h)} \leqslant c \|z\|_{H^1(\Omega_h)}. \quad \text{(B.46)}
$$

By (B.3) and (B.40), we may write

$$
\|r_h^{-1/2} z\|_{L^2(\Gamma_h)} + \|r_h^{-1} z\|_{L^2(\Omega_h)} \leqslant c \|z\|_{H^1(\Omega_h)}. \quad \text{(B.47)}
$$

Thus, we verify that (B.46) holds in a h-neighborhood of $\mathscr{O}$. To this end, using the dilation given by h^{-1}, we verify

$$
\|\rho^{-1/2} \eta\|_{L^2(\partial\Xi_R)} + \|\rho^{-1} \eta\|_{L^2(\Xi_R)} \leqslant c \|\eta\|_{H^1(\Xi_R)}, \quad \text{(B.48)}
$$

in the parameter independent case, where $\Xi_R := \Xi \cap B_R$, B_R is the ball of radius R centered at the origin $\mathscr{O} = \{\rho = 0\}$ and $R > 0$ is such that $\Xi_R \supset \overline{\omega}$. There are three possibilities:

1. if $\mathscr{O}$ is outside $\overline{\Xi_R}$, then $\rho > c > 0$ and (B.48) is satisfied;
2. if $\mathscr{O}$ is inside $\overline{\Xi_R}$, then $\rho > c > 0$ on $\partial\Xi_R$ and the first norm in the left hand side of (B.48) is bounded by $c\|\eta\|_{H^1(\Xi_R)}$ by the standard trace inequality. The estimation of $\|\rho^{-1}\eta\|_{L^2(\Xi_R)}$ in (B.48) follows from the Hardy's inequality (B.17);
3. if $\mathscr{O}$ is on $\partial\Xi_R$, then the boundary $\partial\Xi$ should be rectified.

Note that the boundary $\partial\Xi$ is Lipschitz. Without loss of generality, let us assume that there exists a neighborhood $\mathfrak{N}$ of $\mathscr{O}$ such that $\partial\Xi_R \cap \mathfrak{N}$ is the graph of a Lipschitz function ψ. We rectify the boundary $\partial\Xi_R \cap \mathfrak{N}$ using the transformation

$$T : (\xi_1, \xi_2, \xi_3) \mapsto (\tilde{\xi}_1, \tilde{\xi}_2, \tilde{\xi}_3) = (\xi_1, \xi_2, \xi_3 - \psi(\xi_1, \xi_2)). \tag{B.49}$$

The image of $\partial \Xi_R \cap \mathfrak{N}$ by T is a piece of a plane. Let $(\tilde{\rho}, \tilde{\theta}, \tilde{\phi})$ be the spherical coordinate system associated with $(\tilde{\xi}_1, \tilde{\xi}_2, \tilde{\xi}_3)$. Using the Lipschitz property of ψ, one readily checks that there exist constants $c_1 > 0$ and $c_2 > 0$, dependent on ψ, such that

$$c_1 \rho < \tilde{\rho} < c_2 \rho. \tag{B.50}$$

Using Hardy's inequality (B.17) and the equivalence of ρ and $\tilde{\rho}$, we have

$$\begin{aligned} \|\rho^{-1}\eta\|_{L^2(\Xi_R \cap \mathfrak{N})} &\leqslant c\|\tilde{\rho}^{-1}\tilde{\eta}\|_{L^2(T(\Xi_R \cap \mathfrak{N}))} \\ &\leqslant c\|\tilde{\eta}\|_{H^1(T(\Xi_R \cap \mathfrak{N}))} \\ &\leqslant c\|\eta\|_{H^1(\Xi_R \cap \mathfrak{N})}. \end{aligned} \tag{B.51}$$

For the trace inequality, we separate the radial and angular variables and use the two-dimensional trace inequality in the angular variables:

$$\begin{aligned} \|\rho^{-1/2}\eta\|_{L^2(\partial\Xi_R \cap \mathfrak{N})} &\leqslant c\|\tilde{\rho}^{-1/2}\tilde{\eta}\|_{L^2(T(\partial\Xi_R \cap \mathfrak{N}))} \\ &= c\int_0^{\tilde{R}} \int_0^{2\pi} \tilde{\rho}^{-1}|\tilde{\eta}|^2 \rho \, d\tilde{\theta} \, d\tilde{\rho} \\ &= c\int_0^{\tilde{R}} \int_0^{\pi} \int_0^{2\pi} \left(|\tilde{\eta}|^2 + |\partial_{\tilde{\theta}}\tilde{\eta}|^2 + |\partial_{\tilde{\phi}}\tilde{\eta}|^2\right) d\tilde{\theta} \, d\tilde{\phi} \, d\tilde{\rho}, \end{aligned} \tag{B.52}$$

for some $\tilde{R} > 0$. Then we may use *Friedrich's inequality* to obtain

$$\begin{aligned} \int_0^{\tilde{R}} \int_0^{\pi} \int_0^{2\pi} \left(|\tilde{\eta}|^2 + |\partial_{\tilde{\theta}}\tilde{\eta}|^2 + |\partial_{\tilde{\phi}}\tilde{\eta}|^2\right) d\tilde{\theta} \, d\tilde{\phi} \, d\tilde{\rho} &\leqslant c\|\tilde{\eta}\|_{H^1(T(\Xi_R \cap \mathfrak{N}))} \\ &\leqslant c\|\eta\|_{H^1(\Xi_R \cap \mathfrak{N})}. \end{aligned} \tag{B.53}$$

Therefore, we have proved (B.48) and in view of the previous comments, (B.46) follows. Using (B.46), we get the estimate for $\mathscr{I}_1^2$

$$\begin{aligned} |\mathscr{I}_1^2| &\leqslant c_m \|r^{1/2}\partial_{\mathfrak{n}} v_m^3\|_{L^2(\partial\omega_h \cap \Gamma_h)} \|r^{-1/2} z\|_{L^2(\partial\omega_h \cap \Gamma_h)} \\ &\leqslant c_m \mathfrak{C} h^{1/2} \|r^{1/2}\nabla v_m^3\|_{H^1(\Omega_h)} \leqslant c_m h^{1/2}, \end{aligned} \tag{B.54}$$

where we have also used the estimates

$$|\nabla_x^p v_m^3(x)| \leqslant c_p r^{-p}, \qquad p = 1, 2, ..., \tag{B.55}$$

for the solution of (9.124) which follow from the theory of elliptic boundary problems in the domains with corners or conical points (see [170]) and from the analysis (9.131) of the right hand side of equation (9.124a). By Remark 9.6 and equation (9.122), the following estimates are valid for $\rho \geqslant R_0$

$$|\tilde{w}_m^1(\xi)| = |w_m^1(\xi) - t_m^1(\xi)| \leqslant c\rho^{-3}, \tag{B.56}$$
$$|\tilde{w}_m^2(\xi)| = |w_m^2(\xi) - t_m^2(\xi)| \leqslant c\rho^{-2}, \tag{B.57}$$

which means that

$$\begin{aligned}|\mathscr{I}^5 - h^3\mathscr{I}_3^2| &\leqslant \|r_h^{-1}z\|_{L^2(\Omega_h)} \left(\int_{\Omega_h} \left(r\chi(x)(h\widetilde{w}_m^1 + h^2\widetilde{w}_m^2)\right)^2 dx\right)^{1/2} \\ &\leqslant \mathfrak{C}\left(\int_{\Xi} h^2\rho^2\chi(h\xi)\left(h\widetilde{w}_m^1 + h^2\widetilde{w}_m^2\right)^2 h^3\, d\xi\right)^{1/2} \\ &\leqslant \mathfrak{C}h^{7/2}\left(\int_R^{h^{-1}\mathfrak{r}} \rho^{-4}\rho^2\mathfrak{r}\rho\right)^{1/2} \leqslant \mathfrak{C}h^{7/2},\end{aligned} \tag{B.58}$$

where $\mathfrak{r}$ is the diameter of the support of χ. We denote

$$\begin{aligned}\mathscr{I}^4 = \mathscr{I}_1^4 + \mathscr{I}_2^4 &:= \left(\nabla_x(hw_m^1 + h^2w_m^2), \nabla_x\chi z\right)_{\Omega_h} \\ &- \left([\Delta_x, \chi](hw_m^1 + h^2w_m^2), z\right)_{\Omega_h},\end{aligned} \tag{B.59}$$

$$\begin{aligned}\mathscr{I}_2^2 = \mathscr{I}_4^2 + \mathscr{I}_5^2 &:= \left(\chi\Delta_x(t_m^1 + t_m^2), z\right)_{\Omega_h} \\ &+ \left([\Delta_x, \chi](t_m^1 + t_m^2), z\right)_{\Omega_h}.\end{aligned} \tag{B.60}$$

Here $[\Delta_x, \chi] = 2\nabla_x\chi \cdot \nabla_x + (\Delta_x\chi)$ is the commutator of the Laplace operator with the cut-off function χ. The supports of the coefficients of first order differential operator $[\Delta_x, \chi]$ are contained in the set $\operatorname{supp}\|\nabla_x\chi\|$ which is located at the distance $\mathfrak{r}_\chi$ from the origin. Thus, taking into account Remark 9.6 and relation (9.122), we find

$$\begin{aligned}|\mathscr{I}_2^4 - h^2\mathscr{I}_5^2| &= ([\Delta_x, \chi](h\widetilde{w}_m^1 + h^2\widetilde{w}_m^2), z)_{\Omega_h} \\ &\leqslant c_m\left(\int_{\mathfrak{r}_\chi}^{\mathfrak{r}} \left(h^2\rho^{-6} + h^4\rho^{-4}\right)_{|\rho = r/h} r dr\right)^{1/2} \|z\|_{L^2(\Omega_h)} \leqslant c_m h^4\mathfrak{C}.\end{aligned} \tag{B.61}$$

Moreover,

$$\begin{aligned}\mathscr{I}_1^4 + h^3\mathscr{I}_4^2 &= \mathscr{I}_3^4 + \mathscr{I}_4^4 \\ &:= -\left(\Delta_x(h\widetilde{w}_m^1 + h^2\widetilde{w}_m^2), \chi z\right)_{\Omega_h} + \left(\partial_{n^h}(hw_m^1 + h^2w_m^2), z\right)_{\partial\omega_h \cap \Omega_h}.\end{aligned} \tag{B.62}$$

Remark B.1. The presence of corners on the boundary of domain Ξ may result in the singularities of derivatives of the boundary layers, therefore the inclusions $\chi\Delta_x\widetilde{w}_m^q \in L^2(\Omega_h)$ and $\chi\partial_{n^h}w_m^q \in L^2(\Gamma_h)$, in general are not valid. However, the terms in (B.63) may be well defined in the sense of the *duality pairing* obtained by the extension of scalar products $(\cdot,\cdot)_{\Omega_h}$ and $(\cdot,\cdot)_{\Gamma_h}$ in the Lebesgue spaces to the appropriate weighted Kondratiev spaces (see [117] and also [170, Chapter 2]). Additional weighted factors are local, i.e., the factors are written in fast variables. That is why the norms of test functions z can be bounded as before by the constant $\mathfrak{C}$.

By definition, the function $\widetilde{w}_m^1$ remains harmonic, and according to (9.99) and (9.128), $\widetilde{w}_m^2$ verifies the equation

$$-\Delta_\xi \widetilde{w}_m^2(\xi) = \mathscr{L}^1(\xi_1, \nabla_\xi)\widetilde{w}_m^1(\xi), \quad \xi \in \Xi. \tag{B.63}$$

Therefore,

$$\Delta_x(h\widetilde{w}_m^1 + h^2\widetilde{w}_m^2) = h^2\mathscr{L}^1\widetilde{w}_m^2 + \mathscr{L}^2(h\widetilde{w}_m^1 + h^2\widetilde{w}_m^2). \tag{B.64}$$

In contrast with (B.63), in (B.64) the operators $\mathscr{L}^q$ are written in the slow variables and the function $\widetilde{w}^q$ in fast variables, where $\Delta_\xi = h^2\mathscr{L}^0(\partial_n, \partial_s, \partial_v)$ and $\mathscr{L}^1(\xi_1, \nabla_\xi) = h\mathscr{L}^1(n, \partial_n, \partial_s, \partial_v)$. Owing to (B.64), (9.122) and applying Remark B.1, we have

$$\mathscr{L}^2(h\widetilde{w}_m^1) = h\,O(\rho^{-3}),\ \mathscr{L}^1(\widetilde{w}_m^2) = h^{-1}O(\rho^{-3}),\ \mathscr{L}^2(h^2\widetilde{w}_m^2) = h^2O(\rho^{-2}). \tag{B.65}$$

Thus, it follows that

$$\begin{aligned}
|\mathscr{I}_3^4| &\leqslant \|r_h^{-1}z\|_{L^2(\Omega_h)}\left(\int_{\Omega_h}\left(r\chi(x)\Delta_x(h\widetilde{w}_m^1 + h^2\widetilde{w}_m^2)\right)^2 dx\right)^{1/2}\\
&\leqslant \mathfrak{C}\left(\int_\Xi h^2\rho^2\chi(h\xi)^2\left(\Delta_x(h\widetilde{w}_m^1 + h^2\widetilde{w}_m^2)\right)^2 h^3\,d\xi\right)^{1/2}\\
&\leqslant \mathfrak{C}h^{5/2}\left(\int_{\Xi\setminus B_R}\rho^2\chi(h\xi)^2\left(h\rho^{-3} + h^2\rho^{-2} + h\rho^{-3}\right)^2 d\xi\right)^{1/2}\\
&\leqslant \mathfrak{C}h^{7/2}\left(\int_{\mathfrak{r}_0}^{h^{-1}\mathfrak{r}}\rho^{-4}\rho^2 d\rho\right)^{1/2} \leqslant \mathfrak{C}h^{7/2}.
\end{aligned} \tag{B.66}$$

For the two last terms it suffices to process the difference of integrals from (B.44), (B.45) and (B.63):

$$\mathscr{I}^1 + \mathscr{I}_4^4 = -\left(\partial_{n^h}(hw_m^1 + h^2w_m^2 + v_m^0), z\right)_{\partial\omega_h\cap\Gamma_h}. \tag{B.67}$$

Note that, due to the very construction of w_m^1 and w_m^2 we have $\partial_{n^h}(hw_m^1 + h^2w_m^2 + v_m^0) = O(h^2)$, see (9.99a)-(9.101) for instance. Thus, we get the estimate

$$|\mathscr{I}^1 + \mathscr{I}_4^4| \leqslant c_m\|z\|_{L^2(\partial\omega_h\cap\Gamma_h)}h^2(\mathrm{mes}_2(\partial\omega_h))^{1/2} \leqslant c_m h^{7/2}\mathfrak{C}, \tag{B.68}$$

where mes_2 denotes the two-dimensional Hausdorff measure. Collecting estimates (B.42)-(B.43), (B.54), (B.58), (B.62), (B.66) and (B.68) of the terms in (B.41), we arrive at the following estimate of α in (B.39)

$$\alpha \leqslant c_m h^{7/2}. \tag{B.69}$$

We are ready now to verify the theorem on the asymptotic expansions, which implies the main result of the chapter.

Theorem B.1. *For any positive eigenvalue λ_m^0 in problem* (9.67) *of multiplicity $\varkappa_m$ characterized by* (9.163)*, there exist numbers $c_m > 0$ and $h_m > 0$ such that for $h \in (0, h_m]$ the eigenvalues $\lambda_m^h, \dots, \lambda_{m+\varkappa_m-1}^h$ in problem* (9.63)*, and only those eigenvalues in sequence* (9.64)*, satisfy*

$$|\lambda_q^h - \lambda_m^0 - h^3 \varsigma_q| \leqslant c_m h^{7/2}, \quad q = m, \dots, m + \varkappa_m - 1. \tag{B.70}$$

Moreover, there is a constant C_m and columns $a^{hm}, \dots, a^{hm+\varkappa_m-1}$ which define an unitary matrix of the size $\varkappa_m \times \varkappa_m$ such that

$$\left\| v^{q0} + \chi(hw^{q1} + h^2 w^{q2}) + h^3 v^{q3} - \sum_{p=m}^{m+\varkappa_m-1} a_p^{hq} u_p^h \right\|_{H^1(\Omega_h)} \leqslant C_m h, \tag{B.71}$$

with $q = m, \dots, m + \varkappa_m - 1$. Here v^{q0} denotes the linear combination (9.164) *of eigenfunctions in problem* (9.67)*, constructed in Section 9.3.4, and w^{q1}, w^{q2} and v^{q3} are given functions which are determined for fixed v^{q0} (see Section 9.3.4 for this type of construction). Finally ς_q is an eigenvalue of the matrix Q with entries* (9.168)*. In the case of a simple eigenvalue λ_m^0 (i.e., $\varkappa_m = 1$), we have $v^{m0} = v_m^0$ the corresponding eigenfunction, and $\varsigma_m = \lambda_m'$ is given by* (9.157)*.*

Proof. Given eigenvectors $a^m, \dots, a^{m+\varkappa_m-1}$ of the matrix Q, we construct linear combinations (9.164) and the associated appropriate terms in asymptotic ansätz (9.70). As a result, approximation solutions $\{(\lambda_q^0 + h^3 \varsigma_q)^{-1}, \mathfrak{u}^q\}$ for $q = m, \dots, m + \varkappa_m - 1$ are obtained for the abstract spectral problem (B.35). Let ς_q be an eigenvalue of the matrix Q of multiplicity κ_q, i.e.,

$$\varsigma_{q-1} < \varsigma_q = \dots = \varsigma_{q+\kappa_q-1} < \varsigma_{q+\kappa_q}. \tag{B.72}$$

We choose the factor $c_{\Bbbk}$ in the value $\alpha_{\Bbbk} = c_{\Bbbk} h^3$ in Lemma A.1 so small that the segment

$$\left[(\lambda_m^0 + h^3 \varsigma_q)^{-1} - c_{\Bbbk} h^3, (\lambda_m^0 + h^3 \varsigma_q)^{-1} + c_{\Bbbk} h^3\right] \tag{B.73}$$

does not contain the approximation eigenvalues $(\lambda_m^0 + h^3 \varsigma_p)^{-1}$ when $p \notin \{q, q + \kappa_q - 1\}$. Then Lemma A.1 delivers the eigenvalues $\mu_{i(q)}^h, \dots, \mu_{i(q+\kappa_q-1)}^h$ of the operator K^h such that

$$\left|\mu_{i(p)}^h - (\lambda_m^0 + h^3 \varsigma_p)^{-1}\right| \leqslant \alpha \leqslant c_m h^{7/2}, \quad p = q, \dots, q + \kappa_q - 1. \tag{B.74}$$

We here emphasize that, at the time being, we cannot infer that these eigenvalues are different. At the same moment, the second part of Lemma A.1 gives the normed columns $b^{hp} = (b_{k_{mq}}^{hp}, \dots, b_{k_{mq}+N_{mq}-1}^{hp})$ verifying the inequalities

$$\left\| \mathfrak{u}^p - \sum_{k=k_{mq}}^{k_{mq}+N_{mq}-1} b_k^{hp} u_k^h \right\|_{H^1(\Omega_h)} \leqslant c \frac{\alpha}{\alpha_{\Bbbk}} \leqslant c h^{1/2}. \tag{B.75}$$

Here $\{\mu^h_{k_{mq}}, \ldots, \mu^h_{k_{mq}+N_{mq}-1}\}$ implies the list of all eigenvalues of the operator K^h in segment (B.73). Note that the numbers k_{mq} and N_{mq} can depend on the parameter h but this fact is not reflected in the notation. Since

$$\|h\chi w^1\|_{H^1(\Omega_h)} \leqslant ch^{3/2}, \tag{B.76}$$

$$\|h^2\chi w^2\|_{H^1(\Omega_h)} \leqslant ch^{5/2}, \tag{B.77}$$

$$\|h^2 v^2\|_{H^1(\Omega_h)} \leqslant ch^3, \tag{B.78}$$

the normalization condition (9.68) for the eigenfunctions of problem (9.67) and similar conditions for eigenvectors of the matrix Q ensure that

$$|(\mathrm{u}^p, \mathrm{u}^t)_{\Omega_h} - \delta_{p,t}| \leqslant ch^{3/2}, \quad p,t = q, \ldots, q+\kappa_q+1. \tag{B.79}$$

In a similar way, inequalities (B.75) and the orthogonality and normalization conditions (9.65) for eigenfunctions u^h_k of problem (9.63) lead to the relation

$$\left|(\mathrm{u}^p, \mathrm{u}^t)_{\Omega_h} - \sum_{k=k_{mq}}^{k_{mq}+N_{mq}-1} b^{hp}_k b^{ht}_k\right| \leqslant ch^{1/2}. \tag{B.80}$$

Formulas (B.79) and (B.80) are true simultaneously if and only if

$$N_{mq} \geqslant \kappa_q\,, \tag{B.81}$$

otherwise we arrive at a contradiction where at least one of the coefficients b^{hp}_k has to be close to zero and to one simultaneously. To actually prove that the equality occurs in (B.81), we first of all, notice that, for a sufficiently small $h > 0$, the relations of type (B.81) are valid for all eigenvalues $\lambda^0_1, \ldots, \lambda^0_m$ of problem (9.67) and all eigenvalues ς_q of the associated matrices Q. We have verified above Proposition B.1 that each eigenvalue λ^h_p and the corresponding eigenfunction u^h_p of singularly perturbed problem (9.63) converge to an eigenvalue and an eigenfunction of the limit problem (9.67), respectively. This observation ensures that the number of entries of the eigenvalue sequence (9.64), which lives on the interval $(0, \lambda^0_m)$, does not exceed $m + \varkappa_m - 1$ for a small $h > 0$. Summing up the inequalities (B.81) over all $\lambda^0_1, \ldots, \lambda^0_m$ and ς_q, we conclude that the equalities $N_{mq} = \kappa_q$ are necessary. Moreover, we now are able to confirm that the eigenvalues $\mu^h_{i(q)}, \ldots, \mu^h_{i(q+\kappa_q-1)}$ can be chosen different one from another. Indeed, we take $\alpha_{\Bbbk} = C_{\Bbbk} h^{7/2}$ in Lemma A.1 and fix $C_{\Bbbk}$ so large that the inequality (B.75) with the new bound $c/C_{\Bbbk}$ still guarantees that the segment

$$\Lambda_q(h) = \left[(\lambda^0_m + h^3\varsigma_q)^{-1} - C_{\Bbbk} h^{7/2}, (\lambda^0_m + h^3\varsigma_q)^{-1} + C_{\Bbbk} h^{7/2}\right] \tag{B.82}$$

contains exactly κ_q eigenvalues of the operator K^h. It suffices to mention two facts. First, for a small $h > 0$, the intervals $\Lambda_q(h)$ and $\Lambda_p(h)$ with $\varsigma_q \neq \varsigma_p$ do not intersect. Second, any eigenvalue $\mu^h_k = (\lambda^h_k)^{-1}$ in the interval (B.82) meets the inequality (B.70). □

Remark B.2. Estimates (B.76)-(B.78) show that the bound in (B.71) is larger than the norms of the functions w^{q1}, w^{q2} and v^{q3} included into the approximation solution and, therefore, estimate (B.71) remains valid for the function v^{q0} alone, without three correctors. This is the usual situation in the asymptotic analysis of singular spectral problems: One needs to construct additional asymptotic terms of eigenfunctions in order to prove that the correcting term in the asymptotic expansions of an eigenvalue is found properly. In theory, one can employ the general procedure [143] and construct higher order asymptotic terms of eigenvalues and eigenfunctions. We keep the boundary layer and regular corrections in the estimate (B.71) because they form a so-called asymptotic *conglomerate* which is replicated in the asymptotic series (see [143] and [166]; actually, the notion of asymptotic conglomerates was introduced in [166]).

Appendix C
Spectral Problems in Elasticity

In this appendix we provide the justification for the asymptotic expansions of solutions to the spectral problems in elasticity. In particular, we prove Theorem 9.2 on asymptotic expansions of solutions of singularly perturbed problem [180].

Remark C.1. In our notation the index (j) is attached to the inclusion ω_j, e.g., p^j stands for the center of ω_j, in contrast to the index (p) which is attached to the eigenvalue λ_p , e.g., the asymptotic approximation of the vector eigenfunction $u_{(p)}$ with respect to $h \to 0$ is denoted by $\mathfrak{u}_{(p)}$.

C.1 Justification of Asymptotic Expansions

The following statements are well known for the intact elastic body (see e.g., [118, 181]). In order to cover also the case of defects in the form of cavities (see (9.183)), the general result is given with the proof [179]. We emphasize that a body with small inclusions can be viewed as an intermediate case between a body with cavities and an intact body. Therefore, some of the results presented for an intact body can be applied for a body with foreign inclusions as well.

Proposition C.1. *For a vector function $u \in H^1_\Gamma(\Omega;\mathbb{R}^3)$ the following inequality holds true*

$$\|r_j^{-1}u\|_{L^2(\Omega;\mathbb{R}^3)} + \|\nabla_x u\|_{L^2(\Omega;\mathbb{R}^3)} \leqslant c\|\mathscr{D}(\nabla_x)u\|_{L^2(\Omega;\mathbb{R}^3)}, \tag{C.1}$$

where, according to (9.233), $r_j = \|x - p^j\|$. *The above inequality remains valid with a constant independent of $h \in (0, h_0]$, if the domain Ω is replaced by the domain Ω_h with inclusions or defects.*

Proof. For analysis of displacement fields in the domain Ω_h with cavities (in particular, with cracks) we apply the method described in review paper [167, §2.3]. In this framework the body with elastic inclusions is considered as intact or entire. Let us consider the restriction $\widehat{u}$ of u to the set $\Omega(h) = \Omega \setminus \bigcup_{j=1}^J \overline{B_\ell^j}$, where

$B^j_\ell = \{x : \|x - p^j\| < \ell\}$ and radius $\ell = \ell(h) := Rh$ of the balls is selected in such a way that $\overline{\omega^h_j} \subset B^j_\ell$. We construct an extension $\widetilde{u}$ to Ω of the field $\widehat{u}$. To this end, we introduce the annulae $\Xi^j_h = B^j_{2\ell} \setminus \overline{B^j_\ell}$ and perform the stretching of coordinates $x \mapsto \xi^j = h^{-1}(x - p^j)$. The vector functions $\widehat{u}$ and u written in the ξ^j-coordinates are denoted by $\widehat{u}^j$ and u^j, respectively. It is evident that

$$h\|\mathscr{D}(\nabla_\xi)\widehat{u}^j\|^2_{L^2(\Xi;\mathbb{R}^3)} = \|\mathscr{D}(\nabla_\xi)\widehat{u}\|^2_{L^2(\Xi^j_h;\mathbb{R}^3)} \leqslant \|\mathscr{D}(\nabla_x)u\|^2_{L^2(\Omega_h;\mathbb{R}^3)}, \tag{C.2}$$

where $\Xi = B_{2R} \setminus \overline{B_R}$. Let

$$\widehat{u}^j(\xi^j) = \widehat{u}^j_\perp(\xi^j) + \mathbb{D}(\xi^j)a^j, \tag{C.3}$$

where $\mathbb{D}$ is the matrix (9.174), and the column $a^j \in \mathbb{R}^6$ is selected in such a way that

$$\int_\Xi \mathbb{D}(\xi^j)^\top \widehat{u}^j_\perp(\xi^j)d\xi^j = 0 \in \mathbb{R}^6. \tag{C.4}$$

By the orthogonality condition (C.4), the *Korn's inequality* is valid (see, e.g., [118], [167, §2] and [166, Theorem 2.3.3])

$$\|\widehat{u}^j_\perp\|_{H^1(\Xi;\mathbb{R}^3)} \leqslant c_R\|\mathscr{D}(\nabla_\xi)\widehat{u}^j_\perp\|_{L^2(\Xi;\mathbb{R}^3)} = c_R\|\mathscr{D}(\nabla_\xi)\widehat{u}^j\|_{L^2(\Xi;\mathbb{R}^3)}. \tag{C.5}$$

The last equality follows from the second formulae (9.175) since the rigid motion $\mathbb{D}a^j$ generates null strains (9.171). Let $\widetilde{u}^j_\perp$ denote an extension in the Sobolev class H^1 of the vector function $\widehat{u}^j_\perp$ from Ξ onto B_R, such that

$$\|\widehat{u}^j_\perp\|_{H^1(B_{2R};\mathbb{R}^3)} \leqslant c_R\|\widehat{u}^j_\perp\|_{H^1(\Xi;\mathbb{R}^3)}. \tag{C.6}$$

Now, the required extension of the field u onto the entire domain Ω is given by the formula

$$\widetilde{u}(x) = \begin{cases} \widehat{u}(x), & x \in \Omega(h), \\ \mathbb{D}(\xi^j)a^j + \widetilde{u}^j_\perp(\xi^j), & x \in B^j_\ell, \quad j = 1, \dots, J. \end{cases} \tag{C.7}$$

In addition, according to (C.2), (C.3), (C.5) and (C.6), we have

$$\|\mathscr{D}(\nabla_x)\widetilde{u}\|_{L^2(\Omega;\mathbb{R}^3)} \leqslant c\|\mathscr{D}(\nabla_x)u\|_{L^2(\Omega_h;\mathbb{R}^3)}. \tag{C.8}$$

Applying the Korn's inequality (C.5) in Ω, we obtain

$$\begin{aligned} \|r_j^{-1}u\|_{L^2(\Omega(h);\mathbb{R}^3)} + \|\nabla_x u\|_{L^2(\Omega(h);\mathbb{R}^3)} &\leqslant \|r_j^{-1}\widetilde{u}\|_{L^2(\Omega;\mathbb{R}^3)} + \|\nabla_x \widehat{u}\|_{L^2(\Omega;\mathbb{R}^3)} \\ &\leqslant c\|\mathscr{D}(\nabla_x)\widetilde{u}\|_{L^2(\Omega;\mathbb{R}^3)}. \end{aligned} \tag{C.9}$$

We turn back to the function $\widehat{u}^j$ and find

$$h\|\widehat{u}^j\|^2_{H^1(\Xi;\mathbb{R}^3)} \leqslant c\left(\|r_j^{-1}\widetilde{u}\|^2_{L^2(\Omega;\mathbb{R}^3)} + \|\nabla_x\widetilde{u}\|^2_{L^2(\Omega;\mathbb{R}^3)}\right). \tag{C.10}$$

The other variant of the *Korn's inequality* (see e.g., [118], [166, §3.1] or [167, §2])

$$\|u^j\|^2_{H^1(B_{2R}\setminus\omega_j;\mathbb{R}^3)} \leqslant c\left(\|\mathscr{D}(\nabla_x)u^j\|^2_{L^2(\Xi\setminus\omega_j;\mathbb{R}^3)} + \|u^j\|^2_{L^2(\Xi;\mathbb{R}^3)}\right), \tag{C.11}$$

after returning to the x-coordinates leads to the relations

$$\begin{aligned} h^{-2}\|u\|^2_{L^2(B_{2\ell}\setminus\omega_j^h;\mathbb{R}^3)} &\leqslant c\|\nabla_x u\|^2_{L^2(B_{2\ell}\setminus\omega_j^h;\mathbb{R}^3)} \\ &\leqslant c\left(\|\mathscr{D}(\nabla_x)u\|^2_{L^2(B_{2\ell}\setminus\omega_j^h;\mathbb{R}^3)} + h^{-2}\|u\|^2_{L^2(\Xi_\ell^j;\mathbb{R}^3)}\right). \end{aligned} \tag{C.12}$$

By virtue of $Ch =: \ell^*(h) \geqslant r_j \geqslant \ell(h) = ch > 0$ for $x \in B_{2\ell}\setminus\omega_j^h \supset \Xi_\ell^j$, the multiplier h^{-1} can be inserted into the norm, and transformed to r_j^{-1}, but the norm $\|r_j^{-1}u\|_{L^2(\Xi_\ell^j;\mathbb{R}^3)}$ is already estimated in (C.9), owing to $\widetilde{u} = u$ on Ξ_ℓ^j. Estimates (C.12), $j = 1,\ldots,J$, modified in the indicated way along with relation (C.9) imply the Korn's inequality in the domain Ω_h. □

Remark C.2. If ω_j is a domain, then in the proof of Proposition C.1 we do not need to restrict $\widehat{u}$ to $\Omega(h)$, but operate directly with the sets Ω_h and $B_{2R}\setminus\omega_j$ since there is a bounded extension operator in the class H^1 over the Lipschitz boundary $\partial\omega_j$ with the estimate of type (C.6). The presence of cracks makes the existence of such an extension impossible. However, the Korn's inequality (C.12) is still valid in this case, since it only requires the union of Lipschitz domains (see [118]).

The bilinear form

$$H^1_\Gamma(\Omega;\mathbb{R}^3) \ni (u,v)_\Omega \to \langle u,v\rangle_\Omega = (\mathscr{A}^h\mathscr{D}(\nabla_x)u, \mathscr{D}(\nabla_x)v)_\Omega \in \mathbb{R} \tag{C.13}$$

defines a scalar product in the Hilbert space $H^1_\Gamma(\Omega;\mathbb{R}^3)$. In this way, the integral identity

$$(\mathscr{A}^h\mathscr{D}u, \mathscr{D}v)_\Omega = \lambda(\gamma^h u, v)_\Omega\ , \tag{C.14}$$

can be rewritten as an abstract spectral equation

$$\mathfrak{K}^h u^h = \mu^h u^h\ , \tag{C.15}$$

where $\mu^h = (\lambda^h)^{-1}$ is the new spectral parameter, and $\mathfrak{K}^h$ is a compact, symmetric, and continuous operator, thus selfadjoint,

$$\langle\mathfrak{K}^h u, v\rangle_\Omega = (\gamma^h u, v)_\Omega\ , \quad u, v \in \mathfrak{H}\ . \tag{C.16}$$

Eigenvalues of the operator $\mathfrak{K}^h$ constitute the sequence

$$\mu_1^h \geqslant \mu_2^h \geqslant \cdots \geqslant \mu_p^h \geqslant \cdots \to +0\ , \tag{C.17}$$

with the elements related to the sequence in (9.188) by the first formula in (C.16).

We are going to apply Lemma A.1 on *almost eigenvalues and eigenvectors* for the compact operator $\mathfrak{K}^h$. It means that for given $\mu > 0$ and $\mathfrak{u} \in \mathfrak{H}$, $\|\mathfrak{u}\|_{\mathfrak{H}} = 1$, such that

$$\|\mathfrak{K}^h \mathfrak{u} - \mu \mathfrak{u}\|_{\mathfrak{H}} = \delta, \tag{C.18}$$

there exists an eigenvalue μ_p^h of the operator $\mathfrak{K}^h$, which satisfies the inequality

$$|\mu - \mu_p^h| \leqslant \delta. \tag{C.19}$$

Moreover, for any $\delta_{\mathbb{k}} > \delta$ the following inequality holds

$$\|\mathfrak{u} - \mathfrak{u}_{\mathbb{k}}\|_{\mathfrak{H}} \leqslant 2\delta/\delta_{\mathbb{k}} \tag{C.20}$$

where $\mathfrak{u}_{\mathbb{k}}$ is a linear combination of eigenfunctions of the operator $\mathfrak{K}^h$, associated to the eigenvalues from the segment $[\mu - \delta_{\mathbb{k}}, \mu + \delta_{\mathbb{k}}]$, and $\|\mathfrak{u}_{\mathbb{k}}\|_{\mathfrak{H}} = 1$.

For the asymptotic approximations μ and $\mathfrak{u}$ of solutions to the abstract equation (C.15) we take

$$\mu = (\lambda_p + h^3 \varsigma_p)^{-1}, \quad \mathfrak{u} = \frac{\mathfrak{u}_{(p)}}{\|\mathfrak{u}_{(p)}\|_{\mathfrak{H}}}, \tag{C.21}$$

where

$$\mathfrak{u}_{(p)}(x) := u_{(p)}(x) + h \sum_{j=1}^{J} \chi_j(x) g^j_{(p)}\left(x - p^j\right) + h^3 v_{(p)}(x), \tag{C.22}$$

with $g^j_{(p)}\left(x - p^j\right) := w^{1j}_{(p)}\left(h^{-1}\left(x - p^j\right)\right) + h w^{2j}_{(p)}\left(h^{-1}\left(x - p^j\right)\right)$, stands for the sum of terms separated in the asymptotic ansätz (9.191). Let us evaluate the quantity δ from formula (C.18). By virtue of $\lambda_p > 0$, for $h \in (0, h_p]$ and $h_p > 0$ small enough, we have

$$\begin{aligned}
\delta &= \|\mathfrak{K}^h \mathfrak{u} - \mu \mathfrak{u}\|_{\mathfrak{H}} \\
&= \frac{1}{(\lambda_p + h^3 \varsigma_p)\|\mathfrak{u}_{(p)}\|_{\mathfrak{H}}} \sup_{\upsilon \in \mathfrak{S}} \left| (\lambda_p + h^3 \varsigma_p)\langle \mathfrak{K}^h \mathfrak{u}_{(p)}, \upsilon \rangle_\Omega - \langle \mathfrak{u}_{(p)}, \upsilon \rangle_\Omega \right| \\
&\leqslant c \sup_{\upsilon \in \mathfrak{S}} \left| (\mathscr{A}^h \mathscr{D}(\nabla_x)\mathfrak{u}_{(p)}; \mathscr{D}(\nabla_x)\upsilon)_\Omega - (\lambda_p + h^3 \varsigma_p)(\gamma^h \mathfrak{u}_{(p)}, \upsilon)_\Omega \right|,
\end{aligned} \tag{C.23}$$

where $\mathfrak{S} = \{\upsilon \in \mathfrak{H} : \|\upsilon\|_{\mathfrak{H}} = 1\}$ is the unit sphere in the space $\mathfrak{H}$. In addition, to estimate the norm $\|\mathfrak{u}_{(p)}\|_{\mathfrak{H}}$ the following relations are used

$$\|u_{(p)}\|^2_{\mathfrak{H}} = (\mathscr{A}^h \mathscr{D}(\nabla_x) u_{(p)}, \mathscr{D}(\nabla_x) u_{(p)})_\Omega \geqslant c > 0, \tag{C.24}$$

$$\|h^i \chi_j w^{ij}_{(p)}\|_{\mathfrak{H}} \leqslant c h^{i+1/2}, \quad i = 1, 2, \tag{C.25}$$

$$\|h^3 v_{(p)}\|^2_{\mathfrak{H}} \leqslant c h^3, \tag{C.26}$$

where the first relation follows from the continuity at the points p^j of the second order derivatives of the vector function $u_{(p)}$ combined with the integral identity (9.179) and the normalization condition (9.189). We transform the expression under the sign sup in (C.23). Substituting into the expression the sum of terms in ansätz (9.191), we have

$$\begin{aligned}
\mathscr{I}_0 &= (\mathscr{A}^h\mathscr{D}(\nabla_x)u_{(p)}, \mathscr{D}(\nabla_x)\upsilon)_\Omega - (\lambda_p + h^3\varsigma_p)(\gamma^h u_{(p)}, \upsilon)_\Omega \\
&= \sum_{j=1}^{J}\Big\{((\mathscr{A}_{(j)} - \mathscr{A})\mathscr{D}(\nabla_x)\upsilon)_{\omega_j^h} - \lambda_p((\gamma^h - \gamma)u_{(p)}, \upsilon)_{\omega_j^h}\Big\} - h^3\varsigma_p(\gamma^h u_{(p)}, \upsilon)_\Omega \\
&=: \sum_{j=1}^{J}\mathscr{I}_0^j - \mathscr{I}_0^0, \qquad\qquad (C.27)\\
\mathscr{I}_i^j &= h^i(\mathscr{A}\mathscr{D}(\nabla_x)\chi_j w_{(p)}^{ij}, \mathscr{D}(\nabla_x)\upsilon)_\Omega - h^i(\lambda_p + h^3\varsigma_p)(\gamma^h\chi_j w_{(p)}^{ij}, \upsilon)_\Omega \\
&=: \mathscr{I}_i^{j0} - \mathscr{I}_i^{j0}, \quad i = 1,2, \qquad\qquad (C.28)\\
\mathscr{I}_4 &= h^3((\mathscr{A}\mathscr{D}(\nabla_x)v_{(p)}\mathscr{D}(\nabla_x)\upsilon)_\Omega - \lambda_p(\gamma v_{(p)}, \upsilon)_\Omega) - h^6\varsigma_p(\gamma^h v, \upsilon)_\Omega \\
&+ h^3\sum_{j=1}^{J}\Big\{((\mathscr{A}_{(j)} - \mathscr{A})\mathscr{D}(\nabla_x)v_{(p)}, \mathscr{D}(\nabla_x)\upsilon)_{\omega_j^h} - \lambda_p((\gamma_j - \gamma)v_{(p)}, \upsilon)_{\omega_j^h}\Big\} \\
&=: h^3\mathscr{I}_4^0 + h^6\mathscr{I}_4^{01} + h^3\sum_{j=1}^{J}\mathscr{I}_4^j. \qquad\qquad (C.29)
\end{aligned}$$

In (C.27) we used that $u_{(p)}$ and λ_p verify the integral identity (9.179). Furthermore, by the Taylor formulae (9.205) and (9.208), we obtain

$$\begin{aligned}
\left|\mathscr{I}_0^j - \mathscr{I}_0^{j1} - \mathscr{I}_0^{j2}\right| &\leqslant c\left(h^2\|\mathscr{D}(\nabla_x)\upsilon\|_{L^1(\omega_j^h;\mathbb{R}^3)} + h\|\upsilon\|_{L^1(\omega_j^h;\mathbb{R}^3)} + \int_{\omega_j^h}|\upsilon - \overline{\upsilon}^j|dx\right) \\
&\leqslant ch^2h^{3/2}\|\mathscr{D}(\nabla_x)\upsilon\|_{L^2(\Omega;\mathbb{R}^3)} = ch^{7/2}, \qquad\qquad (C.30)
\end{aligned}$$

with

$$\mathscr{I}_0^{j1} = ((\mathscr{A}_{(j)} - \mathscr{A}(p^j))\vartheta_{(p)}^j, \mathscr{D}(\nabla_x)\upsilon)_{\omega_h^j}, \qquad\qquad (C.31)$$

$$\begin{aligned}
\mathscr{I}_0^{j2} &= ((\mathscr{A}_{(j)} - \mathscr{A}(p^j))\mathscr{D}(\nabla_x)\mathfrak{u}_{(p)}^j, \mathscr{D}(\nabla_x)\upsilon)_{\omega_h^j} \qquad\qquad (C.32)\\
&+ ((x-p^j)^\top\nabla_x\mathscr{A}(p^j)\vartheta_{(p)}^j, \mathscr{D}(\nabla_x)\upsilon)_{\omega_h^j} - \lambda_p((\gamma_j - \gamma(p^j))u_{(p)}(p^j), \upsilon)_{\omega_j^h},
\end{aligned}$$

where the vector functions $\vartheta_{(p)}$ and $\mathfrak{u}_{(p)}$ written in the ξ^j-coordinates (see (9.184)) are denoted by $\vartheta_{(p)}^j$ and $\mathfrak{u}_{(p)}^j$, respectively.

Let explain the derivation of above formulae. The following substitutions are performed

$$\mathscr{D}(\nabla_x)u_{(p)}(x) \rightsquigarrow \vartheta_{(p)}^j + \mathscr{D}(\nabla_x)\mathfrak{u}_{(p)}(x), \qquad\qquad (C.33)$$

$$\mathscr{A}(x) \rightsquigarrow \mathscr{A}(p^j) + (x-p^j)^\top\nabla_x\mathscr{A}(p^j), \qquad\qquad (C.34)$$

$$u_{(p)}(x) \rightsquigarrow u_{(p)}(p^j), \qquad\qquad (C.35)$$

with pointwise estimates for remainders of orders $O(h^2)$, $O(h^2)$ and $O(h)$, respectively. These gave rise to the following multipliers in the majorants

$$\|\mathscr{D}(\nabla_x)\upsilon\|_{L^1(\omega_h^j;\mathbb{R}^3)} \leqslant ch^{3/2}\|\mathscr{D}(\nabla_x)\upsilon\|_{L^2(\Omega;\mathbb{R}^3)}, \tag{C.36}$$

$$\|\upsilon\|_{L^1(\omega_h^j;\mathbb{R}^3)} \leqslant ch^{3/2}\|r_j^{-1}\upsilon\|_{L^2(\Omega;\mathbb{R}^3)}. \tag{C.37}$$

Note that the factor $h^{3/2}$ is proportional to $|\omega_j^h|^{1/2}$, and $h^{-1}r_j$ does not exceed a constant on the inclusion ω_j^h. Besides that, the *Poincaré inequality*

$$\begin{aligned}\int_{\omega_j^h} \|\upsilon(x)-\overline{\upsilon}^j\|dx &\leqslant ch^{3/2}\int_{\omega_j^h} \|\upsilon(x)-\overline{\upsilon}^j\|^2 dx\\ &\leqslant ch^{3/2}h^2\int_{\omega_j^h} \|\nabla_x\upsilon(x)\|^2 dx,\end{aligned} \tag{C.38}$$

is employed together with the relation

$$\int_{\omega_j}(\gamma_j(x)-\overline{\gamma}_j)u_{(p)}(p^j)^\top\upsilon(x)dx = \int_{\omega_j}(\gamma_j(x)-\overline{\gamma}_j)u_{(p)}(p^j)^\top(\upsilon(x)-\overline{\upsilon}^j)dx. \tag{C.39}$$

Here $\overline{\upsilon}^j$ stands for the mean value of υ over ω_j^h. Finally, all the norms of the test function υ are estimated by Proposition C.1.

In similar but much simpler way, by virtue of Remark 9.12, the term $\mathscr{I}_4^j$ from (C.29) satisfies

$$\begin{aligned}h^3\left|\mathscr{I}_4^j\right| &\leqslant ch^3\left(h^{1-\tau}\|r_j^{\tau-1}\nabla_x v_{(p)}\|_{L^2(\omega_j^h;\mathbb{R}^3)} + h^{2-\tau}\|r_j^{\tau-2}v_{(p)}\|_{L^2(\omega_j^h;\mathbb{R}^3)}\right)\|\upsilon\|_{\mathfrak{H}}\\ &\leqslant ch^{4-\tau},\end{aligned} \tag{C.40}$$

where $\tau > 1/2$ is arbitrary. It is clear that $h^6|\mathscr{I}_4^{01}| \leqslant Ch^6$. The integral $h^3\mathscr{I}_4^0$ cancels the integral $-h^3\mathscr{I}_0^0$ in (C.27) and some parts of the integrals $\mathscr{I}_i^j$ from (C.28), which we are going to consider. In the notation of formula (9.235) for $i = 1, 2$, we have

$$\begin{aligned}\mathscr{I}_i^j &= h^i\Big\{(\mathscr{A}_{(j)}\mathscr{D}(\nabla_x)w_{(p)}^{ij}, \mathscr{D}(\nabla_x)\upsilon)_{\omega_j^h} + (\mathscr{A}(p^j)\mathscr{D}(\nabla_x)w_{(p)}^{ij}, \mathscr{D}(\nabla_x)\chi_j\upsilon)_{\Omega\setminus\omega_j^h}\\ &\qquad + h^{-1}\delta_{i2}((x-p^j)^\top\nabla_x\mathscr{A}(p^j)\mathscr{D}(\nabla_x)w_{(p)}^{1j}, \mathscr{D}(\nabla_x)\chi_j\upsilon)_{\Omega\setminus\omega_j^h}\Big\}\\ &\quad + \Big\{(\mathscr{A}[\mathscr{D}(\nabla_x),\chi_j]w_{(p)}^{ij}, \mathscr{D}(\nabla_x)\upsilon)_\Omega - (\mathscr{A}\mathscr{D}(\nabla_x)w_{(p)}^{ij}, [\mathscr{D}(\nabla_x),\chi_j]\upsilon)_\Omega\Big\}\\ &\quad + ((\mathscr{A}-\mathscr{A}(p^j)-\delta_{i1}(x-p^j)^\top\nabla_x\mathscr{A}(p^j))\mathscr{D}(\nabla_x)w_{(p)}^{ij}, \mathscr{D}(\nabla_x)\chi_j\upsilon)_{\Omega\setminus\omega_j^h}\\ &=: h^i\mathscr{I}_i^{j0} + \mathscr{I}_i^{j1} + \mathscr{I}_i^{j2}.\end{aligned} \tag{C.41}$$

Furthermore, the integrals $h^i \mathscr{I}_i^{j0}$ and $\mathscr{I}_i^{ji}$ cancel each other according to the integral identities

$$2E^j(w^{1j}, \chi_j v) = ((\mathscr{A}(p^j) - \mathscr{A}_{(j)})\vartheta^j_{(p)}, \mathscr{D}(\nabla_\xi)\chi_j v)_{\omega_j}, \tag{C.42}$$

$$2E^2(w^{2j}, \chi_j v) = (F^{0j}, \chi_j v)_{\mathbb{R}^3\setminus\omega_j} + (F^j, v)_{\omega_j} + (G^j, v)_{\partial\omega_j}. \tag{C.43}$$

The latter formulae are provided by (9.198), (9.257) and (9.201)-(9.204), (9.206), (9.207), (9.210). We point out that the test function $\xi \mapsto \chi_j(h\xi + p^j)v(h\xi + p^j)$ in (C.42) and (C.43) has a compact support, i.e., the function belongs to the Kondratiev space $V_0^1(\mathbb{R}^3;\mathbb{R}^3)$, and in the analyzed integrals the stretching of coordinates $x \mapsto \xi = h^{-1}(x - p^j)$ has to be performed.

Remark C.3. Variational formulation of problem (9.195a)-(9.195d) for the special fields W^{jk}, which define the elements of the polarization matrix $P^{(j)}$ in decomposition (9.197), are of the form (9.257), where $V_0^1(\mathbb{R}^3;\mathbb{R}^3)$ is the Kondratiev space (see (D.28)), which is the completion of $C_0^\infty(\mathbb{R}^3;\mathbb{R}^3)$ in the weighted norm

$$\|W\|_{V_0^1(\mathbb{R}^3;\mathbb{R}^3)} = \left(\|\nabla_\xi W\|^2_{L^2(\mathbb{R}^3;\mathbb{R}^3)} + \|(1+\rho)^{-1}W\|^2_{L^2(\mathbb{R}^3;\mathbb{R}^3)}\right)^{1/2}. \tag{C.44}$$

The expressions including asymptotic terms $S^{ji}_{(p)}(h^{-1}(x-p^j)) = h^{3-i}S^{ji}_{(p)}(x-p^j)$ are detached from the integrals $\mathscr{I}_i^{j1}$ and $\mathscr{I}_i^{j2}$,

$$\begin{aligned}\mathscr{I}_{i0}^{j1} &= h^3(\mathscr{A}[\mathscr{D}(\nabla_x),\chi_j]S^{ji}_{(p)}, \mathscr{D}(\nabla_x)v)_\Omega - h^3(\mathscr{A}\mathscr{D}(\nabla_x)S^{ji}_{(p)}, [\mathscr{D}(\nabla_x),\chi_j]v)_\Omega,\\ &= h^3([\mathscr{L},\chi_j]S^{ji}, v)_\Omega,\end{aligned} \tag{C.45}$$

$$\mathscr{I}_{i0}^{j2} = h^3((\mathscr{A} - \mathscr{A}(p^j) - \delta_{i1}(x-p^j)^\top\nabla_x\mathscr{A}(p^j))\mathscr{D}(\nabla_x)S^{ji}_{(p)}, \mathscr{D}(\nabla_x)\chi_j v)_{\Omega\setminus\omega_j^h}, \tag{C.46}$$

and the remainders are estimated by virtue of the decompositions (9.199) and (9.220), namely,

$$\left|\mathscr{I}_1^{j1} - \mathscr{I}_{10}^{j1}\right| \leqslant ch\|v\|_{\mathfrak{H}} \left(\int_{\sup|\nabla_x\chi_j|} f_1(x)dx\right)^{1/2} \leqslant ch^4, \tag{C.47}$$

with $f_1(x) := (1+h^{-1}r_j)^{-6} + h^{-2}(1+h^{-1}r_j)^{-8}$,

$$\left|\mathscr{I}_1^{j2} - \mathscr{I}_{10}^{j2}\right| \leqslant ch^2\|v\|_{\mathfrak{H}} \left(\int_{\sup|\nabla_x\chi_j|} f_2(x)dx\right)^{1/2} \leqslant ch^4(1+|\ln h|), \tag{C.48}$$

where $f_2(x) := ((1+h^{-1}r_j)^{-4} + h^{-2}(1+h^{-1}r_j)^{-6})(1+|\ln(h^{-1}r_j)|)^2$,

$$\left|\mathscr{I}_2^{j1} - \mathscr{I}_{20}^{j1}\right| \leqslant ch\|v\|_{\mathfrak{H}} \left(\int_{\Omega\setminus\omega_j^h} r_j^4(1+h^{-1}r_j)^{-6}dx\right)^{1/2} \leqslant ch^4, \tag{C.49}$$

and

$$\left|\mathscr{I}_2^{j2} - \mathscr{I}_{20}^{j2}\right| \leqslant ch^2 \|\upsilon\|_{\mathfrak{H}} \left(\int_{\Omega \setminus \omega_j^h} r_j^2 (1 + h^{-1} r_j)^{-4} (1 + |\ln(h^{-1} r_j)|)^2 dx \right)^{1/2}$$
$$\leqslant ch^4 (1 + |\ln h|). \tag{C.50}$$

Inequalities for the integrals $\mathscr{I}_i^{j0}$ from (C.28) are obtained in a similar way

$$\left|\mathscr{I}_i^{j0} - \mathscr{I}_{i0}^{j0}\right| \leqslant c \|r_j^{-1} \upsilon\|_{L^2(\Omega;\mathbb{R}^3)} h^i h^{4-i} (1 + \delta_{i2} |\ln h|) \leqslant ch^4 (1 + \delta_{i2} |\ln h|), \tag{C.51}$$
$$\mathscr{I}_{i0}^{j0} = h^3 \lambda_p (\rho \chi_j S_{(p)}^{ji}, \upsilon)_\Omega \ . \tag{C.52}$$

According to formula (9.235) for the right hand side f of the problem (9.231) and the associated integral identity (9.241), the sum of the expressions $h^3 \mathscr{I}_4^0$ from (C.29) and $\mathscr{I}_{i0}^{iq}$ from (C.45), (C.46), (C.41) (the latter is summed over $j = 1, \dots, J$ and $i = 0, 1, 2$) turns out to vanish. As a result, collecting the obtained estimates, we conclude that the quantity δ from formula (C.21) (see also (C.18)) satisfies the estimate

$$\delta \leqslant c_\alpha h^{3+\alpha}, \tag{C.53}$$

for any $\alpha \in (0, 1/2)$.

C.2 Proof of Theorem 9.2

Now we are in position to prove the main result on asymptotic expansions of solutions of singularly perturbed elasticity spectral problem given by Theorem 9.2.

Proof. The linear combinations (9.254) of vector eigenfunctions $u_{(p)}, \dots, u_{(p+\varkappa_p-1)}$ as well as the subsequent terms of asymptotic ansätz (9.191) are constructed with the columns $b^{(1)}, \dots, b^{(\varkappa_p)}$ of $\mathsf{Q}^{(p)}$ with entries (9.253). As a result, for $q = p, \dots, p + \varkappa_p - 1$, the approximate solutions $\left\{ (\lambda_p + h^3 \varsigma_p)^{-1}, \|\mathrm{u}_{(p)}^{(q)}\|_{\mathfrak{H}}^{-1} \mathrm{u}_{(p)}^{(q)} \right\}$ of the abstract equation (C.15) are obtained, such that the quantity δ from relations (C.18) verifies the inequality (C.53).

Remark C.4. Here, we denote by $\mathrm{u}_{(p)}^{(q)}$ the approximation of the eigenfunctions $u_{(p)}^{(q)}$. The approximation of the eigenfunction $u_{(p)}$ is defined for a simple eigenvalue of (9.190) in the right hand side of (9.191). However, taking into account the form of approximations of simple eigenfunctions in (9.191), now the approximation for a multiple eigenvalue is defined in the similar way. Let us recall again that in our notation (p) means the *label* of multiple eigenvalue of multiplicity $\varkappa_p$, in contrast to (q), with $q = p, \dots, \varkappa_p - 1$, which stands for the *labels* of the associated normalized eigenfunctions $u_{(p)}^{(q)}$.

We apply the second part of Lemma A.1 and estimate (C.20) with

$$\delta_{\Bbbk} = c_{\Bbbk} h^{3+\alpha_{\Bbbk}} \;, \quad \alpha_{\Bbbk} \in (0,\alpha) \;. \tag{C.54}$$

Let the list

$$\mu_n^h = (\lambda_n^h)^{-1}, \ldots, \mu_{n+N-1}^h = (\lambda_{n+N-1}^h)^{-1} \tag{C.55}$$

includes all eigenvalues of the operator $\mathfrak{K}^h$ from the segment

$$[(\lambda_p)^{-1} - c_{\Bbbk} h^{3+\alpha_{\Bbbk}}, (\lambda_p)^{-1} + c_{\Bbbk} h^{3+\alpha_{\Bbbk}}] \;, \tag{C.56}$$

for sufficiently small $h_{\Bbbk} > 0$, such that $(\lambda_p + h^3 \varsigma_p)^{-1}$ with $h \in (0, h_{\Bbbk}]$ belonging to segment (C.56). Our immediate objective becomes to show that

$$n = p, \quad N = \varkappa_p \;. \tag{C.57}$$

The quantities μ_n^h for $m \geqslant n+N-1$ are uniformly bounded in $h \in (0, h_{\Bbbk}]$. By Proposition C.1, the same assumptions provide the uniform boundedness of the norm $\|\widetilde{u}_{(m)}^h\|_{H_\Gamma^1(\Omega;\mathbb{R}^3)}$ of the vector functions $\widetilde{u}_{(m)}^h \in \mathfrak{H}^h$ constructed for the vector eigenfunctions $u_{(m)}^h$ in (9.185) according to (C.11). Hence, there exists an infinitesimal sequence $\{h_i\}$, such that the limit passage $h_i \to +0$ leads to the convergences

$$\mu_m^h \to \mu_m^0 = (\lambda_m^0)^{-1} \quad \text{and} \quad \widetilde{u}_{(m)}^h \to \widetilde{u}_{(m)}^0, \tag{C.58}$$

weakly in $H^1(\Omega;\mathbb{R}^3)$ and strongly in $L^2(\Omega;\mathbb{R}^3)$. We substitute into the integral identity (9.185) the test function $v \in C_c^\infty(\overline{\Omega} \setminus (\Gamma \cup \{p^1, \cdots, p^J\}); \mathbb{R}^3)$. According to definition (9.184) and for sufficiently small $h > 0$, the stiffness matrix $\mathscr{A}^h$ and the density γ^h coincide on the support of v with $\mathscr{A}$ and γ, respectively. Therefore, the limit passage $h_i \to +0$ in the integral identity (9.185) leads to the equality

$$(\mathscr{A}\mathscr{D}\, \widetilde{u}_{(m)}^0, \mathscr{D}v)_\Omega = \lambda_m^0 (\gamma\, \widetilde{u}_{(m)}^0, v)_\Omega \;. \tag{C.59}$$

Since $C_c^\infty(\overline{\Omega} \setminus (\Gamma \cup \{p^1, \cdots, p^J\}); \mathbb{R}^3)$ is dense in $H_\Gamma^1(\Omega;\mathbb{R}^3)$, the integral identity (C.59) holds true for all test functions $v \in H_\Gamma^1(\Omega;\mathbb{R}^3)$. We observe that the weighted norms $\|r_j^{-1} \widetilde{u}_{(m)}^h\|_{L^2(\Omega;\mathbb{R}^3)}$ are uniformly bounded by virtue of inequality (C.1), thus

$$(\gamma^h\, \widetilde{u}_{(m)}^h, \widetilde{u}_{(l)}^h)_\Omega - (\gamma\, \widetilde{u}_{(m)}^h, \widetilde{u}_{(l)}^h)_\Omega = o(1), \quad \text{for} \quad h \to +0 \;. \tag{C.60}$$

In this way, taking into account formulae (9.189) and (C.58), we find out that

$$(\gamma\, \widetilde{u}_{(m)}^0, \widetilde{u}_{(l)}^0)_\Omega = \delta_{ml} \;. \tag{C.61}$$

Hence, λ_m^0 is an eigenvalue, and $\widetilde{u}_{(m)}^0$ is a normalized vector eigenfunction of the limit problem (9.179). This implies that $p + \varkappa_p \geqslant n + N$. Considering consequently the eigenvalues $\lambda_p, \ldots, \lambda_1$, we conclude that

$$p \geqslant n\,, \quad \varkappa_p \geqslant N\,. \tag{C.62}$$

In order to establish the inequalities $p \leqslant n$ and $\varkappa_p \leqslant N$ we select the factor $c_{\Bbbk}$ in (C.54) such that for $\varsigma_p^{(k)} \neq \varsigma_p^{(q)}$ the number $(\lambda_p + h^3\varsigma_p^{(k)})^{-1}$ is excluded from the segment

$$[(\lambda_p + h^3\varsigma_p^{(q)})^{-1} - c_{\Bbbk}h^{3+\alpha_{\Bbbk}}, (\lambda_p + h^3\varsigma_p^{(q)})^{-1} + c_{\Bbbk}h^{3+\alpha_{\Bbbk}}]\,. \tag{C.63}$$

Let $\kappa_p^{(q)}$ be the multiplicity of the eigenvalue $\varsigma_p^{(q)}$ of matrix Q. By Proposition C.1 and estimate (C.64) there are, not necessarily distinct, eigenvalues $\mu^h_{l(q)}, \ldots,$ $\mu^h_{l(q+\kappa_q-1)}$, here we denote by $l(q)$ the κ_q-tuple of subsequent integers, of the operator $\mathfrak{K}^h$ such that

$$\left|\mu^h_{l(k)} - (\lambda_p + h^3\varsigma_p^{(q)})^{-1}\right| \leqslant c^{\alpha}_{pq}h^{3+\alpha}\,. \tag{C.64}$$

In addition, Proposition C.1 furnishes the normalized columns $\mathfrak{a}^{(k)}$, written in matrix notation as $\mathfrak{a}^{(k)} = (\mathfrak{a}^{(k)}_{n_{\Bbbk}}, \cdots, \mathfrak{a}^{(k)}_{n_{\Bbbk}+N_{\Bbbk}-1})^{\top}$, such that

$$\left\|\mathfrak{u}^{(k)}_{(p)} - \|\mathfrak{u}^{(k)}_{(p)}\|_{\mathfrak{H}} \sum_{i=n_{\Bbbk}}^{n_{\Bbbk}+N_{\Bbbk}-1} \mathfrak{a}^{(k)}_i \mathfrak{u}^h_i\right\|_{\mathfrak{H}} \leqslant \frac{\delta}{\delta_{\Bbbk}} \leqslant \frac{c}{c_{\Bbbk}} h^{\alpha-\alpha_{\Bbbk}}\,, \tag{C.65}$$

where $\mathfrak{u}^h_{n_{\Bbbk}}, \cdots, \mathfrak{u}^h_{n_{\Bbbk}+N_{\Bbbk}-1}$ are normalized in $\mathfrak{H}$ vector eigenfunctions of the operator $\mathfrak{K}^h$ corresponding to all eigenvalues from segment (C.63). By formulae (C.24)-(C.26), (9.179) and (9.181),

$$\left|\langle \mathfrak{u}^{(k)}_{(p)}, \mathfrak{u}^{(l)}_{(p)}\rangle_{\Omega} - \lambda_p\delta_{kl}\right| = o(1), \quad \text{for} \quad h \to +0\,. \tag{C.66}$$

Furthermore, owing to formula (C.65), we have

$$\left|\langle \mathfrak{u}^{(k)}_{(p)}, \mathfrak{u}^{(l)}_{(p)}\rangle_{\Omega} - \lambda_p(\mathfrak{a}^{(k)})^{\top}\mathfrak{a}^{(l)}\right| = o(1), \quad \text{for} \quad h \to +0\,. \tag{C.67}$$

Thus, for sufficiently small h the number $N_{\Bbbk}$ cannot be smaller than $\kappa_p^{(q)}$. Hence, there are eigenvalues $\mu^h_l, \cdots, \mu^h_{l+\kappa_p^{(q)}-1}$ which verify inequality (C.64) with the majorant $c^{\alpha_{\Bbbk}}_{pq}h^{3+\alpha_{\Bbbk}}$ (since the exponent $\alpha \in (0, 1/2)$ is arbitrary, we can choose $\alpha_{\Bbbk} < \alpha$ without loosing of the precision in the final estimate (9.252)). Selecting all eigenvalues of the matrix Q, and subsequently the numbers $\lambda_{p-1}, \cdots, \lambda_1$, it turns out that necessarily the equality in (C.62) occurs, and also $N_{\Bbbk} = \kappa_p^{(q)}$. The proof of Theorem 9.2 is completed. □

Appendix D
Polarization Tensor in Elasticity

The derivation of formulae for topological derivatives in anisotropic elasticity requires the knowledge of integral attributes for singular domain perturbations in the form of cavities, caverns or inclusions [172]. The attributes can be determined by using the asymptotic analysis in singularly perturbed domains [170]. For the purposes of such derivation the polarization tensor in elasticity in three spatial dimensions is characterized. *Polarization matrices* (or tensors) [170] are generalizations of mathematical objects like the *harmonic capacity* or the *virtual mass matrix* [198]. Using results about elliptic problems in domains with a compact complement, polarization matrices can be properly defined in terms of certain coefficients in the asymptotic expansion at infinity of the solution to the homogeneous transmission problem. Representation formulae are derived in [180] from which properties like positivity or negativity can be read of directly.

D.1 Elasticity Boundary Value Problems

D.1.1 Voigt Notation in Elasticity

We recall the *Voigt notation* already introduced in Section 9.4.1. We have

$$\mathscr{D}(\nabla_x)^\top = \begin{bmatrix} \frac{\partial}{\partial x_1} & 0 & 0 & 0 & \frac{1}{\sqrt{2}}\frac{\partial}{\partial x_3} & \frac{1}{\sqrt{2}}\frac{\partial}{\partial x_2} \\ 0 & \frac{\partial}{\partial x_2} & 0 & \frac{1}{\sqrt{2}}\frac{\partial}{\partial x_3} & 0 & \frac{1}{\sqrt{2}}\frac{\partial}{\partial x_1} \\ 0 & 0 & \frac{\partial}{\partial x_3} & \frac{1}{\sqrt{2}}\frac{\partial}{\partial x_2} & \frac{1}{\sqrt{2}}\frac{\partial}{\partial x_1} & 0 \end{bmatrix}, \tag{D.1}$$

and in the *Voigt notation in elasticity*, in view of (9.171)-(9.172), the vectors of *strains* $\vartheta(u(x))$, the vectors of *stresses* $\sigma(u(x))$, and the displacement $u(x)$ are related by the relation,

$$\sigma(u(x)) := \mathscr{A}(x)\vartheta(u(x)) \quad \text{and} \quad \vartheta(u(x)) = \mathscr{D}(\nabla_x)u(x), \tag{D.2}$$

where the matrix $\mathscr{A}$ of elastic material moduli which is called also in the literature the Hooke or stiffness matrix, is defined in (9.169). With the notation it is easy to find:

- the tractions $\sigma^n(u(x))$ in the direction of a unit normal vector field n on an interface or on the boundary of elastic body,

$$\sigma^n(u(x)) = \mathscr{D}(n(x))\sigma(u(x)), \tag{D.3}$$

- the decomposition of the stress tensor in the cartesian basis of $\mathbb{R}^3$,

$$\sigma^j(u(x)) = \mathscr{D}(e^j)\sigma(u(x)), \quad -\sum_{j=1}^{3} \partial x_j \sigma^j(u(x)) = \mathscr{D}(\nabla_x)^\top \sigma(u(x)), \tag{D.4}$$

  where e^1, e^2, e^3 define the cartesian basis in $\mathbb{R}^3$.

In view of the *constitutive relation in the Voigt notation* (D.2) the symmetric bilinear form of the elasticity boundary value problem in the body Ω is given by

$$\begin{aligned} H^1(\Omega;\mathbb{R}^3) \ni (u,v) \to a(u,v) &:= (\sigma(u), \vartheta(v))_\Omega \\ &= (\mathscr{A}\mathscr{D}(\nabla_x)u, \mathscr{D}(\nabla_x)v)_\Omega \in \mathbb{R} \end{aligned} \tag{D.5}$$

and the selfadjoint elliptic operator $\mathscr{L} := \mathscr{D}(\nabla_x)^\top \mathscr{A}\mathscr{D}(\nabla_x)$ associated with the bilinear form

$$a(u,v) := -(\mathscr{L}u, v)_\Omega = -(\mathscr{L}v, u)_\Omega \quad \forall u, v \in H^2(\Omega;\mathbb{R}^3) \cap H_0^1(\Omega;\mathbb{R}^3). \tag{D.6}$$

In the Voigt notation the *Green formula* takes the form

$$(\mathscr{L}u, v)_\Omega - (\mathscr{N}u, v)_{\partial\Omega} = (\mathscr{L}v, u)_\Omega - (\mathscr{N}v, u)_{\partial\Omega} \quad \forall u, v \in H^2(\Omega;\mathbb{R}^3), \tag{D.7}$$

where $\mathscr{N} := \mathscr{D}(n)^\top \mathscr{A}\mathscr{D}(\nabla_x)$.

D.1.2 Korn Inequality

We recall also the classic *Korn inequality* for our purposes. See also Proposition C.1 for another variant.

Theorem D.1. *The following inequalities hold true:*

- *For functions in $H^1(\Omega;\mathbb{R}^3)$, we have*

$$\|u\|_{H^1(\Omega;\mathbb{R}^3)} \leqslant C\left(\|\mathscr{D}(\nabla_x)u\|_{L^2(\Omega;\mathbb{R}^3)} + \|u\|_{L^2(\Omega;\mathbb{R}^3)}\right), \tag{D.8}$$

  where the constant C depends only on Ω.

- *For functions in* $H_0^1(\Omega;\mathbb{R}^3)$, *there is*

$$\|\nabla_x u\|_{L^2(\Omega;\mathbb{R}^3)} \leqslant 2\|\mathscr{D}(\nabla_x)u\|_{L^2(\Omega;\mathbb{R}^3)}. \tag{D.9}$$

- *For functions in* $H_\Gamma^1(\Omega;\mathbb{R}^3)$, *it follows*

$$\|\nabla_x u\|_{L^2(\Omega;\mathbb{R}^3)} \leqslant C\|\mathscr{D}(\nabla_x)u\|_{L^2(\Omega;\mathbb{R}^3)}, \tag{D.10}$$

  where the constant C depend on Γ, *with* $\operatorname{meas}_2(\Gamma) > 0$.

Proposition D.1. *The solution to the elasticity spectral problem presented in Section 9.4 can be characterized as following:*

- *There is existence of a weak solution to Problem 9.8 provided the compatibility conditions* (9.176) *are verified by the element* $g \in L^2(\partial\Omega;\mathbb{R}^3)$.
- *The weak solution of Problem 9.8 minimizes the energy functional*

$$H^1(\Omega;\mathbb{R}^3) \ni v \to \mathscr{E}(\Omega;v) := \frac{1}{2}a(u,v) - l(v) \in \mathbb{R}, \tag{D.11}$$

  where the linear form

$$L^2(\partial\Omega;\mathbb{R}^3) \ni \varphi \mapsto l(\varphi) := \int_{\partial\Omega} g\cdot\varphi ds_x \tag{D.12}$$

  is well defined on the space $H^1(\Omega;\mathbb{R}^3)$ *by the standard trace theorem.*
- *The solution to Problem 9.8 is defined up to the* rigid body motions (9.173)

$$p(x) := \mathbb{D}(x)c = b + d\times x \quad c\in\mathbb{R}^6, \quad b,d\in\mathbb{R}^3, \tag{D.13}$$

  where $c = (c_1,\cdots,c_6)^\top$, $b = (c_1,c_2,c_3)^\top$, $d = 2^{-1/2}(c_4,c_5,c_6)^\top$.

The proof of the proposition is left as an exercise.

D.2 Polarization Matrices in Elasticity

We recall the notation for the ball and the sphere with the center at the origin, $B_R = \{x\in\mathbb{R}^3, \|x\| < R\}$, $S_R = \partial B_R = \{x\in\mathbb{R}^3, \|x\| = R\}$. Let $\Omega\subset\mathbb{R}^3$ be a *Lipschitz domain* with the boundary $\Gamma := \partial\Omega$, with the outward unit normal vector $n(x), x\in\Gamma$, and with a compact connected complement $\Omega^{\mathfrak{c}}$, thus $\mathbb{R}^3 = \Omega^{\mathfrak{c}}\cup\Gamma\cup\Omega$. We recall notation for the Sobolev spaces and the Dirichlet trace:

- For integers $l\in\mathbb{N}$, $H^l(\Omega)$, $H^l(\Omega^{\mathfrak{c}})$ are classic Sobolev spaces.
- For a smooth boundary (interface) Γ the *fractional Sobolev spaces* are denoted by $H^s(\Gamma)$ for $s\in\mathbb{R}$, these spaces are also called *Sobolev-Slobodetskii spaces*.
- If Γ is Lipschitz, then the *Dirichlet trace* operator $\gamma : H^1(\Omega^{\mathfrak{c}}) \to H^{1/2}(\Gamma)$ is continuous.

- For simplicity, the notation $\phi_{|\Gamma}$ instead of $\gamma\phi$ is used for the Dirichlet traces of the Sobolev functions.
- Further the notation $(\cdot,\cdot)_\Xi$ is used for the scalar product in $L^2(\Xi;\mathbb{R}^3)$ for a set $\Xi \subset \mathbb{R}^3$.

Let us present the formulation of the *transmission problem*. We recall that in the matrix-vector notation for the elasticity problems [36, 166], the displacement vector $u = (u_1, u_2, u_3)^\top$ is a column vector or simply a column in $\mathbb{R}^3$ and the strain column of height 6 is defined explicitly in terms of the cartesian components $\varepsilon_{jk}(u)$ of the strain tensor,

$$\vartheta(u) = (\varepsilon_{11}(u), \varepsilon_{22}(u), \varepsilon_{33}(u), \sqrt{2}\varepsilon_{23}(u), \sqrt{2}\varepsilon_{31}(u), \sqrt{2}\varepsilon_{12}(u))^\top, \tag{D.14}$$

where $\alpha = 2^{-1/2}$ and the cartesian components of the strain tensor are given by

$$\varepsilon_{jk}(u) = \frac{1}{2}\left(\frac{\partial u_j}{\partial x_k} + \frac{\partial u_k}{\partial x_j}\right), \quad j = 1,2, \tag{D.15}$$

with $j,k = 1,2,3$. Then we have $\vartheta(u) = \mathscr{D}(\nabla)u$, where $\mathscr{D}$ is matrix (9.170). The stress columns in Ω and Ω^{c} are defined by the Hooke's law,

$$\sigma(u) = \mathscr{A}\vartheta(u) \quad \text{and} \quad \sigma^{\mathrm{c}}(u) = \mathscr{A}^{\mathrm{c}}\vartheta(u), \tag{D.16}$$

where $\mathscr{A}$ and $\mathscr{A}^{\mathrm{c}}$ are symmetric and positive definite 6×6 stiffness matrices, the entries of $\mathscr{A}$ and $\mathscr{A}^{\mathrm{c}}$ are the elastic moduli in Ω and Ω^{c}, respectively.

Remark D.1. For the reader's convenience, we recall the relation between the usual Hooke tensor and the stiffness matrix (see e.g., [36, pp. 42] or [166, Section 2.2]). In tensor notation, Hooke's law reads

$$\sigma_{ij} = \sum_{p,q} a^{ij}_{pq}\varepsilon_{pq}, \quad i,j = 1,2,3. \tag{D.17}$$

We recall that symmetry for a rank four tensor means

$$a^{ij}_{pq} = a^{ji}_{pq} = a^{pq}_{ij}. \tag{D.18}$$

The matrix $\mathscr{A}$ in (D.16) gets the form

$$\mathscr{A} = \begin{pmatrix} a^{11}_{11} & a^{11}_{22} & a^{11}_{33} & \sqrt{2}a^{11}_{23} & \sqrt{2}a^{11}_{31} & \sqrt{2}a^{11}_{12} \\ a^{22}_{11} & a^{22}_{22} & a^{22}_{33} & \sqrt{2}a^{22}_{23} & \sqrt{2}a^{22}_{31} & \sqrt{2}a^{22}_{12} \\ a^{33}_{11} & a^{33}_{22} & a^{33}_{33} & \sqrt{2}a^{33}_{23} & \sqrt{2}a^{33}_{31} & \sqrt{2}a^{33}_{12} \\ \sqrt{2}a^{23}_{11} & \sqrt{2}a^{23}_{22} & \sqrt{2}a^{23}_{33} & 2a^{23}_{23} & 2a^{23}_{31} & 2a^{23}_{12} \\ \sqrt{2}a^{31}_{11} & \sqrt{2}a^{31}_{22} & \sqrt{2}a^{31}_{33} & 2a^{31}_{23} & 2a^{31}_{31} & 2a^{31}_{12} \\ \sqrt{2}a^{12}_{11} & \sqrt{2}a^{12}_{22} & \sqrt{2}a^{12}_{33} & 2a^{12}_{23} & 2a^{12}_{31} & 2a^{12}_{12} \end{pmatrix}. \tag{D.19}$$

In a similar way the matrix $\mathscr{A}$ of the elastic material moduli in two spatial dimensions is transformed into a 3×3 matrix.

Condition D.1. We assume

- *The entries of stiffness matrix in Ω*,

$$\mathscr{A}(x) = \mathscr{A}^0 + \mathscr{A}^e(x) \quad \text{with} \quad \mathscr{A}^e_{ij} \in C^1_0(\overline{\Omega}), \tag{D.20}$$

  with $\mathscr{A}^e(x) = 0$ for $r = \|x\| \geqslant R_0$, where R_0 is such that $\overline{\Omega^{\mathfrak{c}}} \subset B_{R_0}$.
- *The matrix $\mathscr{A}^0$* is constant and positive definite, i.e. the elastic space is homogeneous far away from the inclusion.
- *The entries of stiffness matrix in $\Omega^{\mathfrak{c}}$*, the inclusion $\Omega^{\mathfrak{c}}$ is heterogeneous and the entries of $\mathscr{A}^{\mathfrak{c}}$ are given by C^1 functions in $\overline{\Omega^{\mathfrak{c}}}$.
- *The matrices $\mathscr{A}(x)$ and $\mathscr{A}^{\mathfrak{c}}(x)$* are uniformly positive definite,

$$\xi^\top \mathscr{A}(x)\xi \geq a\|\xi\|^2 \quad \text{and} \quad \xi^\top \mathscr{A}^{\mathfrak{c}}(x)\xi \geq a_{\mathfrak{c}}\|\xi\|^2 \tag{D.21}$$

  for any vector $\xi \in \mathbb{R}^6$ and all $x \in \Omega$ and $x \in \Omega^{\mathfrak{c}}$ with positive constants $a, a_{\mathfrak{c}}$.

We introduce the differential operators for the transmission problem in $\Omega \cup \Omega^{\mathfrak{c}}$:

$$\mathscr{L} := \mathscr{D}(-\nabla)^\top \mathscr{A}(x)\mathscr{D}(\nabla), \quad \mathscr{L}^{\mathfrak{c}} := \mathscr{D}(-\nabla)^\top \mathscr{A}^{\mathfrak{c}}(x)\mathscr{D}(\nabla)u^{\mathfrak{c}}(x), \tag{D.22}$$

$$\mathscr{N}u := \mathscr{D}(n(x))^\top \mathscr{A}(x)\mathscr{D}(\nabla)u(x),\ \mathscr{N}^{\mathfrak{c}}u^{\mathfrak{c}} := \mathscr{D}(n(x))^\top \mathscr{A}^{\mathfrak{c}}(x)\mathscr{D}(\nabla)u^{\mathfrak{c}}. \tag{D.23}$$

The elasticity transmission problem in $\mathbb{R}^3 := \Omega \cup \Omega^{\mathfrak{c}} \cup \Gamma$ reads as follows:

Problem D.1. Find $\{u, u^{\mathfrak{c}}\}$ such that

$$\mathscr{L}u(x) = f(x), \quad x \in \Omega = \mathbb{R}^3 \setminus \overline{\Omega^{\mathfrak{c}}}, \tag{D.24a}$$

$$\mathscr{L}^{\mathfrak{c}}u^{\mathfrak{c}}(x) = f^{\mathfrak{c}}(x), \quad x \in \Omega^{\mathfrak{c}}. \tag{D.24b}$$

Problem (D.24a)-(D.24b) is supplied with the boundary conditions on the interface

$$[\![u]\!](x) := u - u^{\mathfrak{c}} = g^0, \tag{D.24c}$$

$$[\![\mathscr{N}u]\!](x) := \mathscr{N}u(x) - \mathscr{N}^{\mathfrak{c}}u^{\mathfrak{c}}(x) = g^1 \quad \text{on } \Gamma := \partial\Omega^{\mathfrak{c}}. \tag{D.24d}$$

If f decays sufficiently fast we may add the condition at infinity

$$\|u(x)\| = O(\|x\|^{-1}), \qquad \text{as } \|x\| \to \infty. \tag{D.24e}$$

Here f, $f^{\mathfrak{c}}$ are volume forces while g^0 and g^1 stand for jumps of displacements and tractions on the interface Γ.

Remark D.2. Note that the two-dimensional problem can be formulated in just the same way, with stress and strain columns $(\sigma_{11}, \sigma_{22}, \sqrt{2}\sigma_{12})^\top$, $(\varepsilon_{11}, \varepsilon_{22}, \sqrt{2}\varepsilon_{12})^\top$ in $\mathbb{R}^3$ instead of $\mathbb{R}^6$ and 3×3 Hooke matrix, while the matrix $\mathscr{D}(\xi)$ in (9.170) has to be replaced by

$$\mathscr{D}(\xi)^\top = \begin{pmatrix} \xi_1 & 0 & \alpha\xi_2 \\ 0 & \xi_2 & \alpha\xi_1 \end{pmatrix}, \quad \alpha = \frac{1}{\sqrt{2}}, \quad \xi \in \mathbb{R}^2. \tag{D.25}$$

D.3 The Polarization Matrices for Three-Dimensional Anisotropic Elasticity Problems

D.3.1 Solvability of the Transmission Problems

First, a variational formulation of transmission problem is given. By $\mathscr{H}$ is denoted the completion of $C_0^\infty(\mathbb{R}^3;\mathbb{R}^3)$ with respect to the *energy norm*

$$\mathscr{H} \ni u \to \|\mathscr{D}(\nabla)u\|_{L^2(\mathbb{R}^3;\mathbb{R}^3)} \in \mathbb{R}. \tag{D.26}$$

$\mathscr{H}$ is equipped with the scalar product (D.33) which induces an equivalent norm convenient for our purposes.

Using the Fourier transform and Hardy's inequality, the Korn's inequality is obtained (cf. Proposition C.1 and also [118])

$$\|(1+r)^{-1}u\|_{L^2(\mathbb{R}^3;\mathbb{R}^3)} + \|\nabla u\|_{L^2(\mathbb{R}^3;\mathbb{R}^3)} \leqslant \frac{1}{\sqrt{10}} \|\mathscr{D}(\nabla)u\|_{L^2(\mathbb{R}^3;\mathbb{R}^3)}, \qquad u \in \mathscr{H}. \tag{D.27}$$

We recall the definition of norms in *Kondratiev spaces*, well adapted for transmission problems in unbounded domains.

Let $\Upsilon \subseteq \mathbb{R}^3$ an unbounded domain, $\beta \in \mathbb{R}$ and $l \in \mathbb{N}^* = \{0,1,\dots\}$ be fixed. Then the Kondratiev space $V^l_\beta(\Upsilon;\mathbb{R}^3)$ is a subspace of elements in $u \in H^l_{\mathrm{loc}}(\overline{\Upsilon};\mathbb{R}^3)$ with the finite norm

$$\|u\|_{V^l_\beta(\Upsilon;\mathbb{R}^3)} = \left(\sum_{k=0}^{l} \|(1+\|x\|)^{\beta-l+k} \nabla_x^k u\|^2_{L^2(\Upsilon;\mathbb{R}^3)} \right)^{1/2} < \infty. \tag{D.28}$$

The weight is introduced to control the behavior at infinity of the functions under consideration. The Korn inequality (D.27) implies that $\mathscr{H} = V^1_0(\mathbb{R}^3;\mathbb{R}^3)$ and the norms are equivalent.

For vector fields u and v which admit the Dirichlet and Neumann traces, we have the Green's formulae in the domains Ω and Ω^{c}:

$$(\mathscr{L}u,v)_\Omega + (\mathscr{N}u,v)_\Gamma = (\mathscr{A}\mathscr{D}(\nabla)u, \mathscr{D}(\nabla)v)_\Omega, \tag{D.29}$$

$$(\mathscr{L}^{\mathrm{c}}u,v)_\Omega - (\mathscr{N}^{\mathrm{c}}u,v)_\Gamma = (\mathscr{A}^{\mathrm{c}}\mathscr{D}(\nabla)u, \mathscr{D}(\nabla)v)_{\Omega^{\mathrm{c}}}. \tag{D.30}$$

Observe that in (D.29)-(D.30) in the Neumann traces (tractions) $\mathscr{N}(n)u$ and $\mathscr{N}^{\mathrm{c}}(n)u$ on Γ, n stands for the *internal* normal vector to Γ with respect to Ω^{c}. That is the reason for the sign minus in (D.30). In particular, for any vector function $u \in H^2_{\mathrm{loc}}(\overline{\Omega};\mathbb{R}^3)$, $u^{\mathrm{c}} \in H^2(\Omega^{\mathrm{c}};\mathbb{R}^3)$, satisfying (D.24a)-(D.24b) and (D.24e), and $v \in C_0^\infty(\mathbb{R}^3;\mathbb{R}^3)$, the addition of the two formulae leads to

Problem D.2. Find $\{u,u^{\mathrm{c}}\}$, with the prescribed jump of displacement field $[\![u]\!](x) := u - u^{\mathrm{c}} = g^0$ on Γ, and such that

$$(\mathscr{A}\mathscr{D}(\nabla)u, \mathscr{D}(\nabla)v)_\Omega + (\mathscr{A}^\mathrm{c}\mathscr{D}(\nabla)u^\mathrm{c}, \mathscr{D}(\nabla)v)_{\Omega^\mathrm{c}} = (f^\mathrm{c}, v)_{\Omega^\mathrm{c}} + (f, v)_\Omega + (g^1, v)_\Gamma \quad \forall v \in C_0^\infty(\mathbb{R}^3;\mathbb{R}^3). \tag{D.31}$$

If we set $g^0 = 0$ and $u \in V_1^2(\Omega;\mathbb{R}^3)$ in the definition of Problem D.2, then we can glue u, u^c together and obtain a vector field $\mathfrak{u} := \{u, u^\mathrm{c}\} \in V_0^1(\mathbb{R}^3;\mathbb{R}^3) = \mathscr{H}$,

$$\mathfrak{u}(x) = \begin{cases} u(x) = x \in \Omega, \\ u^\mathrm{c}(x) = x \in \Omega^\mathrm{c}. \end{cases} \tag{D.32}$$

Furthermore, due to our assumptions on the stiffness matrices $\mathscr{A}$, $\mathscr{A}^\mathrm{c}$ combined with the Korn's inequality (D.27), the left hand side of (D.31) defines a scalar product on $\mathscr{H}$

$$(\mathfrak{u}, \mathfrak{v})_\mathscr{H} := (\mathscr{A}\mathscr{D}(\nabla)u, \mathscr{D}(\nabla)v)_\Omega + (\mathscr{A}^\mathrm{c}\mathscr{D}(\nabla)u^\mathrm{c}, \mathscr{D}(\nabla)v^\mathrm{c})_{\Omega^\mathrm{c}} \tag{D.33}$$

for all $\mathfrak{u} = \{u, u^\mathrm{c}\}, \mathfrak{v} = \{v, v^\mathrm{c}\} \in \mathscr{H}$, which induces a norm equivalent to the energy norm (D.26). If f and f^c are restrictions of $\mathfrak{f} \in V_1^0(\Omega;\mathbb{R}^3)$,

$$\mathfrak{f}(x) = \begin{cases} f(x) = x \in \Omega, \\ f^\mathrm{c}(x) = x \in \Omega^\mathrm{c}, \end{cases} \tag{D.34}$$

the right hand side of (D.31) defines a continuous linear functional on $\mathscr{H}$,

$$\mathscr{F}(\mathfrak{v}) := (\mathfrak{f}, \mathfrak{v})_\mathscr{H} + (g^1, v)_\Gamma = (f^\mathrm{c}, v)_{\Omega^\mathrm{c}} + (f, v)_\Omega + (g^1, v)_\Gamma, \tag{D.35}$$

where $\mathscr{F} \in \mathscr{H}'$ remains continuous for $g^1 \in H^{-1/2}(\Gamma;\mathbb{R}^3)$. Thus, for $g^0 = 0$, the integral identity (D.31) becomes

$$(\mathfrak{u}, \mathfrak{v})_\mathscr{H} = \mathscr{F}(\mathfrak{v}) \quad \forall \mathfrak{v} \in \mathscr{H}. \tag{D.36}$$

The Neumann traces (tractions) are not defined for an arbitrary displacement field $u \in \mathscr{H}$. However, the tractions on the interface Γ do exist in a weak sense and can be defined by a generalization of the Green formula if in addition we have a sufficient information about one of the elements $\mathscr{L}u$, or $\mathscr{L}^\mathrm{c}u$ in dual spaces, since $\mathscr{L}, \mathscr{L}^\mathrm{c}$ are differential operators in divergence form. Hence we may use a well known weak trace theorem to have the tractions defined on the boundary or an interface in a weak sense (see [216, pp. 9]).

Proposition D.2. *For $u \in H^1(\Omega^\mathrm{c};\mathbb{R}^3)$ such that $\mathscr{L}^\mathrm{c}u \in L^2(\Omega;\mathbb{R}^3)$, there exists the Neumann trace $\mathscr{N}^\mathrm{c}u \in H^{-1/2}(\Gamma;\mathbb{R}^3)$ and*

$$\|\mathscr{N}^\mathrm{c}u\|_{H^{-1/2}(\Gamma;\mathbb{R}^3)} \leqslant C\left(\|\mathscr{D}(\nabla)u\|_{L^2(\Omega;\mathbb{R}^3)} + \|\mathscr{L}^\mathrm{c}u\|_{L^2(\Omega;\mathbb{R}^3)}\right), \tag{D.37}$$

thus the Green's formula (D.30) *is valid for such u. In addition, an analogous result is true for $u \in V_0^1(\Omega;\mathbb{R}^3)$ with $\mathscr{L}u \in V_1^0(\Omega;\mathbb{R}^3)$.*

Remark D.3. Variational formulations are more convenient for analysis. To rewrite the general problem (D.24a)-(D.24d) in the form (D.36), it is necessary to reduce the nonhomogeneous Dirichlet transmission condition (D.24c) to the homogeneous condition $g^0 = 0$. Since a linear problem is considered, we can search for the decomposition $u^{\mathfrak{c}} = \mathfrak{u}^{\mathfrak{c}} - \mathsf{G}$, where G is a suitable extension of g^0 onto $\Omega^{\mathfrak{c}}$ and $\mathfrak{u}^{\mathfrak{c}} = u^{\mathfrak{c}} + \mathsf{G}$ solves a resulting homogeneous problem.

Condition D.2. *Extension to $\Omega^{\mathfrak{c}}$ of the Dirichlet condition g^0 on the interface Γ:*

- If $g^0 \in H^{3/2}(\Gamma;\mathbb{R}^3)$, a continuous extension $H^{3/2}(\Gamma;\mathbb{R}^3) \ni g^0 \to \mathsf{G} \in H^2(\Omega^{\mathfrak{c}};\mathbb{R}^3)$ can be constructed.
- For $g^0 \in H^{1/2}(\Gamma;\mathbb{R}^3)$ the harmonic extension can be employed, so the extension is given by a weak solution $\mathsf{G} \in H^1(\Omega^{\mathfrak{c}};\mathbb{R}^3)$ of

$$\mathscr{L}^{\mathfrak{c}}\mathsf{G} = 0 \quad \text{in } \Omega^{\mathfrak{c}}, \qquad \mathsf{G} = g^0 \quad \text{on } \Gamma, \tag{D.38}$$

  with

$$\|\mathsf{G}\|_{H^1(\Omega^{\mathfrak{c}};\mathbb{R}^3)} \leqslant C\|g^0\|_{H^{1/2}(\Gamma;\mathbb{R}^3)}, \tag{D.39}$$

  where the constant C is independent of g^0.
- By the standard elliptic regularity [72, 199], inequality (D.39) extends to

$$\|\mathsf{G}\|_{H^{l+2}(\Omega^{\mathfrak{c}};\mathbb{R}^3)} \leqslant C\|g^0\|_{H^{l+3/2}(\Gamma;\mathbb{R}^3)}, \quad l \in \mathbb{N}^*, \tag{D.40}$$

  provided the surface Γ as well as the coefficient functions in $\mathscr{A}^{\mathfrak{c}}$ are sufficiently smooth and $g^0 \in H^{l+3/2}(\Gamma;\mathbb{R}^3)$.

Definition D.1. Let $f^{\mathfrak{c}} \in L^2(\Omega^{\mathfrak{c}};\mathbb{R}^3)$, $f \in V_1^0(\Omega;\mathbb{R}^3)$, $g^0 \in H^{1/2}(\Gamma;\mathbb{R}^3)$ and $g^1 \in H^{-1/2}(\Gamma;\mathbb{R}^3)$ be given, and let $\mathsf{G} \in H^1(\Omega^{\mathfrak{c}};\mathbb{R}^3)$ be the extension of g^0 into $\Omega^{\mathfrak{c}}$ defined by (D.38). We call a pair $\{u, u^{\mathfrak{c}}\}$ of vector fields defined on Ω and $\Omega^{\mathfrak{c}}$, respectively, a weak solution of the boundary value problem (D.24a)-(D.24d), if $\{u, u^{\mathfrak{c}} + \mathsf{G}\} \in \mathscr{H}$ and

$$\begin{aligned}(\mathscr{A}\mathscr{D}(\nabla)u, \mathscr{D}(\nabla)v)_{\Omega} + (\mathscr{A}^{\mathfrak{c}}\mathscr{D}(\nabla)u^{\mathfrak{c}}, \mathscr{D}(\nabla)v)_{\Omega^{\mathfrak{c}}} = \\ (f^{\mathfrak{c}}, v)_{\Omega^{\mathfrak{c}}} + (f, v)_{\Omega} + \langle g^1, v\rangle_{\Gamma} \quad \forall v \in \mathscr{H} = V_0^1(\mathbb{R}^3;\mathbb{R}^3).\end{aligned} \tag{D.41}$$

The Riesz representation theorem leads to the following result.

Proposition D.3. *Problem D.2 has a unique weak solution $\{u^{\mathfrak{c}}, u\} \in H^1(\Omega^{\mathfrak{c}};\mathbb{R}^3) \times V_0^1(\Omega;\mathbb{R}^3)$, and*

$$\begin{aligned}&\|u\|_{V_0^1(\Omega;\mathbb{R}^3)} + \|u^{\mathfrak{c}}\|_{H^1(\Omega^{\mathfrak{c}};\mathbb{R}^3)} \leqslant \\ &c\left(\|f^{\mathfrak{c}}\|_{L^2(\Omega^{\mathfrak{c}};\mathbb{R}^3)} + \|f\|_{V_1^0(\Omega;\mathbb{R}^3)} + \|g^0\|_{H^{1/2}(\Gamma;\mathbb{R}^3)} + \|g^1\|_{H^{-1/2}(\Gamma;\mathbb{R}^3)}\right).\end{aligned} \tag{D.42}$$

If the surface Γ and the matrix functions $\mathscr{A}$, $\mathscr{A}^{\mathfrak{c}}$ are smooth and for some $l \in \mathbb{N}$ we have

$$\begin{gathered}f \in V_l^{l-1}(\Omega;\mathbb{R}^3), \quad f^{\mathfrak{c}} \in H^{l-1}(\Omega^{\mathfrak{c}};\mathbb{R}^3), \\ g^0 \in H^{l+1/2}(\Gamma;\mathbb{R}^3), \quad g^1 \in H^{l-1/2}(\Gamma;\mathbb{R}^3).\end{gathered} \tag{D.43}$$

Then $u \in V_l^{l+1}(\Omega;\mathbb{R}^3)$, $u^{\mathrm{c}} \in H^{l+1}(\Omega^{\mathrm{c}};\mathbb{R}^3)$ *and the pair* $\{u,u^{\mathrm{c}}\}$ *is a strong solution to the elliptic transmission problem* (D.24a)-(D.24b), (D.24e). *Moreover,*

$$\|u\|_{V_l^{l+1}(\Omega;\mathbb{R}^3)} + \|u^{\mathrm{c}}\|_{H^{l+1}(\Omega^{\mathrm{c}};\mathbb{R}^3)} \leqslant \tag{D.44}$$
$$C\Big(\|f\|_{V_l^{l-1}(\Omega;\mathbb{R}^3)} + \|f^{\mathrm{c}}\|_{H^{l-1}(\Omega^{\mathrm{c}};\mathbb{R}^3)} + \|g^0\|_{\in H^{l+1/2}(\Gamma;\mathbb{R}^3)} + \|g^1\|_{H^{l-1/2}(\Gamma;\mathbb{R}^3)}\Big),$$

where C *depends on* Γ.

Proof. By Proposition D.37 the trace $\mathscr{N}^{\mathrm{c}}\mathsf{G} \in H^{-1/2}(\Gamma;\mathbb{R}^3)$, and

$$(\mathscr{A}^{\mathrm{c}}\mathscr{D}(\nabla)\mathsf{G}, \mathscr{D}(\nabla)v)_{\Omega^{\mathrm{c}}} + \langle \mathscr{N}^{\mathrm{c}}\mathsf{G}, v\rangle_\Gamma = 0. \tag{D.45}$$

Thus (D.41) is fulfilled if $\mathfrak{u} = \{u, u^{\mathrm{c}} + \mathsf{G}\}$ solves

$$(\mathfrak{u}, v)_{\mathscr{H}} = (f^{\mathrm{c}}, v)_{\Omega^{\mathrm{c}}} + (f, v)_\Omega + \langle g^1 - \mathscr{N}^{\mathrm{c}}\mathsf{G}, v\rangle_\Gamma \quad \forall v \in \mathscr{H}. \tag{D.46}$$

Clearly, (D.46) is again of the form (D.36), thus application of the Riesz representation theorem for a linear functional in a Hilbert space ensures the existence of a unique solution while estimates (D.27) and (D.39) lead to estimate (D.42). The estimate (D.44) follows from (D.40) and regularity results for elliptic problems. □

Remark D.4. Let $\{u, u^{\mathrm{c}}\}$ be a weak solution to (D.31) given by Proposition D.3 with $f \in V_\gamma^{l-1}(\Omega;\mathbb{R}^3)$, $\gamma \in (l+3/2, l+5/2)$. We have $u \in V_l^{l+1}(\Omega;\mathbb{R}^3)$ in view of the embedding $V_\gamma^{l-1}(\Omega;\mathbb{R}^3) \subset V_l^{l-1}(\Omega;\mathbb{R}^3)$.

Remark D.5. Let us observe that equation (D.36) admits a unique solution for any $\mathscr{F} \in \mathscr{H}'$,

$$\|u\|_{\mathscr{H}} \leqslant \|\mathscr{F}\|_{\mathscr{H}'}. \tag{D.47}$$

We recall that a continuous linear functional on the Hilbert space $V_0^1(\mathbb{R}^3;\mathbb{R}^3)$ takes the form

$$\mathscr{F}(v) = (f, v)_{\mathbb{R}^3} + \sum_{i=1}^3 (F_i, \partial_{x_i} v)_{\mathbb{R}^3}, \tag{D.48}$$

where $f \in V_1^0(\mathbb{R}^3;\mathbb{R}^3)$, $F_i \in L^2(\mathbb{R}^3), i = 1,2,3$, and with the norm bounded by

$$\|\mathscr{F}\|^2_{V_0^1(\mathbb{R}^3;\mathbb{R}^3)'} \leqslant \left(\|f\|^2_{V_1^0(\mathbb{R}^3;\mathbb{R}^3)} + \sum_{i=1}^3 \|F_i\|^2_{L^2(\mathbb{R}^3)}\right). \tag{D.49}$$

Let us consider the *weak transmission problem*:

Problem D.3. Given $\mathscr{F} \in \mathscr{H}'$ and $g^0 \in H^{1/2}(\Gamma;\mathbb{R}^3)$, let G be the solution to (D.38). We call $\{u, u^{\mathrm{c}}\}$ a solution to the weak transmission problem (D.24a)-(D.24b) and (D.24e), if $\mathfrak{u} = \{u, u^{\mathrm{c}} + \mathsf{G}\} \in \mathscr{H}$ and $\mathfrak{u}$ solves (D.36).

Proposition D.4. *There is a solution to Problem D.3. In view of* (D.39), (D.47) *and* (D.49) *it follows*

$$\|u\|^2_{V^1_0(\Omega;\mathbb{R}^3)} + \|u^{\mathrm{c}}\|^2_{H^1(\Omega^{\mathrm{c}};\mathbb{R}^3)} \leqslant \\ c\left(\|f\|^2_{V^0_1(\mathbb{R}^3;\mathbb{R}^3)} + \sum_{i=1}^{3}\|F_i\|^2_{L^2(\mathbb{R}^3;\mathbb{R}^3)} + \|g^0\|^2_{H^{1/2}(\Gamma;\mathbb{R}^3)}\right). \tag{D.50}$$

D.3.2 Asymptotic Behavior of the Solutions

In order to characterize the asymptotic behavior of the solution u to transmission problem D.2 for $\|x\| \to \infty$ we can apply a general result for elliptic boundary values in domains with conical boundary points (see e.g., [170, Chapter 6.4]) since the stiffness matrix $\mathscr{A}$ is constant in the unbounded set $\|x\| > R_0$ with a suitable radius $R_0 > 0$. Thereby, let $\boldsymbol{\Phi}$ denote the *fundamental matrix* in $\mathbb{R}^3$ of the differential operator

$$\mathscr{L}^0 := \mathscr{D}(-\nabla)^\top \mathscr{A}^0 \mathscr{D}(\nabla) \tag{D.51}$$

hence $\boldsymbol{\Phi}$ is given by a solution to

$$\mathscr{L}^0 \boldsymbol{\Phi}(x) = \delta(x)\mathrm{I}_3, \quad x \in \mathbb{R}^3, \tag{D.52}$$

where $\delta(x)$ is the *Dirac measure* concentrated at the origin.

Since $u \in V^{l+1}_l(\Omega;\mathbb{R}^3)$ can be regarded as a solution to the exterior Dirichlet problem in the unbounded domain $\Xi = \{x : \|x\| > R_0\}$, the asymptotic representation of such a solution for $\|x\| > R_0$ takes the form

$$u(x) = (\mathbb{D}(-\nabla)\boldsymbol{\Phi}(x)^\top)^\top a + (\mathscr{D}(-\nabla)\boldsymbol{\Phi}(x)^\top)^\top b + \widetilde{u}(x) =: \mathrm{u}(x) + \widetilde{u}(x), \tag{D.53}$$

with $\widetilde{u} \in V^{l+1}_\gamma(\Xi;\mathbb{R}^3)$. The vectors $a, b \in \mathbb{R}^6$ are coefficient columns, $\mathscr{D}(\xi)$ is matrix (9.170) and $\mathbb{D}(\xi)$ is matrix (9.174). If the right hand side f vanishes on Ξ, then u solves the homogeneous system (D.24a) in Ξ, and due to general results in [153] (see also [170, Chapter 3.6]), the remainder in (D.53) fulfills

$$\|\nabla^k_x \widetilde{u}(x)\| \leqslant c_k\,(1 + \|x\|)^{-3-k}, \quad x \in \Xi, \quad k \in \mathbb{N}^*. \tag{D.54}$$

We emphasize that the matrices (9.170) and (9.174) satisfy the relations (9.175).

Lemma D.1. *The coefficient column* $a \in \mathbb{R}^6$ *in the representation* (D.53) *is given by the integral formula*

$$a = \int_{\Omega^{\mathrm{c}}} \mathbb{D}(x) f^{\mathrm{c}}(x)\,dx + \int_{\Omega} \mathbb{D}(x) f(x)\,dx + \int_{\Gamma} \mathbb{D}(x) g^1(x)\,ds_x\,. \tag{D.55}$$

Proof. Let $\{\chi_R\} \subset C^\infty_0(\mathbb{R}^3)$ be a family of cut-off functions with $\chi_R(x) = 1$ for $\|x\| \leqslant R+1$, and $\chi_R(x) = 0$ for $\|x\| \geq R+2$. We denote simply $\chi := \chi_R$ keeping in mind that χ depends on R. Let $\{u, u^{\mathrm{c}}\}$ be a weak solution according to Definition D.1. We use (D.31) with $v = \chi\mathbb{D}_j$, where $\mathbb{D}_j$ is the j-th row of the matrix $\mathbb{D}$, and $R \geq R_0 + 2$, so that $\Omega^{\mathrm{c}} \subset B_{R-2}$. With (9.175), we obtain

$$(\mathscr{A}\mathscr{D}(\nabla)u,\mathscr{D}(\nabla)(\chi\mathbb{D}_j))_\Omega = (f^{\mathrm{c}},\mathbb{D}_j)_{\Omega^{\mathrm{c}}} + (f,\chi\mathbb{D}_j)_\Omega + (g^1,\mathbb{D}_j)_\Gamma. \tag{D.56}$$

Again due to (9.175), we have $\mathscr{D}(\nabla)(\chi\mathbb{D}_j) = -[\mathscr{D}(\nabla),\chi]\mathbb{D}_j$, thus the integrand on the left hand side of (D.56) vanishes outside the annulus $\{x \,:\, R < \|x\| < R+2\}$. Moreover we have $\chi\mathbb{D}_j = \mathbb{D}_j$ on the sphere S_R, while this expression vanishes on S_{R+2}. Thus, integration by parts leads to

$$\begin{aligned}(\mathscr{A}\mathscr{D}(\nabla)u,\mathscr{D}(\nabla)(\chi\mathbb{D}_j))_\Omega &= (\mathscr{A}\mathscr{D}(\nabla)u,\mathscr{D}(\nabla)\chi\mathbb{D}_j)_{B_{R+2}\setminus\overline{B}_R}\\ &= (\mathscr{N}u,\chi\mathbb{D}_j)_{\partial(B_{R+2}\setminus\overline{B}_R)} + (\mathscr{L}u,\chi\mathbb{D}_j)_{B_{R+2}\setminus\overline{B}_R}\\ &= (\mathscr{N}u,\mathbb{D}_j)_{S_R} + (f,\chi\mathbb{D}_j)_{B_{R+2}\setminus\overline{B}_R},\end{aligned} \tag{D.57}$$

where the Neumann operator $\mathscr{N}$ is defined in (D.23) for $n = -R^{-1}x$. We have $\mathscr{A}(x) = \mathscr{A}^0$ for $\|x\| \geq R_0$, hence it follows for $R \geq R_0$

$$\begin{aligned}(\mathscr{N}^0u,\mathbb{D}_j)_{S_R} &= (f^{\mathrm{c}},\mathbb{D}_j)_{\Omega^{\mathrm{c}}} + (g^1,\mathbb{D}_j)_\Gamma\\ &\quad + (f,\chi\mathbb{D}_j)_\Omega - (f,\chi\mathbb{D}_j)_{B_{R+2}\setminus\overline{B}_R}.\end{aligned} \tag{D.58}$$

Since $f(1+r)^{5/2} \in L^2(\Omega;\mathbb{R}^3)$ the integral $(f,\mathbb{D}_j)_\Omega$ converges and we may pass to the limit $R \to \infty$ in the right hand side of (D.58), note that the last integral in (D.58) vanishes then. To calculate the limit of the left hand side, we insert the asymptotic representation (D.53) of u into (D.58), then by (D.54), $(\mathscr{N}\tilde{u},\mathbb{D}_j)_{S_R} = O(R^{-1})$ as $R \to \infty$, and we are left with the terms $(\mathscr{N}^0\mathfrak{u},\mathbb{D}_j)_{S_R}$, which can be interpreted as a distribution with compact support applied to the C^∞ function $\mathbb{D}_j$. Here we mention that due continuity arguments in spaces of distributions, Green's formula

$$(\mathscr{L}^0\varphi,\psi)_{B_R} - (\varphi,\mathscr{L}^0\psi)_{B_R} = (\mathscr{N}^0\varphi,\psi)_{S_R} - (\varphi,\mathscr{N}^0\psi)_{S_R} \tag{D.59}$$

can be extended from $\varphi,\psi \in C^\infty(\mathbb{R}^3;\mathbb{R}^3)$ to $\varphi = \partial^\alpha\Phi_k$, where Φ_k is a column of the *fundamental solution* Φ. Then the first integral has to be replaced by $\langle\partial^\alpha\delta,\psi_k\rangle = (-1)^{|\alpha|}\partial^\alpha\psi_k(0)$. We apply this argument for $\varphi = \mathfrak{u}$, and $\psi = \mathbb{D}_j$, together with formulae (9.175), this leads to

$$\begin{aligned}\left(\mathscr{N}^0\mathfrak{u},\mathbb{D}_j\right)_{S_R} &= \left\langle\left\{\mathbb{D}(-\nabla)^\top a\mathrm{I}_3\right\}\delta,\mathbb{D}_j\right\rangle + \left\langle\left\{\mathscr{D}(-\nabla)^\top b\mathrm{I}_3\right\}\delta,\mathbb{D}_j\right\rangle\\ &= \left(\mathbb{D}(\nabla)\mathbb{D}_j^\top(x)\cdot a + \mathscr{D}(\nabla)\mathbb{D}_j(x)^\top\cdot b\right)\Big|_{x=0} = a_j,\end{aligned} \tag{D.60}$$

which leads to the result. □

In order to derive an integral formula for the coefficient vector b in the asymptotic representation (D.53), we consider problem (D.24a)-(D.24d) with the special right hand sides

$$\begin{aligned}&f^{\mathrm{c}}_{(k)}(x) = \mathscr{D}(\nabla)^\top\mathscr{A}^{\mathrm{c}}(x)e_{(k)}, \quad f_{(k)}(x) = \mathscr{D}(\nabla)^\top\mathscr{A}(x)e_{(k)},\\ &g^0_{(k)} = 0, \qquad g^1_{(k)}(x) = \mathscr{D}(n(x))^\top(\mathscr{A}^{\mathrm{c}}(x) - \mathscr{A})e_{(k)},\end{aligned} \tag{D.61}$$

where $e_{(k)}$ is the k-th unit vector in $\mathbb{R}^6$. Note that $f_{(k)}$ has a compact support contained in B_{R_0} due to the choice of the matrix $\mathscr{A}(x) = \mathscr{A}^0 + \mathscr{A}^e(x)$. The data in (D.61) arise if we replace u in the transmission problem (D.24a)-(D.24b), (D.24e) by the rows of the matrix $-\mathscr{D}(x)$. We denote the corresponding unique weak solutions to (D.24a)-(D.24d) by $\{\mathsf{Z}_{(k)}, \mathsf{Z}^{\mathfrak{c}}_{(k)}\}$. Note, that the rows of $\mathscr{D}(x)$ are solutions to the transmission problem which grow at infinity while $\{\mathsf{Z}_{(k)}, \mathsf{Z}^{\mathfrak{c}}_{(k)}\}$ decays at infinity. Since

$$\int_{\Omega^{\mathfrak{c}}} \mathbb{D}(x) f^{\mathfrak{c}}_{(k)}(x)\,dx + \int_{\Omega} \mathbb{D}(x) f_{(k)}(x)\,dx + \int_{\Gamma} \mathbb{D}(x) g^1_{(k)}(x)\,ds_x = 0 \in \mathbb{R}^6, \quad \text{(D.62)}$$

Lemma D.1 turns the asymptotic form (D.53) for the solution $\mathsf{Z}_{(k)}$ into

$$\mathsf{Z}_{(k)}(x) = (\mathscr{D}(\nabla)\boldsymbol{\Phi}(x)^\top)^\top \mathsf{P}_{(k)} + \widetilde{\mathsf{Z}}_{(k)}(x), \quad \text{(D.63)}$$

where the remainder $\widetilde{\mathsf{Z}}_{(k)}$ satisfies (D.54) and $\mathsf{P}_{(k)} (= -b)$ denotes a column of height 6. Regarding $\mathsf{Z}_{(k)}(x)$ as a column for each x, we define the 3×6-matrix $\mathsf{Z}(x) = (\mathsf{Z}_{(1)}(x), \ldots, \mathsf{Z}_{(6)}(x))$, and, analogously, $\mathsf{Z}^{\mathfrak{c}}(x)$. Hence, due to (D.61) and (9.175), the columns of the matrix

$$\zeta(x) = \mathscr{D}(x)^\top + \{\mathsf{Z}(x), \mathsf{Z}^{\mathfrak{c}}(x)\} \quad \text{(D.64)}$$

are formal solutions of the homogeneous problem (D.24a)-(D.24b), (D.24e) (as well as the columns of the matrix $\mathbb{D}(x)^\top$), although they do not belong to the energy space $\mathscr{H}$. A slight modification of the proof of Lemma D.1 (cf. [165, 172]) provides the following assertion.

Lemma D.2. *The coefficient column $b \in \mathbb{R}^6$ in* (D.53) *is given by the integral formula*

$$b = \int_{\Omega^{\mathfrak{c}}} \zeta(x)^\top f^{\mathfrak{c}}(x)\,dx + \int_{\Omega} \zeta(x)^\top f(x)\,dx + \int_{\Gamma} \zeta(x)^\top g^1(x)\,ds_x - \int_{\Gamma} \left\{ \mathscr{D}(n(x))^\top \mathscr{A}\mathscr{D}(\nabla)\zeta(x) \right\}^\top g^0(x)\,ds_x. \quad \text{(D.65)}$$

D.3.3 The Polarization Matrix and Its Properties

Rewriting the asymptotic representation (D.63) in the condensed form

$$\mathsf{Z}(x) = (\mathscr{D}(\nabla)\boldsymbol{\Phi}(x)^\top)^\top \mathsf{P} + \widetilde{\mathsf{Z}}(x), \quad \text{(D.66)}$$

there appears the matrix P of size 6×6 composed of the coefficient columns $\mathsf{P}_{(1)}, \ldots, \mathsf{P}_{(6)}$ in (D.63). As in [165, 220] and others, we call P *the polarization matrix for the elastic inclusion $\Omega^{\mathfrak{c}}$.*

By Lemma D.2 and formula (D.61) we obtain the integral representation

$$\begin{aligned}\mathsf{P} = &-\int_{\Omega^c} \Big(\mathscr{D}(x)^\top + \mathsf{Z}^c(x)\Big)^\top \mathscr{D}(\nabla)^\top \mathscr{A}^c(x)\,dx \\ &-\int_{\Omega} \Big(\mathscr{D}(x)^\top + \mathsf{Z}(x)\Big)^\top \mathscr{D}(\nabla)^\top \mathscr{A}(x)\,dx \\ &-\int_{\Gamma} \Big(\mathscr{D}(x)^\top + \mathsf{Z}(x)\Big)^\top \mathscr{D}(n(x))^\top \Big(\mathscr{A}^c(x) - \mathscr{A}(x)\Big)\,ds_x. \qquad \text{(D.67)}\end{aligned}$$

Let us transform the right hand side of (D.67). Using $\mathscr{D}(\nabla)^\top\mathscr{D}(x) = \mathrm{I}_6$ and integrating by parts, we find

$$\begin{aligned}&\int_{\Omega^c} \Big(\mathscr{A}^c(x) - \mathscr{A}^0\Big)\,dx + \int_{\Omega} \mathscr{A}^e(x)dx = \\ &\int_{\Omega^c} \Big(\mathscr{D}(\nabla)\mathscr{D}(x)^\top\Big)\Big(\mathscr{A}^c(x) - \mathscr{A}^0\Big)\,dx + \int_{\Omega} \Big(\mathscr{D}(\nabla)\mathscr{D}(x)^\top\Big)\mathscr{A}^e(x)dx = \\ &-\int_{\Omega^c} \mathscr{D}(x)^\top\mathscr{D}(\nabla)^\top\Big(\mathscr{A}^c(x) - \mathscr{A}^0\Big)\,dx - \int_{\Gamma} \mathscr{D}(x)^\top\mathscr{D}(n(x))^\top\Big(\mathscr{A}^c - \mathscr{A}^0\Big)\,ds_x \\ &-\int_{\Omega} \mathscr{D}(x)^\top\mathscr{D}(\nabla)^\top\mathscr{A}^e(x)\,dx + \int_{\Gamma} \mathscr{D}(x)^\top\mathscr{D}(n(x))^\top\mathscr{A}^e(x)\,ds_x = \\ &-\int_{\Omega^c} \mathscr{D}(x)^\top\mathscr{D}(\nabla)^\top\mathscr{A}^c(x)dx - \int_{\Omega} \mathscr{D}(x)^\top\mathscr{D}(\nabla)^\top\mathscr{A}(x)dx \\ &-\int_{\Gamma} \mathscr{D}(x)^\top\mathscr{D}(n)^\top(\mathscr{A}^c(x) - \mathscr{A}(x))ds_x. \qquad \text{(D.68)}\end{aligned}$$

The last equality holds true due to $\mathscr{D}(\nabla)^\top\mathscr{A}^0 = 0$. Since the columns of $\{\mathsf{Z},\mathsf{Z}^c\}$ are contained in $\mathscr{H}$ and fulfill definition D.1 with data given in (D.61) we may use identity (D.41) with $\{u,u^c\} = \{\mathsf{Z},\mathsf{Z}^c\} = v$ and obtain further

$$\begin{aligned}&-\int_{\Omega^c} \mathsf{Z}^{c\top}\mathscr{D}(\nabla)^\top\mathscr{A}^c\,dx - \int_{\Omega} \mathsf{Z}^\top\mathscr{D}(\nabla)^\top\mathscr{A}\,dx - \int_{\Gamma} \mathsf{Z}^\top\mathscr{D}(n)^\top\Big(\mathscr{A} - \mathscr{A}^c\Big)\,ds_x = \\ &\quad -\int_{\Omega^c} \Big(\mathscr{D}(\nabla)\mathsf{Z}^c\Big)^\top\mathscr{A}^c\mathscr{D}(\nabla)\mathsf{Z}^c\,dx - \int_{\Omega} \Big(\mathscr{D}(\nabla)\mathsf{Z}\Big)^\top\mathscr{A}\mathscr{D}(\nabla)\mathsf{Z}\,dx. \qquad \text{(D.69)}\end{aligned}$$

Thus, we have another integral representation of the polarization matrix

$$\begin{aligned}\mathsf{P} = &-\int_{\Omega^c} \Big(\mathscr{A}^0 - \mathscr{A}^c(x)\Big)\,dx + \int_{\Omega} \mathscr{A}^e(x)dx \\ &-\int_{\Omega} \Big(\mathscr{D}(\nabla)\mathsf{Z}\Big)^\top\mathscr{A}\mathscr{D}(\nabla)\mathsf{Z}\,dx - \int_{\Omega^c} \Big(\mathscr{D}(\nabla)\mathsf{Z}^c\Big)^\top\mathscr{A}^c\mathscr{D}(\nabla)\mathsf{Z}^c\,dx. \qquad \text{(D.70)}\end{aligned}$$

The last two matrices are Gram's matrices for the sets of vector functions $\{\mathsf{Z}_{(k)}\}$ and $\{\mathsf{Z}^c_{(k)}\}$, hence in particular, they are symmetric and nonnegative. Thus we can formulate two intrinsic properties of the polarization matrix.

Theorem D.2. *The polarization matrix* P *is always symmetric. If* $\mathscr{A}^e = 0$*, i.e.* $\mathscr{A}(x) = \mathscr{A}^0$ *everywhere in* Ω*, and* $\mathscr{A}^{\mathfrak{c}}(x) < \mathscr{A}^0$ *for* $x \in \Omega^{\mathfrak{c}}$ *then* P *is negative definite.*

D.3.4 Homogeneous Inclusion

In this section we assume that the inclusion $\Omega^{\mathfrak{c}}$ as well as the elastic space are homogeneous, i.e., $\mathscr{A}^{\mathfrak{c}}$, $\mathscr{A}$ are constant matrices. We put

$$\mathsf{Z}^{\mathfrak{c}}(x) = \mathsf{Z}^{\mathfrak{a}}(x) - \mathsf{Z}^0(x) \quad \text{and} \quad \mathsf{Z}^0(x) = \mathscr{D}(x)^\top(\mathscr{A}^{\mathfrak{c}})^{-1}(\mathscr{A} - \mathscr{A}^{\mathfrak{c}}). \tag{D.71}$$

Then the columns of $\{\mathsf{Z}, \mathsf{Z}^{\mathfrak{a}}\}$ satisfy problem (D.24a)-(D.24d) with

$$f = 0, \quad f^{\mathfrak{c}} = 0, \quad g^1 = 0, \quad g^0(x) = -\mathsf{Z}^0_{(k)}(x). \tag{D.72}$$

Applying Lemma D.2 to this problem, we derive

$$\begin{aligned} -\mathsf{P} &= \int_\Gamma \Big(\mathscr{D}(n)^\top \mathscr{A}\mathscr{D}(\nabla)\zeta\Big)^\top \mathsf{Z}^0\, ds_x \qquad\qquad (D.73)\\ &= -\int_\Gamma \Big(\mathscr{D}(n)^\top \mathscr{A}\mathscr{D}(\nabla)(\mathscr{D}^\top + \mathsf{Z})\Big)^\top \mathsf{Z}\, ds_x \\ &\quad + \int_\Gamma \Big(\mathscr{D}(n)^\top \mathscr{A}^{\mathfrak{c}}\mathscr{D}(\nabla)\big(\mathscr{D}^\top + \mathsf{Z}^{\mathfrak{a}} + \mathsf{Z}^0\big)\Big)^\top \mathsf{Z}^{\mathfrak{a}} ds_x \\ &= -\int_\Gamma \Big(\mathscr{D}(n)^\top \mathscr{A}\mathscr{D}(\nabla)\mathsf{Z}\Big)^\top \mathsf{Z}\, ds_x + \int_\Gamma \Big(\mathscr{D}(n)^\top \mathscr{A}^{\mathfrak{c}}\mathscr{D}(\nabla)\mathsf{Z}^{\mathfrak{a}}\Big)^\top \mathsf{Z}^{\mathfrak{a}} ds_x \\ &\quad - \int_\Gamma \Big(\mathscr{D}(n)^\top \mathscr{A}\Big)^\top \mathsf{Z}\, ds_x + \int_\Gamma \Big(\mathscr{D}(n)^\top \mathscr{A}^{\mathfrak{c}}\Big(\mathrm{I}_6 + (\mathscr{A}^{\mathfrak{c}})^{-1}(\mathscr{A} - \mathscr{A}^{\mathfrak{c}})\Big)\Big)^\top \mathsf{Z}^{\mathfrak{a}}\, ds_x. \end{aligned}$$

The sum of the first two integrals in the right hand side of (D.73) is equal to

$$-\int_\Omega \Big(\mathscr{D}(\nabla)\mathsf{Z}\Big)^\top \mathscr{A}\mathscr{D}(\nabla)\mathsf{Z}\, dx - \int_{\Omega^{\mathfrak{c}}} \Big(\mathscr{D}(\nabla)\mathsf{Z}^{\mathfrak{a}}\Big)^\top \mathscr{A}^{\mathfrak{c}}\, \mathscr{D}(\nabla)\mathsf{Z}^{\mathfrak{a}}\, dx \tag{D.74}$$

and gives rise to a nonpositive symmetric 6×6-matrix. The sum of the last two integrals in (D.73) coincides with

$$\begin{aligned} \int_\Gamma \Big(\mathscr{D}(n(x))^\top \mathscr{A}\Big)^\top \mathsf{Z}^0(x)\, ds_x &= \int_{\Omega^{\mathfrak{c}}} \mathscr{A}\mathscr{D}(\nabla)\mathscr{D}(x)^\top(\mathscr{A}^{\mathfrak{c}})^{-1}(\mathscr{A} - \mathscr{A}^{\mathfrak{c}})\, dx \\ &= \mathscr{A}\,(\mathscr{A}^{\mathfrak{c}})^{-1}\,(\mathscr{A} - \mathscr{A}^{\mathfrak{c}})\,\big|\Omega^{\mathfrak{c}}\big| \\ &= \mathscr{A}\,\Big[(\mathscr{A}^{\mathfrak{c}})^{-1} - \mathscr{A}^{-1}\Big]\,\mathscr{A}\,\big|\Omega^{\mathfrak{c}}\big|, \end{aligned} \tag{D.75}$$

where $\big|\Omega^{\mathfrak{c}}\big|$ denotes the volume of the domain $\Omega^{\mathfrak{c}}$. Thus we have proved the following assertion.

Theorem D.3. *If the matrix* $\mathscr{A}^{\mathrm{c}}$ *is constant and* $(\mathscr{A}^{\mathrm{c}})^{-1} < \mathscr{A}^{-1}$*, then the polarization matrix* P *is positive definite.*

Certain positivity/negativity properties of the polarization matrix P can be expressed in terms of the eigenvalues $\lambda_1, \dots, \lambda_6$ of the matrix $\mathscr{A}^{-1/2}\mathscr{A}^{\mathrm{c}}\mathscr{A}^{-1/2}$. This matrix is symmetric and positive definite, and hence $\lambda_j > 0$ and the eigenvectors $a^j \in \mathbb{R}^6$ can be normalized by the condition $\left(a^k\right)^\top a^j = \delta_{j,k}$, $j,k = 1,\dots,6$. Then the columns $b^j = \mathscr{A}^{-1/2} a^j$ satisfy the formulae

$$\mathscr{A}^{\mathrm{c}} b^j = \lambda_j \mathscr{A} b^j, \qquad \left(b^k\right)^\top \mathscr{A} b^j = \delta_{k,j}\,. \tag{D.76}$$

Theorem D.4. *The following three results holds true:*

1. *If* $\lambda_j > 1$ *then* $\left(b^j\right)^\top \mathsf{P} b^j > 0$.
2. *If* $\lambda_j < 1$ *then* $\left(b^j\right)^\top \mathsf{P} b^j < 0$.
3. *If* $\lambda_j = 1$ *then* $\left(b^j\right)^\top \mathsf{P} b^j = 0$.

Proof. The proof for each item are respectively given as follows:

1. Recalling (D.73)-(D.75), we see that $-\mathsf{P} \leqslant \left(\mathscr{A}(\mathscr{A}^{\mathrm{c}})^{-1}\mathscr{A} - \mathscr{A}\right)\left|\Omega^{\mathrm{c}}\right|$. Thus, in virtue of (D.76),

$$\begin{aligned} -\left(b^j\right)^\top \mathsf{P} b^j &\leqslant \left(b^j\right)^\top \left(\mathscr{A}(\mathscr{A}^{\mathrm{c}})^{-1}\mathscr{A} - \mathscr{A}\right) b^j \\ &= \left(b^j\right)^\top \mathscr{A}(\lambda_j^{-1} - 1) b^j \left|\Omega^{\mathrm{c}}\right| \\ &= (\lambda_j^{-1} - 1)\left|\Omega^{\mathrm{c}}\right| < 0. \end{aligned} \tag{D.77}$$

2. By (D.70), we have $\mathsf{P} \leqslant (\mathscr{A}^{\mathrm{c}} - \mathscr{A})\left|\Omega^{\mathrm{c}}\right|$ and

$$\begin{aligned} \left(b^j\right)^\top \mathsf{P} b^j &\leqslant \left(b^j\right)^\top \left(\mathscr{A}^{\mathrm{c}} - \mathscr{A}\right) b^j \left|\Omega^{\mathrm{c}}\right| \\ &= \left(b^j\right)^\top \mathscr{A}(\lambda_j - 1) b^j \left|\Omega^{\mathrm{c}}\right| \\ &= (\lambda_j - 1)\left|\Omega^{\mathrm{c}}\right| < 0. \end{aligned} \tag{D.78}$$

3. Repeating calculations (D.77) and (D.78), we change "< 0" for "$= 0$" to see the assertion. □

Appendix E
Compound Asymptotic Expansions for Semilinear Problems

Let Ω be a bounded domain in $\mathbb{R}^3$ with $C^{2,\alpha}$ boundary $\partial\Omega$, and Ω_ε be a singularly perturbed domain with $C^{2,\alpha}$ boundary $\partial\Omega \cup \partial\omega_\varepsilon$. The small domain ω_ε is a cavity far from the boundary $\partial\Omega$ in singularly perturbed domain Ω_ε. In the limit passage $\varepsilon \to 0$, the perturbed domain becomes punctured i.e., $\Omega \setminus \{\mathscr{O}\}$ is obtained. This means, that at the origin $\mathscr{O}$ there are singularities of solutions for the linear boundary value problems under consideration. The asymptotics of solutions to the semilinear boundary value problem in Ω_ε with the Dirichlet boundary conditions are investigated or constructed in the framework of the compound asymptotics expansions.

Condition E.1. Beside Condition 10.1 we need the following assumptions collected here in one condition:

Assumption E.1. The limit problem (10.51) has a solution $v \in C^{2,\alpha}(\Omega)$ for a certain $\alpha \in (0,1)$.

Assumption E.2. Given $v \in C^{2,\alpha}(\overline{\Omega})$, the linear problem

$$\begin{cases} -\Delta\zeta(x) - F_v'(x,v(x))\zeta(x) = G(x),\ x \in \Omega, \\ \zeta(x) = g(x),\ \ x \in \partial\Omega, \end{cases} \tag{E.1}$$

with $G \in C^{0,\alpha}(\Omega)$, $g \in C^{2,\alpha}(\partial\Omega)$ has a unique solution $\zeta \in C^{2,\alpha}(\Omega)$,

$$\|\zeta\|_{C^{2,\alpha}(\Omega)} \leqslant C\left(\|G\|_{C^{0,\alpha}(\Omega)} + \|g\|_{C^{2,\alpha}(\partial\Omega)}\right). \tag{E.2}$$

Assumption E.3. With a certain $\kappa \in (0,1)$ and for $|\eta(x)| \leqslant C$, $x \in \Omega$, the inequality $|F_{vv}(x,\eta(x))| \leqslant C|\eta(x)|^{1+\kappa}$ and the following relations are valid:

$$\begin{aligned} &|F_{vv}(x,\eta_1(x)) - F_{vv}(y,\eta_2(y))| \\ &\leqslant C\left(\|x-y\|^\alpha\left(|\eta_1(x)| + |\eta_2(y)|\right)^{1+\kappa} + |\eta_1(x)-\eta_2(y)|\left(|\eta_1(x)|^\kappa + |\eta_2(y)|^\kappa\right)\right), \end{aligned} \tag{E.3}$$

as well as

$$
\begin{aligned}
&|F_{vv}(x,\eta_1(x)) - F_{vv}(x,\eta_2(x)) - (F_{vv}(y,\eta_1(y)) - F_{vv}(y,\eta_2(y)))| \\
&\leqslant C(|\eta_1(x)-\eta_2(x)-(\eta_1(y)-\eta_2(y))|\eta_{12}(x,y)^{\kappa} \\
&+\|x-y\|^{\alpha}(|\eta_1(x)-\eta_2(x)|+|\eta_1(y)-\eta_2(y)|)\eta_{12}(x,y)^{\kappa} \\
&+F_{12}(x,y)(1+\eta_{12}(x,y))^{\kappa-1}\,, \qquad \text{(E.4)}
\end{aligned}
$$

where

$$\eta_{12}(x,y) := |\eta_1(x)|+|\eta_2(x)|+|\eta_1(y)|+|\eta_2(y)|\,, \qquad \text{(E.5)}$$

and

$$
\begin{aligned}
F_{12}(x,y) :=\ & (|\eta_1(x)-\eta_2(x)|+|\eta_1(y)-\eta_2(y)|) \\
\times\ & (|\eta_1(x)-\eta_2(y)|+|\eta_1(y)-\eta_2(y)|)\,, \qquad \text{(E.6)}
\end{aligned}
$$

with C standing for a positive constant that may change from place to place but never depends on ε. We recall the norm in the *Hölder space* $C^{l,\alpha}(\Omega)$:

$$
\begin{aligned}
\|\zeta\|_{C^{l,\alpha}(\Omega)} =\ & \sum_{k=0}^{l}\sup_{x\in\Omega}\|\nabla_x^k\zeta(x)\| \\
&+ \sup_{x,y\in\Omega,\|x-y\|<\frac{\|x\|}{2}} \|x-y\|^{-\alpha}\|\nabla_x^l\zeta(x)-\nabla_y^l\zeta(y)\|\,. \qquad \text{(E.7)}
\end{aligned}
$$

Here $l\in\{0,1,...\}$ and $\alpha\in(0,1)$.

E.1 Linearized Problem in Weighted Hölder Spaces

In Chapter 10 the approximate solutions to problem (10.49) are constructed by the method of compound asymptotic expansions and for a given shape functional (10.84), the first order expansion with respect to ε is formally obtained, namely,

$$\mathscr{J}_{\Omega_\varepsilon}(u_\varepsilon) = \mathscr{J}_{\Omega}(v) + \varepsilon\mathscr{T}(\widehat{x}) + o(\varepsilon)\,, \qquad \text{(E.8)}$$

where $\mathscr{T}(\widehat{x})$ is the topological derivative (10.96) of the shape functional (10.2) in the three spatial dimensions at an arbitrary point $\widehat{x}\in\Omega$ far from the boundary $\partial\Omega$.

In this appendix the proof of the asymptotic approximation (E.8) is given in the scale of weighted Hölder spaces [99, 213]. This means that the remainder $\widetilde{u}_\varepsilon(x)$ of the approximation (10.73) is estimated in the weighted Hölder spaces by an application of the Banach fixed point theorem to the nonlinear boundary value problem (10.80). Namely, the obtained estimate for the solutions to (10.73) shows that the constructed approximation (10.74) is sufficiently precise to replace the exact solution in (10.84) by its approximation, and in this way derive expansion (E.8) of the shape functional under consideration.

The regular correctors in the asymptotic approximation of solutions to (10.49) are given by solutions of the linearized problem (E.1). In particular, for an appropriate choice of source terms, the solution to (E.1) is named the adjoint state. The adjoint state is introduced in order to simplify the expression obtained for the topological derivative. Since the solutions to the linearized equation are considered in the punctured domain, the solutions admit singularities at the origin, and the *a priori* estimates for the solutions to (E.1) can be established in the weighted spaces, introduced in the scale of Sobolev spaces in bounded domains by Kondratiev in his famous paper [117]. We use however, the weighted Hölder spaces and the results given in [152]. Weighted Hölder spaces are employed to analyze the solvability of linearized boundary value problems introduced in Chapter 10.

Definition E.1. Let $C_c^\infty(\overline{\Omega} \setminus \{\mathcal{O}\})$ be the set of smooth functions vanishing in the vicinity of $\mathcal{O}$. The *weighted Hölder spaces* $\Lambda_\beta^{l,\alpha}(\Omega)$ are defined [152] as the closure of $C_c^\infty(\overline{\Omega} \setminus \{\mathcal{O}\})$ in the norm

$$\begin{aligned} \|\zeta\|_{\Lambda_\beta^{l,\alpha}(\Omega)} &= \sum_{k=0}^{l} \sup_{x\in\Omega} \|x\|^{\beta-l-\alpha+k} \|\nabla_x^k \zeta(x)\| \\ &+ \sup_{x,y\in\Omega, \|x-y\|<\frac{\|x\|}{2}} \|x\|^\beta \|x-y\|^{-\alpha} \|\nabla_x^l \zeta(x) - \nabla_y^l \zeta(y)\| . \end{aligned} \tag{E.9}$$

Here $l \in \{0,1,...\}, \alpha \in (0,1)$ and $\beta \in \mathbb{R}$.

We recall the classic results on solvability of linear elliptic problems in the scale of weighted spaces given in [152]. Assumption E.2 assures the existence and uniqueness of classical solutions to the linearized problem in Hölder spaces $C^{2,\alpha}(\Omega)$ with the a priori estimate (E.2). It turns out that the linear mapping for problem (E.1)

$$S : \{G, g\} \longmapsto V \tag{E.10}$$

is an isomorphism in the Hölder spaces $C^{0,\alpha}(\Omega) \times C^{2,\alpha}(\partial\Omega) \to C^{2,\alpha}(\Omega)$. By a general result found in [152], the operator remains to be an isomorphism in the weighted Hölder spaces under a proper choice of indices (see also [170, Chapters 3 and 4]).

Theorem E.1. *Under Assumptions E.2 and 10.1, the mapping* (E.10) *considered in the weighted Hölder spaces*

$$S : \Lambda_\beta^{0,\alpha}(\Omega) \times C^{2,\alpha}(\partial\Omega) \longmapsto \Lambda_\beta^{2,\alpha}(\Omega) \tag{E.11}$$

is an isomorphism if and only if $\beta - \alpha \in (2,3)$.

The following result on asymptotics is due to [117, 152] (see also [150] and, e.g., [170, Chapters 3 and 4]).

Theorem E.2. *If the right hand side* G *in* (E.1) *belongs to* $\Lambda_\gamma^{0,\alpha}(\Omega)$ *and* $\gamma - \alpha \in (1,2)$, *then the solution* V *to* (E.1) *can be decomposed as* $V(x) = V(\mathcal{O}) + \widetilde{V}(x)$ *and the following estimate holds*

$$|V(\mathscr{O})| + \|\widetilde{V}\|_{\Lambda^{2,\alpha}_{\gamma}(\Omega)} \leqslant C\left(\|G\|_{\Lambda^{0,\alpha}_{\gamma}(\Omega)} + \|g\|_{C^{2,\alpha}(\partial\Omega)}\right). \tag{E.12}$$

An assertion, similar to Theorem E.1, is valid for the perforated domain Ω_ε as well. The following result is due to [146] (see also [148, Section 2.4] and [170, Chapter 6]).

Theorem E.3. *Under Assumptions E.2 and 10.1, the linearized problem*

$$\begin{cases} -\Delta V^\varepsilon(x) - F'_v(x,v(x))V^\varepsilon(x) = G^\varepsilon(x),\ x \in \Omega_\varepsilon, \\ \qquad\qquad\qquad\qquad\quad V^\varepsilon(x) = g^\varepsilon(x),\ \ x \in \partial\Omega_\varepsilon, \end{cases} \tag{E.13}$$

is uniquely solvable and the solution operator

$$S_\varepsilon : \{G^\varepsilon, g^\varepsilon\} \to v^\varepsilon \tag{E.14}$$

is bounded in the weighted Hölder spaces

$$S_\varepsilon : \Lambda^{0,\alpha}_{\beta}(\Omega_\varepsilon) \times \Lambda^{2,\alpha}_{\beta}(\partial\Omega_\varepsilon) \to \Lambda^{2,\alpha}_{\beta}(\Omega_\varepsilon). \tag{E.15}$$

Moreover, in the case $\beta - \alpha \in (2,3)$ the estimate

$$\|V^\varepsilon\|_{\Lambda^{2,\alpha}_{\beta}(\Omega_\varepsilon)} \leqslant C_\beta \left(\|G^\varepsilon\|_{\Lambda^{0,\alpha}_{\beta}(\Omega_\varepsilon)} + \|g^\varepsilon\|_{\Lambda^{2,\alpha}_{\beta}(\partial\Omega_\varepsilon)}\right) \tag{E.16}$$

is valid, where the constant C_β is independent of $\varepsilon \in (0, \varepsilon_0]$.

Remark E.1. Since $\|x\| \geqslant C\varepsilon > 0$ in Ω_ε, the weighted norm $\|\cdot\|_{\Lambda^{2,\alpha}_{\beta}(\Omega_\varepsilon)}$ is equivalent to the usual norm $\|\cdot\|_{C^{2,\alpha}(\Omega_\varepsilon)}$. However, the equivalence constants depend on ε. Thus $\Lambda^{2,\alpha}_{\beta}(\Omega_\varepsilon)$ and $C^{2,\alpha}(\Omega_\varepsilon)$ coincide algebraically and topologically but are normed in different way. The norm of operator S_ε is uniformly bounded for $\varepsilon \in (0, \varepsilon_0]$ for any β, although the constant C_β in (E.16) depends on ε provided $\beta \notin (2,3)$. That is, the norm of the inverse operator is uniformly bounded in $\varepsilon \in (0, \varepsilon_1]$ only in the case of $\beta \in (2,3)$.

For the nonlinear boundary value problem (10.49), we shall use the classical solutions, which means that for given $F \in C^{0,\alpha}(\overline{\Omega} \times \mathbb{R})$, $\alpha \in (0,1)$, the solutions lives in $C^{2,\alpha}(\overline{\Omega})$. We refer to [72] and [124] for a result on the existence and uniqueness of solutions to semilinear elliptic boundary value problems. It means, in particular, that problem (10.49) admits the unique solution $u_\varepsilon \in C^{2,\alpha}(\Omega_\varepsilon)$ for some $0 < \alpha < 1$ and for all $\varepsilon \in [0, \varepsilon_0)$.

E.2 Estimates for the Remainders

The method of compound asymptotic expansions is described in Chapter 10 in application to the singular perturbations of the semilinear elliptic boundary value problem leading to (10.49). For the solution u_ε to the perturbed boundary value problem we have proposed the expansion (10.72), where v, w, v' and $\widetilde{u}_\varepsilon$ are solutions to (10.51), (10.57), (10.71) and (10.80), respectively. We recall that v and v' are components of regular type, w is a boundary layer and $\widetilde{u}_\varepsilon \in \Lambda_\beta^{2,\alpha}(\Omega_\varepsilon)$ is the remainder which we are going to estimate, by showing that it is of order $o(\varepsilon)$ in the sense to be precised. Therefore, the functions v and v' are defined in Ω and depend on the spatial variable x. The boundary layer term w depends on the fast variable $\xi = \varepsilon^{-1}x$, thus w is given by a solution of an exterior boundary value problem in $\mathbb{R}^3 \setminus \overline{\varpi}$. The remainder $\widetilde{u}_\varepsilon$ is defined in the domains Ω_ε depending on the parameter $\varepsilon \to 0$.

We are going to employ the Banach contraction principle and, thus, we need to estimate the norms of $\widetilde{u}_\varepsilon$. Owing to (10.80), $x \mapsto g_\Omega^\varepsilon(x) = -w(\varepsilon^{-1}x) - c\varepsilon\phi(x)$ is smooth function on the boundary $\partial\Omega$, where $\|x\| \geqslant C > 0$, and

$$|w(\varepsilon^{-1}x) + c\varepsilon\phi(x)| \leqslant C\varepsilon^2\|x\|^{-2} \leqslant C\varepsilon^2 , \tag{E.17}$$

with $w(\varepsilon^{-1}x)$ given by (10.65) and $\phi(x)$ standing for the fundamental solution in $\mathbb{R}^3$, and

$$\|\nabla_x^k w(\varepsilon^{-1}x) + c\varepsilon\nabla_x^k\phi(x)\| \leqslant C\varepsilon^{-k}\varepsilon^{2+k}\|x\|^{-2-k} = C\varepsilon^2\|x\|^{-2-k} \leqslant C\varepsilon^2 . \tag{E.18}$$

The above inequalities for $x \mapsto g_\Omega^\varepsilon(x)$ lead to the following estimates of the norm of g_Ω^ε in the weighted Hölder space:

$$\|g_\Omega^\varepsilon\|_{\Lambda_\beta^{2,\alpha}(\partial\Omega)} \leqslant C\|g_\Omega^\varepsilon\|_{C^{2,\alpha}(\partial\Omega)} \leqslant C\|g_\Omega^\varepsilon\|_{C^3(\partial\Omega)} \leqslant C\varepsilon^2. \tag{E.19}$$

Moreover, owing again to (10.80), $x \mapsto g_\omega^\varepsilon(x) = -v(x) + v(\mathscr{O}) - \varepsilon v'(x)$ is smooth function on the boundary $\partial\omega$, we have, for $\beta - \beta' > 0$,

$$\begin{aligned}
\|g_\omega^\varepsilon\|_{\Lambda_\beta^{2,\alpha}(\partial\Omega)} &\leqslant C\Bigg(\sup_{x\in\partial\omega_\varepsilon}\sum_{k=0}^{2}\|x\|^{\beta-2-\alpha+k}\Big(\|\nabla_x^k(v(x)-v(\mathscr{O}))\| + \varepsilon\|\nabla_x^k v'(x)\|\Big)\\
&+ \sup_{x,y\in\partial\omega_\varepsilon}\|x\|^\beta\|x-y\|^{-\alpha}\left(\|\nabla_x^2 v(x) - \nabla_y^2 v(y)\| + \varepsilon\|\nabla_x^2 v'(x) - \nabla_y^2 v'(y)\|\right)\Bigg)\\
&\leqslant C\left(\varepsilon^{\beta-1-\alpha}\|v\|_{C^{2,\alpha}(\Omega)} + \varepsilon^{1+\beta-\beta'}\|v'\|_{\Lambda_{\beta'}^{2,\alpha}(\Omega)}\right) .
\end{aligned} \tag{E.20}$$

Notice that $v' \in \Lambda_{\beta'}^{2,\alpha}(\partial\Omega)$ with arbitrary $\beta' \in (2+\alpha, 3+\alpha)$, we shall further select the indices β and β' in an appropriate way. Let us denote

$$F_{vv}(x,V(x)) := F(x,v(x)+V(x)) - F(x,v(x)) - V(x)F_v'(x,v(x)) , \tag{E.21}$$

so that

$$\begin{aligned}
F^\varepsilon(x;\widetilde{u}_\varepsilon) = &\ F_{vv}(x, w(\varepsilon^{-1}x) + \varepsilon v'(x) + \widetilde{u}_\varepsilon(x))\\
&+ (w(\varepsilon^{-1}x) + \varepsilon c\phi(x) + \widetilde{u}_\varepsilon(x))F_v'(x,v(x)) .
\end{aligned} \tag{E.22}$$

Since $F_v' \in C^{0,\alpha}(\Omega \times \mathbb{R})$, by Assumption 10.1, we take into account representation (10.62) together with the inequality $\beta - \alpha > 2$ and, as a result, we obtain

$$\begin{aligned}
&\|(w+\varepsilon c\phi)F_v'\|_{\Lambda_\beta^{0,\alpha}(\Omega_\varepsilon)} \\
&\leqslant C\varepsilon^2 \left(\sup_{x\in\Omega_\varepsilon} \|x\|^{\beta-\alpha}\|x\|^{-2} + \sup_{x,y\in\Omega_\varepsilon, \|x-y\|<\|x\|/2} \|x\|^{\beta}\|x-y\|^{1-\alpha}\|x\|^{-3} \right) \\
&\leqslant C\varepsilon^2 \sup_{x\in\Omega_\varepsilon} \left(\|x\|^{\beta-\alpha}\|x\|^{-2} + \|x\|^{\beta+1-\alpha}\|x\|^{-3} \right) \leqslant C\varepsilon^2 . \qquad \text{(E.23)}
\end{aligned}$$

To estimate the first term on the right-hand side of (E.22), we need the Assumption E.3 which states that the mapping F_{vv} enjoys the Hölder continuity in two variables and has a power-law growth in the second variable. Moreover, the second order difference satisfies estimate given by Assumption E.3.

Lemma E.1. *Let* $V \in \Lambda_\beta^{2,\alpha}(\Omega_\varepsilon)$ *and* $\beta - \alpha \in (2,3), \alpha \in (0,1), \kappa \in (0,1)$. *Then, for* $x \in \Omega_\varepsilon$ *and* $\|x-y\| < \|x\|/2$*, the estimates*

$$\|x\|^{\beta-\alpha}|V(x)|^{1+\kappa} \leqslant C\|V\|^{1+\kappa}_{\Lambda_\beta^{2,\alpha}(\Omega_\varepsilon)} , \qquad \text{(E.24)}$$

$$\|x\|^{\beta-(\beta-\alpha)\frac{\kappa}{1+\kappa}}\|x-y\|^{-\alpha}|V(x)-V(y)|^{1+\kappa} \leqslant C\|V\|^{1+\kappa}_{\Lambda_\beta^{2,\alpha}(\Omega_\varepsilon)} \qquad \text{(E.25)}$$

are valid. In addition, under the same restrictions on α, β, κ *and* x, y *as above*

$$\|x\|^{\beta-\alpha}|w(\varepsilon^{-1}x)|^{1+\kappa} \leqslant C\varepsilon^{1+\kappa} , \qquad \text{(E.26)}$$

$$\|x\|^{\beta-(\beta-\alpha)\frac{\kappa}{1+\kappa}}\|x-y\|^{-\alpha}|w(\varepsilon^{-1}x)-w(\varepsilon^{-1}y)|^{1+\kappa} \leqslant C\varepsilon . \qquad \text{(E.27)}$$

Proof. First, we readily show the first assertion:

$$\begin{aligned}
\|x\|^{\beta-\alpha}|V(x)|^{1+\kappa} &\leqslant \|x\|^{\beta-\alpha}\|x\|^{-(1+\kappa)(\beta-2-\alpha)}(\|x\|^{\beta-2-\alpha}|V(x)|)^{1+\kappa} \\
&\leqslant \|x\|^{2-\kappa(\beta-2-\alpha)}\|V\|^{1+\kappa}_{\Lambda_\beta^{2,\alpha}(\Omega_\varepsilon)} . \qquad \text{(E.28)}
\end{aligned}$$

The second inequality follows from the relation

$$2-\kappa(\beta-2-\alpha) \geqslant 2-1(3-2-\alpha) > 1 > 0 . \qquad \text{(E.29)}$$

Since

$$\frac{1}{2}\|x\| < \|y\| < \frac{3}{2}\|x\| , \qquad \text{(E.30)}$$

in view of

$$\|x-y\| < \frac{\|x\|}{2} , \qquad \text{(E.31)}$$

and using the Newton-Leibnitz formula, we conclude that

$$\begin{aligned}
&\|x\|^{\beta-(\beta-\alpha)\frac{\kappa}{1+\kappa}}\|x-y\|^{-\alpha}|V(x)-V(y)|^{1+\kappa} \\
&\leqslant C\|x\|^{\beta-(\beta-\alpha)\frac{\kappa}{1+\kappa}}\|x-y\|^{-\alpha}\|x\|^{-\beta+1+\alpha}\|x-y\|\sup_{x\in\Omega_\varepsilon}\left(\|x\|^{\beta-1-\alpha}\|\nabla_x V(x)\|\right) \\
&\leqslant C\|x\|^{\beta-(\beta-\alpha)\frac{\kappa}{1+\kappa}}\|x\|^{1-\alpha}\|x\|^{-\beta+1+\alpha}\|V\|_{\Lambda^{2,\alpha}_\beta(\Omega_\varepsilon)}\,,
\end{aligned} \tag{E.32}$$

while applying the inequalities

$$\begin{aligned}
&\beta-(\beta-\alpha)\frac{\kappa}{1+\kappa}+1-\alpha-\beta+1+\alpha \\
&=2-(\beta-\alpha)\frac{\kappa}{1+\kappa}\geqslant\frac{2-(\beta-\alpha-2)\kappa}{1+\kappa}>0\,.
\end{aligned} \tag{E.33}$$

Based on the assumptions $\beta-\alpha>2$ and $1+\kappa<2$, we prove the second assertion. We have

$$\begin{aligned}
\|x\|^{\beta-\alpha}|w(\varepsilon^{-1}x)|^{1+\kappa} &\leqslant C\|x\|^{\beta-\alpha}(1+\|\varepsilon^{-1}x\|)^{-1-\kappa} \\
&=C\varepsilon^{1+\kappa}\frac{\|x\|^{\beta-\alpha}}{(\varepsilon+\|x\|)^{1+\kappa}}\leqslant C\varepsilon^{1+\kappa}\,.
\end{aligned} \tag{E.34}$$

Owing to the estimate $|\wp(\xi)|\leqslant C(1+\|\xi\|)^{-1}$ for the *capacity potential*, it follows that

$$\begin{aligned}
&\|x\|^{\beta-(\beta-\alpha)\frac{\kappa}{1+\kappa}}\|x-y\|^{-\alpha}|w(\varepsilon^{-1}x)-w(\varepsilon^{-1}y)| \\
&\leqslant C\|x\|^{\beta-(\beta-\alpha)\frac{\kappa}{1+\kappa}}\|x-y\|^{-\alpha}\|\varepsilon^{-1}x-\varepsilon^{-1}y\|(1+\|\varepsilon^{-1}x\|)^{-2}\sup_{\xi\in\mathbb{R}^3\setminus\overline{\omega}}c(\xi) \\
&\leqslant C\varepsilon\|x\|^{\beta-(\beta-\alpha)\frac{\kappa}{1+\kappa}}\|x\|^{1-\alpha}(\varepsilon+\|x\|)^{-2}\leqslant C\varepsilon\,,
\end{aligned} \tag{E.35}$$

where $c(\xi)=(1+\|\xi\|)^2\|\nabla_\xi w(\xi)\|$. Indeed, in the second inequality we have used that

$$\|\nabla_\xi\wp(\xi)\|\leqslant C(1+\|\xi\|)^{-2}\quad\text{and}\quad\beta-\alpha-(\beta-\alpha)\frac{\kappa}{1+\kappa}=\frac{\beta-\alpha}{1+\kappa}\geqslant 1\,, \tag{E.36}$$

and in the first one we applied again the Newton-Leibnitz formula. □

We now list the necessary estimates based on Assumption E.3 and Lemma E.1. We start with the boundedness of the first term in (E.22) multiplied by a weight. We obtain

$$\begin{aligned}
&\|x\|^{\beta-\alpha}\|F_{vv}(x,w(\varepsilon^{-1}x)+\varepsilon v'(x)+\widetilde{u}_\varepsilon(x))| \\
&\leqslant C\|x\|^{\beta-\alpha}\left(|w(\varepsilon^{-1}x)|^{1+\kappa}+\varepsilon^{1+\kappa}|v'(x)|^{1+\kappa}+|\widetilde{u}_\varepsilon(x)|^{1+\kappa}\right) \\
&\leqslant C\left(\varepsilon^{1+\kappa}+\|\widetilde{u}_\varepsilon\|^{1+\kappa}_{\Lambda^{2,\alpha}_\beta(\Omega_\varepsilon)}\right)\,.
\end{aligned} \tag{E.37}$$

We verify the boundedness of the weighted difference, namely,

$$
\begin{aligned}
&\|x\|^{\beta}\|x-y\|^{-\alpha}|F_{vv}(x,\overbrace{w(\varepsilon^{-1}x)+\varepsilon v'(x)+\widetilde{u}_{\varepsilon}(x)}^{V(x)})-F_{vv}(y,V(y))|\\
&\leqslant C\|x\|^{\beta}\left(|V(x)|^{1+\kappa}+\|x-y\|^{-\alpha}|V(x)-V(y)|(|V(x)|^{\kappa}+|V(y)|^{\kappa})\right)\\
&\leqslant C\left(\varepsilon^{1+\kappa}+\|\widetilde{u}_{\varepsilon}\|^{1+\kappa}_{\Lambda^{2,\alpha}_{\beta}(\Omega_{\varepsilon})}\right)\\
&+C\left(\varepsilon^{\kappa}+\|\widetilde{u}_{\varepsilon}\|^{\kappa}_{\Lambda^{2,\alpha}_{\beta}(\Omega_{\varepsilon})}\right)\|x\|^{\beta-(\beta-\alpha)\frac{\kappa}{1+\kappa}}\|x-y\|^{-\alpha}\eta_{\varepsilon}(x,y)\\
&\leqslant C\left(\varepsilon^{1+\kappa}+\|\widetilde{u}_{\varepsilon}\|^{1+\kappa}_{\Lambda^{2,\alpha}_{\beta}(\Omega_{\varepsilon})}\right),
\end{aligned}
\tag{E.38}
$$

where we denote

$$
\eta_{\varepsilon}(x,y):=|w(\varepsilon^{-1}x)-w(\varepsilon^{-1}y)|+\varepsilon|v'(x)-v'(y)|+|\widetilde{u}_{\varepsilon}(x)-\widetilde{u}_{\varepsilon}(y)|. \tag{E.39}
$$

Now, we deduce the local Lipschitz continuity of the first part of mapping (E.22):

$$
\begin{aligned}
&\|x\|^{\beta-\alpha}|F_{vv}(x,\overbrace{w(\varepsilon^{-1}x)+\varepsilon v'(x)+\widetilde{u}^{(1)}_{\varepsilon}(x)}^{V_1(x)})-F_{vv}(x,\overbrace{w(\varepsilon^{-1}x)+\varepsilon v'(x)+\widetilde{u}^{(2)}_{\varepsilon}(x)}^{V_2(x)})|\\
&\leqslant C\|x\|^{\beta-\alpha}|\widetilde{u}^{(1)}_{\varepsilon}(x)-\widetilde{u}^{(2)}_{\varepsilon}(x)|(|V_1(x)|^{\kappa}+|V_2(x)|^{\kappa})\\
&\leqslant C\|\widetilde{u}^{(1)}_{\varepsilon}-\widetilde{u}^{(2)}_{\varepsilon}\|_{\Lambda^{2,\alpha}_{\beta}(\Omega_{\varepsilon})}\left(\varepsilon^{\kappa}+\|\widetilde{u}^{(1)}_{\varepsilon}\|^{\kappa}_{\Lambda^{2,\alpha}_{\beta}(\Omega_{\varepsilon})}+\|\widetilde{u}^{(2)}_{\varepsilon}\|^{\kappa}_{\Lambda^{2,\alpha}_{\beta}(\Omega_{\varepsilon})}\right).
\end{aligned}
\tag{E.40}
$$

Finally, we prove the local Lipschitz continuity for the weighted second order differences of the mapping F_{vv}. For example, the first term on the right-hand side of (E.4) gets the bound

$$
\begin{aligned}
&C\|x\|^{\beta-(\beta-\alpha)\frac{\kappa}{1+\kappa}}\|x-y\|^{-\alpha}|\widetilde{V}_{12}(x,y)|\left(\varepsilon^{\kappa}+\|\widetilde{u}^{(1)}_{\varepsilon}\|_{\Lambda^{2,\alpha}_{\beta}(\Omega_{\varepsilon})}+\|\widetilde{u}^{(2)}_{\varepsilon}\|_{\Lambda^{2,\alpha}_{\beta}(\Omega_{\varepsilon})}\right)\\
&\leqslant C\|\widetilde{u}^{(1)}_{\varepsilon}-\widetilde{u}^{(2)}_{\varepsilon}\|_{\Lambda^{2,\alpha}_{\beta}(\Omega_{\varepsilon})}\left(\varepsilon^{\kappa}+\|\widetilde{u}^{(1)}_{\varepsilon}\|^{\kappa}_{\Lambda^{2,\alpha}_{\beta}(\Omega_{\varepsilon})}\right),
\end{aligned}
\tag{E.41}
$$

where we denote

$$
\widetilde{V}_{12}(x,y):=(V_1(x)-V_2(x))-(V_1(y)-V_2(y)). \tag{E.42}
$$

Other two terms in (E.4) are estimated in the same way as in (E.2) and (E.16), respectively.

The above estimates allow us to apply the Banach fixed point theorem to verify the existence of the remainder $\widetilde{u}_{\varepsilon}$. To this end, we rewrite problem (10.80) in the form of an abstract equation in the Banach space $\mathscr{R}=\Lambda^{2,\alpha}_{\beta}(\Omega_{\varepsilon})$, namely,

$$
\widetilde{u}_{\varepsilon}=\mathfrak{G}\widetilde{u}_{\varepsilon}\,, \tag{E.43}
$$

where

$$\mathfrak{G}\widetilde{u}_\varepsilon = S_\varepsilon(F^\varepsilon(\cdot;\widetilde{u}_\varepsilon), g^\varepsilon_\Omega, g^\varepsilon_\omega) \tag{E.44}$$

and S_ε denotes isomorphism (E.14). Let $\widetilde{u}_\varepsilon$ belong to the ball $\mathscr{B} \subset \mathscr{R}$ of radius $R\varepsilon^{1+\kappa}$, where R is a constant independent of ε. We further need to verify two properties. First, that the mapping $\mathfrak{G}$ maps the ball $\mathscr{B}$ into itself,

$$\mathscr{B} \ni \widetilde{u}_\varepsilon \Rightarrow \mathfrak{G}\widetilde{u}_\varepsilon \in \mathscr{B}\,, \tag{E.45}$$

and, second, that the mapping is a strict contraction in the ball, i.e.,

$$\|\mathfrak{G}V - \mathfrak{G}W\|_{\mathscr{R}} \leqslant k\|V - W\|_{\mathscr{R}}\,, \quad V, W \in \mathscr{B} \subset \mathscr{R} \text{ with } k < 1\,. \tag{E.46}$$

By (E.19), (E.20), (E.23) and (E.2), (E.16), we have

$$\begin{aligned}\|\mathfrak{G}\widetilde{u}_\varepsilon\|_{\mathscr{R}} &\leqslant C\left(\|F^\varepsilon\|_{\Lambda^{0,\alpha}_\beta(\Omega_\varepsilon)} + \|g^\varepsilon_\Omega\|_{\Lambda^{2,\alpha}_\beta(\Omega_\varepsilon)} + \|g^\varepsilon_\omega\|_{\Lambda^{2,\alpha}_\beta(\Omega_\varepsilon)}\right)\\ &\leqslant C\left(\varepsilon^{1+\kappa} + \|\widetilde{u}_\varepsilon\|^{1+\kappa}_{\mathscr{R}} + \varepsilon^2 + \varepsilon^{\beta-1-\alpha} + \varepsilon^{1+\beta-\beta'}\right)\,.\end{aligned} \tag{E.47}$$

Let us fix β, α and β', κ such that

$$(1,2) \ni \beta - \alpha - 1 \geqslant 1 + \kappa\,, \tag{E.48}$$

and

$$\beta - \beta' \geqslant \kappa\,. \tag{E.49}$$

Recall that $\beta - \alpha$ and $\beta' - \alpha$ belong to the interval $(2,3)$. Thus, to satisfy (E.49), we must put $\beta - \alpha$ near 3 (satisfying (E.48) as well) and $\beta' - \alpha$ near 2. This allows to create a gap of any length $\kappa \in (0,1)$. If (E.48) and (E.49) hold true, we obtain

$$\|\mathfrak{G}\widetilde{u}_\varepsilon\|_{\mathscr{R}} \leqslant C\left(4\varepsilon^{1+\kappa} + \|\widetilde{u}_\varepsilon\|^{1+\kappa}_{\mathscr{R}}\right) \leqslant R\varepsilon^{1+\kappa}\,, \tag{E.50}$$

while the desired inequality $R \geqslant C(4 + R^{1+\kappa}\varepsilon^{(1+\kappa)\kappa})$ is achieved by a proper choice of the constant R (e.g., $R = 5C$) and the bound for the parameter ε_0 in the condition $\varepsilon \in (0, \varepsilon_0]$. By virtue of (E.40) and (E.41), the estimate

$$\|\mathfrak{G}V - \mathfrak{G}W\|_{\mathscr{R}} \leqslant \underbrace{C\left(\varepsilon^\kappa + 2R^\kappa\varepsilon^{(1+\kappa)\kappa}\right)}_{k}\|V - W\|_{\mathscr{R}} \tag{E.51}$$

is valid. The strict inequality $k < 1$ can be achieved by diminishing, if necessary, the upper bound ε_0 for ε again.

Theorem E.4. *Let the indices* β, α *and* $\kappa \in (0,1)$ *satisfy* (E.48) *and* $\beta - 2 > \kappa$, *while Assumptions E.2 and E.3 hold true. Then there exist positive constants* R *and* ε_0 *such that for* $\varepsilon \in (0, \varepsilon_0]$, *the nonlinear problem* (10.80) *has a unique small solution* $\widetilde{u}_\varepsilon$, *namely,*

$$\|\widetilde{u}_\varepsilon\|_{\Lambda^{2,\alpha}_\beta(\Omega_\varepsilon)} \leqslant R\varepsilon^{1+\kappa}\,. \tag{E.52}$$

Consequently, the singularly perturbed problem (10.49) *has at least one solution of the form* (10.73).

In the theorem we have proven the existence of a small remainder $\widetilde{u}_\varepsilon$ in (10.73), i.e., we have verified that problem (10.49) has a unique solution in a small ball centered at the approximate asymptotic solution. If the uniqueness of the solution $\widetilde{u}_\varepsilon$ is known, for example, F in (10.49) gives rise to a monotone operator, the remainder is unique without any smallness assumption.

Appendix F
Sensitivity Analysis for Variational Inequalities

In this section we recall an abstract result on shape differentiability of solutions to variational inequalities. The abstract result is applied to establish the first and second order differentiability of the energy functional with respect to the parameter. In our application to variational inequalities the nonpenetration unilateral condition is prescribed in the contact zone on the boundary of a rigid obstacle or on the crack. This condition is translated in the associated energy minimization problem into a cone constraints. It means that the weak solution of nonlinear boundary value problem is given by a minimization problem of the form:

$$\mathscr{J}(u) := \inf_{\varphi \in \mathscr{K} \subset \mathscr{V}} \left\{ \frac{1}{2} a(\varphi, \varphi) - l(\varphi) \right\} , \tag{F.1}$$

where we denote

- $\varphi \mapsto a(\varphi, \varphi)$ is a bilinear form on the Hilbert space $\mathscr{V}$;
- $\varphi \mapsto l(\varphi)$ is a linear form on $\mathscr{V}$;
- $\mathscr{K} \subset \mathscr{V}$ is a convex, closed subset, in our applications $\mathscr{K}$ is a cone, i.e. $\lambda \mathscr{K} \subset \mathscr{K}$ for all $\lambda > 0$;
- $u \in \mathscr{K}$ is a minimizer, hence

  $$\mathscr{J}(u) = \frac{1}{2} a(u, u) - l(u) , \tag{F.2}$$

  and the optimal value $\mathscr{J}_{\Omega}(u) := \mathscr{J}(u)$ of the minimization problem (F.1), depending on the domain of integration Ω for the space $\mathscr{V} := \mathscr{V}(\Omega)$ of functions defined in Ω, is called energy shape functional;
- $\mathscr{J}(\varphi)$ is a quadratic energy functional and the minimizer u is a weak solution of the variational inequality

  $$u \in \mathscr{K} \ : \ a(u, \varphi - u) \geqslant l(\varphi - u) \quad \forall \varphi \in \mathscr{K} , \tag{F.3}$$

- for a cone $\mathscr{K} \subset \mathscr{V}$ given by pointwise inequality constraints on a subset of Ω the minimization problem (F.1) becomes a quadratic programming problem.

If the domain of integration Ω_t is parameterized by the shape parameter t, the parametric optimization problem arises in the spaces $\mathscr{V}_t := \mathscr{V}(\Omega_t)$, thus the minimization problem also becomes parametric

$$\mathscr{J}_{\Omega_t}(u(\Omega_t)) := \inf_{\varphi \in \mathscr{K} \subset \mathscr{V}_t} \left\{ \frac{1}{2} a_{\Omega_t}(\varphi, \varphi) - l_{\Omega_t}(\varphi) \right\} . \tag{F.4}$$

There are two questions for the parametric problem (F.4):

- if the optimal value function or the energy shape functional

$$t \mapsto \mathscr{J}_{\Omega_t}(u(\Omega_t)) = \frac{1}{2} a_{\Omega_t}(u(\Omega_t), u(\Omega_t)) - l_{\Omega_t}(u(\Omega_t)) \tag{F.5}$$

  is differentiable at $t = 0^+$;
- if the minimizer

$$t \mapsto u(\Omega_t) \in \mathscr{V}_t \tag{F.6}$$

  is differentiable at $t = 0^+$;

We use throughout the book the positive answer to the first question which is obtained under strong convergence of minimizers. In Section F.1 the positive answer for the second question is obtained for a class of convex sets in the Dirichlet-Sobolev spaces.

F.1 Polyhedral Convex Sets in Sobolev Spaces of the Dirichlet Type

For the convenience of the reader we recall here the abstract result [210] which is a generalization of the implicit function theorem for variational inequalities.

Let $\mathscr{K} \subset \mathscr{V}$ be a convex and closed subset of a Hilbert space $\mathscr{V}$, and let $\langle \cdot, \cdot \rangle$ denote the duality pairing between $\mathscr{V}'$ and $\mathscr{V}$, where $\mathscr{V}'$ denotes the dual of $\mathscr{V}$. We shall consider the following family of variational inequalities depending on a parameter $t \in [0, t_0)$, $t_0 > 0$,

$$u_t \in \mathscr{K} \ : \ a_t(u_t, \varphi - u_t) \geq \langle b_t, \varphi - u_t \rangle \qquad \forall \varphi \in \mathscr{K} \ . \tag{F.7}$$

Moreover, let $u_t = \mathscr{P}_t(b_t)$ be a solution to (F.7). For $t = 0$ we denote

$$u \in \mathscr{K} \ : \ a(u, \varphi - u) \geq \langle b, \varphi - u \rangle \qquad \forall \varphi \in \mathscr{K} \ , \tag{F.8}$$

with $u = \mathscr{P}(b)$ solution to (F.8).

Theorem F.1. *Let us assume that:*

- *The bilinear form $a_t(\cdot, \cdot) : \mathscr{V} \times \mathscr{V} \to \mathbb{R}$ is coercive and continuous uniformly with respect to $t \in [0, t_0)$. Let $\mathscr{Q}_t \in \mathscr{L}(\mathscr{V}; \mathscr{V}')$ be the linear operator defined as follows*

$a_t(\phi,\varphi) = \langle \mathscr{Q}_t(\phi),\varphi\rangle \ \forall\phi,\varphi \in \mathscr{V}$; it is supposed that there exists $\mathscr{Q}' \in \mathscr{L}(\mathscr{V};\mathscr{V}')$ such that

$$\mathscr{Q}_t = \mathscr{Q} + t\mathscr{Q}' + o(t) \quad in \quad \mathscr{L}(\mathscr{V};\mathscr{V}')\,. \tag{F.9}$$

- *For $t > 0$, t small enough, the following equality holds*

$$b_t = b + tb' + o(t) \quad in \quad \mathscr{V}'\,, \tag{F.10}$$

where $b_t, b, b' \in \mathscr{V}'$.

- *The set $\mathscr{K} \subset \mathscr{V}$ is convex and closed, and for the solutions to the variational inequality*

$$\Pi b = \mathscr{P}(b) \in \mathscr{K}: \quad a(\Pi b, \varphi - \Pi b) \geq \langle b, \varphi - \Pi b\rangle \quad \forall \varphi \in \mathscr{K} \tag{F.11}$$

the following differential stability result holds

$$\forall h \in \mathscr{V}': \quad \Pi(b + sh) = \Pi b + s\Pi' h + o(s) \quad in \quad \mathscr{V} \tag{F.12}$$

for $s > 0$, s small enough, where the mapping $\Pi' : \mathscr{V}' \to \mathscr{V}$ is continuous and positively homogeneous and $o(s)$ is uniform, with respect to $h \in \mathscr{V}'$, on compact subsets of $\mathscr{V}'$.

Then the solutions to the variational inequality (F.7) *are right-differentiable with respect to t at $t = 0$, i.e. for $t > 0$, t small enough,*

$$u_t = u + tu' + o(t) \quad in \quad \mathscr{V}\,, \tag{F.13}$$

where

$$u' = \Pi'(b' - \mathscr{Q}' u)\,. \tag{F.14}$$

Let us note, that for $b_t = 0$ and $u_t = \mathscr{P}_t(0)$ we obtain $u' = \Pi'(-\mathscr{Q}'u)$.

F.2 Compactness of the Asymptotic Energy Expansion

The main result we obtain is based on the Condition 11.1 for the expansion of the Steklov-Poincaré operator with respect to the parameter ε. The expansion is established in this section by an application of elementary Fourier analysis. We consider the mapping $\mathscr{A}_\varepsilon : H^{1/2}(\Gamma_R) \mapsto H^{-1/2}(\Gamma_R)$ given in Definition 11.1. By taking into account the relation which follows by integration by parts in (11.19), we find that

$$\langle \mathscr{A}_\varepsilon(v), v\rangle_{\Gamma_R} = \int_{C(R,\varepsilon)} \|\nabla w_\varepsilon\|^2\,, \tag{F.15}$$

and for $\varepsilon > 0$, ε small enough,

$$\int_{C(R,\varepsilon)} \|\nabla w_\varepsilon\|^2 = \int_{B_R} \|\nabla w\|^2 - 2\varepsilon^2 \langle \mathscr{B}(v), v\rangle_{\Gamma_R} + O(\varepsilon^4)\,, \tag{F.16}$$

with the remainder $O(\varepsilon^4)$ uniformly bounded on bounded sets in the space $H^{1/2}(\Gamma_R)$, where w is solution to (11.19) for $\varepsilon = 0$.

By the properties of harmonic functions the second term can be represented in two spatial dimensions in the equivalent form of a line integral over the circle $\Gamma_R = \{x \in \mathbb{R}^2 : \|x - \widehat{x}\| = R\}$ with the center at the arbitrary point $\widehat{x} \in \Omega$, as given by (11.13). Therefore, we obtain the expansion

$$\mathscr{A}_\varepsilon = \mathscr{A} - 2\varepsilon^2 \mathscr{B} + O(\varepsilon^4) , \tag{F.17}$$

in the operator norm $\mathscr{L}(H^{1/2}(\Gamma_R); H^{-1/2}(\Gamma_R))$.

In order to apply the abstract results of Proposition 11.4 and Theorem F.1 to the energy functional for specific variational inequality we require the expansion of the related Steklov-Poincaré operator with an appropriate estimate for the remainder with respect to the small parameter ε. We start with the analysis of such an expansion for the Signorini problem by providing a simple proof of (F.17), which is equivalent to (F.16).

Let $\widehat{x} \in \Omega$ and B_R be a ball around $\widehat{x}$, while the ring $C(R,\varepsilon) = \{x \in \mathbb{R}^2 : \varepsilon < \|x - \widehat{x}\| < R\}$ with inner boundary ∂B_ε and outer boundary Γ_R. Additionally we use the notation $\Omega_R = \Omega \setminus \overline{B_R}$. We consider functions $v \in H^1(\Omega_R)$ with traces (still denoted by v) on Γ_R belonging to $H^{1/2}(\Gamma_R)$. The following implication is true

$$\|v\|_{H^1(\Omega_R)} \leqslant C_0 \quad \Rightarrow \quad \|v\|_{H^{1/2}(\Gamma_R)} \leqslant C_R , \tag{F.18}$$

and since R is fixed, we shall omit it, writing C instead of C_R (by C we shall denote a generic constant depending only on C_0). Finally, we denote by (r,θ) a polar coordinate system around $\widehat{x}$, which we assume that coincides with the origin $\mathscr{O}$. From the fact that $v \in H^{1/2}(\Gamma_R)$ follows the existence of the Fourier series expansion in terms of θ:

$$v(\theta) = \frac{1}{2} a_0 + \sum_{k=1}^{\infty} (a_k \sin k\theta + b_k \cos k\theta) , \tag{F.19}$$

with coefficients satisfying

$$\sum_{k=1}^{\infty} \sqrt{1+k^2}(a_k^2 + b_k^2) \leqslant C . \tag{F.20}$$

This implies two important properties for us:

$$\sum_{k=1}^{\infty} (a_k^2 + b_k^2) \leqslant C \qquad \text{and} \qquad \sum_{k=1}^{\infty} k(a_k^2 + b_k^2) \leqslant C . \tag{F.21}$$

Now we shall consider in B_R the solution of the Laplace equation with Dirichlet boundary condition on Γ_R coinciding with v, denoted by w, and the solution of the same equation in $C(R,\varepsilon)$, with the same condition on Γ_R and homogeneous Neumann condition on ∂B_ε, denoted by w_ε. We define energies

$$\mathscr{E}(v) = \int_{B_R} \|\nabla w\|^2 \qquad \text{and} \qquad \mathscr{E}_\varepsilon(v) = \int_{C(R,\varepsilon)} \|\nabla w_\varepsilon\|^2 \,, \tag{F.22}$$

which depend on v via boundary conditions. Our goal is to prove that $\mathscr{E}_\varepsilon$ has an expansion in which the remainder is uniformly bounded. More precisely this can be expressed as follows.

Theorem F.2. *The energy $\mathscr{E}_\varepsilon(v)$ admits the expansion, for $\varepsilon > 0$, ε small enough,*

$$\mathscr{E}_\varepsilon(v) = \mathscr{E}(v) - 2\varepsilon^2 \langle \mathscr{B}(v), v\rangle_{\Gamma_R} + \mathscr{R}_\varepsilon(v) \,, \tag{F.23}$$

where

$$|\mathscr{R}_\varepsilon(v)| \leqslant C\varepsilon^4 \tag{F.24}$$

uniformly on any fixed compact set in $H^1(\Omega_R)$, i.e. C depends on this set only.

Proof. Since any compact set may be covered by finite number of balls, it is enough to prove the Lemma for a fixed ball in $H^1(\Omega_R)$. We may therefore assume that (F.21) holds. The proof will consist in obtaining explicit formulas for w and w_ε as Fourier series, using the well known methods, similarly as in [204]. Then the energies may be computed exactly and the desired property of the remainder $\mathscr{R}_\varepsilon(v)$ proven. By constructing w from the Fourier series of its boundary condition we get

$$w(r,\theta) = \frac{1}{2}a_0 + \sum_{k=1}^{\infty} \left(\frac{r}{R}\right)^k (a_k \sin k\theta + b_k \cos k\theta) \,. \tag{F.25}$$

Similarly, for w_ε in $C(R,\varepsilon)$ holds

$$w_\varepsilon(r,\theta) = \frac{1}{2}a_0 + \sum_{k=1}^{\infty} \varphi_k(r)(a_k \sin k\theta + b_k \cos k\theta) \,, \tag{F.26}$$

where

$$\varphi_k(r) = A_k r^k + B_k r^{-k} \tag{F.27}$$

with A_k and B_k determined by the boundary conditions on Γ_R and ∂B_ε, namely

$$A_k R^k + B_k \frac{1}{R^k} = 1 \quad \text{and} \quad A_k \varepsilon^{k-1} - B_k \frac{1}{\varepsilon^{k+1}} = 0 \,. \tag{F.28}$$

Hence

$$A_k = \frac{R^k}{R^{2k} + \varepsilon^{2k}} \quad \text{and} \quad B_k = A_k \varepsilon^{2k} \,, \tag{F.29}$$

and finally

$$\varphi_k(r) = \frac{r^k}{R^k} + \frac{\varepsilon^{2k}}{R^{2k} + \varepsilon^{2k}} \left(\frac{R^k}{r^k} - \frac{r^k}{R^k}\right) \,. \tag{F.30}$$

Substituting this into the expansion for w_ε gives

$$w_\varepsilon(r,\theta) = w(r,\theta) + z_\varepsilon(r,\theta) \,, \tag{F.31}$$

with

$$z_\varepsilon(r,\theta) = \sum_{k=1}^{\infty} \frac{\varepsilon^{2k}}{R^{2k}+\varepsilon^{2k}} \left(\frac{R^k}{r^k} - \frac{r^k}{R^k}\right)(a_k \sin k\theta + b_k \cos k\theta) \, . \tag{F.32}$$

Therefore

$$\begin{aligned}
\mathscr{E}_\varepsilon(v) &= \int_{C(R,\varepsilon)} \|\nabla w + \nabla z_\varepsilon\|^2 \\
&= \int_{C(R,\varepsilon)} \|\nabla w\|^2 + 2\int_{C(R,\varepsilon)} \nabla w \cdot \nabla z_\varepsilon + \int_{C(R,\varepsilon)} \|\nabla z_\varepsilon\|^2 \pm \int_{B_\varepsilon} \|\nabla w\|^2 \\
&= \mathscr{E}(v) + \int_{C(R,\varepsilon)} \|\nabla z_\varepsilon\|^2 + 2\int_{C(R,\varepsilon)} \nabla w \cdot \nabla z_\varepsilon - \int_{B_\varepsilon} \|\nabla w\|^2 \\
&= \mathscr{E}(v) + \mathscr{I}_1 + \mathscr{I}_2 + \mathscr{I}_3 \, ,
\end{aligned} \tag{F.33}$$

where we define the integrals

$$\mathscr{I}_1 := \int_{C(R,\varepsilon)} \|\nabla z_\varepsilon\|^2 \, , \tag{F.34}$$

$$\mathscr{I}_2 := 2\int_{C(R,\varepsilon)} \nabla w \cdot \nabla z_\varepsilon \, , \tag{F.35}$$

$$\mathscr{I}_3 := -\int_{B_\varepsilon} \|\nabla w\|^2 \, . \tag{F.36}$$

Now we have

$$\partial_r z_\varepsilon(r,\theta) = -\sum_{k=1}^{\infty} \frac{\varepsilon^{2k}}{R^{2k}+\varepsilon^{2k}} k \frac{1}{r} \left(\frac{R^k}{r^k} + \frac{r^k}{R^k}\right)(a_k \sin k\theta + b_k \cos k\theta) \, , \tag{F.37}$$

$$\frac{1}{r}\partial_\theta z_\varepsilon(r,\theta) = \sum_{k=1}^{\infty} \frac{\varepsilon^{2k}}{R^{2k}+\varepsilon^{2k}} k \frac{1}{r} \left(\frac{R^k}{r^k} - \frac{r^k}{R^k}\right)(a_k \cos k\theta - b_k \sin k\theta) \, . \tag{F.38}$$

After taking into account the orthogonality of trigonometric functions on $[0,2\pi]$ and integrating with respect to θ one gets

$$\mathscr{I}_1 = \pi \sum_{k=1}^{\infty} \left(\frac{\varepsilon^{2k}}{R^{2k}+\varepsilon^{2k}}\right)^2 k^2 (a_k^2 + b_k^2) \mathscr{I}_k(\varepsilon) \, , \tag{F.39}$$

where the integral $\mathscr{I}_k(\varepsilon)$ is defined as

$$\begin{aligned}
\mathscr{I}_k(\varepsilon) &= \int_\varepsilon^R \left[\left(\frac{R^k}{r^{k+1}} + \frac{r^{k-1}}{R^k}\right)^2 + \left(\frac{R^k}{r^{k+1}} - \frac{r^{k-1}}{R^k}\right)^2\right] r dr \\
&= \frac{1}{k}\left(\frac{R^{2k}}{\varepsilon^{2k}} - \frac{\varepsilon^{2k}}{R^{2k}}\right) \, ,
\end{aligned} \tag{F.40}$$

which leads to

$$\begin{aligned}\mathscr{I}_1 &= \pi \sum_{k=1}^{\infty} \left(\frac{\varepsilon^{2k}}{R^{2k}+\varepsilon^{2k}} \right)^2 k(a_k^2+b_k^2) \left(\frac{R^{2k}}{\varepsilon^{2k}} - \frac{\varepsilon^{2k}}{R^{2k}} \right) \\ &= \pi\varepsilon^2 \frac{a_1^2+b_1^2}{R^2} + O(\varepsilon^4)\,. \end{aligned} \tag{F.41}$$

In order to compute the second integral $\mathscr{I}_2$ we observe that

$$\partial_r w(r,\theta) = \sum_{k=1}^{\infty} k \frac{r^{k-1}}{R^k} \left(a_k \sin k\theta + b_k \cos k\theta\right)\,, \tag{F.42}$$

$$\frac{1}{r}\partial_\theta w(r,\theta) = \sum_{k=1}^{\infty} k \frac{r^{k-1}}{R^k} \left(a_k \cos k\theta - b_k \sin k\theta\right)\,, \tag{F.43}$$

and after easy computations, we have

$$\mathscr{I}_2 = 2\pi \sum_{k=1}^{\infty} \left(\frac{\varepsilon}{R}\right)^{2k} k(a_k^2+b_k^2) \frac{R^{2k}-\varepsilon^{2k}}{R^{2k}+\varepsilon^{2k}} = -2\pi\varepsilon^2 \frac{a_1^2+b_1^2}{R^2} + O(\varepsilon^4)\,. \tag{F.44}$$

There remains the last integral $\mathscr{I}_3$, which leads to

$$\mathscr{I}_3 = -\pi \sum_{k=1}^{\infty} \left(\frac{\varepsilon}{R}\right)^{2k} k(a_k^2+b_k^2) = -\pi\varepsilon^2 \frac{a_1^2+b_1^2}{R^2} + O(\varepsilon^4)\,. \tag{F.45}$$

Finally, after collecting formulas (F.41), (F.44) and (F.45), we may single out the first terms containing ε^2 and the rest of $O(\varepsilon^4)$, namely

$$\mathscr{E}_\varepsilon(v) = \mathscr{E}(v) - 2\pi\varepsilon^2 \frac{a_1^2+b_1^2}{R^2} + O(\varepsilon^4)\,, \tag{F.46}$$

which in view of the regularity of boundary conditions and implied by the inequalities (F.21) is uniformly bounded by $C\varepsilon^4$. □

Appendix G
Tensor Calculus

In this appendix some basic results of tensor calculus are recalled, which are useful for the development presented in this monograph. We follow the book by Gurtin 1981 [82]. Let us introduce the following notation:

- $a, b, c, d, e \in \mathbb{R}^3$;
- $A, B, C, S, W \in \mathbb{R}^3 \times \mathbb{R}^3$;
- φ scalar field;
- u, v vector fields;
- T, U second order tensor fields.

G.1 Inner, Vector and Tensor Products

The scalar or inner product of two vectors a and b is defined as

$$a \cdot b = b^\top a \,, \tag{G.1}$$

with $\|a\| = (a \cdot a)^{1/2}$. The tensor A is a linear map that assigns to each vector a a vector $b = Aa$. The transpose $A^\top$ of a tensor A is the unique tensor with the property

$$a \cdot Ab = A^\top a \cdot b \,, \tag{G.2}$$

for all vectors a and b. An important tensor is the identity I defined by $\mathrm{I}a = a$ for every vector a. The product of two tensors A and B is a tensor $C = AB$. In general $AB \neq BA$. When $AB = BA$, we say that A and B commute. The scalar or inner product of two tensors A and B is defined as

$$A \cdot B = \mathrm{tr}(B^\top A) = \mathrm{tr}(A^\top B) \quad \Rightarrow \quad \mathrm{tr}(AB) = \mathrm{tr}(BA) \,, \tag{G.3}$$

where the trace of a tensor A is defined as

$$\mathrm{tr}(A) = \mathrm{I} \cdot A \,. \tag{G.4}$$

It then follows that

$$A \cdot (BC) = (B^\top A) \cdot C = (AC^\top) \cdot B \,. \tag{G.5}$$

The vector product of two vectors a and b is defined as

$$a \times b = -b \times a \,. \tag{G.6}$$

Furthermore

$$a \times a = 0 \,, \tag{G.7}$$

and

$$a \cdot (b \times c) = c \cdot (a \times b) = b \cdot (c \times a) = \mathrm{vol}(\mathfrak{P}) \,, \tag{G.8}$$

where $\mathfrak{P}$ is the parallelepiped defined by the vectors a, b and c. Finally, the determinant of a second order tensor is defined as

$$\det A = \frac{Aa \cdot (Ab \times Ac)}{a \cdot (b \times c)} \,. \tag{G.9}$$

The tensor product of two vectors a and b is a second order tensor $A = a \otimes b$ that assigns to each vector c the vector $(b \cdot c)a$, namely

$$(a \otimes b)c = (b \cdot c)a \,. \tag{G.10}$$

Then it follows that

$$(a \otimes b)^\top = (b \otimes a) \,, \tag{G.11}$$

$$(a \otimes b)(c \otimes d) = (b \cdot c)(a \otimes d) \,, \tag{G.12}$$

$$(a \otimes b) \cdot (c \otimes d) = (a \cdot c)(b \cdot d) \,, \tag{G.13}$$

$$\mathrm{tr}(a \otimes b) = a \cdot b \,, \tag{G.14}$$

$$a \cdot Ab = A \cdot (a \otimes b) \,, \tag{G.15}$$

$$A(a \otimes b) = (Aa) \otimes b \,. \tag{G.16}$$

G.2 Gradient, Divergence and Curl

Let us consider the smooth enough fields φ, u, v, T and U, where φ is scalar, u, v are vectors and T, U are tensors. Here, we do not state smoothness hypotheses, since standard differentiability assumptions sufficient to make an argument rigorous are generally obvious to mathematicians and of little interest to engineers and physicists. Then the following identities hold:

$$\nabla(\varphi u) = \varphi \nabla u + u \otimes \nabla \varphi \tag{G.17}$$
$$\operatorname{div}(\varphi u) = \varphi \operatorname{div}(u) + \nabla \varphi \cdot u \tag{G.18}$$
$$\operatorname{rot}(\varphi u) = \varphi \operatorname{rot} u + \nabla \varphi \times u \tag{G.19}$$
$$\nabla(u \cdot v) = (\nabla u)^\top v + (\nabla v)^\top u \tag{G.20}$$
$$\operatorname{div}(u \times v) = u \cdot \operatorname{rot}(v) - v \cdot \operatorname{rot}(u) \tag{G.21}$$
$$\operatorname{div}(u \otimes v) = u \operatorname{div}(v) + (\nabla u) v \tag{G.22}$$
$$\operatorname{div}(T^\top u) = \operatorname{div}(T) \cdot u + T \cdot \nabla u \tag{G.23}$$
$$\operatorname{div}(\varphi T) = \varphi \operatorname{div} T + T \nabla \varphi \tag{G.24}$$
$$\operatorname{div}(\nabla u^\top) = \nabla \operatorname{div}(u) \tag{G.25}$$
$$\operatorname{div}(TU) = (\nabla T) U + T \operatorname{div}(U) \tag{G.26}$$
$$\nabla(T \cdot U) = (\nabla T)^\top U + (\nabla U)^\top T \tag{G.27}$$

G.3 Integral Theorems

Let Ω be an open and bounded domain in $\mathbb{R}^d$, $d \geqslant 2$, whose boundary is denoted by $\partial\Omega$. Let n denote the outward unit normal vector field on the boundary $\partial\Omega$ of Ω. Here, we state the integral theorems without proofs and without smoothness assumptions regarding the underlying functions and the domain of integration as well. Then, given scalar φ, vector v and tensor T fields, the following integral identities hold:

$$\int_\Omega \nabla \varphi = \int_{\partial\Omega} \varphi\, n\,, \tag{G.28}$$
$$\int_\Omega \nabla v = \int_{\partial\Omega} v \otimes n\,, \tag{G.29}$$
$$\int_\Omega \operatorname{div}(v) = \int_{\partial\Omega} v \cdot n\,, \tag{G.30}$$
$$\int_\Omega \operatorname{div}(T) = \int_{\partial\Omega} T n\,. \tag{G.31}$$

Divergence theorems are deep mathematical results central to the derivations presented in this monograph. In particular, let us state the divergence theorems in their useful forms, namely

$$\int_\Omega (T \cdot \nabla v + \operatorname{div}(T) \cdot v) = \int_\Omega \operatorname{div}(T^\top v) = \int_{\partial\Omega} T n \cdot v\,. \tag{G.32}$$

If $T = S$, with S a symmetric tensor field ($S = S^\top$), then

$$\int_\Omega (S \cdot \nabla v^s + \operatorname{div}(S) \cdot v) = \int_\Omega \operatorname{div}(S v) = \int_{\partial\Omega} S n \cdot v\,. \tag{G.33}$$

In addition, we have

$$\int_\Omega (\varphi \mathrm{div}(v) + \nabla\varphi \cdot v) = \int_\Omega \mathrm{div}(\varphi v) = \int_{\partial\Omega} \varphi\, v \cdot n\,. \tag{G.34}$$

If $v = \nabla\phi$, with ϕ a scalar field, then

$$\int_\Omega (\varphi\Delta\phi + \nabla\varphi \cdot \nabla\phi) = \int_\Omega \mathrm{div}(\varphi\nabla\phi) = \int_{\partial\Omega} \varphi\partial_n\phi\,. \tag{G.35}$$

G.4 Some Useful Decompositions

Every tensor A can be expressed uniquely as the sum of a symmetric tensor S and a skew tensor W, namely

$$A = S + W\,, \tag{G.36}$$

where

$$S = \frac{1}{2}(A + A^\top) \quad \text{and} \quad W = \frac{1}{2}(A - A^\top)\,. \tag{G.37}$$

We call S the symmetric part of A and W the skew part of A. Therefore there is a one-to-one correspondence between vectors and skew tensors

$$Wa = w \times a, \quad \text{with} \quad w_1 = W_{32}\,, \quad w_2 = W_{13}\,, \quad w_3 = W_{21}\,, \tag{G.38}$$

where $W = -W^\top$ is a skew or anti-symmetric second order tensor. In addition,

$$[(a \otimes b) - (b \otimes a)]c = -[(a \cdot c)b - (b \cdot c)a] = -(a \times b) \times c\,. \tag{G.39}$$

Finally, we have:

- If S is symmetric,

$$S \cdot A = S \cdot A^\top = S \cdot \left[\frac{1}{2}(A + A^\top)\right]\,. \tag{G.40}$$

- If W is skew,

$$W \cdot A = -W \cdot A^\top = W \cdot \left[\frac{1}{2}(A - A^\top)\right]\,. \tag{G.41}$$

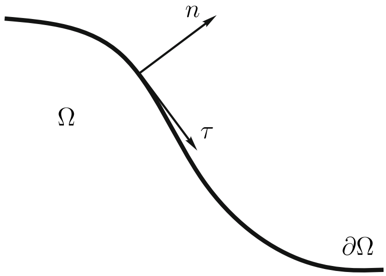
- If S is symmetric and W is skew,

$$S \cdot W = 0\,. \tag{G.42}$$

- If $A \cdot B = 0$, for every B, then $A = 0$.
- If $A \cdot S = 0$, for every S, then A is skew.
- If $A \cdot W = 0$, for every W, then A is symmetric.

Let us consider a two-dimensional open and bounded domain $\Omega \subset \mathbb{R}^2$, whose boundary is denoted by $\partial\Omega$. Let us also introduce two orthonormal vectors n and τ,

Fig. G.1 Curvilinear coordinate system on $\partial\Omega$



such that $n\cdot n = 1$, $\tau\cdot\tau = 1$ and $n\cdot\tau = 0$, defined on the boundary $\partial\Omega$, as shown in fig. G.1. Then, we have that a vector a defined on $\partial\Omega$ can be decomposed as following

$$a = (n\otimes n)a + (\tau\otimes\tau)a = (a\cdot n)n + (a\cdot\tau)\tau = a^n n + a^\tau \tau\,, \tag{G.43}$$

where $a^n := a\cdot n$ and $a^\tau := a\cdot\tau$ are the normal and tangential components of the vector a, respectively. In other words, a^τ is the projection of a into the tangential plane to Ω and a^n is the projection of a orthogonal to the referred tangent plane. In addition, the identity tensor I can be written in the basis (n,τ), namely

$$\mathrm{I} = n\otimes n + \tau\otimes\tau\,. \tag{G.44}$$

Thus, the projections operators into the tangential and normal directions can respectively be defined as

$$(\mathrm{I} - n\otimes n)a = a - (a\cdot n)n = a^\tau\tau\,, \tag{G.45}$$
$$(\mathrm{I} - \tau\otimes\tau)a = a - (a\cdot\tau)\tau = a^n n\,. \tag{G.46}$$

Let A be a second order tensor. Then, A can be decomposed in the basis (n,τ) in the following form

$$A = A^{nn}(n\otimes n) + A^{n\tau}(n\otimes\tau) + A^{\tau n}(\tau\otimes n) + A^{\tau\tau}(\tau\otimes\tau)\,, \tag{G.47}$$

whose components A^{nn}, $A^{n\tau}$, $A^{\tau n}$ and $A^{\tau\tau}$ are defined as

$$\begin{aligned} An &= [A^{nn}(n\otimes n) + A^{n\tau}(n\otimes\tau) + A^{\tau n}(\tau\otimes n) + A^{\tau\tau}(\tau\otimes\tau)]\,n \\ &= A^{nn}(n\cdot n)n + A^{n\tau}(\tau\cdot n)n + A^{\tau n}(n\cdot n)\tau + A^{\tau\tau}(\tau\cdot n)\tau \\ &= A^{nn}n + A^{\tau n}\tau \;\Rightarrow\; A^{nn} = n\cdot An \quad \text{and} \quad A^{\tau n} = \tau\cdot An\,, \end{aligned} \tag{G.48}$$

$$\begin{aligned} A\tau &= [A^{nn}(n\otimes n) + A^{n\tau}(n\otimes\tau) + A^{\tau n}(\tau\otimes n) + A^{\tau\tau}(\tau\otimes\tau)]\,\tau \\ &= A^{nn}(n\cdot\tau)n + A^{n\tau}(\tau\cdot\tau)n + A^{\tau n}(n\cdot\tau)\tau + A^{\tau\tau}(\tau\cdot\tau)\tau \\ &= A^{n\tau}n + A^{\tau\tau}\tau \;\Rightarrow\; A^{n\tau} = n\cdot A\tau \quad \text{and} \quad A^{\tau\tau} = \tau\cdot A\tau\,. \end{aligned} \tag{G.49}$$

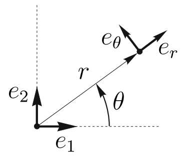


Fig. G.2 Polar coordinate system (r, θ)

In the same way, we have that the gradient of a scalar field $\nabla\varphi$ defined on $\partial\Omega$ can be decomposed as

$$\begin{aligned}\nabla\varphi &= (\nabla\varphi\cdot n)n + (\nabla\varphi\cdot\tau)\tau\\ &= (\partial_n\varphi)n + (\partial_\tau\varphi)\tau \;\Rightarrow\; \partial_n\varphi = \nabla\varphi\cdot n \quad \text{and} \quad \partial_\tau\varphi = \nabla\varphi\cdot\tau\,, \end{aligned} \tag{G.50}$$

where $\partial_n\varphi$ and $\partial_\tau\varphi$ are the normal and tangential derivatives of the scalar field φ. In addition, the gradient of a vector field ∇u defined on $\partial\Omega$ can be decomposed as

$$\nabla u = \partial_n u^n (n\otimes n) + \partial_\tau u^n (n\otimes\tau) + \partial_n u^\tau (\tau\otimes n) + \partial_\tau u^\tau (\tau\otimes\tau)\,, \tag{G.51}$$

whose components $\partial_n u^n$, $\partial_\tau u^n$, $\partial_n u^\tau$ and $\partial_\tau u^\tau$ are defined as

$$\begin{aligned}(\nabla u)n &= [\partial_n u^n (n\otimes n) + \partial_\tau u^n (n\otimes\tau) + \partial_n u^\tau (\tau\otimes n) + \partial_\tau u^\tau (\tau\otimes\tau)]\,n\\ &= (\partial_n u^n)n + (\partial_n u^\tau)\tau \;\Rightarrow\; \partial_n u^n = n\cdot(\nabla u)n \quad \text{and} \quad \partial_n u^\tau = \tau\cdot(\nabla u)n\,, \end{aligned} \tag{G.52}$$

$$\begin{aligned}(\nabla u)\tau &= [\partial_n u^n (n\otimes n) + \partial_\tau u^n (n\otimes\tau) + \partial_n u^\tau (\tau\otimes n) + \partial_\tau u^\tau (\tau\otimes\tau)]\,\tau\\ &= (\partial_\tau u^n)n + (\partial_\tau u^\tau)\tau \;\Rightarrow\; \partial_\tau u^n = n\cdot(\nabla u)\tau \quad \text{and} \quad \partial_\tau u^\tau = \tau\cdot(\nabla u)\tau\,. \end{aligned} \tag{G.53}$$

G.5 Polar and Spherical Coordinate Systems

Let us consider a polar coordinate system of the form (r, θ) with center at the origin $\mathscr{O}$, as shown in fig. G.2. The oriented basis defining this system is denoted by e_r and e_θ, with $e_r\cdot e_\theta = 0$ and $\|e_r\| = \|e_\theta\| = 1$. Thus, we have the representations below.

- Gradient of a scalar field φ:

$$\nabla\varphi = \frac{\partial\varphi}{\partial r}e_r + \frac{1}{r}\frac{\partial\varphi}{\partial\theta}e_\theta\,. \tag{G.54}$$

- Laplacian of a scalar field φ:

$$\Delta\varphi = \frac{\partial^2\varphi}{\partial r^2} + \frac{1}{r}\frac{\partial\varphi}{\partial r} + \frac{1}{r^2}\frac{\partial^2\varphi}{\partial\theta^2}\,. \tag{G.55}$$

- Gradient of a vector field v:

$$\nabla v = \frac{\partial v^r}{\partial r} e_r \otimes e_r + \frac{1}{r}\left(\frac{\partial v^r}{\partial \theta} - v^\theta\right) e_r \otimes e_\theta + \frac{\partial v^\theta}{\partial r} e_\theta \otimes e_r + \frac{1}{r}\left(\frac{\partial v^\theta}{\partial \theta} + v^r\right) e_\theta \otimes e_\theta \,. \tag{G.56}$$

- Divergence of a vector field v:

$$\text{div}(v) = \frac{\partial v^r}{\partial r} + \frac{1}{r}\left(\frac{\partial v^\theta}{\partial \theta} + v^r\right) \,. \tag{G.57}$$

- Divergence of a second order tensor field T:

$$\text{div}(T) = \left(\frac{\partial T^{rr}}{\partial r} + \frac{1}{r}\frac{\partial T^{\theta r}}{\partial \theta} + \frac{T^{rr} - T^{\theta\theta}}{r}\right) e_r + \left(\frac{\partial T^{r\theta}}{\partial r} + \frac{1}{r}\frac{\partial T^{\theta\theta}}{\partial \theta} + \frac{T^{r\theta} + T^{\theta r}}{r}\right) e_\theta \,. \tag{G.58}$$

- Transformation of a vector v from cartesian to polar:

$$\begin{pmatrix} v^r \\ v^\theta \end{pmatrix} = \begin{pmatrix} \cos\theta & \sin\theta \\ -\sin\theta & \cos\theta \end{pmatrix} \begin{pmatrix} v^1 \\ v^2 \end{pmatrix}, \tag{G.59}$$

  where $v^i = v \cdot e_i$ are the components of vector v in the cartesian coordinate system.
- Transformation of a second order tensor T from cartesian to polar:

$$\begin{pmatrix} T^{rr} & T^{r\theta} \\ T^{\theta r} & T^{\theta\theta} \end{pmatrix} = \begin{pmatrix} \cos\theta & \sin\theta \\ -\sin\theta & \cos\theta \end{pmatrix}^\top \begin{pmatrix} T^{11} & T^{12} \\ T^{21} & T^{22} \end{pmatrix} \begin{pmatrix} \cos\theta & \sin\theta \\ -\sin\theta & \cos\theta \end{pmatrix}, \tag{G.60}$$

  where $T^{ij} = e_i \cdot T e_j$ are the components of tensor T in the cartesian coordinate system.

Let us consider a ball $B_\rho(\mathscr{O}) \subset \mathbb{R}^2$ of radius ρ and center at the origin $\mathscr{O}$, whose boundary is denoted by ∂B_ρ. Then, the integral of a scalar field φ over B_ρ is evaluated as

$$\int_{B_\rho} \varphi = \int_0^{2\pi} \left(\int_0^\rho \varphi(r,\theta) r dr\right) d\theta \,. \tag{G.61}$$

The integral of φ over the boundary ∂B_ρ is written as

$$\int_{\partial B_\rho} \varphi = \rho \int_0^{2\pi} \varphi(\rho,\theta)\, d\theta \,. \tag{G.62}$$

Let us now consider a spherical coordinate system centered at the origin $\mathscr{O}$ given by (r,θ,ϕ), as shown in fig. G.3. We define an oriented basis for the system of the

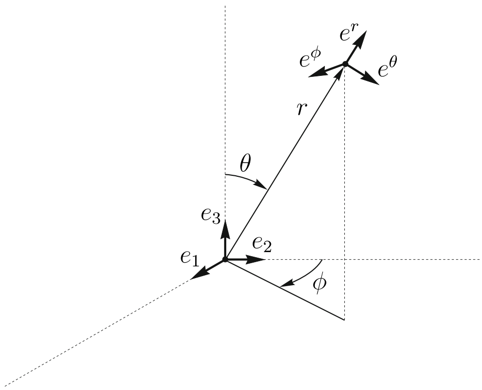


Fig. G.3 Spherical coordinate system (r, θ, ϕ)

form e_r, e_θ and e_ϕ, with $e_r \cdot e_\theta = e_r \cdot e_\phi = e_\theta \cdot e_\phi = 0$ and $\|e_r\| = \|e_\theta\| = \|e_\phi\| = 1$. By taking into account this system, we have the representations below.

- Gradient of a scalar field φ:

$$\nabla\varphi = \frac{\partial\varphi}{\partial r} e_r + \frac{1}{r}\frac{\partial\varphi}{\partial\theta} e_\theta + \frac{1}{r\sin\theta}\frac{\partial\varphi}{\partial\phi} e_\phi \, . \tag{G.63}$$

- Laplacian of a scalar field φ:

$$\Delta\varphi = \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial\varphi}{\partial r}\right) + \frac{1}{r^2\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial\varphi}{\partial\theta}\right) + \frac{1}{r^2\sin^2\theta}\frac{\partial^2\varphi}{\partial\phi^2} \, . \tag{G.64}$$

- Transformation of a vector v from cartesian to spherical:

$$\begin{pmatrix} v^r \\ v^\theta \\ v^\phi \end{pmatrix} = \begin{pmatrix} \sin\theta\cos\phi & \sin\theta\sin\phi & \cos\theta \\ \cos\theta\cos\phi & \cos\theta\sin\phi & -\sin\theta \\ -\sin\phi & \cos\phi & 0 \end{pmatrix} \begin{pmatrix} v^1 \\ v^2 \\ v^3 \end{pmatrix}, \tag{G.65}$$

  where $v^i = v \cdot e_i$ are the components of vector v in the cartesian coordinate system.

Let us consider a ball $B_\rho(\mathscr{O}) \subset \mathbb{R}^3$ of radius ρ and center at the origin $\mathscr{O}$, with boundary denoted by ∂B_ρ. Then, the integral of a scalar field φ over B_ρ is evaluated as

$$\int_{B_\rho} \varphi = \int_0^{2\pi}\left(\int_0^{\pi}\left(\int_0^{\rho}\varphi(r,\theta,\phi)r^2 dr\right)\sin\theta d\theta\right)d\phi \, . \tag{G.66}$$

The integral of φ over the boundary ∂B_ρ is given by

$$\int_{\partial B_\rho} \varphi = \rho^2\int_0^{2\pi}\left(\int_0^{\pi}\varphi(\rho,\theta,\phi)\sin\theta d\theta\right)d\phi \, . \tag{G.67}$$

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Index