

Mathematics for Physics I

A set of lecture notes by

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Preface

These notes were prepared for the first semester of a year-long mathematical methods course for beginning graduate students in physics. The emphasis is on linear operators and stresses the analogy between such operators acting on function spaces and matrices acting on finite dimensional spaces. The operator language then provides a unified framework for investigating ordinary and partial differential equations, and integral equations.

The mathematical prerequisites for the course are a sound grasp of undergraduate calculus (including the vector calculus needed for electricity and magnetism courses), linear algebra (the more the better), and competence at complex arithmetic. Fourier sums and integrals, as well as basic ordinary differential equation theory receive a quick review, but it would help if the reader had some prior experience to build on. Contour integration is not required.

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Chapter 1

Calculus of Variations

We begin our tour of useful mathematics with what is called the *calculus of variations*. Many physics problems can be formulated in the language of this calculus, and once they are there are useful tools to hand. In the text and associated exercises we will meet some of the equations whose solution will occupy us for much of our journey.

1.1 What is it good for?

The classical problems that motivated the creators of the calculus of variations include:

- i) *Dido's problem*: In Virgil's *Aeneid* we read how Queen Dido of Carthage must find largest area that can be enclosed by a curve (a strip of bull's hide) of fixed length.
- ii) *Plateau's problem*: Find the surface of minimum area for a given set of bounding curves. A soap film on a wire frame will adopt this minimal-area configuration.
- iii) *Johann Bernoulli's Brachistochrone*: A bead slides down a curve with fixed ends. Assuming that the total energy $\frac{1}{2}mv^2 + V(x)$ is constant, find the curve that gives the most rapid descent.
- iv) *Catenary*: Find the form of a hanging heavy chain of fixed length by minimizing its potential energy.

These problems all involve finding maxima or minima, and hence equating some sort of derivative to zero. In the next section we will define this derivative, and show how to compute it.

1.2 Functionals

In variational problems we are provided with an expression $J[y]$ that “eats” whole functions $y(x)$ and returns a single number. Such objects are often called *functionals* to distinguish them from ordinary functions. An ordinary function is a map $f : \mathbb{R} \rightarrow \mathbb{R}$. A functional J is a map $J : C^\infty(\mathbb{R}) \rightarrow \mathbb{R}$ where $C^\infty(\mathbb{R})$ is the space of smooth (having derivatives of all orders) functions. To find the function $y(x)$ that maximizes or minimizes a given functional $J[y]$ we need to define, and evaluate, its *functional derivative*.

1.2.1 The functional derivative

We will restrict ourselves to expressions of the form

$$J[y] = \int_{x_1}^{x_2} f(x, y, y', y'', \dots y^{(n)}) dx, \quad (1.1)$$

where f depends on the value of $y(x)$ and only finitely many of its derivatives. Such functionals are said to be *local* in x .

Consider first a functional $J = \int f dx$ in which f depends only x , y and y' , and suppose that we vary $y(x) \rightarrow y(x) + \varepsilon \eta(x)$ where ε is a (small) x -independent constant. The resultant change in J is then

$$\begin{aligned} J[y + \varepsilon \eta] - J[y] &= \int_{x_1}^{x_2} \{f(x, y + \varepsilon \eta, y' + \varepsilon \eta') - f(x, y, y')\} dx \\ &= \int_{x_1}^{x_2} \left\{ \varepsilon \eta \frac{\partial f}{\partial y} + \varepsilon \frac{d\eta}{dx} \frac{\partial f}{\partial y'} + O(\varepsilon^2) \right\} dx \\ &= \left[\varepsilon \eta \frac{\partial f}{\partial y'} \right]_{x_1}^{x_2} + \int_{x_1}^{x_2} (\varepsilon \eta(x)) \left\{ \frac{\partial f}{\partial y} - \frac{d}{dx} \left(\frac{\partial f}{\partial y'} \right) \right\} dx + O(\varepsilon^2). \end{aligned}$$

For the moment we assume that $\eta(x_1) = \eta(x_2) = 0$. The change $\delta y(x) \equiv \varepsilon \eta(x)$ that we have made in $y(x)$ is therefore a “fixed-endpoint variation.” For such variations the integrated-out part $[\dots]_{x_1}^{x_2}$ vanishes and, defining δJ to be the $O(\varepsilon)$ part of $J[y + \varepsilon \eta] - J[y]$, we have

$$\begin{aligned} \delta J &= \int_{x_1}^{x_2} (\varepsilon \eta(x)) \left\{ \frac{\partial f}{\partial y} - \frac{d}{dx} \left(\frac{\partial f}{\partial y'} \right) \right\} dx \\ &= \int_{x_1}^{x_2} \delta y(x) \left(\frac{\delta J}{\delta y(x)} \right) dx. \end{aligned} \quad (1.2)$$

The function

$$\frac{\delta J}{\delta y(x)} \equiv \frac{\partial f}{\partial y} - \frac{d}{dx} \left(\frac{\partial f}{\partial y'} \right) \quad (1.3)$$

is called the *functional* (or *Fréchet*) derivative of J with respect to $y(x)$. We can think of it as a generalization of the partial derivative $\partial J/\partial y_i$, where the discrete subscript “ i ” on y is replaced by a continuous label “ x ,” and sums over i are replaced by integrals over x :

$$\delta J = \sum_i \frac{\partial J}{\partial y_i} \delta y_i \rightarrow \int_{x_1}^{x_2} dx \left(\frac{\delta J}{\delta y(x)} \right) \delta y(x). \quad (1.4)$$

1.2.2 The Euler-Lagrange equation

Suppose that we have a differentiable function $J(y_1, y_2, \dots, y_n)$ of n variables and seek its *stationary points* — these being the locations at which J has its maxima, minima and saddlepoints. At a stationary point (y_1, y_2, \dots, y_n) the variation

$$\delta J = \sum_{i=1}^n \frac{\partial J}{\partial y_i} \delta y_i \quad (1.5)$$

is zero for all possible δy_i . We know that this will be so if, and only if, all partial derivatives $\partial J/\partial y_i$, $i = 1, \dots, n$, are zero. By analogy, we expect that a functional $J[y]$ will be stationary under any variation $y(x) \rightarrow y(x) + \delta y(x)$, if, and only if, we are at a point $y(x)$ in function space where the functional derivative $\delta J/\delta y(x)$ vanishes for all x . In other words, when

$$\boxed{\frac{\partial f}{\partial y(x)} - \frac{d}{dx} \left(\frac{\partial f}{\partial y'(x)} \right) = 0, \quad x_1 < x < x_2.} \quad (1.6)$$

This condition for $y(x)$ to be a stationary point is usually called the *Euler-Lagrange equation*¹.

¹That $\delta J/\delta y(x) \equiv 0$ is a *sufficient* condition for δJ to be zero is clear from its definition in (1.2). That it is also a *necessary* condition can be seen by imagining a point $y(x)$ at which J is stationary but where $\delta J/\delta y(x)$ is non-zero at some $x_0 \in [x_1, x_2]$. Because $f(y, y', x)$ is assumed smooth, the functional derivative $\delta J/\delta y(x)$ is also a smooth function of x . Therefore, by continuity, it will have the same sign throughout some open interval containing x_0 . By taking $\delta y(x)$ to be zero outside this interval, and of one sign within it, we obtain a non-zero δJ — in contradiction to stationarity.

If the functional depends on more than one function y , then stationarity under all possible variations requires one equation

$$\frac{\delta J}{\delta y_i(x)} = \frac{\partial f}{\partial y_i} - \frac{d}{dx} \left(\frac{\partial f}{\partial y'_i} \right) = 0 \quad (1.7)$$

for each function $y_i(x)$.

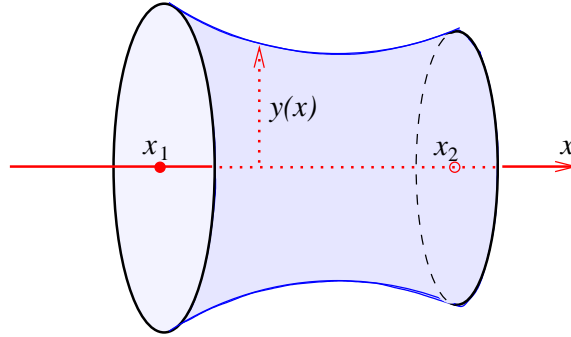
If the function depends on higher derivatives, y'' , $y^{(3)}$, etc., then we have to integrate by parts more times, and we end up with

$$\frac{\delta J}{\delta y(x)} = \frac{\partial f}{\partial y} - \frac{d}{dx} \left(\frac{\partial f}{\partial y'} \right) + \frac{d^2}{dx^2} \left(\frac{\partial f}{\partial y''} \right) - \frac{d^3}{dx^3} \left(\frac{\partial f}{\partial y^{(3)}} \right) + \dots \quad (1.8)$$

1.2.3 Some applications

Now we use our new functional derivative to address some of the classic problems mentioned in the introduction.

Example: Soap film supported by a pair of coaxial rings.



Soap film between two rings.

This is a simple case of Plateau's problem. The free energy of the soap film is equal to twice (once for each liquid-air interface) the surface tension σ of the soap solution times the area of the film. The film can therefore minimize its free energy by minimizing its area, and the axial symmetry suggests that the minimal surface will be a surface of revolution about the x axis. We therefore seek the profile $y(x)$ that makes the area

$$J[y] = 2\pi \int_{x_1}^{x_2} y \sqrt{1 + y'^2} dx \quad (1.9)$$

of the surface of revolution the least among all such surfaces bounded by the circles of radii $y(x_1) = y_1$ and $y(x_2) = y_2$. Since a minimum is a stationary point, we seek candidates for the minimizing profile $y(x)$ by setting the functional derivative $\delta J/\delta y(x)$ to zero.

We begin by forming the partial derivatives

$$\frac{\partial f}{\partial y} = 4\pi\sigma\sqrt{1+y'^2}, \quad \frac{\partial f}{\partial y'} = \frac{4\pi\sigma yy'}{\sqrt{1+y'^2}} \quad (1.10)$$

and use them to write down the Euler-Lagrange equation

$$\sqrt{1+y'^2} - \frac{d}{dx} \left(\frac{yy'}{\sqrt{1+y'^2}} \right) = 0. \quad (1.11)$$

Performing the indicated derivative with respect to x gives

$$\sqrt{1+y'^2} - \frac{(y')^2}{\sqrt{1+y'^2}} - \frac{yy''}{\sqrt{1+y'^2}} + \frac{y(y')^2 y''}{(1+y'^2)^{3/2}} = 0. \quad (1.12)$$

After collecting terms, this simplifies to

$$\frac{1}{\sqrt{1+y'^2}} - \frac{yy''}{(1+y'^2)^{3/2}} = 0. \quad (1.13)$$

The differential equation (1.13) still looks a trifle intimidating. To simplify further, we multiply by y' to get

$$\begin{aligned} 0 &= \frac{y'}{\sqrt{1+y'^2}} - \frac{yy'y''}{(1+y'^2)^{3/2}} \\ &= \frac{d}{dx} \left(\frac{y}{\sqrt{1+y'^2}} \right). \end{aligned} \quad (1.14)$$

The solution to the minimization problem therefore reduces to solving

$$\frac{y}{\sqrt{1+y'^2}} = \kappa, \quad (1.15)$$

where κ is an as yet undetermined integration constant. Fortunately this non-linear, first order, differential equation is elementary. We recast it as

$$\frac{dy}{dx} = \sqrt{\frac{y^2}{\kappa^2} - 1} \quad (1.16)$$

and separate variables

$$\int dx = \int \frac{dy}{\sqrt{\frac{y^2}{\kappa^2} - 1}}. \quad (1.17)$$

We now make the natural substitution $y = \kappa \cosh t$, whence

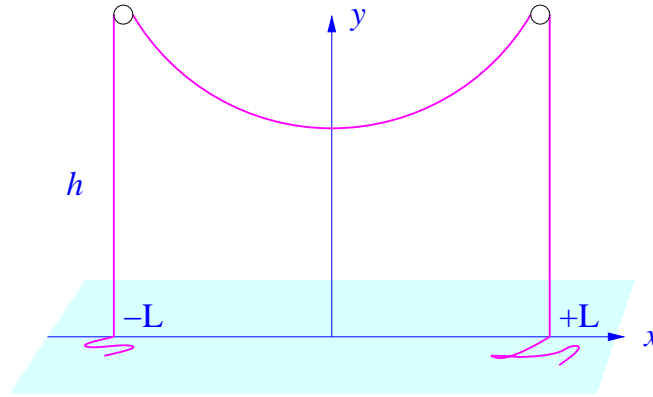
$$\int dx = \kappa \int dt. \quad (1.18)$$

Thus we find that $x + a = \kappa t$, leading to

$$y = \kappa \cosh \frac{x + a}{\kappa}. \quad (1.19)$$

We select the constants κ and a to fit the endpoints $y(x_1) = y_1$ and $y(x_2) = y_2$.

Example: Heavy Chain over Pulleys. We cannot yet consider the form of the catenary, a hanging chain of fixed length, but we can solve a simpler problem of a heavy cable draped over a pair of pulleys located at $x = \pm L$, $y = h$, and with the excess cable resting on a horizontal surface.



Hanging chain.

The potential energy of the system is

$$P.E. = \sum mgy = \rho g \int_{-L}^L y \sqrt{1 + (y')^2} dx + \text{const}. \quad (1.20)$$

Here the constant refers to the unchanging potential energy of the vertically hanging cable and the cable on the horizontal surface. Notice that the tension in the cable is being tacitly determined by the weight of the vertical segments.

The Euler-Lagrange equations coincide with those of the soap film, so

$$y = \kappa \cosh \frac{(x + a)}{\kappa} \quad (1.21)$$

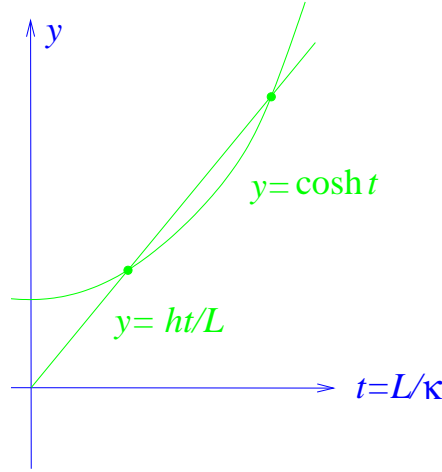
where we have to find κ and a . We have

$$\begin{aligned} h &= \kappa \cosh(-L + a)/\kappa, \\ &= \kappa \cosh(L + a)/\kappa, \end{aligned} \quad (1.22)$$

so $a = 0$ and $h = \kappa \cosh L/\kappa$. Setting $t = L/\kappa$ this reduces to

$$\left(\frac{h}{L}\right) t = \cosh t. \quad (1.23)$$

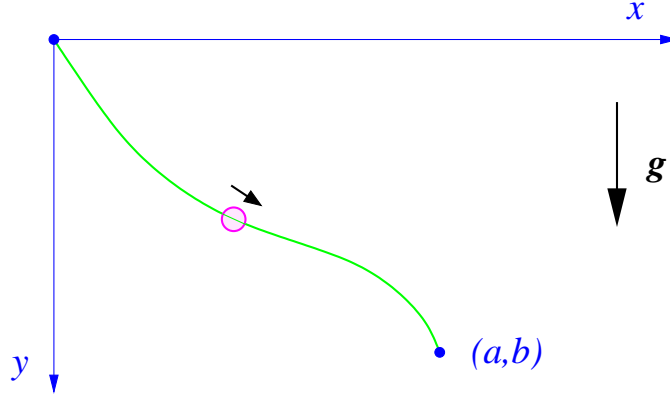
By considering the intersection of the line $y = ht/L$ with $y = \cosh t$ we see that if h/L is too small there is no solution (the weight of the suspended cable is too big for the tension supplied by the dangling ends) and once h/L is large enough there will be two possible solutions.



Intersection of $y = ht/L$ with $y = \cosh t$.

Further investigation will show that only one of these is stable.

Example: The Brachistochrone. This problem was posed as a challenge by Johann Bernoulli in 1696. He asked what shape should a wire with endpoints $(0, 0)$ and (a, b) take in order that a frictionless bead will slide from rest down the wire in the shortest possible time ($\beta\rho\alpha\chi\iota\sigma\tau\omicron\varsigma$: shortest, $\chi\rho\omicron\nu\omicron\varsigma$: time).



Bead on a wire.

When presented with an ostensibly anonymous solution, Johann made his famous remark: “*Tanquam ex unguem leonem*” (I recognize the lion by his clawmark) meaning that he recognized that the author was Isaac Newton.

Johann gave a solution himself, but that of his brother Jacob Bernoulli was superior and Johann tried to pass it off as his. This was not atypical. Johann later misrepresented the publication date of his book on hydraulics to make it seem that he had priority in this field over his own son, Daniel Bernoulli.

We begin *our* solution of the problem by observing that the total energy

$$E = \frac{1}{2}m(\dot{x}^2 + \dot{y}^2) - mgy = \frac{1}{2}m\dot{x}^2(1 + y'^2) - mgy, \quad (1.24)$$

of the bead will be constant. From the initial condition we see that this constant is zero. We therefore wish to minimize

$$T = \int_0^T dt = \int_0^a \frac{1}{\dot{x}} dx = \int_0^a \sqrt{\frac{1 + y'^2}{2gy}} dx \quad (1.25)$$

so as find $y(x)$, given that $y(0) = 0$ and $y(a) = b$. The Euler-Lagrange equation is

$$yy'' + \frac{1}{2}(1 + y'^2) = 0. \quad (1.26)$$

Again this looks intimidating, but we can use the same trick of multiplying through by y' to get

$$y' \left(yy'' + \frac{1}{2}(1 + y'^2) \right) = \frac{1}{2} \frac{d}{dx} \{ y(1 + y'^2) \} = 0. \quad (1.27)$$

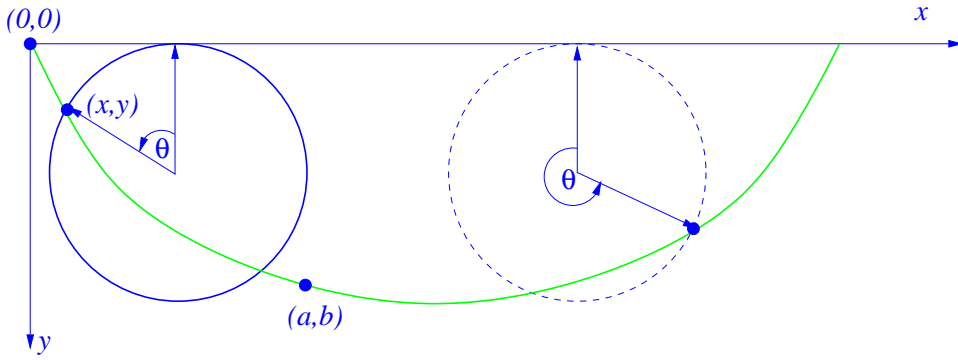
Thus

$$2c = y(1 + y'^2). \quad (1.28)$$

This has a parametric solution

$$\begin{aligned} x &= c(\theta - \sin \theta), \\ y &= c(1 - \cos \theta), \end{aligned} \quad (1.29)$$

(as you should verify) and the solution is a cycloid.



A wheel rolls on the x axis. The dot, which is fixed to the rim of the wheel, traces out a cycloid.

The parameter c is determined by requiring that the curve does in fact pass through the point (a, b) .

1.2.4 First integral

How did we know that we could simplify both the soap-film problem and the brachistochrone by multiplying the Euler equation by y' ? The answer is that there is a general principle, closely related to energy conservation in mechanics, that tells us when and how we can make such a simplification. It works when the f in $\int f dx$ is of the form $f(y, y')$, *i.e.* has no *explicit* dependence on x . In this case the last term in

$$\frac{df}{dx} = y' \frac{\partial f}{\partial y} + y'' \frac{\partial f}{\partial y'} + \frac{\partial f}{\partial x} \quad (1.30)$$

is absent. We then have

$$\frac{d}{dx} \left(f - y' \frac{\partial f}{\partial y'} \right) = y' \frac{\partial f}{\partial y} + y'' \frac{\partial f}{\partial y'} - y'' \frac{\partial f}{\partial y'} - y' \frac{d}{dx} \left(\frac{\partial f}{\partial y'} \right)$$

$$= y' \left(\frac{\partial f}{\partial y} - \frac{d}{dx} \left(\frac{\partial f}{\partial y'} \right) \right), \quad (1.31)$$

and this is zero if the Euler-Lagrange equation is satisfied.

The quantity

$$I = f - y' \frac{\partial f}{\partial y'} \quad (1.32)$$

is called a *first integral* of the Euler-Lagrange equation. In the soap-film case

$$f - y' \frac{\partial f}{\partial y'} = y \sqrt{1 + (y')^2} - \frac{y(y')^2}{\sqrt{1 + (y')^2}} = \frac{y}{\sqrt{1 + (y')^2}}. \quad (1.33)$$

When there are a number of dependent variables y_i , so that we have

$$J[y_1, y_2, \dots, y_n] = \int f(y_1, y_2, \dots, y_n; y'_1, y'_2, \dots, y'_n) dx \quad (1.34)$$

then the first integral becomes

$$I = f - \sum_i y'_i \frac{\partial f}{\partial y'_i}. \quad (1.35)$$

Again

$$\begin{aligned} \frac{dI}{dx} &= \frac{d}{dx} \left(f - \sum_i y'_i \frac{\partial f}{\partial y'_i} \right) \\ &= \sum_i \left(y'_i \frac{\partial f}{\partial y_i} + y''_i \frac{\partial f}{\partial y'_i} - y''_i \frac{\partial f}{\partial y'_i} - y'_i \frac{d}{dx} \left(\frac{\partial f}{\partial y'_i} \right) \right) \\ &= \sum_i y'_i \left(\frac{\partial f}{\partial y_i} - \frac{d}{dx} \left(\frac{\partial f}{\partial y'_i} \right) \right), \end{aligned} \quad (1.36)$$

and this zero if the Euler-Lagrange equation is satisfied for each y_i .

Note that there is only *one* first integral, no matter how many y 's there are.

1.3 Lagrangian Mechanics

In his *Mécanique Analytique* (1788) Joseph-Louis de La Grange, following Jean le Ronde d'Alembert (1742) and Pierre Louis Moreau de Maupertuis

(1744), showed that most of classical mechanics can be recast as a variational condition: the *principle of least action*. The idea is to introduce the *Lagrangian* function $L = T - V$ where T is the kinetic energy of the system and V the potential energy, both expressed in terms of *generalized co-ordinates* q^i and their time derivatives \dot{q}^i . Then Lagrange showed that the multitude of Newton's $\mathbf{F} = m\mathbf{a}$ equations, one for each particle in the system, could be reduced to

$$\frac{d}{dt} \left(\frac{\partial L}{\partial \dot{q}^i} \right) - \frac{\partial L}{\partial q^i} = 0, \quad (1.37)$$

one equation for each generalized coordinate q . Quite remarkably — given that Lagrange's derivation contains no mention of maxima or minima — we recognise that this is the precisely the condition that the *action functional*

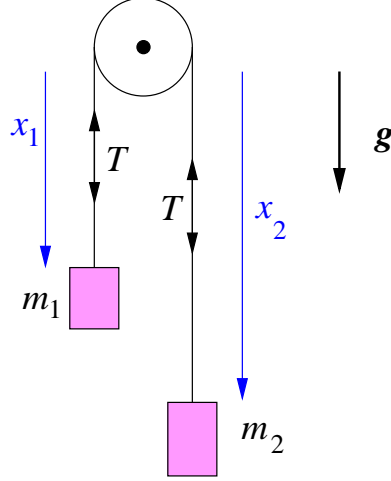
$$S[q] = \int_{t_{\text{initial}}}^{t_{\text{final}}} L(t, q^i; \dot{q}^i) dt \quad (1.38)$$

be stationary with respect to variations of the trajectory $q^i(t)$ that leave the initial and final points fixed. This fact so impressed its discoverers that they believed they had uncovered the unifying principle of the universe. Maupertuis, for one, tried to base a proof of the existence of God on it. Today the action integral, through its starring role in the Feynman path-integral formulation of quantum mechanics, remains at the heart of theoretical physics.

1.3.1 One degree of freedom

We will not attempt to derive Lagrange's equations from d'Alembert's extension of the principle of virtual work — leaving this task to a mechanics course — but will satisfy ourselves with some examples which illustrate the computational advantages of Lagrange's approach, as well as a subtle pitfall.

Consider, for example, *Atwood's Machine*. This device, invented in 1784 but still a familiar sight in teaching laboratories, is used to demonstrate Newton's laws of motion and to measure g . It consists of two weights connected by a light string which passes over a light and frictionless pulley.

*Atwood's machine.*

The elementary approach is to write an equation of motion for each of the two weights

$$\begin{aligned} m_1 \ddot{x}_1 &= m_1 g - T, \\ m_2 \ddot{x}_2 &= m_2 g - T. \end{aligned} \quad (1.39)$$

We then take into account the constraint $\dot{x}_1 = -\dot{x}_2$ to get

$$\begin{aligned} m_1 \ddot{x}_1 &= m_1 g - T, \\ -m_2 \ddot{x}_1 &= m_2 g - T. \end{aligned} \quad (1.40)$$

Finally we eliminate the constraint force, the tension T , to get the acceleration

$$(m_1 + m_2) \ddot{x}_1 = (m_1 - m_2)g. \quad (1.41)$$

The Lagrangian solution takes the constraint into account from the very beginning by introducing a single generalized coordinate $q = x_1 = -x_2$, and writing

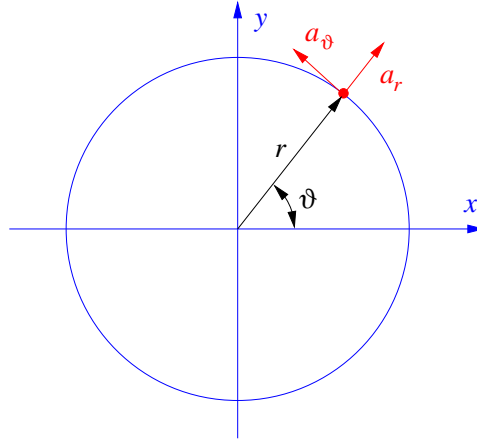
$$L = T - V = \frac{1}{2}(m_1 + m_2)\dot{q}^2 - (m_2 - m_1)gq. \quad (1.42)$$

From this we obtain a single equation of motion

$$\frac{d}{dt} \left(\frac{\partial L}{\partial \dot{q}^i} \right) - \frac{\partial L}{\partial q^i} = 0 \quad \Rightarrow \quad (m_1 + m_2)\ddot{q} = (m_1 - m_2)g. \quad (1.43)$$

The advantage of the the Lagrangian method is that constraint forces, which do no net work, never appear. The disadvantage is exactly the same: if we need to find the constraint forces – in this case the tension in the string — we cannot use Lagrange alone.

Lagrange provides a convenient way to derive the equations of motion in non-cartesian co-ordinate systems, such as plane polar co-ordinates.



Polar components of acceleration.

Consider the central force problem with $F_r = -\partial_r V(r)$. The Newtonian method begins by computing the acceleration in polar coordinates. This is most easily done by setting $z = re^{i\theta}$ and differentiating twice:

$$\begin{aligned}\dot{z} &= (\dot{r} + ir\dot{\theta})e^{i\theta}, \\ \ddot{z} &= (\ddot{r} - r\dot{\theta}^2)e^{i\theta} + i(2\dot{r}\dot{\theta} + r\ddot{\theta})e^{i\theta}.\end{aligned}\tag{1.44}$$

Reading off the components parallel and perpendicular to $e^{i\theta}$ gives the radial and angular acceleration

$$\begin{aligned}a_r &= \ddot{r} - r\dot{\theta}^2, \\ a_\theta &= r\ddot{\theta} + 2\dot{r}\dot{\theta}.\end{aligned}\tag{1.45}$$

Newton's equations therefore become

$$\begin{aligned}m(\ddot{r} - r\dot{\theta}^2) &= -\frac{\partial V}{\partial r} \\ m(r\ddot{\theta} + 2\dot{r}\dot{\theta}) &= 0, \quad \Rightarrow \quad \frac{d}{dt}(mr^2\dot{\theta}) = 0.\end{aligned}\tag{1.46}$$

Setting $l = mr^2\dot{\theta}$, the conserved angular momentum, and eliminating $\dot{\theta}$ gives

$$m\ddot{r} - \frac{l^2}{mr^3} = -\frac{\partial V}{\partial r}. \quad (1.47)$$

(If this were Kepler's problem, where $V = GmM/r$, we would now proceed to simplify this equation by substituting $r = 1/u$, but that is another story.)

Following Lagrange we first compute the kinetic energy in polar coordinates (this requires less thought than computing the acceleration) and set

$$L = T - V = \frac{1}{2}m(\dot{r}^2 + r^2\dot{\theta}^2) - V(r). \quad (1.48)$$

The Euler-Lagrange equations are now

$$\begin{aligned} \frac{d}{dt} \left(\frac{\partial L}{\partial \dot{r}} \right) - \frac{\partial L}{\partial r} &= 0, \Rightarrow m\ddot{r} - r^2\dot{\theta}^2 + \frac{\partial V}{\partial r} = 0, \\ \frac{d}{dt} \left(\frac{\partial L}{\partial \dot{\theta}} \right) - \frac{\partial L}{\partial \theta} &= 0, \Rightarrow \frac{d}{dt}(mr^2\dot{\theta}) = 0. \end{aligned} \quad (1.49)$$

The first integral for this problem is

$$\begin{aligned} E &= \dot{r} \frac{\partial L}{\partial \dot{r}} + \dot{\theta} \frac{\partial L}{\partial \dot{\theta}} - L \\ &= \frac{1}{2}m(\dot{r}^2 + r^2\dot{\theta}^2) + V(r). \end{aligned} \quad (1.50)$$

which is the total energy. Thus the constancy of the first integral states that

$$\frac{dE}{dt} = 0, \quad (1.51)$$

or that energy is conserved.

Warning: We might realize, without having gone to the trouble of deriving it from the Lagrange equations, that rotational invariance guarantees that the angular momentum $l = mr^2\dot{\theta}$ will be a constant. Having done so, it is almost irresistible to try to short-circuit some of the arithmetic by plugging this prior knowledge into

$$L = \frac{1}{2}m(\dot{r}^2 + r^2\dot{\theta}^2) - V(r) \quad (1.52)$$

so as to eliminate the variable $\dot{\theta}$ in favour of the constant l . If we try this we get

$$L \overset{?}{\rightarrow} \frac{1}{2}m\dot{r}^2 + \frac{l^2}{mr^2} - V(r). \quad (1.53)$$

We can now directly write down the Lagrange equation r , which is

$$m\ddot{r} + \frac{l^2}{mr^3} \overset{?}{=} -\frac{\partial V}{\partial r}. \quad (1.54)$$

Unfortunately this has the wrong sign before the l^2/mr^3 term! The lesson is that we must be very careful in using consequences of a variational principle to modify the principle. It can be done, and in mechanics it leads to the *Routhian* or, in more modern language to *Hamiltonian reduction*, but it requires using a Legendre transform. The reader should consult a book on mechanics for details.

1.3.2 Noether's theorem

The time-independence of the first integral

$$\frac{d}{dt} \left\{ \dot{q} \frac{\partial L}{\partial \dot{q}} - L \right\} = 0, \quad (1.55)$$

and of angular momentum

$$\frac{d}{dt} \{mr^2\dot{\theta}\} = 0, \quad (1.56)$$

are examples of *conservation laws*. We obtained them both by manipulating the Euler-Lagrange equations of motion, but also indicated that they were in some way connected with symmetries. One of the chief advantages of a variational formulation of a physical problem is that this connection

Symmetry \Leftrightarrow Conservation Law

can be made explicit by exploiting a strategy due to Emmy Noether. She showed how to proceed directly from the action integral to the conserved quantity without having to fiddle about with the individual equations of motion. We begin by illustrating her technique in the case of angular momentum, whose conservation is a consequence the rotational symmetry of

the central force problem. The action integral for the central force problem is

$$S = \int_0^T \left\{ \frac{1}{2} m (\dot{r}^2 + r^2 \dot{\theta}^2) - V(r) \right\} dt. \quad (1.57)$$

Noether observes that the integrand is left unchanged if we make the variation

$$\theta(t) \rightarrow \theta(t) + \varepsilon \alpha \quad (1.58)$$

where α is a fixed angle and ε is a small, time-independent, parameter. This invariance is the symmetry we shall exploit. It is a mathematical identity: it does not require that r and θ obey the equations of motion. She next observes that since the *equations of motion* are equivalent to the statement that S is left stationary under *any* infinitesimal variations in r and θ , they necessarily imply that S is stationary under the specific variation

$$\theta(t) \rightarrow \theta(t) + \varepsilon(t) \alpha \quad (1.59)$$

where now ε is allowed to be time-dependent. This stationarity of the action is no longer a mathematical identity, but, because it requires r , θ , to obey the equations of motion, has physical content. Inserting $\delta\theta = \varepsilon(t)\alpha$ into our expression for S gives

$$\delta S = \alpha \int_0^T \left\{ r^2 \dot{\theta} \right\} \dot{\varepsilon} dt. \quad (1.60)$$

Note that this variation depends only on the time derivative of ε , and not ε itself. This is because of the invariance of S under time-independent rotations. We now assume that $\varepsilon(t) = 0$ at $t = 0$ and $t = T$, and integrate by parts to take the time derivative off ε and put it on the rest of the integrand:

$$\delta S = -\alpha \int \left\{ \frac{d}{dt} (r^2 \dot{\theta}) \right\} \varepsilon(t) dt. \quad (1.61)$$

Since the equations of motion say that $\delta S = 0$ under all infinitesimal variations, and in particular those due to any time dependent rotation $\varepsilon(t)\alpha$, we deduce that the equations of motion imply that the coefficient of $\varepsilon(t)$ must be zero, and so, provided $r(t)$, $\theta(t)$, obey the equations of motion, we have

$$0 = \frac{d}{dt} (r^2 \dot{\theta}). \quad (1.62)$$

As a second illustration we derive energy (first integral) conservation for the case that the system is invariant under time translations — meaning

that L does not depend explicitly on time. In this case the action integral is invariant under constant time shifts $t \rightarrow t + \varepsilon$ in the argument of the dynamical variable:

$$q(t) \rightarrow q(t + \varepsilon) \approx q(t) + \varepsilon \dot{q}. \quad (1.63)$$

The equations of motion tell us that the action will be stationary under the variation

$$\delta q(t) = \varepsilon(t) \dot{q}, \quad (1.64)$$

where again we now permit the parameter ε to depend on t . We insert this variation into

$$S = \int_0^T L dt \quad (1.65)$$

and find

$$\delta S = \int_0^T \left\{ \frac{\partial L}{\partial q} \dot{q} \varepsilon + \frac{\partial L}{\partial \dot{q}} (\ddot{q} \varepsilon + \dot{q} \dot{\varepsilon}) \right\} dt. \quad (1.66)$$

This expression contains undotted ε 's. Because of this the change in S is not obviously zero when ε is time independent — but the absence of any explicit t dependence in L tells us that

$$\frac{dL}{dt} = \frac{\partial L}{\partial q} \dot{q} + \frac{\partial L}{\partial \dot{q}} \ddot{q}. \quad (1.67)$$

As a consequence, for time independent ε , we have

$$\delta S = \int_0^T \left\{ \varepsilon \frac{dL}{dt} \right\} dt = \varepsilon [L]_0^T, \quad (1.68)$$

showing that the change in S comes entirely from the endpoints of the time interval. These fixed endpoints explicitly break time-translation invariance, but in a trivial manner. For general $\varepsilon(t)$ we have

$$\delta S = \int_0^T \left\{ \varepsilon(t) \frac{dL}{dt} + \frac{\partial L}{\partial \dot{q}} \dot{q} \dot{\varepsilon} \right\} dt. \quad (1.69)$$

This equation is an identity. It does not rely on q obeying the equation of motion. After an integration by parts, taking $\varepsilon(t)$ to be zero at $t = 0, T$, it is equivalent to

$$\delta S = \int_0^T \varepsilon(t) \frac{d}{dt} \left\{ L - \frac{\partial L}{\partial \dot{q}} \dot{q} \right\} dt. \quad (1.70)$$

Now we assume that $q(t)$ does obey the equations of motion. The variation principle then says that $\delta S = 0$ for any $\varepsilon(t)$, and we deduce that for $q(t)$ satisfying the equations of motion we have

$$\frac{d}{dt} \left\{ L - \frac{\partial L}{\partial \dot{q}} \dot{q} \right\} = 0. \quad (1.71)$$

The general strategy that constitutes “Noether’s theorem” must now be obvious: we look for an invariance of the action under a symmetry transformation with a time-independent parameter. We then observe that if the dynamical variables obey the equations of motion, then the action principle tells us that the action will remain stationary under such a variation of the dynamical variables even after the parameter is promoted to being time dependent. The resultant variation of S can only depend on time derivatives of the parameter. We integrate by parts so as to take all the time derivatives off it, and on to the rest of the integrand. Since the parameter is arbitrary, we deduce that the equations of motion tell us that that its coefficient in the integral must be zero. Since this coefficient is the time derivative of something, this something is conserved.

1.3.3 Many degrees of freedom

The extension of the action principle to many degrees of freedom is straightforward. As an example consider the small oscillations about equilibrium of a system with N degrees of freedom. We parametrize the system in terms of deviations from the equilibrium position and expand out to quadratic order. We obtain a Lagrangian

$$L = \sum_{i,j=1}^N \left\{ \frac{1}{2} M_{ij} \dot{q}^i \dot{q}^j - \frac{1}{2} V_{ij} q^i q^j \right\}, \quad (1.72)$$

where M_{ij} and V_{ij} are $N \times N$ symmetric matrices encoding the inertial and potential energy properties of the system. Now we have one equation

$$0 = \frac{d}{dt} \left(\frac{\partial L}{\partial \dot{q}^i} \right) - \frac{\partial L}{\partial q^i} = \sum_{j=1}^N (M_{ij} \ddot{q}^j + V_{ij} q^j) \quad (1.73)$$

for each i .

1.3.4 Continuous systems

The action principle can be extended to field theories and to continuum mechanics. Here one has a continuous infinity of dynamical degrees of freedom, either one for each point in space and time or one for each point in the material, but the extension of the variational derivative to functions of more than one variable should possess no conceptual difficulties.

Suppose we are given an action functional $S[\varphi]$ depending on a field $\varphi(x^\mu)$ and its first derivatives

$$\varphi_\mu \equiv \frac{\partial \varphi}{\partial x^\mu}. \quad (1.74)$$

Here x^μ , $\mu = 0, 1, \dots, d$, are the coordinates of $d + 1$ dimensional space-time. It is traditional to take $x^0 \equiv t$ and the other coordinates spacelike. Suppose further that

$$S[\varphi] = \int L dt = \int \mathcal{L}(x^\mu, \varphi, \varphi_\mu) d^{d+1}x, \quad (1.75)$$

where \mathcal{L} is the *Lagrangian density*, in terms of which

$$L = \int \mathcal{L} d^d x, \quad (1.76)$$

and the integral is over the space coordinates. Now

$$\begin{aligned} \delta S &= \int \left\{ \delta \varphi(x) \frac{\partial \mathcal{L}}{\partial \varphi(x)} + \delta(\varphi_\mu(x)) \frac{\partial \mathcal{L}}{\partial \varphi_\mu(x)} \right\} d^{d+1}x \\ &= \int \delta \varphi(x) \left\{ \frac{\partial \mathcal{L}}{\partial \varphi(x)} - \frac{\partial}{\partial x^\mu} \left(\frac{\partial \mathcal{L}}{\partial \varphi_\mu(x)} \right) \right\} d^{d+1}x. \end{aligned} \quad (1.77)$$

In going from the first line to the second, we have observed that

$$\delta(\varphi_\mu(x)) = \frac{\partial}{\partial x^\mu} \delta \varphi(x) \quad (1.78)$$

and used the divergence theorem,

$$\int_\Omega \left(\frac{\partial A^\mu}{\partial x^\mu} \right) d^{d+1}x = \int_{\partial\Omega} A^\mu n_\mu dS, \quad (1.79)$$

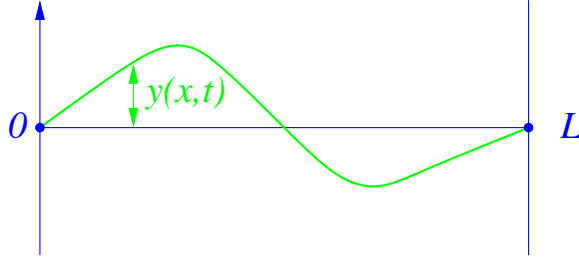
where Ω is some space-time region and $\partial\Omega$ its boundary, to integrate by parts. Here dS is the element of area on the boundary, and n_μ the outward

normal. As before, we take $\delta\varphi$ to vanish on the boundary, and hence there is no boundary contribution to variation of S . The result is that

$$\frac{\delta S}{\delta\varphi(x)} = \frac{\partial\mathcal{L}}{\partial\varphi(x)} - \frac{\partial}{\partial x^\mu} \left(\frac{\partial\mathcal{L}}{\partial\varphi_\mu(x)} \right), \quad (1.80)$$

and the equation of motion comes from setting this to zero. Note that a sum over the repeated coordinate index μ is implied. In practice it is easier not to use this formula. Instead, make the variation by hand—as in the following examples.

Example: The Vibrating string. The simplest continuous dynamical system is the transversely vibrating string. We describe the string displacement by $y(x, t)$.



Let us suppose that the string has fixed ends, a mass per unit length of ρ , and is under tension T . If we assume only small displacements from equilibrium, the Lagrangian is

$$L = \int_0^L dx \left\{ \frac{1}{2}\rho\dot{y}^2 - \frac{1}{2}Ty'^2 \right\}. \quad (1.81)$$

The variation of the action is

$$\begin{aligned} \delta S &= \iint_0^L dt dx \{ \rho\dot{y}\delta\dot{y} - Ty'\delta y' \} \\ &= \iint_0^L dt dx \{ \delta y(x, t) (-\rho\ddot{y} + Ty'') \}. \end{aligned} \quad (1.82)$$

To reach the second line we have integrated by parts, and, because the ends are fixed, and therefore $\delta y = 0$ at $x = 0$ and L , there is no boundary term. Requiring that $\delta S = 0$ for all allowed variations δy then gives the equation of motion

$$\rho \frac{\partial^2 y}{\partial t^2} - T \frac{\partial^2 y}{\partial x^2} = 0. \quad (1.83)$$

This is the wave equation describing transverse waves propagating with speed $c = \sqrt{T/\rho}$. Observe that from (1.82) we can read off the functional derivative of S with respect to the variable $y(x, t)$ as being

$$\frac{\delta S}{\delta y(x, t)} = -\rho \ddot{y}(x, t) + T y''(x, t). \quad (1.84)$$

In writing down the first integral for this continuous system, we must replace the sum over discrete indices by an integral:

$$E = \sum_i \dot{q}_i \frac{\partial L}{\partial \dot{q}_i} - L \rightarrow \int dx \left\{ \dot{y}(x) \frac{\delta L}{\delta \dot{y}(x)} \right\} - L. \quad (1.85)$$

When computing $\delta L / \delta \dot{y}(x)$ from

$$L = \int_0^L dx \left\{ \frac{1}{2} \rho \dot{y}^2 - \frac{1}{2} T y'^2 \right\},$$

we must remember that it is the continuous analogue of $\partial L / \partial \dot{q}_i$, and so, in contrast to what we do when computing $\delta S / \delta y(x)$, we must treat $\dot{y}(x)$ as a variable independent of $y(x)$. We then have

$$\frac{\delta L}{\delta \dot{y}(x)} = \rho \dot{y}(x), \quad (1.86)$$

leading to

$$E = \int_0^L dx \left\{ \frac{1}{2} \rho \dot{y}^2 + \frac{1}{2} T y'^2 \right\}. \quad (1.87)$$

This, as expected, is the total energy, kinetic plus potential, of the string.

The energy-momentum tensor

If we consider an action of the form

$$S = \int \mathcal{L}(\varphi, \varphi_\mu) d^{d+1}x, \quad (1.88)$$

which does not depend *explicitly* on any of the co-ordinates x^μ , we may refine Noether's derivation of the law of conservation total energy and obtain

accounting information about the position-dependent energy *density*. To do this we make a variation of the form

$$\varphi(x) \rightarrow \varphi(x^\mu + \varepsilon^\mu(x)) = \varphi(x^\mu) + \varepsilon^\mu(x) \partial_\mu \varphi + O(|\varepsilon|^2), \quad (1.89)$$

where ε depends on $x \equiv (x^0, \dots, x^d)$. The resulting variation in S is

$$\begin{aligned} \delta S &= \int \left\{ \frac{\partial \mathcal{L}}{\partial \varphi} \varepsilon^\mu \partial_\mu \varphi + \frac{\partial \mathcal{L}}{\partial \varphi_\nu} \partial_\nu (\varepsilon^\mu \partial_\mu \varphi) \right\} d^{d+1}x \\ &= \int \varepsilon^\mu(x) \frac{\partial}{\partial x^\nu} \left\{ \mathcal{L} \delta_\mu^\nu - \frac{\partial \mathcal{L}}{\partial \varphi_\nu} \partial_\mu \varphi \right\} d^{d+1}x. \end{aligned} \quad (1.90)$$

When φ satisfies the equations of motion this δS will be zero for arbitrary $\varepsilon^\mu(x)$. We conclude that

$$\frac{\partial}{\partial x^\nu} \left\{ \mathcal{L} \delta_\mu^\nu - \frac{\partial \mathcal{L}}{\partial \varphi_\nu} \partial_\mu \varphi \right\} = 0. \quad (1.91)$$

The d -by- d array of functions

$$T^\nu{}_\mu \equiv \frac{\partial \mathcal{L}}{\partial \varphi_\nu} \partial_\mu \varphi - \delta_\mu^\nu \mathcal{L} \quad (1.92)$$

is known as the *canonical energy-momentum tensor*, and the statement

$$\partial_\nu T^\nu{}_\mu = 0 \quad (1.93)$$

usually provides book-keeping for the flow of energy and momentum.

In the case of the vibrating string, the $\mu = 0, 1$ components of $\partial_\nu T^\nu{}_\mu = 0$ become the two following *local* conservation equations:

$$\frac{\partial}{\partial t} \left\{ \frac{\rho}{2} \dot{y}^2 + \frac{T}{2} y'^2 \right\} + \frac{\partial}{\partial x} \{-T \dot{y} y'\} = 0, \quad (1.94)$$

and

$$\frac{\partial}{\partial t} \{-\rho \dot{y} y'\} + \frac{\partial}{\partial x} \left\{ \frac{\rho}{2} \dot{y}^2 + \frac{T}{2} y'^2 \right\} = 0. \quad (1.95)$$

It is easy to verify that these are indeed consequences of the wave equation. They are “local” conservation laws because they are of the form

$$\frac{\partial q}{\partial t} + \nabla \cdot \mathbf{J} = 0, \quad (1.96)$$

where q is the local density, and \mathbf{J} the flux, of the globally conserved quantity $Q = \int q d^d x$. In the first case, the local density q is

$$T^0_0 = \frac{\rho}{2} \dot{y}^2 + \frac{T}{2} y'^2, \quad (1.97)$$

which is the energy density. The energy flux is given by $T^1_0 \equiv -T \dot{y} y'$, which is the rate of working by one piece of string on its neighbour. Integrating over x , and observing that the fixed-end boundary conditions are such that

$$\int_0^L \frac{\partial}{\partial x} \{-T \dot{y} y'\} dx = [-T \dot{y} y']_0^L = 0, \quad (1.98)$$

gives us

$$\frac{d}{dt} \int_0^L \left\{ \frac{\rho}{2} \dot{y}^2 + \frac{T}{2} y'^2 \right\} dx = 0, \quad (1.99)$$

which is the global energy conservation law we obtained earlier.

The physical interpretation of $T^0_1 = -\rho \dot{y} y'$, the locally conserved quantity in the second case, is less obvious. If this were a relativistic system, we would have no difficulty in identifying $\int T^0_1 dx$ as the x -component of the energy-momentum 4-vector, and therefore T^0_1 as the density of x -momentum. Now a physical string will have some motion in the x direction, but the magnitude of this motion will depend on the string's elastic constants and other quantities unknown to our Lagrangian. Thus the T^0_1 derived from L cannot be the string's x -momentum density. Instead, it is the density of something called *pseudo-momentum*. The distinction between true and pseudo-momentum is best understood by considering the corresponding Noether symmetry. The symmetry associated with Newtonian momentum is the invariance of the action integral under an x translation of the entire apparatus: the string, and any wave on it. The symmetry associated with pseudo-momentum is the invariance of the action under a shift $y(x) \rightarrow y(x - a)$ of the location of the wave on the string — the string itself not being translated. Newtonian momentum is conserved if the *ambient space* is translationally invariant. Pseudo-momentum is conserved only if the *string* is translationally invariant — *i.e.* if ρ and T are position independent. A failure to realize that the presence of a medium (here the string) requires us to distinguish between these two symmetries is the origin of much confusion involving “wave momentum.”

Maxwell's equations

Michael Faraday and James Clerk Maxwell's description of electromagnetism in terms of dynamical vector fields gave us the first modern field theory. D' Alembert and Maupertuis would have been delighted to discover that the famous equations of Maxwell's *A Treatise on Electricity and Magnetism* (1873) follow from an action principle. There is a slight complication stemming from gauge invariance but, as long as we are not interested in exhibiting the covariance of Maxwell under Lorentz transformations, we can sweep this under the rug by working in the *axial gauge*, where the scalar electric potential does not appear.

We will start from Maxwell's equations

$$\begin{aligned}\nabla \cdot \mathbf{B} &= 0, \\ \nabla \times \mathbf{E} &= -\dot{\mathbf{B}}, \\ \nabla \times \mathbf{H} &= \mathbf{J} + \dot{\mathbf{D}}, \\ \nabla \cdot \mathbf{D} &= \rho,\end{aligned}\tag{1.100}$$

and show that they can be obtained from an action principle. For convenience we shall use *natural* units in which $\mu_0 = \varepsilon_0 = 1$, and so $c = 1$ and $\mathbf{D} \equiv \mathbf{E}$ and $\mathbf{B} \equiv \mathbf{H}$.

The first equation $\nabla \cdot \mathbf{B} = 0$ contains no time derivatives. It is a constraint which we satisfy by introducing a vector potential \mathbf{A} such that $\mathbf{B} = \nabla \times \mathbf{A}$. If we set

$$\mathbf{E} = -\dot{\mathbf{A}},\tag{1.101}$$

then this automatically implies Faraday's law of induction

$$\nabla \times \mathbf{E} = -\dot{\mathbf{B}}.\tag{1.102}$$

We now guess that the Lagrangian is

$$L = \int d^3x \left[\frac{1}{2} \{ \mathbf{E}^2 - \mathbf{B}^2 \} + \mathbf{J} \cdot \mathbf{A} \right].\tag{1.103}$$

The motivation is that L looks very like $T - V$ if we regard $\frac{1}{2}\mathbf{E}^2 \equiv \frac{1}{2}\dot{\mathbf{A}}^2$ as being the kinetic energy and $\frac{1}{2}\mathbf{B}^2 = \frac{1}{2}(\nabla \times \mathbf{A})^2$ as being the potential energy. The term in \mathbf{J} represents the interaction of the fields with an external current

source. In the axial gauge the electric charge density ρ does not appear in the Lagrangian. The corresponding action is therefore

$$S = \int L dt = \iint d^3x \left[\frac{1}{2} \dot{\mathbf{A}}^2 - \frac{1}{2} (\nabla \times \mathbf{A})^2 + \mathbf{J} \cdot \mathbf{A} \right] dt. \quad (1.104)$$

Now vary \mathbf{A} to $\mathbf{A} + \delta\mathbf{A}$, whence

$$\delta S = \iint d^3x \left[-\ddot{\mathbf{A}} \cdot \delta\mathbf{A} - (\nabla \times \mathbf{A}) \cdot (\nabla \times \delta\mathbf{A}) + \mathbf{J} \cdot \delta\mathbf{A} \right] dt. \quad (1.105)$$

Here, we have already removed the time derivative from $\delta\mathbf{A}$ by integrating by parts in the time direction. Now we do the integration by parts in the space directions by using the identity

$$\nabla \cdot (\delta\mathbf{A} \times (\nabla \times \mathbf{A})) = (\nabla \times \mathbf{A}) \cdot (\nabla \times \delta\mathbf{A}) - \delta\mathbf{A} \cdot (\nabla \times (\nabla \times \mathbf{A})) \quad (1.106)$$

and taking $\delta\mathbf{A}$ to vanish at spatial infinity, so the surface term, which would come from the integral of the total divergence, is zero. We end up with

$$\delta S = \iint d^3x \left\{ \delta\mathbf{A} \cdot \left[-\ddot{\mathbf{A}} - \nabla \times (\nabla \times \mathbf{A}) + \mathbf{J} \right] \right\} dt. \quad (1.107)$$

Demanding that the variation of S be zero thus requires

$$\ddot{\mathbf{A}} = -\nabla \times (\nabla \times \mathbf{A}) + \mathbf{J}, \quad (1.108)$$

or, in terms of the physical fields,

$$\nabla \times \mathbf{B} = \mathbf{J} + \dot{\mathbf{E}}. \quad (1.109)$$

This is Ampère's law, as modified by Maxwell so as to include the displacement current.

How do we deal with the last Maxwell equation, Gauss' law, which asserts that $\nabla \cdot \mathbf{E} = \rho$? If ρ were equal to zero, this equation would hold if $\nabla \cdot \mathbf{A} = 0$, *i.e.* if \mathbf{A} were solenoidal. In this case we might be tempted to impose the constraint $\nabla \cdot \mathbf{A} = 0$ on the vector potential, but doing so would undo all our good work, as we have been assuming that we can vary \mathbf{A} freely.

We notice, however, that the three Maxwell equations we already have tell us that

$$\frac{\partial}{\partial t} (\nabla \cdot \mathbf{E} - \rho) = \nabla \cdot (\nabla \times \mathbf{B}) - \left(\nabla \cdot \mathbf{J} + \frac{\partial \rho}{\partial t} \right). \quad (1.110)$$

Since $\nabla \cdot (\nabla \times \mathbf{B}) = 0$, the left-hand side is zero provided charge is conserved, *i.e.* provided

$$\dot{\rho} + \nabla \cdot \mathbf{J} = 0, \quad (1.111)$$

and we assume that this is so. Thus, if Gauss' law holds initially, it holds eternally. We arrange for it to hold at $t = 0$ by imposing initial conditions on \mathbf{A} . We first choose $\mathbf{A}|_{t=0}$ by requiring it to satisfy

$$\mathbf{B}|_{t=0} = \nabla \times (\mathbf{A}|_{t=0}). \quad (1.112)$$

The solution is not unique, because may we add any $\nabla\phi$ to $\mathbf{A}|_{t=0}$, but this does not affect the physical \mathbf{E} and \mathbf{B} fields. The initial “velocities” $\dot{\mathbf{A}}|_{t=0}$ are then fixed uniquely by $\dot{\mathbf{A}}|_{t=0} = -\mathbf{E}|_{t=0}$, where the initial \mathbf{E} satisfies Gauss' law. The subsequent evolution of \mathbf{A} is then uniquely determined by integrating the second-order equation (1.108).

The first integral for Maxwell is

$$\begin{aligned} E &= \sum_{i=1}^3 \int d^3x \left\{ \dot{A}_i \frac{\delta L}{\delta \dot{A}_i} \right\} - L \\ &= \int d^3x \left[\frac{1}{2} \{ \mathbf{E}^2 + \mathbf{B}^2 \} - \mathbf{J} \cdot \mathbf{A} \right]. \end{aligned} \quad (1.113)$$

This will be conserved if \mathbf{J} is time independent. If $\mathbf{J} = 0$, it is the total field energy.

Suppose \mathbf{J} is neither zero nor time independent. Then, looking back at the derivation of the time-independence of the first integral, we see that if L *does* depend on time, we instead have

$$\frac{dE}{dt} = -\frac{\partial L}{\partial t}. \quad (1.114)$$

In the present case we have

$$-\frac{\partial L}{\partial t} = -\int \dot{\mathbf{J}} \cdot \mathbf{A} d^3x, \quad (1.115)$$

so that

$$-\int \dot{\mathbf{J}} \cdot \mathbf{A} d^3x = \frac{dE}{dt} = \frac{d}{dt}(\text{Field Energy}) - \int \{ \mathbf{J} \cdot \dot{\mathbf{A}} + \dot{\mathbf{J}} \cdot \mathbf{A} \} d^3x. \quad (1.116)$$

Thus, cancelling the duplicated term and using $\mathbf{E} = -\dot{\mathbf{A}}$, we find

$$\frac{d}{dt}(\text{Field Energy}) = - \int \mathbf{J} \cdot \mathbf{E} d^3x. \quad (1.117)$$

Now $\int \mathbf{J} \cdot (-\mathbf{E}) d^3x$ is the rate at which the power source driving the current is doing work against the field. The result is therefore physically sensible.

Continuum mechanics

Since the mechanics of discrete objects can be derived from an action principle, it seems obvious that so must the mechanics of continua. This is certainly true if we use the *Lagrangian* description where we follow the history of each particle composing the continuous material as it moves through space. In fluid mechanics, though, it is more natural to describe the motion by using the *Eulerian* description in which we focus on what is going on at a particular point in space by introducing a velocity field $\mathbf{v}(\mathbf{r}, t)$. Eulerian action principles can still be found, but they seem to be logically distinct from the Lagrangian mechanics action principle, and mostly were not discovered until the 20th century.

We begin by showing that Euler's equation for the irrotational motion of an inviscid compressible fluid can be obtained from the Lagrangian

$$L = \int d^3x \left\{ \rho \dot{\phi} + \frac{1}{2} \rho (\nabla \phi)^2 + u(\rho) \right\}, \quad (1.118)$$

Here, ρ is the mass density, the flow velocity is determined from the velocity potential ϕ by $\mathbf{v} = \nabla \phi$, and the function u is the internal energy density.

Varying with respect to ρ is straightforward, and gives a time dependent generalization of (Daniel) Bernoulli's equation

$$\dot{\phi} + \frac{1}{2} \mathbf{v}^2 + h(\rho) = 0. \quad (1.119)$$

Here $h(\rho) \equiv du/d\rho$, is the specific enthalpy². Varying with respect to ϕ requires an integration by parts, based on

$$\nabla \cdot (\rho \delta \phi \nabla \phi) = \rho (\nabla \delta \phi) \cdot (\nabla \phi) - \delta \phi \nabla \cdot (\rho \nabla \phi), \quad (1.120)$$

²The enthalpy, $H = U + PV$, per unit mass. In general u and h will be functions of both the density and the specific entropy. By taking u to depend only on ρ we are tacitly assuming that specific entropy is constant. This makes the resultant flow *barotropic*, meaning that the pressure is a function of the density only.

and gives the equation of mass conservation

$$\dot{\rho} + \nabla \cdot (\rho \mathbf{v}) = 0. \quad (1.121)$$

Taking the gradient of Bernoulli's equation, and using the fact that for potential flow the *vorticity* $\boldsymbol{\omega} \equiv \nabla \times \mathbf{v}$ is zero and so $\partial_i v_j = \partial_j v_i$, we find that

$$\dot{\mathbf{v}} + (\mathbf{v} \cdot \nabla) \mathbf{v} = -\nabla h. \quad (1.122)$$

We now introduce the pressure P , which is related to h by

$$h(P) = \int_0^P \frac{dP}{\rho(P)}. \quad (1.123)$$

We see that $\rho \nabla h = \nabla P$, and so obtain Euler's equation

$$\rho \left(\dot{\mathbf{v}} + (\mathbf{v} \cdot \nabla) \mathbf{v} \right) = -\nabla P. \quad (1.124)$$

For future reference, we observe that combining the mass-conservation equation

$$\partial_t \rho + \partial_j \{ \rho v_j \} = 0 \quad (1.125)$$

with Euler's equation

$$\rho (\partial_t v_i + v_j \partial_j v_i) = -\partial_i P \quad (1.126)$$

yields

$$\partial_t \{ \rho v_i \} + \partial_j \{ \rho v_i v_j + \delta_{ij} P \} = 0, \quad (1.127)$$

which expresses the local conservation of momentum. The quantity

$$\Pi_{ij} = \rho v_i v_j + \delta_{ij} P \quad (1.128)$$

is the *momentum-flux tensor*, and is the j -th component of the flux of the i -th component $p_i = \rho v_i$ of momentum density.

The relations $h = du/d\rho$ and $\rho = dP/dh$ show that P and u are related by a Legendre transformation: $P = \rho h - u(\rho)$. From this, and the Bernoulli equation, we see that the integrand in the Lagrangian (1.118) is equal to minus the pressure:

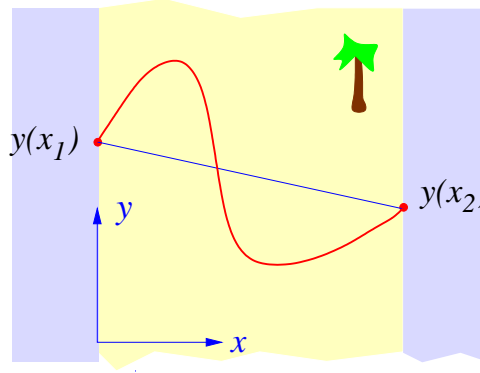
$$-P = \rho \dot{\phi} + \frac{1}{2} \rho (\nabla \phi)^2 + u(\rho). \quad (1.129)$$

This Eulerian formulation cannot be a “follow the particle” action principle in a clever disguise. The mass conservation law is only a consequence of the equation of motion, and is not built in from the beginning as a constraint. Our variations in ϕ are therefore conjuring up new matter rather than merely moving it around.

1.4 Variable End Points

We now relax our previous assumption that all boundary or surface terms coming from integrations by parts may be ignored. We will find that variation principles can be very useful for figuring out what boundary conditions we should impose on our differential equations.

Consider the problem of building a railway across a parallel sided isthmus.



Suppose that the cost of construction is proportional to the length of the track, but the cost of sea transport being negligible, we may locate the terminal seaports wherever we like. We therefore wish to minimize the length

$$L[y] = \int_{x_1}^{x_2} \sqrt{1 + (y')^2} dx, \quad (1.130)$$

by allowing both the path $y(x)$ and the endpoints $y(x_1)$ and $y(x_2)$ to vary. Then

$$\begin{aligned} L[y + \delta y] - L[y] &= \int_{x_1}^{x_2} (\delta y') \frac{y'}{\sqrt{1 + (y')^2}} dx \\ &= \int_{x_1}^{x_2} \left\{ \frac{d}{dx} \left(\delta y \frac{y'}{\sqrt{1 + (y')^2}} \right) - \delta y \frac{d}{dx} \left(\frac{y'}{\sqrt{1 + (y')^2}} \right) \right\} dx \\ &= \delta y(x_1) \frac{y'(x_1)}{\sqrt{1 + (y')^2}} - \delta y(x_2) \frac{y'(x_1)}{\sqrt{1 + (y')^2}} \\ &\quad + \int_{x_1}^{x_2} \delta y \frac{d}{dx} \left(\frac{y'}{\sqrt{1 + (y')^2}} \right) dx. \end{aligned} \quad (1.131)$$

We have stationarity when both

i) the coefficient of $\delta y(x)$ in the integral,

$$\frac{d}{dx} \left(\frac{y'}{\sqrt{1 + (y')^2}} \right), \quad (1.132)$$

is zero. This requires that $y' = \text{const.}$, *i.e.* the track should be straight.

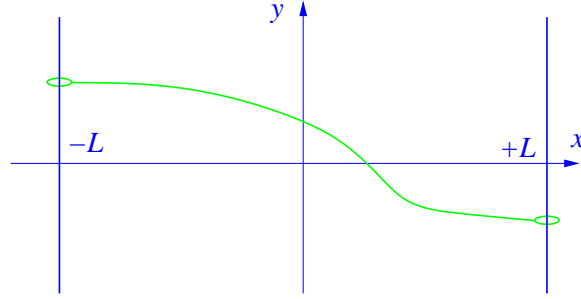
ii) The coefficients of $\delta y(x_1)$ and $\delta y(x_2)$ vanish. For this we need

$$0 = \frac{y'(x_1)}{\sqrt{1 + (y')^2}} = \frac{y'(x_2)}{\sqrt{1 + (y')^2}}. \quad (1.133)$$

This in turn requires that $y'(x_1) = y'(x_2) = 0$.

The integrated-out bits have determined the boundary conditions that are to be imposed on the solution of the differential equation. In the present case they require us to build perpendicular to the coastline, and so we go straight across the isthmus. When boundary conditions are obtained from endpoint variations in this way, they are called *natural boundary conditions*.

Example: Sliding String. A massive string of linear density ρ is stretched between two smooth posts separated by distance $2L$. The string is under tension T , and is free to slide up and down the posts. We will consider only a small deviations of the string from the horizontal.



As we saw earlier, the Lagrangian for a stretched string is

$$L = \int_{-L}^L \left\{ \frac{1}{2} \rho \dot{y}^2 - \frac{1}{2} T (y')^2 \right\} dx. \quad (1.134)$$

Now, Lagrange's principle says that the equation of motion is found by requiring the action

$$S = \int_{t_i}^{t_f} L dt \quad (1.135)$$

to be stationary under variations of $y(x, t)$ that vanish at the initial and final times, t_i and t_f . It does *not* demand that δy vanish at ends of the string, $x = \pm L$. So, when we make the variation, we must not assume this. Taking care not to discard the results of the integration by parts in the x direction, we find

$$\begin{aligned} \delta S = & \int_{t_i}^{t_f} \int_{-L}^L \delta y(x, t) \{ \rho \ddot{y} - T y'' \} dx dt - \int_{t_i}^{t_f} \delta y(L, t) T y'(L) dt \\ & + \int_{t_i}^{t_f} \delta y(-L, t) T y'(-L) dt. \end{aligned} \quad (1.136)$$

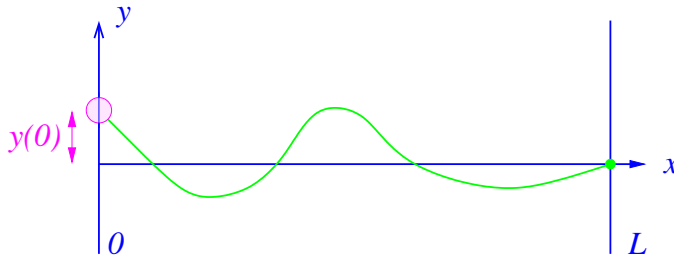
The equation of motion, which arises from the variation within the interval, is therefore the wave equation

$$\rho \ddot{y} - T y'' = 0. \quad (1.137)$$

The boundary conditions, which come from the variations at the endpoints, are

$$y'(L, t) = y'(-L, t) = 0, \quad (1.138)$$

at all times t . These are the physically correct boundary conditions, because any up-or-down component of the tension would provide a finite force on an infinitesimal mass. The string must therefore be horizontal at its endpoints. *Example: Bead and String.* Suppose now that a bead of mass M is free to slide up and down the y axis,



A bead connected to a string.

and is attached to the $x = 0$ end of our string. The Lagrangian for the string-bead contraption is

$$L = \frac{1}{2} M [\dot{y}(0)]^2 + \int_0^L \left\{ \frac{1}{2} \rho \dot{y}^2 - \frac{1}{2} T y'^2 \right\} dx. \quad (1.139)$$

Here, as before, ρ is the mass per unit length of the string and T is its tension. The end of the string at $x = L$ is fixed. By varying the action $S = \int L dt$, and taking care not to throw away the boundary part at $x = 0$ we find that

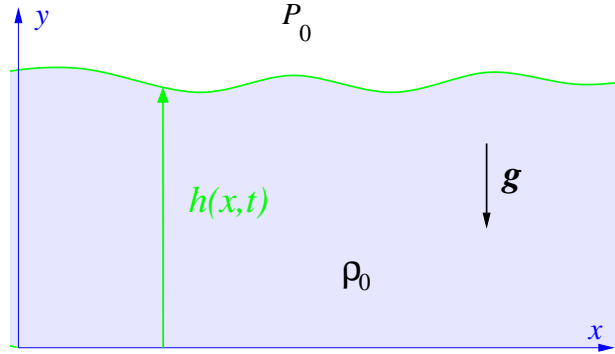
$$\delta S = \int_{t_i}^{t_f} [Ty' - M\ddot{y}]_{x=0} \delta y(0, t) dt + \int_{t_i}^{t_f} \int_0^L \{Ty'' - \rho\ddot{y}\} \delta y(x, t) dx dt. \quad (1.140)$$

The Euler-Lagrange equations are therefore

$$\begin{aligned} \rho\ddot{y}(x) - Ty''(x) &= 0, & 0 < x < L, \\ M\ddot{y}(0) - Ty'(0) &= 0, & y(L) = 0. \end{aligned} \quad (1.141)$$

The boundary condition at $x = 0$ is the equation of motion for the bead. It is clearly correct, because $Ty'(0)$ is the vertical component of the force that the string tension exerts on the bead.

These examples led to boundary conditions that we could easily have figured out for ourselves without the variational principle. The next example shows that a variational formulation can be exploited to obtain a set of boundary conditions that might be difficult to write down by purely “physical” reasoning.



Harder example: Surface Waves on Water. An action suitable for describing waves on the surface of water is given by³ $S = \int L dt$, where

$$L = \int dx \int_0^{h(x,t)} \rho_0 \left\{ \dot{\phi} + \frac{1}{2}(\nabla\phi)^2 + gy \right\} dy. \quad (1.142)$$

³J. C. Luke, *J. Fluid Dynamics*, **27** (1967) 395.

Here ρ_0 is the density of the water, which is being treated as being incompressible, and the flow velocity is $\mathbf{v} = \nabla\phi$. By varying $\phi(x, y, t)$ and the depth $h(x, t)$, and taking care not to throw away any integrated-out parts of the variation at the physical boundaries, we obtain:

$$\begin{aligned}\nabla^2\phi &= 0, & \text{within the fluid.} \\ \dot{\phi} + \frac{1}{2}(\nabla\phi)^2 + gy &= 0, & \text{on the free surface.} \\ \frac{\partial\phi}{\partial y} &= 0, & \text{on } y = 0. \\ \dot{h} - \frac{\partial\phi}{\partial y} + \frac{\partial h}{\partial x} \frac{\partial\phi}{\partial x} &= 0, & \text{on the free surface.}\end{aligned}\tag{1.143}$$

The first equation comes from varying ϕ within the fluid, and it simply confirms that the flow is incompressible, *i.e.* obeys $\nabla \cdot \mathbf{v} = 0$. The second comes from varying h , and is the Bernoulli equation stating that we have $P = P_0$ (atmospheric pressure) everywhere on the free surface. The third, from the variation of ϕ at $y = 0$, states that no fluid escapes through the lower boundary.

Obtaining and interpreting the last equation, involving \dot{h} , is somewhat trickier. It comes from the variation of ϕ on the upper boundary. The variation of S due to $\delta\phi$ is

$$\delta S = \int \rho_0 \left\{ \frac{\partial}{\partial t} \delta\phi + \frac{\partial}{\partial x} \left(\delta\phi \frac{\partial\phi}{\partial x} \right) + \frac{\partial}{\partial y} \left(\delta\phi \frac{\partial\phi}{\partial y} \right) - \delta\phi \nabla^2\phi \right\} dt dx dy.\tag{1.144}$$

The first three terms in the integrand constitute the three-dimensional divergence $\nabla \cdot (\delta\phi \mathbf{\Phi})$ where, listing components in the order t, x, y ,

$$\mathbf{\Phi} = \left[1, \frac{\partial\phi}{\partial x}, \frac{\partial\phi}{\partial y} \right].\tag{1.145}$$

The integrated-out part on the upper surface is therefore $\int (\mathbf{\Phi} \cdot \mathbf{n}) \delta\phi d|S|$. Here, the outward normal is

$$\mathbf{n} = \left(1 + \left(\frac{\partial h}{\partial t} \right)^2 + \left(\frac{\partial h}{\partial x} \right)^2 \right)^{-1/2} \left[-\frac{\partial h}{\partial t}, -\frac{\partial h}{\partial x}, 1 \right],\tag{1.146}$$

and the element of area

$$d|S| = \left(1 + \left(\frac{\partial h}{\partial t} \right)^2 + \left(\frac{\partial h}{\partial x} \right)^2 \right)^{1/2} dt dx.\tag{1.147}$$

The boundary variation is thus

$$\delta S|_{y=h} = - \int \left\{ \frac{\partial h}{\partial t} - \frac{\partial \phi}{\partial y} + \frac{\partial h}{\partial x} \frac{\partial \phi}{\partial x} \right\} \delta \phi(x, h(x, t), t) dx dt. \quad (1.148)$$

Requiring this to be zero for arbitrary $\delta \phi(x, h(x, t), t)$ leads to

$$\frac{\partial h}{\partial t} - \frac{\partial \phi}{\partial y} + \frac{\partial h}{\partial x} \frac{\partial \phi}{\partial x} = 0. \quad (1.149)$$

This last boundary condition expresses the geometrical constraint that the surface moves with the fluid it bounds, or, in other words, that a fluid particle initially on the surface stays on the surface. To see this define $f(x, y, t) = h(x, t) - y$, so the free surface is given by $f(x, y, t) = 0$. If the surface particles are carried with the flow then the convective derivative of f ,

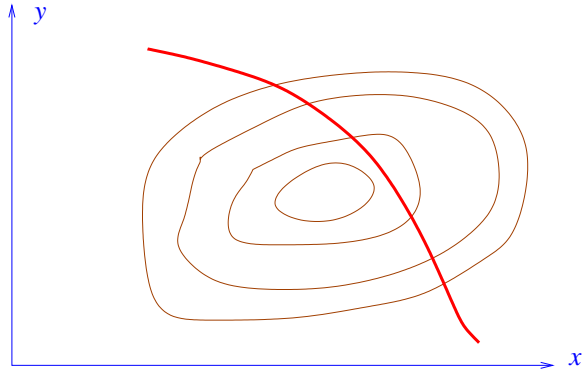
$$\frac{df}{dt} \equiv \frac{\partial f}{\partial t} + (\mathbf{v} \cdot \nabla) f, \quad (1.150)$$

must vanish on the free surface. Using $\mathbf{v} = \nabla \phi$ and the definition of f , this reduces to

$$\frac{\partial h}{\partial t} + \frac{\partial \phi}{\partial x} \frac{\partial h}{\partial x} - \frac{\partial \phi}{\partial y} = 0, \quad (1.151)$$

which is indeed the last boundary condition.

1.5 Lagrange Multipliers



The figure shows the contour map of hill of height $h = f(x, y)$ traversed by a road given by the equation $g(x, y) = 0$. Our problem is to find the highest point on the road.

When \mathbf{r} changes by $d\mathbf{r} = (dx, dy)$, the height f changes by

$$df = \nabla f \cdot d\mathbf{r}, \quad (1.152)$$

where $\nabla f = (\partial_x f, \partial_y f)$. The highest point will have $df = 0$ for all displacements $d\mathbf{r}$ that stay on the road — that is for all $d\mathbf{r}$ such that $dg = 0$. Thus $\nabla f \cdot d\mathbf{r}$ must be zero for those $d\mathbf{r}$ such that $0 = \nabla g \cdot d\mathbf{r}$. In other words, ∇f must be orthogonal to all vectors that are orthogonal to ∇g . This is possible only if the vectors ∇f and ∇g are parallel, and so $\nabla f = \lambda \nabla g$ for some λ . To find the stationary point, therefore, we solve the equations

$$\begin{aligned} \nabla f - \lambda \nabla g &= 0, \\ g(x, y) &= 0, \end{aligned} \quad (1.153)$$

simultaneously.

Example: Let $f = x^2 + y^2$ and $g = x + y - 1$. Then $\nabla f = 2(x, y)$ and $\nabla g = (1, 1)$. So

$$\begin{aligned} 2(x, y) - \lambda(1, 1) &= 0, \quad \Rightarrow \quad (x, y) = \frac{\lambda}{2}(1, 1) \\ x + y &= 1, \quad \Rightarrow \quad \lambda = 1, \quad \Rightarrow \quad (x, y) = \left(\frac{1}{2}, \frac{1}{2}\right). \end{aligned}$$

In general, if there are n constraints, $g_1 = g_2 = \cdots = g_n = 0$, we will want ∇f to lie in

$$(< \nabla g_i >^\perp)^\perp = < \nabla g_i >, \quad (1.154)$$

where $< \mathbf{e}_i >$ denotes the space spanned by the vectors \mathbf{e}_i and $< \mathbf{e}_i >^\perp$ is the its orthogonal complement. Thus ∇f lies in the space spanned by the vectors ∇g_i , so there must exist n numbers λ_i such that

$$\nabla f = \sum_{i=1}^n \lambda_i \nabla g_i. \quad (1.155)$$

The numbers λ_i are called *Lagrange multipliers*. We can therefore regard our problem as one of finding the stationary points of an auxilliary function

$$F = f - \sum_i \lambda_i g_i, \quad (1.156)$$

with the *undetermined multipliers* λ_i subsequently being fixed by imposing the requirement that $g_i = 0$.

Example: Find the stationary points of

$$F(\mathbf{x}) = \frac{1}{2} \mathbf{x} \cdot \mathbf{A} \mathbf{x} = \frac{1}{2} x_i A_{ij} x_j \quad (1.157)$$

on the surface $\mathbf{x} \cdot \mathbf{x} = 1$. Here A_{ij} is a symmetric matrix.

Solution: We look for stationary points of

$$G(\mathbf{x}) = F(\mathbf{x}) - \frac{1}{2} \lambda |\mathbf{x}|^2. \quad (1.158)$$

The derivatives we need are

$$\begin{aligned} \frac{\partial F}{\partial x^k} &= \frac{1}{2} \delta_{ki} A_{ij} x_j + \frac{1}{2} x_i A_{ij} \delta_{jk} \\ &= A_{kj} x_j, \end{aligned} \quad (1.159)$$

and

$$\frac{\partial}{\partial x_k} \left(\frac{\lambda}{2} x_j x_j \right) = \lambda x_k. \quad (1.160)$$

Thus, the stationary points must satisfy

$$\begin{aligned} A_{kj} x_j &= \lambda x_k, \\ x^i x^i &= 1, \end{aligned} \quad (1.161)$$

and so are the normalized eigenvectors of the matrix \mathbf{A} . The Lagrange multiplier at each stationary point is the corresponding eigenvalue.

Example: Statistical Mechanics. Let Γ denote the classical phase space of a mechanical system of n particles governed by Hamiltonian $H(p, q)$. Let $d\Gamma$ be the Liouville measure $d^{3n}p d^{3n}q$. In statistical mechanics we work with a probability density $\rho(p, q)$ such that $\rho(p, q) d\Gamma$ is the probability of the system being in a state in the small region $d\Gamma$. The *entropy* associated with the probability distribution is the functional

$$S[\rho] = - \int_{\Gamma} \rho \ln \rho d\Gamma. \quad (1.162)$$

We wish to find the $\rho(p, q)$ that maximizes the entropy for a given total energy

$$E = \int_{\Gamma} \rho H d\Gamma. \quad (1.163)$$

We cannot vary ρ freely as we should preserve both the energy and the normalization condition

$$\int_{\Gamma} \rho d\Gamma = 1 \quad (1.164)$$

that is required of any probability distribution. We therefore introduce two Lagrange multipliers, $1 + \alpha$ and β , to enforce the normalization and energy conditions, and look for stationary points of

$$F[\rho] = \int_{\Gamma} \{-\rho \ln \rho + (\alpha + 1)\rho - \beta \rho H\} d\Gamma. \quad (1.165)$$

Now we can vary ρ freely, and hence find that

$$\delta F = \int_{\Gamma} \{-\ln \rho + \alpha - \beta H\} \delta \rho d\Gamma. \quad (1.166)$$

Requiring this to be zero gives us

$$\rho(p, q) = e^{\alpha - \beta H(p, q)}, \quad (1.167)$$

where α, β are determined by imposing the normalization and energy constraints. This probability density is known as the *canonical distribution*, and the parameter β is the inverse temperature $\beta = 1/T$.

Example: The Catenary. At long last we can solve the problem of the hanging chain of fixed length. We wish to minimize the potential energy

$$E[y] = \int_{-L}^L y \sqrt{1 + (y')^2} dx, \quad (1.168)$$

subject to the constraint

$$l[y] = \int_{-L}^L \sqrt{1 + (y')^2} dx = \text{const.}, \quad (1.169)$$

where the constant is the length of the chain. We introduce a Lagrange multiplier λ and find the stationary points of

$$F[y] = \int_{-L}^L (y - \lambda) \sqrt{1 + (y')^2} dx, \quad (1.170)$$

so, following our earlier methods, we find

$$y = \lambda + \kappa \cosh \frac{(x + a)}{\kappa}. \quad (1.171)$$

We choose κ, λ, a to fix the two endpoints (two conditions) and the length (one condition).

Example: Sturm-Liouville Problem. We wish to find the stationary points of the quadratic functional

$$J[y] = \int_{x_1}^{x_2} \frac{1}{2} \{p(x)(y')^2 + q(x)y^2\} dx, \quad (1.172)$$

subject to the boundary conditions $y(x) = 0$ at the endpoints x_1, x_2 and the normalization

$$K[y] = \int_{x_1}^{x_2} y^2 dx = 1. \quad (1.173)$$

Taking the variation of $J - \lambda K$, we find

$$\delta J = \int_{x_1}^{x_2} \{-(py')' + qy - \lambda y\} \delta y dx. \quad (1.174)$$

Stationarity therefore requires

$$-(py')' + qy = \lambda y, \quad y(x_1) = y(x_2) = 0. \quad (1.175)$$

This is the *Sturm-Liouville eigenvalue problem*. It is an infinite dimensional analogue of the $F(\mathbf{x}) = \frac{1}{2}\mathbf{x} \cdot \mathbf{A}\mathbf{x}$ problem.

Example: Irrotational Flow Again. Consider the Lagrange density

$$L = \int \left\{ -\frac{1}{2}\rho\mathbf{v}^2 + u(\rho) - \phi(\dot{\rho} + \nabla \cdot \rho\mathbf{v}) \right\} d^3x \quad (1.176)$$

This is similar to our previous Lagrangian for the irrotational barotropic flow of an inviscid fluid, but here ϕ is playing the role of a Lagrange multiplier enforcing the condition of mass conservation. Varying \mathbf{v} shows that $\mathbf{v} = \nabla\phi$, and the Bernoulli and Euler equations follow almost as before. Because the equation $\mathbf{v} = \nabla\phi$ does not involve time derivatives, this is one of the cases where it is legitimate to substitute a consequence of the action principle back into the action, and this gives us back our previous formulation.

1.6 Maximum or Minimum?

We have provided many examples of stationary points in function space. We have said almost nothing about whether these stationary points are maxima

or minima. There is a reason for this: investigating the character of the stationary point requires the computation of the second functional derivative.

$$\frac{\delta^2 J}{\delta y(x_1)\delta y(x_2)}$$

and the use of the functional version of Taylor's theorem to expand about the stationary point $y(x)$:

$$\begin{aligned} J[y + \varepsilon\eta] &= J[y] + \varepsilon \int \eta(x) \left. \frac{\delta J}{\delta y(x)} \right|_y dx \\ &\quad + \frac{\varepsilon^2}{2} \int \eta(x_1)\eta(x_2) \left. \frac{\delta^2 J}{\delta y(x_1)\delta y(x_2)} \right|_y dx_1 dx_2 + \cdots \end{aligned} \quad (1.177)$$

Since $y(x)$ is a stationary point, the term with $\delta J/\delta y(x)|_y$ vanishes. Whether $y(x)$ is a maximum, a minimum, or a saddle therefore depends on the number of positive and negative eigenvalues of $\delta^2 J/\delta(y(x_1))\delta(y(x_2))$, a matrix with a continuous infinity of rows and columns, these being labeled by x_1 and x_2 respectively. It is not easy to diagonalize such a continuously infinite matrix! Consider, for example, the functional

$$J[y] = \int_a^b \frac{1}{2} \{p(x)(y')^2 + q(x)y^2\} dx, \quad (1.178)$$

with $y(a) = y(b) = 0$. Here, as we already know,

$$\frac{\delta J}{\delta y(x)} = Ly \equiv -\frac{d}{dx} \left(p(x) \frac{d}{dx} y(x) \right) + q(x)y(x), \quad (1.179)$$

and, except in degenerate cases, this will be zero only if $y(x) \equiv 0$. We might reasonably expect the second derivative to be

$$\frac{\delta}{\delta y}(Ly) \stackrel{?}{=} L, \quad (1.180)$$

where L is the Sturm-Liouville differential operator

$$L = -\frac{d}{dx} \left(p(x) \frac{d}{dx} \right) + q(x). \quad (1.181)$$

How can a differential operator be a matrix like $\delta^2 J / \delta(y(x_1)) \delta(y(x_2))$?

We can formally compute the second derivative by exploiting the Dirac delta “function” $\delta(x)$ which has the property that

$$y(x_2) = \int \delta(x_2 - x_1) y(x_1) dx_1. \quad (1.182)$$

Thus

$$\delta y(x_2) = \int \delta(x_2 - x_1) \delta y(x_1) dx_1, \quad (1.183)$$

from which we read off that

$$\frac{\delta y(x_2)}{\delta y(x_1)} = \delta(x_2 - x_1). \quad (1.184)$$

Using (1.184), we find that

$$\frac{\delta}{\delta y(x_1)} \left(\frac{\delta J}{\delta y(x_2)} \right) = -\frac{d}{dx_2} \left(p(x_2) \frac{d}{dx_2} \delta(x_2 - x_1) \right) + q(x_2) \delta(x_2 - x_1). \quad (1.185)$$

How are we to make sense of this expression? We begin in the next chapter where we explain what it means to differentiate $\delta(x)$, and show that (1.185) does indeed correspond to the differential operator L . In subsequent chapters we will explore the manner in which differential operators and matrices are related. We will learn that just as some matrices can be diagonalized so can some differential operators, and that the class of diagonalizable operators includes (1.181).

If all the eigenvalues of L are positive, our stationary point was a minimum. For each negative eigenvalue, there is direction in which $J[y]$ decreases as we move away from the stationary point.

1.7 Exercises and Problems

Here is a collection of problems relating to the calculus of variations. Some date back to the 16th century, others are quite recent in origin.

Exercise 1.1: Fermat’s principle. A medium is characterised optically by its *refractive index* n , such that the speed of light in the medium is c/n . According to Fermat, the path taken by a ray of light between any two points makes stationary the travel time between those points. Assume that the ray

propagates in the x, y plane in a layered medium with refractive index $n(x)$. Use Fermat's principle to establish Snell's law in its general form $n(x) \sin \psi = \text{constant}$ by finding the equation giving the stationary paths $y(x)$ for

$$F_1[y] = \int n(x) \sqrt{1 + y'^2} dx.$$

(Here the prime denotes differentiation with respect to x .) Repeat this exercise for the case that n depends only on y and find a similar equation for the stationary paths of

$$F_2[y] = \int n(y) \sqrt{1 + y'^2} dx.$$

By using suitable definitions of the angle of incidence ψ , in each case show that the two formulations of the problem give physically equivalent answers. In the second formulation you will find it easiest to use the first integral of Euler's equation.

Exercise 1.2: Hyperbolic Geometry. This problem introduces a version of the Poincaré model for the non-Euclidean geometry of Lobachevski.

a) Show that the stationary paths for the functional

$$F_3[y] = \int \frac{1}{y} \sqrt{1 + y'^2} dx,$$

with $y(x)$ restricted to lying in the upper half plane are semi-circles of arbitrary radius and with centres on the x axis. These paths are the *geodesics*, or minimum length paths, in a space with Riemann metric

$$ds^2 = \frac{1}{y^2} (dx^2 + dy^2), \quad y > 0.$$

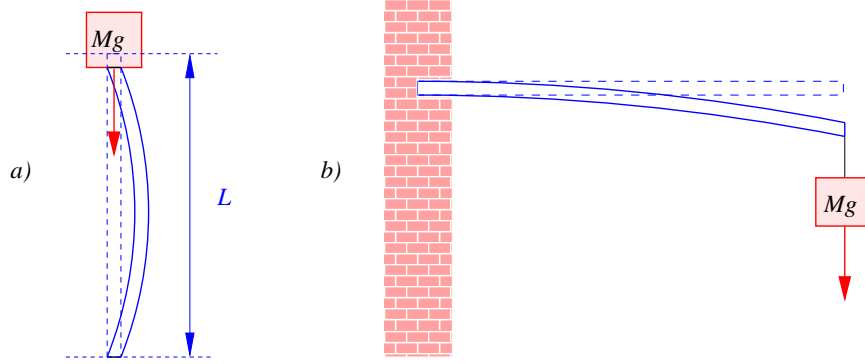
- b) Show that if we call these geodesics “lines”, then one and only one line can be drawn through two given points.
- c) Two lines are said to be *parallel* if, and only if, they meet at “infinity”, *i.e.* on the x axis. (Verify that the x axis is indeed infinitely far from any point with $y > 0$.) Show that given a line q and a point A not lying on that line, that there are *two* lines passing through A that are parallel to q , and that between these two lines lies a pencil of lines passing through A that never meet q .

Exercise 1.3: Elastic Rods. The elastic energy per unit length of a bent steel rod is given by $\frac{1}{2}YI/R^2$. Here R is the radius of curvature due to the bending,

Y is the Young's modulus of the steel and $I = \iint y^2 dx dy$ is the moment of inertia of the rod's cross section about an axis through its centroid and perpendicular to the plane in which the rod is bent. If the rod is only slightly bent into the yz plane and lies close to the z axis, show that this elastic energy can be approximated as

$$U[y] = \int_0^L \frac{1}{2} Y I (y'')^2 dz,$$

where the prime denotes differentiation with respect to z and L is the length of the rod. We will use this approximate energy functional to discuss two practical problems.



- a) *Euler's problem: the buckling of a slender column.* The rod is used as a column which supports a compressive load Mg directed along the z axis (which is vertical). Show that when the rod buckles slightly (*i.e.* deforms with both ends remaining on the z axis) the total energy, including the gravitational potential energy of the loading mass M , can be approximated by

$$U[y] = \int_0^L \left\{ \frac{YI}{2} (y'')^2 - \frac{Mg}{2} (y')^2 \right\} dz.$$

By considering small deformations of the form

$$y(z) = \sum_{n=1}^{\infty} a_n \sin \frac{n\pi z}{L}$$

show that the column is unstable to buckling and collapse if $Mg \geq \pi^2 Y I / L^2$.

b) *Leonardo da Vinci's problem: the light cantilever.* Here we take the z axis as horizontal and the y axis as being vertical. The rod is used as a beam or cantilever and is fixed into a wall so that $y(0) = 0 = y'(0)$. A weight Mg is hung from the end $z = L$ and the beam sags in the $-y$ direction. We wish to find $y(z)$ for $0 < z < L$. We will ignore the weight of the beam itself.

- Write down the complete expression for the energy, including the gravitational potential energy of the weight.
- Find the differential equation and boundary conditions at $z = 0, L$ that arise from minimizing the total energy. In doing this take care not to throw away any term arising from the integration by parts. You may find the following identity to be of use:

$$\frac{d}{dz}(f'g'' - fg''') = f''g'' - fg''''.$$

- Solve the equation. You should find that the displacement of the end of the beam is $y(L) = -\frac{1}{3}MgL^3/YI$.

Exercise 1.4: Suppose that an elastic body Ω of density ρ is slightly deformed so that the point that was at cartesian co-ordinate x_i is moved to $x_i + \eta_i(x)$. We define the resulting *strain tensor* e_{ij} by

$$e_{ij} = \frac{1}{2} \left(\frac{\partial \eta_j}{\partial x_i} + \frac{\partial \eta_i}{\partial x_j} \right).$$

It is automatically symmetric in its indices. The Lagrangian for small-amplitude elastic motion of the body is

$$L[\boldsymbol{\eta}] = \int_{\Omega} \left\{ \frac{1}{2} \rho \dot{\eta}_i^2 - \frac{1}{2} e_{ij} c_{ijkl} e_{kl} \right\} d^3x.$$

Here, c_{ijkl} is the tensor of *elastic constants*, which has the symmetries

$$c_{ijkl} = c_{klij} = c_{jikl} = c_{ijlk}.$$

By varying the η_i , show that the equation of motion for the body is

$$\rho \frac{\partial^2 \eta_i}{\partial t^2} - \frac{\partial}{\partial x_j} \sigma_{ji} = 0,$$

where

$$\sigma_{ij} = c_{ijkl} e_{kl}$$

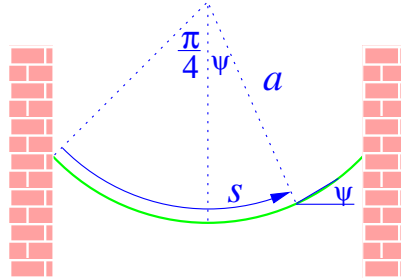
is the *stress tensor*. Show that variations of η_i on the boundary $\partial\Omega$ give as boundary conditions

$$\sigma_{ij}n_j = 0,$$

where n_i are the components of the outward normal on $\partial\Omega$.

Exercise 1.5: The Catenary Again. We can describe a catenary curve in parametric form as $x(s)$, $y(s)$, where s is the arc-length. The potential energy is then simply $\int_0^L \rho g y(s) ds$ where ρ is the mass per unit length of the hanging chain. The x , y are not independent functions of s , however, because $\dot{x}^2 + \dot{y}^2 = 1$ at every point on the curve.

- a) Introduce infinitely many Lagrange multipliers $\lambda(s)$ to enforce the $\dot{x}^2 + \dot{y}^2$ constraint, one for each point s on the curve. From the resulting functional derive two coupled equations for the catenary, one for $x(s)$ and one for $y(s)$. By thinking about the forces acting on a small section of the cable, and perhaps by introducing the angle ψ where $\dot{x} = \cos \psi$ and $\dot{y} = \sin \psi$, so that s and ψ are *intrinsic coordinates* for the curve, interpret these equations and relate $\lambda(s)$ to the position-dependent tension $T(s)$ in the chain.



Weighted line.

- b) You are provided with a light-weight line of length $\pi a/2$ and some lead shot of total mass M . By using equations from the previous part (suitably modified to take into account the position dependent $\rho(s)$) or otherwise, determine how the lead should be distributed along the line if the loaded line is to hang in an arc of a circle of radius a when its ends are attached to two points at the same height.

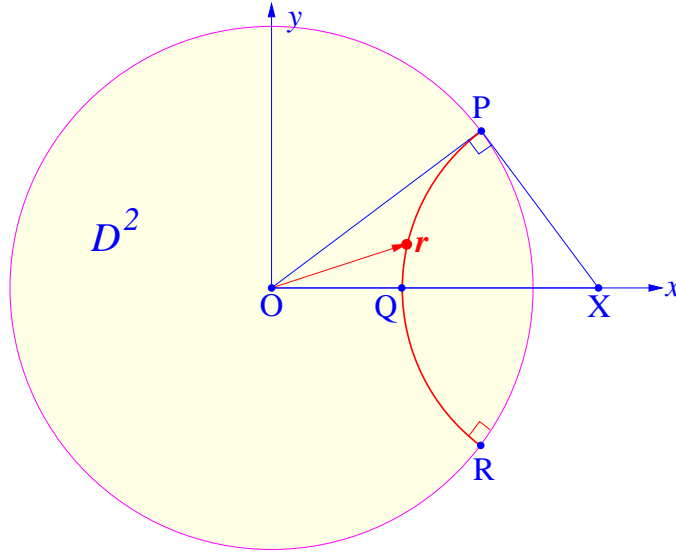
Exercise 1.6: Another model for Lobachevski geometry (see exercise 1.2) is the *Poincaré disc*. This space consists of the interior of the unit disc $D^2 = \{x, y \in \mathbb{R} : x^2 + y^2 \leq 1\}$ equipped with Riemann metric

$$ds^2 = \frac{dx^2 + dy^2}{(1 - x^2 - y^2)^2}.$$

The geodesic paths are therefore found by minimizing the arc-length functional

$$s[\mathbf{r}] \equiv \int ds = \int \left\{ \frac{1}{1-x^2-y^2} \sqrt{\dot{x}^2 + \dot{y}^2} \right\} dt.$$

Here $\mathbf{r}(t) = (x(t), y(t))$ is a function of a parameter t , and a dot indicates a derivative with respect to t .



The Poincaré disc and the construction of the geodesic PQR. The radius OP of the Poincare disc is unity, while the radius of the geodesic arc is $PX = QX = RX = R$. The distance between the centres of the disc and arc is $OX = x_0$. Your task in part c) is to show that $\angle OPX = \angle ORX = 90^\circ$.

- a) Either by manipulating the two Euler-Lagrange equations that give the conditions for $s[\mathbf{r}]$ to be stationary under variations in $\mathbf{r}(t)$, or, more efficiently, by observing that $s[\mathbf{r}]$ is invariant under the infinitesimal rotation

$$\begin{aligned} \delta x &= \varepsilon y \\ \delta y &= -\varepsilon x \end{aligned}$$

and applying Noether's theorem, show that the parameterised geodesics obey

$$\frac{d}{dt} \left(\frac{1}{1-x^2-y^2} \frac{x\dot{y} - y\dot{x}}{\sqrt{\dot{x}^2 + \dot{y}^2}} \right) = 0.$$

- b) Given a point (x_0, y_0) within D^2 , and a direction through it, show that the equation you derived in part a) determines a unique geodesic curve passing through (x_0, y_0) in the given direction, but does not determine the parametrization of the curve.
- c) Show that there exists a solution to the equation in part a) in the form

$$\begin{aligned} x(t) &= R \cos t + x_0 \\ y(t) &= R \sin t. \end{aligned}$$

Find a relation between x_0 and R , and from it deduce that the geodesics are circular arcs that cut the bounding unit circle (which plays the role of the line at infinity in the Lobachevski plane) at right angles.

Exercise 1.7: The Lagrangian for a particle of charge q is

$$L[\mathbf{x}] = \frac{1}{2}m\dot{\mathbf{x}}^2 - q\phi + q\dot{\mathbf{x}} \cdot \mathbf{A}.$$

Show that Lagrange's equation is

$$m\ddot{\mathbf{x}} = q(\mathbf{E} + \dot{\mathbf{x}} \times \mathbf{B}),$$

where

$$\mathbf{E} = -\nabla\phi - \dot{\mathbf{A}}, \quad \mathbf{B} = \nabla \times \mathbf{A}.$$

Exercise 1.8: Consider the action functional

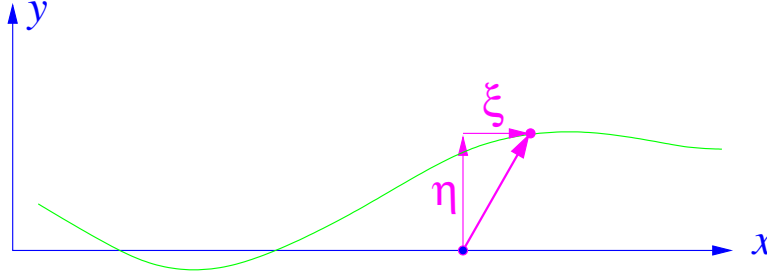
$$S[\boldsymbol{\omega}, \mathbf{p}, \mathbf{r}] = \int \left(\frac{1}{2}I_1\omega_1^2 + \frac{1}{2}I_2\omega_2^2 + \frac{1}{2}I_3\omega_3^2 + \mathbf{p} \cdot (\dot{\mathbf{r}} + \boldsymbol{\omega} \times \mathbf{r}) \right) dt,$$

where \mathbf{r} and \mathbf{p} are three-vectors, as is $\boldsymbol{\omega} = (\omega_1, \omega_2, \omega_3)$. Apply the action principle to obtain the equations of motion for $\mathbf{r}, \mathbf{p}, \boldsymbol{\omega}$ and show that they lead to Euler's equations for the motion of a rigid body:

$$\begin{aligned} I_1\dot{\omega}_1 + (I_2 - I_3)\omega_2\omega_3 &= 0, \\ I_2\dot{\omega}_2 + (I_3 - I_1)\omega_3\omega_1 &= 0, \\ I_3\dot{\omega}_3 + (I_1 - I_2)\omega_1\omega_2 &= 0. \end{aligned}$$

Exercise 1.9: Piano String. A elastic piano string can vibrate both transversely and longitudinally, and the two vibrations influence one another. A Lagrangian that takes into account the lowest-order effect of stretching on the local string tension, and can therefore model this coupled motion, is

$$L[\xi, \eta] = \int dx \left\{ \frac{1}{2}\rho_0 \left[\left(\frac{\partial \xi}{\partial t} \right)^2 + \left(\frac{\partial \eta}{\partial t} \right)^2 \right] - \frac{\lambda}{2} \left[\frac{\tau_0}{\lambda} + \frac{\partial \xi}{\partial x} + \frac{1}{2} \left(\frac{\partial \eta}{\partial x} \right)^2 \right]^2 \right\}.$$



Vibrating piano string.

Here $\xi(x, t)$ is the longitudinal displacement and $\eta(x, t)$ the transverse displacement of the string. Thus, the point that in the undisturbed string had co-ordinates $[x, 0]$ is moved to the point with co-ordinates $[x + \xi(x, t), \eta(x, t)]$. The parameter τ_0 represents the tension in the undisturbed string, λ is the product of Young's modulus and the cross-sectional area of the string, and ρ_0 is the mass per unit length.

- Use the action principle to derive the two coupled equations of motion, one involving $\frac{\partial^2 \xi}{\partial t^2}$ and one involving $\frac{\partial^2 \eta}{\partial t^2}$.
- Show that when we linearize these two equations of motion, the longitudinal and transverse motions decouple. Find expressions for the longitudinal (c_L) and transverse (c_T) wave velocities in terms of τ_0 , ρ_0 and λ .
- Assume that a given transverse pulse $\eta(x, t) = \eta_0(x - c_T t)$ propagates along the string. Show that this induces a concurrent longitudinal pulse of the form $\xi(x - c_T t)$. Show further that the longitudinal Newtonian momentum density in this concurrent pulse is given by

$$\rho_0 \frac{\partial \xi}{\partial t} = \frac{1}{2} \frac{c_L^2}{c_L^2 - c_T^2} T^0{}_1$$

where

$$T^0{}_1 \equiv -\rho_0 \frac{\partial \eta}{\partial x} \frac{\partial \eta}{\partial t}$$

is the associated pseudo-momentum density.

The forces that created the transverse pulse will also have created other longitudinal waves that travel at c_L . Consequently the Newtonian x -momentum moving at c_T is not the only x -momentum on the string, and the total “true” longitudinal momentum density is not simply proportional to the pseudo-momentum density.

Exercise 1.10: Obtain the canonical energy-momentum tensor T^ν_μ for the barotropic fluid described by (1.118). Show that its conservation leads to both the momentum conservation equation (1.127), and to the energy conservation equation

$$\partial_t \mathcal{E} + \partial_i \{v_i (\mathcal{E} + P)\},$$

where the energy density is

$$\mathcal{E} = \frac{1}{2} \rho (\nabla \phi)^2 + u(\rho).$$

Interpret the energy flux as being the sum of the convective transport of energy together with the rate of working by an element of fluid on its neighbours.

Exercise 1.11: Consider the action functional⁴

$$S[\mathbf{v}, \rho, \phi, \beta, \gamma] = \int d^4x \left\{ -\frac{1}{2} \rho \mathbf{v}^2 - \phi (\dot{\rho} + \nabla \cdot (\rho \mathbf{v})) + \rho \beta (\dot{\gamma} + (\mathbf{v} \cdot \nabla) \gamma) + u(\rho) \right\},$$

which is a generalization of (1.176) to include two new scalar fields β and γ . Show that varying \mathbf{v} leads to

$$\mathbf{v} = \nabla \phi + \beta \nabla \gamma.$$

This is the *Clebsch representation* of the velocity field. It allows for flows with non-zero vorticity

$$\boldsymbol{\omega} = \nabla \times \mathbf{v} = \nabla \beta \times \nabla \gamma.$$

Show that the equations that arise from varying the remaining fields ρ , ϕ , β , γ , together imply the mass conservation equation

$$\dot{\rho} + \nabla \cdot (\rho \mathbf{v}) = 0,$$

and Bernoulli's equation in the form

$$\dot{\mathbf{v}} - \boldsymbol{\omega} \times \mathbf{v} = -\nabla \left(\frac{1}{2} \mathbf{v}^2 + h \right).$$

(Recall that $h = du/d\rho$.) Show that this form of Bernoulli's equation is equivalent to Euler's equation

$$\dot{\mathbf{v}} + (\mathbf{v} \cdot \nabla) \mathbf{v} = -\nabla h.$$

Consequently S provides an action principle for a general inviscid barotropic flow.

⁴H. Bateman, *Proc. Roy. Soc. Lond. A* **125** (1929) 598-618; C. C. Lin, *Liquid Helium* in *Proc. Int. Sch. Phys. "Enrico Fermi"*, Course XXI (Academic Press 1965).

Chapter 2

Function Spaces

We are going to consider the differential equations of physics as relations involving *linear differential operators*. These operators, like matrices, are linear maps acting on vector spaces, but the elements of the vector spaces are functions. Such spaces are infinite dimensional. We will try to survive by relying on our experience in finite dimensions, but sometimes this fails, and more sophistication is required.

2.1 Motivation

In the previous chapter we looked at two variational problems:

- 1) Find the stationary points of

$$F(\mathbf{x}) = \frac{1}{2} \mathbf{x} \cdot \mathbf{A} \mathbf{x} = \frac{1}{2} x_i A_{ij} x_j \quad (2.1)$$

on the surface $\mathbf{x} \cdot \mathbf{x} = 1$. This led to the matrix eigenvalue equation

$$\mathbf{A} \mathbf{x} = \lambda \mathbf{x}. \quad (2.2)$$

- 2) Find the stationary points of

$$J[y] = \int_a^b \frac{1}{2} \{p(x)(y')^2 + q(x)y^2\} dx, \quad (2.3)$$

subject to the conditions $y(a) = y(b) = 0$ and

$$K[y] = \int_a^b y^2 dx = 1. \quad (2.4)$$

This led to the differential equation

$$-(py')' + qy = \lambda y, \quad y(a) = y(b) = 0. \quad (2.5)$$

There will be a solution that satisfies the boundary conditions only for a discrete set of values of λ .

The stationary points of both function and functional are therefore determined by *linear eigenvalue problems*. The only difference is that the finite matrix in the first is replaced in the second by a linear differential operator. The theme of the next few chapters is an exploration of the similarities and differences between finite matrices and linear differential operators. In this chapter we will focus on how the functions on which the derivatives act can be thought of as vectors.

2.1.1 Functions as vectors

Consider $F[a, b]$, the set of all real (or complex) valued functions $f(x)$ on the interval $[a, b]$. This is a *vector space* over the field of the real (or complex) numbers because, given two functions $f_1(x)$ and $f_2(x)$, and two numbers λ_1 and λ_2 , we can form the sum $\lambda_1 f_1(x) + \lambda_2 f_2(x)$ and the result is still a function on the same interval. Examination of the axioms listed in appendix A will show that $F[a, b]$ possesses all the other attributes of a vector space as well. We may think of the array of numbers $(f(x))$ for $x \in [a, b]$ as being the components of the vector. Since there is an infinity of independent components, the space of functions is infinite dimensional.

The set of *all* functions is usually too large for us. We will restrict ourselves to subspaces of functions with nice properties, such as being continuous or differentiable. There is some fairly standard notation for these spaces: The space of C^n functions (those which have n continuous derivatives) is called $C^n[a, b]$. For smooth functions (those with derivatives of all orders) we write $C^\infty[a, b]$. For the space of analytic functions (those whose Taylor expansion actually converges to the function) we write $C^\omega[a, b]$. For C^∞ functions defined on the whole real line we write $C^\infty(\mathbb{R})$. For the subset of functions with compact support (those that vanish outside some finite interval) we write $C_0^\infty(\mathbb{R})$. There are no non-zero analytic functions with compact support: $C_0^\omega(\mathbb{R}) = \{0\}$.

2.2 Norms and Inner Products

We are often interested in “how large” a function is. This leads to the idea of *normed* function spaces. There are many measures of function size. Suppose $R(t)$ is the number of inches per hour of rainfall. If you are a farmer you are probably most concerned with the total amount of rain that falls. A big rain has big $\int |R(t)| dt$. If you are the Urbana city engineer worrying about the capacity of the sewer system to cope with a downpour, you are primarily concerned with the maximum value of $R(t)$. For you a big rain has a big “sup $|R(t)|$ ”¹.

2.2.1 Norms and convergence

We can seldom write down an exact solution function to a real-world problem. We are usually forced to use numerical methods, or to expand as a power series in some small parameter. The result is a sequence of approximate solutions $f_n(x)$, which we hope will converge to the desired exact solution $f(x)$ as we make the numerical grid smaller, or take more terms in the power series.

Because there is more than one way to measure of the “size” of a function, the convergence of a sequence of functions, f_n , to a limit function f is not as simple a concept as the convergence of a sequence of numbers, x_n , to a limit x . Convergence means that the distance between the f_n and the limit function f gets smaller and smaller as n increases, so each different measure of how “large” the distance is provides a new notion of what it means to converge. We are not going to make much use of formal “ ε , δ ” analysis, but you must realize that this distinction between different forms of convergence is not merely academic: real-world engineers must be precise about the kind of errors they are prepared to tolerate, or else a bridge they design might collapse. If you look, therefore, at the syllabus of graduate-level *engineering* courses in mathematical methods you will see that they devote much time to these issues. While physicists do not normally face the same legal liabilities as engineers, we should at least have it clear in our own minds what we mean

¹Here “sup”, short for *supremum*, is synonymous with the “least upper bound” of a set of numbers, *i.e.* the smallest number that is exceeded by no number in the set. This concept is more useful than “maximum” because the supremum need not be an element of the set. It is an axiom of the real number system that any bounded set of real numbers has a least upper bound. The “greatest lower bound” is denoted “inf”, for *infimum*.

when we write that $f_n \rightarrow f$.

Here are some common forms of convergence:

- i) If, for each x in its domain of definition \mathcal{D} , the set of numbers $f_n(x)$ converges to $f(x)$, then we say the sequence converges *pointwise*.
- ii) If the maximum separation

$$\sup_{x \in \mathcal{D}} |f_n(x) - f(x)| \quad (2.6)$$

goes to zero as $n \rightarrow \infty$, then we say that f_n converges to f *uniformly* on \mathcal{D} .

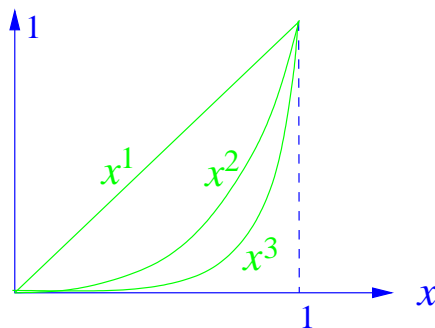
- iii) If

$$\int_{\mathcal{D}} |f_n(x) - f(x)| dx \quad (2.7)$$

goes to zero as $n \rightarrow \infty$, then we say that f_n converges *in the mean* to f on \mathcal{D} .

Uniform convergence implies pointwise convergence, but not *vice versa*. If \mathcal{D} is a finite interval, then uniform convergence implies convergence in the mean, but convergence in the mean implies neither uniform nor pointwise convergence.

Example: Consider the sequence $f_n = x^n$ ($n = 1, 2, \dots$) and $\mathcal{D} = [0, 1)$. Here, the round bracket means that the point $x = 1$ is excluded from the interval.



$x^n \rightarrow 0$ on $[0, 1)$, but not uniformly.

As n becomes large we have $f_n(x) \rightarrow 0$ pointwise in \mathcal{D} , but the convergence is *not* uniform because

$$\sup_{x \in \mathcal{D}} |f_n(x) - 0| = 1 \quad (2.8)$$

for all n .

Example: Let $f_n = x^n$ with $\mathcal{D} = [0, 1]$. Here, the square bracket means that the point $x = 1$ is included in the interval. In this case, we have neither uniform nor pointwise convergence of the f_n to zero, but $f_n \rightarrow 0$ in the mean.

We can describe uniform convergence by means of a *norm* — a generalization of the usual measure of the length of a vector. A norm, denoted by $\|f\|$, of a vector f (a function, in our case) is a real number that obeys

- i) positivity: $\|f\| \geq 0$, and $\|f\| = 0 \Leftrightarrow f = 0$,
- ii) the *triangle inequality*: $\|f + g\| \leq \|f\| + \|g\|$,
- iii) linear homogeneity: $\|\lambda f\| = |\lambda| \|f\|$.

One example is the “sup” norm, which is defined by

$$\|f\|_\infty = \sup_{x \in \mathcal{D}} |f(x)|. \quad (2.9)$$

This number is guaranteed to be finite if f is continuous and \mathcal{D} is compact. In terms of the sup norm, uniform convergence is the statement that

$$\lim_{n \rightarrow \infty} \|f_n - f\|_\infty = 0. \quad (2.10)$$

2.2.2 Norms from integrals

The space $L^p[a, b]$, for $1 \leq p < \infty$, is defined to be our $F[a, b]$ equipped with

$$\|f\|_p = \left(\int_a^b |f(x)|^p dx \right)^{1/p}, \quad (2.11)$$

as the measure of length, and with a restriction to functions for which $\|f\|_p$ is finite.

We say that $f_n \rightarrow f$ in L^p if the L^p distance $\|f - f_n\|_p$ tends to zero. We have already seen the L^1 measure of distance in the definition of convergence in the mean. As in that case, convergence in L^p says nothing about pointwise convergence.

We would like to regard $\|f\|_p$ as a norm. It is possible, however, for a function to have $\|f\|_p = 0$ without f being identically zero — a function that vanishes at all but a finite set of points, for example. This pathology violates number i) in our list of requirements for something to be called a norm, but we circumvent the problem by simply declaring such functions to be zero. This means that elements of the L^p spaces are not really functions, but only *equivalence classes* of functions — two functions being regarded as

the same is they differ by a function of zero length. Clearly these spaces are not for use when anything significant depends on the value of the function at any precise point. They *are* useful in physics, however, because we can never measure a quantity at an exact position in space or time. We usually measure some sort of local average.

All the L^p norms satisfy the triangle inequality, although, for general p , this is not exactly trivial to prove.

An important property for any space to have is that of being *complete*. Roughly speaking, a space is complete if when some sequence of elements of the space look as if they are converging, then they are indeed converging, and their limit is an element of the space. To make this concept precise, we need to say what we mean by the phrase “look as if they are converging”. This we do by introducing the idea of a *Cauchy sequence*.

Definition: A sequence f_n in a normed vector space is said to be *Cauchy* if for any $\varepsilon > 0$ we can find an N such that $n, m > N$ implies that $\|f_m - f_n\| < \varepsilon$. Loosely speaking, the elements of a Cauchy sequence get arbitrarily close to each other as $n \rightarrow \infty$. A normed vector space is then *complete* with respect to its norm if every Cauchy sequence actually converges to some element in the space.

Consider, for example, the normed vector space \mathbb{Q} of rational numbers with distance measured in the usual way as $\|q_1 - q_2\| \equiv |q_1 - q_2|$. The sequence

$$\begin{aligned} q_0 &= 1.0, \\ q_1 &= 1.4, \\ q_2 &= 1.41, \\ q_3 &= 1.414, \\ &\vdots \end{aligned}$$

consisting of successive decimal approximations to $\sqrt{2}$, obeys

$$|q_n - q_m| < \frac{1}{10^{\min(n,m)}} \quad (2.12)$$

and so is Cauchy. Pythagoras famously showed that $\sqrt{2}$ is irrational, however, and so this sequence has no limit in \mathbb{Q} . Thus \mathbb{Q} is not complete. The space \mathbb{R} of real numbers is constructed by filling in the gaps between the rationals, and so *completing* \mathbb{Q} . A real number such as $\sqrt{2}$ is defined as a Cauchy sequence of rational numbers (by specifying, for example, its infinite decimal

expansion), with two rational sequences q_n and q'_n defining the same real number if $q_n - q'_n$ converges to zero.

A complete normed vector space is called a *Banach space*. If we interpret the norms as Lebesgue integrals² then the $L^p[a, b]$ are complete, and therefore Banach spaces. The theory of Lebesgue integration is rather complicated, however, and is not really necessary. One way of avoiding it is explained in exercise 2.2.

Exercise 2.1: Show that any convergent sequence is Cauchy.

2.2.3 Hilbert space

The Banach space L^2 is special in that it is also a *Hilbert space*. This means that its norm is derived from an inner product. If we define the inner product

$$\langle f, g \rangle = \int_a^b f^* g \, dx \quad (2.13)$$

then the L^2 norm can be written

$$\|f\|_2 = \sqrt{\langle f, f \rangle}. \quad (2.14)$$

When we omit the subscript on a norm, we mean it to be this one. You are probably familiar with this Hilbert space from your quantum mechanics classes.

Being positive definite, the inner product satisfies the *Cauchy-Schwarz-Bunyakovsky inequality*

$$|\langle f, g \rangle| \leq \|f\| \|g\|. \quad (2.15)$$

That this is so can be seen by looking at

$$0 \leq \langle \lambda f + \mu g, \lambda f + \mu g \rangle = \begin{pmatrix} \lambda^* & \mu^* \end{pmatrix} \begin{pmatrix} \|f\|^2 & \langle f, g \rangle \\ \langle f, g \rangle^* & \|g\|^2 \end{pmatrix} \begin{pmatrix} \lambda \\ \mu \end{pmatrix}, \quad (2.16)$$

and observing that if the matrix is to be positive definite, then its determinant

$$\|f\|^2 \|g\|^2 - |\langle f, g \rangle|^2 \quad (2.17)$$

²The “ L ” in L^p honours Henri Lebesgue. Banach spaces are named after Stefan Banach, who was one of the founders of functional analysis, a subject largely developed by him and the other habitués of the Scottish Café in Lvów, Poland.

must be positive.

From Cauchy-Schwarz-Bunyakovsky we can establish the triangle inequality:

$$\begin{aligned}
 \|f + g\|^2 &= \|f\|^2 + \|g\|^2 + 2\operatorname{Re}\langle f, g \rangle \\
 &\leq \|f\|^2 + \|g\|^2 + 2|\langle f, g \rangle|, \\
 &\leq \|f\|^2 + \|g\|^2 + 2\|f\|\|g\|, \\
 &= (\|f\| + \|g\|)^2,
 \end{aligned} \tag{2.18}$$

so

$$\|f + g\| \leq \|f\| + \|g\|. \tag{2.19}$$

A second important consequence of Cauchy-Schwarz-Bunyakovsky is that if $f_n \rightarrow f$ in the sense that $\|f_n - f\| \rightarrow 0$, then

$$\begin{aligned}
 |\langle f_n, g \rangle - \langle f, g \rangle| &= |\langle f_n - f, g \rangle| \\
 &\leq \|f_n - f\| \|g\|
 \end{aligned} \tag{2.20}$$

tends to zero, and so

$$\langle f_n, g \rangle \rightarrow \langle f, g \rangle. \tag{2.21}$$

This means that the inner product $\langle f, g \rangle$ is a *continuous* functional of f and g . Take care to note that this continuity hinges on $\|g\|$ being finite. It for this reason that we do not permit $\|g\| = \infty$ functions to be elements of our Hilbert space.

Orthonormal sets

Once we are in possession of an inner product, we can introduce the notion of an *orthonormal set*. A set of functions $\{u_n\}$ is orthonormal if

$$\langle u_n, u_m \rangle = \delta_{nm}. \tag{2.22}$$

For example,

$$2 \int_0^1 \sin(n\pi x) \sin(m\pi x) dx = \delta_{nm}, \quad n, m = 1, 2, \dots \tag{2.23}$$

so the set of functions $u_n = \sqrt{2} \sin n\pi x$ is orthonormal on $[0, 1]$. This set of functions is also *complete* — in a different sense, however, from our earlier

use of this word. A orthonormal set of functions is said to be complete if any function f for which $\|f\|^2$ is finite, and hence f an element of the Hilbert space, has a convergent expansion

$$f(x) = \sum_{n=0}^{\infty} a_n u_n(x).$$

If we assume that such an expansion exists, and that we can freely interchange the order of the sum and integral, we can multiply both sides of this expansion by $u_m^*(x)$ and use the orthonormality of the u_n 's to read off the expansion coefficients as $a_n = \langle u_n, f \rangle$. When

$$\|f\|^2 = \int_0^1 |f(x)|^2 dx \quad (2.24)$$

and $u_n = \sqrt{2} \sin(n\pi x)$, the result is the (sine) Fourier series.

Example: Expanding unity. Suppose $f(x) = 1$. Since $\int_0^1 |f|^2 dx = 1$ is finite, the function $f(x) = 1$ can be represented as a convergent sum of the $u_n = \sqrt{2} \sin(n\pi x)$.

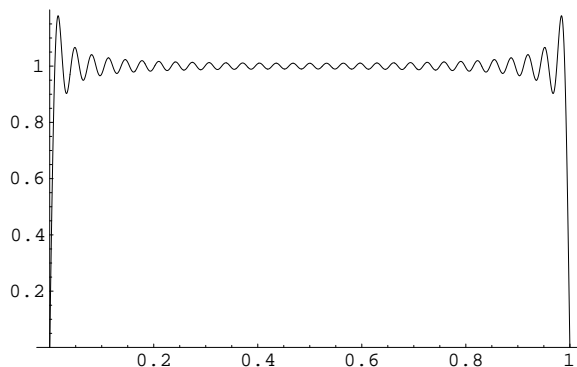
The inner product of f with the u_n 's is

$$\langle u_n, f \rangle = \int_0^1 \sqrt{2} \sin(n\pi x) dx = \begin{cases} 0, & n \text{ even,} \\ \frac{2\sqrt{2}}{n\pi}, & n \text{ odd.} \end{cases}$$

Thus,

$$1 = \sum_{n=0}^{\infty} \frac{4}{(2n+1)\pi} \sin((2n+1)\pi x), \quad \text{in } L^2[0, 1]. \quad (2.25)$$

It is important to understand that the sum converges to the left hand side in the closed interval $[0, 1]$ only in the L^2 sense. The series does not converge pointwise to unity at $x = 0$ or $x = 1$ — every term is zero at these points.



The sum of the first 31 terms in the sine expansion of $f(x) = 1$

The figure shows the sum of the series up to and including the term with $n = 30$. The L^2 measure of the distance between $f(x) = 1$ and this sum is

$$\int_0^1 \left| 1 - \sum_{n=0}^{30} \frac{4}{(2n+1)\pi} \sin((2n+1)\pi x) \right|^2 dx = 0.00654. \quad (2.26)$$

We can make this number as small as we like by taking sufficiently many terms.

It is perhaps surprising that a set of functions that vanish at the endpoints of the interval can be used to expand a function that does not vanish at the ends. This exposes an important technical point: Any finite sum of continuous functions vanishing at the endpoints is also a continuous function vanishing at the endpoints. It is therefore tempting to talk about the “subspace” of such functions. This set is indeed a vector space, and a subset of the Hilbert space, but it is not itself a Hilbert space. As the example above shows, a Cauchy sequence of functions vanishing at the endpoints of an interval can converge to a function that does *not* vanish there. The “subspace” is therefore not complete in our original meaning of the term. The set of continuous functions vanishing at the endpoints fits into the whole Hilbert space much as the rational numbers fit into the real numbers. A finite sum of rationals is a rational number, but an infinite sum of rationals is not in general a rational number. Furthermore, we can express any real number as the limit of a sequence of rational numbers. We say that the rationals \mathbb{Q} are a *dense* subset of the reals, and, as explained earlier, the reals are obtained by completing the set of rationals by adding to this set its limit points. In

the same sense, the set of continuous functions vanishing at the endpoints is a dense subset of the whole Hilbert space and the whole Hilbert space is its completion.

Exercise 2.2: In this exercise we will explain in more detail how we “complete” a Hilbert space. The idea is to mirror the construction to the real numbers and *define* the elements of the Hilbert space to be Cauchy sequences of continuous functions. To specify a general element of $L^2[a, b]$ we must therefore exhibit a Cauchy sequence $f_n \in C[a, b]$. The choice is not unique: two Cauchy sequences $f_n^{(1)}(x)$ and $f_n^{(2)}(x)$ will specify the the same element if

$$\lim_{n \rightarrow \infty} \|f_n^{(1)} - f_n^{(2)}\| = 0.$$

Such sequences are said to be *equivalent*. For convenience, we will write “ $\lim_{n \rightarrow \infty} f_n = f$ ” but bear in mind that, in this exercise, this means that the sequence f_n *defines* the symbol f , and not that f is the limit of the sequence, as this limit need have no prior existence. We have deliberately written “ f ”, and not “ $f(x)$ ”, for the “limit function” to warn us that f is assigned no unique numerical value at any x . A continuous function $f(x)$ can still be considered to be an element of $L^2[a, b]$ —take a sequence in which every $f_n(x)$ is equal to $f(x)$ —but an equivalent sequence of $f_n(x)$ can alter the limiting $f(x)$ on a set of measure zero without changing the resulting element $f \in L^2[a, b]$.

- i) If f_n and g_n are Cauchy sequences defining f , g , respectively, it is natural to try to define the inner product $\langle f, g \rangle$ by setting

$$\langle f, g \rangle \equiv \lim_{n \rightarrow \infty} \langle f_n, g_n \rangle.$$

Use the Cauchy-Schwarz-Bunyakovsky inequality to show that the numbers $F_n = \langle f_n, g_n \rangle$ form a Cauchy sequence in \mathbb{C} . Since \mathbb{C} is complete, deduce that this limit exists. Next show that the limit is unaltered if either f_n or g_n is replaced by an equivalent sequence. Conclude that our tentative inner product is well defined.

- ii) The next, and harder, task is to show that the “completed” space is indeed complete. The problem is to show that given a Cauchy sequence $f_k \in L^2[a, b]$, where the f_k are *not* necessarily in $C[a, b]$, has a limit in $L^2[a, b]$. Begin by taking Cauchy sequences $f_{ki} \in C[a, b]$ such that $\lim_{i \rightarrow \infty} f_{ki} = f_k$. Use the triangle inequality to show that the diagonal subsequence f_{kk} is Cauchy, and so defines the desired limit.

Later we will show that the elements of $L^2[a, b]$ can be given a concrete meaning as *distributions*.

Best approximation

Let $u_n(x)$ be an orthonormal set of functions. The sum of the first N terms of the Fourier expansion of $f(x)$ in the u_n , is the closest—measuring distance with the L^2 norm—that one can get to f whilst remaining in the space spanned by u_1, u_2, \dots, u_N .

To see this, consider

$$\begin{aligned}
 \Delta &\equiv \left\| f - \sum_{n=1}^N a_n u_n \right\|^2 = \left\langle f - \sum_{m=1}^N a_m u_m, f - \sum_{n=1}^N a_n u_n \right\rangle \\
 &= \|f\|^2 - \sum_{n=1}^N a_n \langle f, u_n \rangle - \sum_{m=1}^N a_m^* \langle u_m, f \rangle + \sum_{n,m=1}^N a_m^* a_n \langle u_m, u_n \rangle \\
 &= \|f\|^2 - \sum_{n=1}^N a_n \langle f, u_n \rangle - \sum_{m=1}^N a_m^* \langle u_m, f \rangle + \sum_{n=1}^N |a_n|^2, \tag{2.27}
 \end{aligned}$$

where at the last line we have used the orthonormality of the u_n . We can complete the squares, and rewrite this as

$$\Delta = \|f\|^2 - \sum_{n=1}^N |\langle u_n, f \rangle|^2 + \sum_{n=1}^N |a_n - \langle u_n, f \rangle|^2. \tag{2.28}$$

We seek to minimize Δ by a suitable choice of coefficients a_n . The smallest we can make Δ is

$$\Delta_{\min} = \|f\|^2 - \sum_{n=1}^N |\langle u_n, f \rangle|^2, \tag{2.29}$$

and we attain this bound by setting each of the $|a_n - \langle u_n, f \rangle|$ equal to zero. That is by taking

$$a_n = \langle u_n, f \rangle. \tag{2.30}$$

Thus the Fourier coefficients $\langle u_n, f \rangle$ are the optimal choice for the a_n .

Suppose we have some *non-orthogonal* collection of functions g_n , $n = 1, \dots, N$, and we have found the best approximation $\sum_{n=1}^N a_n g_n(x)$ to $f(x)$. Now suppose we are given a g_{N+1} to add to our collection. We may then seek an improved approximation $\sum_{n=1}^{N+1} a'_n g_n(x)$ by including this new function—but finding this better fit will generally involve tweaking *all* the a_n , not just

trying different values of a_{N+1} . The great advantage of approximating by orthogonal functions is that, given another member of an orthonormal family, we can improve the precision of the fit by adjusting only the coefficient of the new term. We do not have to perturb the previously obtained coefficients.

Parseval's theorem

The “best approximation” result from the previous section allows us to give an alternative definition of a “complete orthonormal set”, and to obtain the formula $a_n = \langle u_n, f \rangle$ for the expansion coefficients without having to assume that we can integrate the infinite series $\sum a_n u_n$ term-by-term. Recall that we said that a set of points S is a *dense* subset of a space T if any given point $x \in T$ is the limit of a sequence of points in S , *i.e.* there are elements of S lying arbitrarily close to x . For example, the set of rational numbers \mathbb{Q} is a dense subset of \mathbb{R} . Using this language, we say that a set of orthonormal functions $\{u_n(x)\}$ is complete if the set of all finite linear combinations of the u_n is a dense subset of the entire Hilbert space. This guarantees that, by taking N sufficiently large, our best approximation will approach arbitrarily close to our target function $f(x)$. Since the best approximation containing all the u_n up to u_N is the N -th partial sum of the Fourier series, this shows that the Fourier series actually converges to f .

We have therefore proved that if we are given $u_n(x)$, $n = 1, 2, \dots$, a complete orthonormal set of functions on $[a, b]$, then any function for which $\|f\|^2$ is finite can be expanded as a convergent Fourier series

$$f(x) = \sum_{n=1}^{\infty} a_n u_n(x), \quad (2.31)$$

where

$$a_n = \langle u_n, f \rangle = \int_a^b u_n^*(x) f(x) dx. \quad (2.32)$$

The convergence is guaranteed only in the L^2 sense that

$$\lim_{N \rightarrow \infty} \int_a^b \left| f(x) - \sum_{n=1}^N a_n u_n(x) \right|^2 dx = 0. \quad (2.33)$$

Equivalently

$$\Delta_N = \|f - \sum_{n=1}^N a_n u_n\|^2 \rightarrow 0 \quad (2.34)$$

as $N \rightarrow \infty$. Now, we showed in the previous section that

$$\begin{aligned}\Delta_N &= \|f\|^2 - \sum_{n=1}^N |\langle u_n, f \rangle|^2 \\ &= \|f\|^2 - \sum_{n=1}^N |a_n|^2,\end{aligned}\tag{2.35}$$

and so the L^2 convergence is equivalent to the statement that

$$\|f\|^2 = \sum_{n=1}^{\infty} |a_n|^2.\tag{2.36}$$

This last result is called *Parseval's theorem*.

Example: In the expansion (2.25), we have $\|f^2\| = 1$ and

$$|a_n|^2 = \begin{cases} 8/(n^2\pi^2), & n \text{ odd}, \\ 0, & n \text{ even}. \end{cases}\tag{2.37}$$

Parseval therefore tells us that

$$\sum_{n=0}^{\infty} \frac{1}{(2n+1)^2} = 1 + \frac{1}{3^2} + \frac{1}{5^2} + \cdots = \frac{\pi^2}{8}.\tag{2.38}$$

Example: The functions $u_n(x) = \frac{1}{\sqrt{2\pi}}e^{inx}$, $n \in \mathbb{Z}$ form a complete orthonormal set on the interval $[-\pi, \pi]$. Let $f(x) = \frac{1}{\sqrt{2\pi}}e^{i\zeta x}$. Then its Fourier expansion is

$$e^{i\zeta x} = \sum_{n=-\infty}^{\infty} c_n e^{inx}, \quad -\pi < x < \pi,\tag{2.39}$$

where

$$c_n = \frac{1}{2\pi} \int_{-\pi}^{\pi} e^{i\zeta x} e^{-inx} dx = \frac{\sin(\pi(\zeta - n))}{\pi(\zeta - n)}.\tag{2.40}$$

We also have that

$$\|f\|^2 = \int_{-\pi}^{\pi} \frac{1}{2\pi} dx = 1.\tag{2.41}$$

Now Parseval tells us that

$$\|f\|^2 = \sum_{n=-\infty}^{\infty} \frac{\sin^2(\pi(\zeta - n))}{\pi^2(\zeta - n)^2},\tag{2.42}$$

the left hand side being unity.

Finally, as $\sin^2(\pi(\zeta - n)) = \sin^2(\pi\zeta)$, we have

$$\operatorname{cosec}^2(\pi\zeta) \equiv \frac{1}{\sin^2(\pi\zeta)} = \sum_{n=-\infty}^{\infty} \frac{1}{\pi^2(\zeta - n)^2}. \quad (2.43)$$

The end result is a quite non-trivial expansion for the square of the cosecant.

2.2.4 Orthogonal polynomials

A useful class of orthonormal functions are the sets of *orthogonal polynomials* associated with an interval $[a, b]$ and a positive weight function $w(x)$ such that $\int_a^b w(x) dx$ is finite. We introduce the Hilbert space $L_w^2[a, b]$ with the real inner product

$$\langle u, v \rangle_w = \int_a^b w(x) u(x) v(x) dx, \quad (2.44)$$

and apply the *Gram-Schmidt procedure* to the monomial powers $1, x, x^2, x^3, \dots$ so as to produce an orthonormal set. We begin with

$$P_0(x) \equiv 1/\|1\|_w, \quad (2.45)$$

where $\|1\|_w = \sqrt{\int_a^b w(x) dx}$, and define recursively

$$P_{n+1}(x) = \frac{xP_n(x) - \sum_0^n P_i(x) \langle P_i, xP_n \rangle_w}{\|xP_n - \sum_0^n P_i \langle P_i, xP_n \rangle_w\|_w}. \quad (2.46)$$

Clearly $P_n(x)$ is an n -th order polynomial, and by construction

$$\langle P_n, P_m \rangle_w = \delta_{nm}. \quad (2.47)$$

All such sets of polynomials obey a three-term recurrence relation

$$xP_n(x) = b_n P_{n+1}(x) + a_n P_n(x) + b_{n-1} P_{n-1}(x). \quad (2.48)$$

That there are only three terms, and that the coefficients of P_{n+1} and P_{n-1} are related, is due to the identity

$$\langle P_n, xP_m \rangle_w = \langle xP_n, P_m \rangle_w. \quad (2.49)$$

This means that the matrix (in the P_n basis) representing the operation of multiplication by x is symmetric. Since multiplication by x takes us from P_n only to P_{n+1} , the matrix has just one non-zero entry above the main diagonal, and hence, by symmetry, only one below.

The completeness of a family of polynomials orthogonal on a finite interval is guaranteed by the *Weierstrass approximation theorem* which asserts that for any continuous real function $f(x)$ on $[a, b]$, and for any $\varepsilon > 0$, there exists a polynomial $p(x)$ such that $|f(x) - p(x)| < \varepsilon$ for all $x \in [a, b]$. This means that polynomials are dense in the space of continuous functions equipped with the $\|\dots\|_\infty$ norm. Because

$$\int_a^b |f(x) - p(x)|^2 w(x) dx \leq \varepsilon^2 \int_a^b w(x) dx, \quad (2.50)$$

they are also a dense subset of the continuous functions in the sense of $L_w^2[a, b]$ convergence. Because the Hilbert space $L_w^2[a, b]$ is defined to be the completion of the space of continuous functions, the continuous functions are automatically dense in $L_w^2[a, b]$. Now a dense subset of a dense set is dense in the larger set, so the polynomials are dense in $L_w^2[a, b]$ itself. The normalized orthogonal polynomials therefore constitute a complete orthonormal set.

For later use, we here summarize the properties of the families of polynomials named after Legendre, Hermite and Tchebychef.

Legendre polynomials

These are defined by $a = -1$, $b = 1$ and $w = 1$. The standard Legendre polynomials are not normalized by the scalar product, but instead by setting $P_n(1) = 1$. They are given by *Rodriguez'* formula

$$P_n(x) = \frac{1}{2^n n!} \frac{d^n}{dx^n} (x^2 - 1)^n. \quad (2.51)$$

The first few are

$$\begin{aligned} P_0(x) &= 1, \\ P_1(x) &= x, \\ P_2(x) &= \frac{1}{2}(3x^2 - 1), \\ P_3(x) &= \frac{1}{2}(5x^3 - 3x), \\ P_4(x) &= \frac{1}{8}(35x^4 - 30x^2 + 3). \end{aligned}$$

Their inner product is

$$\int_{-1}^1 P_n(x)P_m(x) dx = \frac{2}{2n+1}\delta_{nm}. \quad (2.52)$$

The three-term recurrence relation is

$$(2n+1)xP_n(x) = (n+1)P_{n+1}(x) + nP_{n-1}(x). \quad (2.53)$$

The P_n form a complete set for expanding functions on $[-1, 1]$.

Hermite polynomials

The Hermite polynomials have $a = -\infty$, $b = +\infty$ and $w(x) = e^{-x^2}$, and are defined by the generating function

$$e^{2tx-t^2} = \sum_0^{\infty} \frac{1}{n!} H_n(x) t^n. \quad (2.54)$$

If we write

$$e^{2tx-t^2} = e^{x^2-(x-t)^2}, \quad (2.55)$$

we may use Taylor's theorem to find

$$H_n(x) = \left. \frac{d^n}{dt^n} e^{x^2-(x-t)^2} \right|_{t=0} = (-1)^n e^{x^2} \frac{d^n}{dx^n} e^{-x^2}, \quad (2.56)$$

which is a useful alternative definition. The first few Hermite polynomials are

$$\begin{aligned} H_1(x) &= 1, \\ H_2(x) &= 2x, \\ H_3(x) &= 8x^3 - 12x, \\ H_4(x) &= 16x^4 - 48x^2 + 12, \\ H_5(x) &= 32x^5 - 160x^3 + 120x. \end{aligned}$$

The normalization is such that

$$\int_{-\infty}^{\infty} H_n(x)H_m(x)e^{-x^2} dx = 2^n n! \sqrt{\pi} \delta_{nm}, \quad (2.57)$$

as may be proved by using the generating function. The three-term recurrence relation is

$$2xH_n(x) = H_{n+1}(x) - 2nH_{n-1}(x). \quad (2.58)$$

Exercise 2.3: Evaluate the integral

$$F(s, t) = \int_{-\infty}^{\infty} e^{-x^2} e^{2sx-s^2} e^{2tx-t^2} dx$$

and expand the result as a double power series in s and t . By examining the coefficient of $s^n t^m$, show that

$$\int_{-\infty}^{\infty} H_n(x) H_m(x) e^{-x^2} dx = 2^n n! \sqrt{\pi} \delta_{nm}.$$

Exercise 2.4: Let

$$\varphi_n(x) = \frac{1}{\sqrt{2^n n! \sqrt{\pi}}} H_n(x) e^{-x^2/2}$$

be the *normalized Hermite functions*. They form a complete orthonormal set in $L^2(\mathbb{R})$. Starting from the generating function for the Hermite polynomials, show that

$$\sum_{n=0}^{\infty} t^n \varphi_n(x) \varphi_n(y) = \frac{1}{\sqrt{\pi(1-t^2)}} \exp \left\{ \frac{4xyt - (x^2 + y^2)(1+t^2)}{2(1-t^2)} \right\}, \quad 0 \leq t < 1.$$

This is *Mehler's formula*.

Exercise 2.5: Let $\varphi_n(x)$ be the same functions as in the previous exercise. Define a Fourier-transform operator $F : L^2(\mathbb{R}) \rightarrow L^2(\mathbb{R})$ by

$$F(f) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} e^{ixs} f(s) ds.$$

With this normalization of the Fourier transform, F^4 is the identity map. The possible eigenvalues of F are therefore $\pm 1, \pm i$. Starting from (2.56), show that the $\varphi_n(x)$ are eigenfunctions of F , and that

$$F(\varphi_n) = i^n \varphi_n(x).$$

Tchebychef polynomials

These are defined by taking $a = -1$, $b = +1$ and $w(x) = (1 - x^2)^{\pm 1/2}$. The *Tchebychef polynomials of the first kind* are

$$T_n(x) = \cos(n \cos^{-1} x). \quad (2.59)$$

The first few are

$$\begin{aligned} T_0(x) &= 1, \\ T_1(x) &= x, \\ T_2(x) &= 2x^2 - 1, \\ T_3(x) &= 4x^3 - 3x. \end{aligned}$$

The *Tchebychef polynomials of the second kind* are

$$U_{n-1}(x) = \frac{\sin(n \cos^{-1} x)}{\sin(\cos^{-1} x)} = \frac{1}{n} T'_n(x). \quad (2.60)$$

and the first few are

$$\begin{aligned} U_{-1}(x) &= 0, \\ U_0(x) &= 1, \\ U_1(x) &= 2x, \\ U_2(x) &= 4x^2 - 1, \\ U_3(x) &= 8x^3 - 4x. \end{aligned}$$

T_n and U_n obey the same recurrence relation

$$\begin{aligned} 2xT_n &= T_{n+1} + T_{n-1}, \\ 2xU_n &= U_{n+1} + U_{n-1}, \end{aligned}$$

which are disguised forms of elementary trigonometric identities. Their orthogonality is also a disguised form of the orthogonality of the functions $\cos n\theta$ and $\sin n\theta$. After setting $x = \cos \theta$ we have

$$\int_0^\pi \cos n\theta \cos m\theta \, d\theta = \int_{-1}^1 \frac{1}{\sqrt{1-x^2}} T_n(x) T_m(x) \, dx = h_n \delta_{nm}, \quad n, m, \geq 0, \quad (2.61)$$

where $h_0 = \pi$, $h_n = \pi/2$, $n > 0$, and

$$\int_0^\pi \sin n\theta \sin m\theta \, d\theta = \int_{-1}^1 \sqrt{1-x^2} U_{n-1}(x) U_{m-1}(x) \, dx = \frac{\pi}{2} \delta_{nm}, \quad n, m > 0. \quad (2.62)$$

The set $\{T_n(x)\}$ is therefore orthogonal and complete in $L^2_{(1-x^2)^{-1/2}}[-1, 1]$, and the set $\{U_n(x)\}$ is orthogonal and complete in $L^2_{(1-x^2)^{1/2}}[-1, 1]$. Any function continuous on the closed interval $[-1, 1]$ lies in both of these spaces, and can therefore be expanded in terms of either set.

2.3 Linear Operators and Distributions

Our theme is the analogy between linear differential operators and matrices. It is therefore useful to understand how we can think of a differential operator as a continuously indexed “matrix”.

2.3.1 Linear operators

The action of a finite matrix on a vector $\mathbf{y} = \mathbf{A}\mathbf{x}$ is given in components by

$$y_i = A_{ij}x_j. \quad (2.63)$$

The function-space analogue of this, $g = Af$, is naturally to be thought of as

$$g(x) = \int_a^b A(x, y)f(y) dy, \quad (2.64)$$

where the summation over adjacent indices has been replaced by an integration over the dummy variable y . If $A(x, y)$ is an ordinary function then $A(x, y)$ is called an *integral kernel*. We will study such linear operators in the chapter on integral equations.

The identity operation is

$$f(x) = \int_a^b \delta(x - y)f(y) dy, \quad (2.65)$$

and so the Dirac delta function, which is **not** an ordinary function, plays the role of the identity matrix. Once we admit *distributions* such as $\delta(x)$, we can think of differential operators as continuously indexed matrices by using the distribution

$$\delta'(x) = \left\langle \frac{d}{dx} \delta(x) \right\rangle. \quad (2.66)$$

The quotes are to warn us that we are not really taking the derivative of the highly singular delta function. The symbol $\delta'(x)$ is properly defined by its behaviour in an integral

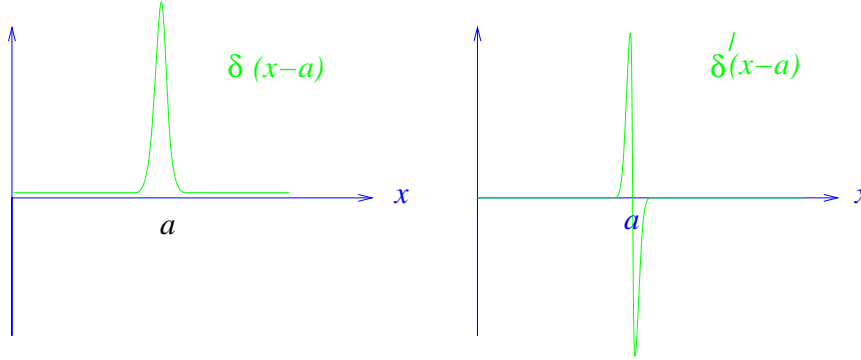
$$\begin{aligned} \int_a^b \delta'(x - y)f(y) dy &= \int_a^b \frac{d}{dx} \delta(x - y)f(y) dy \\ &= - \int_a^b f(y) \frac{d}{dy} \delta(x - y) dy \end{aligned}$$

$$\begin{aligned}
&= \int_a^b f'(y) \delta(x-y) dy, \quad (\text{Integration by parts}) \\
&= f'(x).
\end{aligned}$$

The manipulations here are purely formal, and serve only to motivate the defining property

$$\int_a^b \delta'(x-y) f(y) dy = f'(x). \quad (2.67)$$

It is, however, sometimes useful to think of a smooth approximation to $\delta'(x-a)$ being the genuine derivative of a smooth approximation to $\delta(x-a)$.



Smooth approximations to $\delta(x-a)$ and $\delta'(x-a)$.

We can now define higher “derivatives” of $\delta(x)$ by

$$\int_a^b \delta^{(n)}(x) f(x) dx = (-1)^n f^{(n)}(0), \quad (2.68)$$

and use them to represent any linear differential operator as a formal integral kernel.

Example: In chapter one we formally evaluated a second functional derivative and ended up with the distributional kernel (1.185), which we here write as

$$\begin{aligned}
k(x, y) &= -\frac{d}{dy} \left(p(y) \frac{d}{dy} \delta(y-x) \right) + q(y) \delta(y-x) \\
&= -p(y) \delta''(y-x) - p'(y) \delta'(y-x) + q(y) \delta(y-x). \quad (2.69)
\end{aligned}$$

When k acts on a function u , it gives

$$\int k(x, y) u(y) dy = \int \{ -p(y) \delta''(y-x) - p'(y) \delta'(y-x) + q(y) \delta(y-x) \} u(y) dy$$

$$\begin{aligned}
&= \int \delta(y-x) \{-[p(y)u(y)]'' + [p'(y)u(y)]' + q(y)u(y)\} dy \\
&= \int \delta(y-x) \{-p(y)u''(y) - p'(y)u'(y) + q(y)u(y)\} dy \\
&= -\frac{d}{dx} \left(p(x) \frac{du}{dx} \right) + q(x)u(x). \tag{2.70}
\end{aligned}$$

The continuous matrix (1.185) therefore does, as indicated in chapter one, represent the Sturm-Liouville operator L defined in (1.181).

Exercise 2.6: Consider the distributional kernel

$$k(x, y) = a_2(y)\delta''(x-y) + a_1(y)\delta'(x-y) + a_0(y)\delta(x-y). \tag{2.71}$$

Show that

$$\int k(x, y)u(y) dy = (a_2(x)u(x))'' + (a_1(x)u(x))' + a_0(x)u(x), \tag{2.72}$$

and that

$$k(x, y) = a_2(x)\delta''(x-y) + a_1(x)\delta'(x-y) + a_0(x)\delta(x-y), \tag{2.73}$$

leads to

$$\int k(x, y)u(y) dy = a_2(x)u''(x) + a_1(x)u'(x) + a_0(x)u(x). \tag{2.74}$$

Exercise 2.7: The distributional kernel (2.69) was originally obtained as a second functional derivative

$$\begin{aligned}
k(x_1, x_2) &= \frac{\delta}{\delta y(x_1)} \left(\frac{\delta J[y]}{\delta y(x_2)} \right) \\
&= -\frac{d}{dx_2} \left(p(x_2) \frac{d}{dx_2} \delta(x_2 - x_1) \right) + q(x_2)\delta(x_2 - x_1).
\end{aligned}$$

By analogy with conventional partial derivatives, we would expect that

$$\frac{\delta}{\delta y(x_1)} \left(\frac{\delta J[y]}{\delta y(x_2)} \right) = \frac{\delta}{\delta y(x_2)} \left(\frac{\delta J[y]}{\delta y(x_1)} \right),$$

but x_1 and x_2 appear asymmetrically in $k(x_1, x_2)$. Define

$$k^T(x_1, x_2) = k(x_2, x_1),$$

and show that

$$\int k^T(x_1, x_2)u(x_2) dx_2 = \int k(x_1, x_2)u(x_2) dx_2.$$

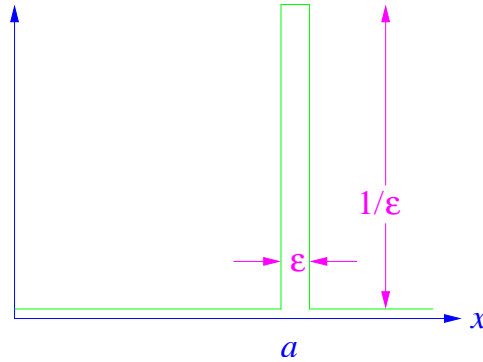
Conclude that, superficial appearance notwithstanding, we do have $k(x_1, x_2) = k(x_2, x_1)$.

The example and exercises show that linear differential operators correspond to continuously-infinite matrices having entries only infinitesimally close to their main diagonal.

2.3.2 Distributions and test-functions

It is possible to work most the problems in this book with no deeper understanding of what a delta-function is than that presented in section 2.3.1. At some point however, the more careful reader will wonder about the logical structure of what we are doing, and will soon discover that too free a use of $\delta(x)$ and its derivatives can lead to paradoxes. How do such creatures fit into the function-space picture, and what sort of manipulations with them are valid?

We often think of $\delta(x)$ as being a “limit” of a sequence of functions whose graphs are getting narrower and narrower while their height grows to keep the area under the curve fixed. An example would be the spike function $\delta_\varepsilon(x - a)$ in the figure



Approximation $\delta_\varepsilon(x - a)$ to $\delta(x - a)$.

The L^2 norm of δ_ε ,

$$\|\delta_\varepsilon\|^2 = \int |\delta_\varepsilon(x)|^2 dx = \frac{1}{\varepsilon}, \quad (2.75)$$

tends to infinity as $\varepsilon \rightarrow 0$, so δ_ε cannot be tending to any function in L^2 . This delta function has infinite “length,” and so is *not* an element of our Hilbert space.

The simple spike is not the only way to construct a delta function. In Fourier theory we meet

$$\delta_\Lambda(x) = \int_{-\Lambda}^{\Lambda} e^{ikx} \frac{dk}{2\pi} = \frac{1}{\pi} \frac{\sin \Lambda x}{x}, \quad (2.76)$$

which becomes a delta-function when Λ becomes large. In this case

$$\|\delta_\Lambda\|^2 = \int_{-\infty}^{\infty} \frac{\sin^2 \Lambda x}{\pi^2 x^2} dx = \Lambda/\pi. \quad (2.77)$$

Again the “limit” has infinite length and cannot be accommodated in Hilbert space. This $\delta_\Lambda(x)$ is even more pathological than δ_ε . It provides a salutary counter-example to the often asserted “fact” that $\delta(x) = 0$ for $x \neq 0$. As Λ becomes large $\delta_\Lambda(0)$ diverges to infinity. At any fixed non-zero x , however, $\delta_\Lambda(x)$ oscillates between $\pm 1/x$ as Λ grows. Consequently the limit $\lim_{\Lambda \rightarrow \infty} \delta_\Lambda(x)$ exists nowhere. It therefore makes no sense to assign a numerical value to $\delta(x)$ at any x .

Given its wild behaviour, is not surprising that mathematicians looked askance at Dirac’s $\delta(x)$. It was only in 1944, long after its effectiveness in solving physics and engineering problems had become an embarrassment, that Laurent Schwartz was able to tame $\delta(x)$ by creating his *theory of distributions*. Using the language of distributions we can state precisely the conditions under which a manoeuvre involving singular objects such as $\delta'(x)$ is legitimate.

Schwartz’ theory is built on a concept from linear algebra. Recall that the *dual space* V^* of a vector space V is the vector space of linear functions from the original vector space V to the field over which it is defined. We consider $\delta(x)$ to be an element of the dual space of a vector space \mathcal{T} of *test functions*. When a test function $\varphi(x)$ is plugged in, the δ -machine returns the number $\varphi(0)$. This operation is a linear map because the action of δ on $\lambda\varphi(x) + \mu\chi(x)$ is to return $\lambda\varphi(0) + \mu\chi(0)$. Test functions are smooth (infinitely differentiable) functions that tend rapidly to zero at infinity. Exactly what class of function we chose for \mathcal{T} depends on the problem at hand. If we are going to make extensive use of Fourier transforms, for example, we might

select the *Schwartz space*, $\mathcal{S}(\mathbb{R})$. This is the space of infinitely differentiable functions $\varphi(x)$ such that the *seminorms*³

$$|\varphi|_{m,n} = \sup_{x \in \mathbb{R}} \left\{ |x|^n \left| \frac{d^m \varphi}{dx^m} \right| \right\} \quad (2.78)$$

are finite for all positive integers m and n . The Schwartz space has the advantage that if φ is in $\mathcal{S}(\mathbb{R})$, then so is its Fourier transform. Another popular space of test functions is \mathcal{D} consisting of C^∞ functions of *compact support*—meaning that each function is identically zero outside some finite interval. Only if we want to prove theorems is a precise specification of \mathcal{T} essential. For most physics calculations infinite differentiability and a rapid enough decrease at infinity for us to be able to ignore boundary terms is all that we need.

The “nice” behaviour of the test functions compensates for the “nasty” behaviour of $\delta(x)$ and its relatives. The objects, such as $\delta(x)$, composing the dual space \mathcal{T}^* are called *generalized functions*, or *distributions*. Actually, not every linear map $\mathcal{T} \rightarrow \mathbb{R}$ is to be included in \mathcal{T}^* , because, for technical reasons, we must require the maps in the dual space to be *continuous*. In other words, if $\varphi_n \rightarrow \varphi$, we want all distributions u to obey $u(\varphi_n) \rightarrow u(\varphi)$. Making precise what we mean by $\varphi_n \rightarrow \varphi$ is part of the task of specifying \mathcal{T} . In the Schwartz space, for example, we declare that $\varphi_n \rightarrow \varphi$ if $|\varphi_n - \varphi|_{n,m} \rightarrow 0$, for all positive m, n .

When they wish to stress the dual-space aspect of distribution theory, mathematically minded authors use the notation

$$\delta(\varphi) = \varphi(0), \quad (2.79)$$

or

$$(\delta, \varphi) = \varphi(0), \quad (2.80)$$

in place of the common, but purely formal,

$$\int \delta(x) \varphi(x) dx = \varphi(0). \quad (2.81)$$

The expression (δ, φ) here represents the *pairing* of the element φ of the vector space \mathcal{T} with the element δ of its dual space \mathcal{T}^* . It should not be

³A seminorm $|\cdots|$ is like a norm, except that $|\varphi| = 0$ does not imply that $\varphi = 0$.

thought of as an inner product as the distribution and the test function lie in different spaces. The “integral” in the common notation is purely symbolic, of course, but the common notation should not be despised even by those in quest of rigour. It suggests correct results, such as

$$\int \delta(ax - b)\varphi(x) dx = \frac{1}{|a|}\varphi(b/a), \quad (2.82)$$

which would look quite unmotivated in the dual-space notation.

The distribution $\delta'(x)$ is now defined by the pairing

$$(\delta', \varphi) = -\varphi'(0), \quad (2.83)$$

where the minus sign comes from imagining an integration by parts that takes the “derivative” off $\delta(x)$ and puts it on to the smooth function $\varphi(x)$:

$$“\int \delta'(x)\varphi(x) dx” = -\int \delta(x)\varphi'(x) dx. \quad (2.84)$$

Similarly $\delta^{(n)}(x)$ is now defined by the pairing

$$(\delta^{(n)}, \varphi) = (-1)^n \varphi^{(n)}(0). \quad (2.85)$$

The “nicer” the class of test function we take, the “nastier” the class of distributions we can handle. For example, the Hilbert space L^2 is its own dual: the *Riesz-Fréchet theorem* (see exercise 2.10) asserts that any continuous linear map $F : L^2 \rightarrow \mathbb{R}$ can be written as $F[f] = \langle l, f \rangle$ for some $l \in L^2$. The delta-function map is not continuous when considered as a map from $L^2 \rightarrow \mathbb{R}$ however. An arbitrarily small change, $f \rightarrow f + \delta f$, in a function (small in the L^2 sense of $\|\delta f\|$ being small) can produce an arbitrarily large change in $f(0)$. Thus L^2 functions are not “nice” enough for their dual space to be able accommodate the delta function. Another way of understanding this is to remember that we regard two L^2 functions as being the same whenever $\|f_1 - f_2\| = 0$. This distance will be zero even if f_1 and f_2 differ from one another on a countable set of points. As we have remarked earlier, this means that elements of L^2 are not really functions at all — they do not have an assigned value at each point. They are, instead, only *equivalence classes* of functions. Since $f(0)$ is undefined, any attempt to interpret the statement $\int \delta(x)f(x) dx = f(0)$ for f an arbitrary element L^2 is necessarily doomed to failure. Continuous functions, however,

do have well-defined values at every point. If we take the space of test functions \mathcal{T} to consist of all continuous functions, but not demand that they be differentiable, then \mathcal{T}^* will include the delta function, but not its “derivative” $\delta'(x)$, as this requires us to evaluate $f'(0)$. If we require the test functions to be once-differentiable, then \mathcal{T}^* will include $\delta'(x)$ but not $\delta''(x)$, and so on.

When we add suitable spaces \mathcal{T} and \mathcal{T}^* to our toolkit, we are constructing what is called a *rigged*⁴ Hilbert space. In such a rigged space we have the inclusion

$$\mathcal{T} \subset L^2 \equiv [L^2]^* \subset \mathcal{T}^*. \quad (2.86)$$

The idea is to take the space \mathcal{T}^* big enough to contain objects such as the limit of our sequence of “approximate” delta functions δ_ε , which does not converge to anything in L^2 .

Ordinary functions can also be regarded as distributions, and this helps illuminate the different senses in which a sequence u_n can converge. For example, we can consider the functions

$$u_n = \sin n\pi x, \quad 0 < x < 1, \quad (2.87)$$

as being either elements of $L^2[0, 1]$ or as distributions. As distributions we evaluate them on a smooth function φ as

$$(u_n, \varphi) = \int_0^1 \varphi(x) u_n(x) dx. \quad (2.88)$$

Now

$$\lim_{n \rightarrow \infty} (u_n, \varphi) = 0, \quad (2.89)$$

since the high-frequency Fourier coefficients of any smooth function tend to zero. We deduce that *as a distribution* we have $\lim_{n \rightarrow \infty} u_n = 0$. Considered as elements of L^2 , however, the u_n do not tend to zero. Their norm obeys $\|u_n\| = 1/2$ and so all the u_n remain at the same fixed distance from 0.

Exercise 2.8: Here we show that the elements of $L^2[a, b]$, which we defined in exercise 2.2 to be the formal limits of Cauchy sequences of continuous functions, may be thought of as distributions.

⁴“Rigged” as in a sailing ship ready for sea, not “rigged” as in a corrupt election.

- i) Let $\varphi(x)$ be a test function and $f_n(x)$ a Cauchy sequence of continuous functions defining $f \in L^2$. Use the Cauchy-Schwarz-Bunyakovsky inequality to show that the sequence of numbers $\langle \varphi, f_n \rangle$ is Cauchy and so deduce that $\lim_{n \rightarrow \infty} \langle \varphi, f_n \rangle$ exists.
- ii) Let $\varphi(x)$ be a test function and $f_n^{(1)}(x)$ and $f_n^{(2)}(x)$ be a pair of equivalent sequences defining the same element $f \in L^2$. Use Cauchy-Schwarz-Bunyakovsky to show that

$$\lim_{n \rightarrow \infty} \langle \varphi, f_n^{(1)} - f_n^{(2)} \rangle = 0.$$

Combine this result with that of the preceding exercise to deduce that we can set

$$(\varphi, f) \equiv \lim_{n \rightarrow \infty} \langle \varphi, f_n \rangle,$$

and so define $f \equiv \lim_{n \rightarrow \infty} f_n$ as a distribution.

The interpretation of elements of L^2 as distributions is simultaneously simpler and more physical than the classical interpretation *via* the Lebesgue integral.

Weak derivatives

By exploiting the infinite differentiability of our test functions, we were able to make mathematical sense of the “derivative” of the highly singular delta function. The same idea of a formal integration by parts can be used to define the “derivative” for any distribution, and also for ordinary functions that would not usually be regarded as being differentiable.

We therefore define the *weak* or *distributional* derivative $v(x)$ of a distribution $u(x)$ by requiring its evaluation on a test function $\varphi \in \mathcal{T}$ to be

$$\int v(x) \varphi(x) dx \stackrel{\text{def}}{=} - \int u(x) \varphi'(x) dx. \quad (2.90)$$

In the more formal pairing notation we write

$$(v, \varphi) \stackrel{\text{def}}{=} -(u, \varphi'). \quad (2.91)$$

The right hand side of (2.91) is a continuous linear function of φ , and so, therefore, is the left hand side. Thus the weak derivative $u' \equiv v$ is a well-defined distribution for any u .

When $u(x)$ is an ordinary function and differentiable in the conventional sense, its weak derivative coincides with the usual derivative. When the

function is not conventionally differentiable the weak derivative still exists, but does not assign a numerical value to the derivative at each point. It is therefore a distribution and not a function.

The elements of L^2 are not quite functions — having no well-defined value at a point — but are particularly mild-mannered distributions, and their weak derivatives may themselves be elements of L^2 . It is this weak sense that we will, in later chapters, allow differential operators to act on L^2 “functions”.

Example: In the weak sense

$$\frac{d}{dx}|x| = \operatorname{sgn}(x), \quad (2.92)$$

$$\frac{d}{dx}\operatorname{sgn}(x) = 2\delta(x). \quad (2.93)$$

The object $|x|$ is an ordinary function, but $\operatorname{sgn}(x)$ has no definite value at $x = 0$, whilst $\delta(x)$ has no definite value at any x .

Example: As a more subtle illustration, consider the weak derivative of the function $\ln|x|$. With $\varphi(x)$ a test function, the improper integral

$$I = - \int_{-\infty}^{\infty} \varphi'(x) \ln|x| dx \equiv - \lim_{\varepsilon, \varepsilon' \rightarrow 0} \left(\int_{-\infty}^{-\varepsilon} + \int_{\varepsilon'}^{\infty} \right) \varphi'(x) \ln|x| dx \quad (2.94)$$

is convergent and defines the pairing $(-\ln|x|, \varphi')$. We wish to integrate by parts and interpret the result as $([\ln|x|]', \varphi)$. The logarithm is differentiable in the conventional sense away from $x = 0$, and

$$[\ln|x|\varphi(x)]' = \frac{1}{x}\varphi(x) + \ln|x|\varphi'(x), \quad x \neq 0. \quad (2.95)$$

From this we find that

$$-(\ln|x|, \varphi') = \lim_{\varepsilon, \varepsilon' \rightarrow 0} \left\{ \left(\int_{-\infty}^{-\varepsilon} + \int_{\varepsilon'}^{\infty} \right) \frac{1}{x}\varphi(x) dx + \left(\varphi(\varepsilon') \ln|\varepsilon'| - \varphi(-\varepsilon) \ln|\varepsilon| \right) \right\}. \quad (2.96)$$

So far ε and ε' are unrelated except in that they are both being sent to zero. If, however, we choose to make them equal, $\varepsilon = \varepsilon'$, then the integrated-out part becomes

$$\left(\varphi(\varepsilon) - \varphi(-\varepsilon) \right) \ln|\varepsilon| \sim 2\varphi'(0)\varepsilon \ln|\varepsilon|, \quad (2.97)$$

and this tends to zero as ε becomes small. In this case

$$-(\ln |x|, \varphi') = \lim_{\varepsilon \rightarrow 0} \left\{ \left(\int_{-\infty}^{-\varepsilon} + \int_{\varepsilon}^{\infty} \right) \frac{1}{x} \varphi(x) dx \right\}. \quad (2.98)$$

By the definition of the weak derivative, the left hand side of (2.98) is the pairing $(\ln |x|', \varphi)$. We conclude that

$$\frac{d}{dx} \ln |x| = P \left(\frac{1}{x} \right), \quad (2.99)$$

where $P(1/x)$, the *principal-part* distribution, is defined by the right-hand-side of (2.98). It is evaluated on the test function $\varphi(x)$ by forming $\int \varphi(x)/x dx$, but with an infinitesimal interval from $-\varepsilon$ to $+\varepsilon$, omitted from the range of integration. It is essential that this omitted interval lie symmetrically about the dangerous point $x = 0$. Otherwise the integrated-out part will not vanish in the $\varepsilon \rightarrow 0$ limit. The resulting *principal-part integral*, written $P \int \varphi(x)/x dx$, is then convergent and $P(1/x)$ is a well-defined distribution despite the singularity in the integrand. Principal-part integrals are common in physics. We will next meet them when we study Green functions.

For further reading on distributions and their applications we recommend M. J. Lighthill *Fourier Analysis and Generalised Functions*, or F. G. Friedlander *Introduction to the Theory of Distributions*. Both books are published by Cambridge University Press.

2.4 Exercises and Problems

The first two problems lead to a proof of the Riesz-Fréchet theorem. Although not an essential part of our story, they demonstrate how “completeness” is used in Hilbert space theory, and provide some practice with “ ϵ, δ ” arguments for those who desire it.

Exercise 2.9: Show that if a norm $\| \cdot \|$ is derived from an inner product, then it obeys the *parallelogram law*

$$\|f + g\|^2 + \|f - g\|^2 = 2(\|f\|^2 + \|g\|^2).$$

Let N be a complete linear subspace of a Hilbert space H . Let $g \notin N$, and let

$$\inf_{f \in N} \|g - f\| = d.$$

Show that there exists a sequence $f_n \in N$ such that $\lim_{n \rightarrow \infty} \|f_n - g\| = d$. Use the parallelogram law to show that the sequence f_n is Cauchy, and hence deduce that there is a unique $f \in N$ such that $\|g - f\| = d$. Conclude that $d > 0$. Show also that $\langle (g - f), h \rangle = 0$ for all $h \in N$.

Exercise 2.10: Riesz-Fréchet theorem. Let $L[h]$ be a continuous linear functional on a Hilbert space H . Here *continuous* means that

$$\|h_n - h\| \rightarrow 0 \Rightarrow L[h_n] \rightarrow L[h].$$

Show that the set $N = \{f \in H : L[f] = 0\}$ is a complete linear subspace of H .

Suppose now that there is a $g \in H$ such that $L[g] \neq 0$, and let $l \in H$ be the vector “ $g - f$ ” from the previous problem. Show that

$$L[h] = \langle \alpha l, h \rangle, \quad \alpha = L[g] / \langle l, g \rangle = L[g] / \|l\|^2.$$

A continuous linear functional can therefore be expressed as an inner product.

Next we have some problems on orthogonal polynomials and three-term recurrence relations. They provide an excuse for reviewing some linear algebra, and also serve to introduce the theory behind some practical numerical methods.

Exercise 2.11: Let $\{P_n(x)\}$ be a family of polynomials orthonormal on $[a, b]$ with respect to a positive weight function $w(x)$, and with $\deg[P_n(x)] = n$. Let us also scale $w(x)$ so that $\int_a^b w(x) dx = 1$, and $P_0(x) = 1$.

a) Suppose that the $P_n(x)$ obey the three-term recurrence relation

$$xP_n(x) = b_n P_{n+1}(x) + a_n P_n(x) + b_{n-1} P_{n-1}(x); \quad P_{-1}(x) = 0, \quad P_0(x) = 1.$$

Define

$$p_n(x) = P_n(x)(b_{n-1}b_{n-2} \cdots b_0),$$

and show that

$$xp_n(x) = p_{n+1}(x) + a_n p_n(x) + b_{n-1}^2 p_{n-1}(x); \quad p_{-1}(x) = 0, \quad p_0(x) = 1.$$

Conclude that the $p_n(x)$ are *monic* — i.e. the coefficient of their leading power of x is unity.

b) Show also that the functions

$$q_n(x) = \int_a^b \frac{p_n(x) - p_n(\xi)}{x - \xi} w(\xi) d\xi$$

are degree $n-1$ monic polynomials that obey the same recurrence relation as the $p_n(x)$, but with initial conditions $q_0(x) = 0$, $q_1(x) \equiv \int_a^b w dx = 1$.

Warning: While the $q_n(x)$ polynomials defined in part b) turn out to be very useful, they are *not* mutually orthogonal with respect to $\langle \cdot, \cdot \rangle_w$.

Exercise 2.12: Gaussian quadrature. Orthogonal polynomials have application to numerical integration. Let the polynomials $\{P_n(x)\}$ be orthonormal on $[a, b]$ with respect to the positive weight function $w(x)$, and let x_ν , $\nu = 1, \dots, N$ be the zeros of $P_N(x)$. We will show that if we define the weights

$$w_\nu = \int_a^b \frac{P_N(x)}{P'_N(x_\nu)(x - x_\nu)} w(x) dx$$

then *Gauss' quadrature rule*

$$\int_a^b f(x)w(x) dx \approx w_1f(x_1) + w_2f(x_2) + \cdots w_Nf(x_N)$$

is *exact* for $f(x)$ any polynomial of degree less than or equal to $2N - 1$.

- a) Let $\pi(x) = (x - \xi_1)(x - \xi_2) \cdots (x - \xi_N)$ be a polynomial of degree N . Given a function $F(x)$, show that

$$F_L(x) \stackrel{\text{def}}{=} \sum_{\nu=1}^N F(\xi_\nu) \frac{\pi(x)}{\pi'(\xi_\nu)(x - \xi_\nu)}$$

is a polynomial of degree $N - 1$ that coincides with $F(x)$ at $x = \xi_\nu$, $\nu = 1, \dots, N$. (This is *Lagrange's interpolation formula*.)

- b) Show that if $F(x)$ is polynomial of degree $N - 1$ or less then $F_L(x) = F(x)$.
 c) Let $f(x)$ be polynomial of degree $2N - 1$ or less. Cite the polynomial division algorithm to show that there exist polynomials $Q(x)$ and $R(x)$, each of degree $N - 1$ or less, such that

$$f(x) = P_N(x)Q(x) + R(x).$$

- d) Show that $f(x_\nu) = R(x_\nu)$, and that

$$\int_a^b f(x)w(x) dx = \int_a^b R(x)w(x) dx.$$

- e) Combine parts a), b) and d) to establish Gauss' result.
 f) Show that if we normalize $w(x)$ so that $\int w dx = 1$ then the weights w_ν can be expressed as $w_\nu = q_N(x_\nu)/p'_N(x_\nu)$, where $p_n(x)$, $q_n(x)$ are the monic polynomials defined in the preceding problem.

The ultimate large- N exactness of Gaussian quadrature can be expressed as

$$w(x) = \lim_{N \rightarrow \infty} \left\{ \sum_{\nu} \delta(x - x_{\nu}) w_{\nu} \right\}.$$

Of course, a sum of Dirac delta-functions can never become a continuous function in any ordinary sense. The equality holds only after both sides are integrated against a smooth test function, *i.e.* when it is considered as a statement about distributions.

Exercise 2.13: The completeness property of a set of polynomials $\{P_n(x)\}$, orthonormal set with respect to the positive weight function $w(x)$, is equivalent to the statement that

$$\sum_{n=0}^{\infty} P_n(x) P_n(y) = \frac{1}{w(x)} \delta(x - y).$$

It is useful to have a formula for the partial sums of this infinite series.

Suppose that the polynomials $P_n(x)$ obey the three-term recurrence relation

$$xP_n(x) = b_n P_{n+1}(x) + a_n P_n(x) + b_{n-1} P_{n-1}(x); \quad P_{-1}(x) = 0, \quad P_0(x) = 1.$$

Use this recurrence relation, together with its initial conditions, to obtain the *Christoffel-Darboux* formula

$$\sum_{n=0}^{N-1} P_n(x) P_n(y) = \frac{b_{N-1} [P_N(x) P_{N-1}(y) - P_{N-1}(x) P_N(y)]}{x - y}.$$

Exercise 2.14: Again suppose that the polynomials $P_n(x)$ obey the three-term recurrence relation

$$xP_n(x) = b_n P_{n+1}(x) + a_n P_n(x) + b_{n-1} P_{n-1}(x); \quad P_{-1}(x) = 0, \quad P_0(x) = 1.$$

Consider the N -by- N tridiagonal matrix eigenvalue problem

$$\begin{bmatrix} a_{N-1} & b_{N-2} & 0 & 0 & \dots & 0 \\ b_{N-2} & a_{N-2} & b_{N-3} & 0 & \dots & 0 \\ 0 & b_{N-3} & a_{N-3} & b_{N-4} & \dots & 0 \\ \vdots & \ddots & \ddots & \ddots & \ddots & \vdots \\ 0 & \dots & b_2 & a_2 & b_1 & 0 \\ 0 & \dots & 0 & b_1 & a_1 & b_0 \\ 0 & \dots & 0 & 0 & b_0 & a_0 \end{bmatrix} \begin{bmatrix} u_{N-1} \\ u_{N-2} \\ u_{N-3} \\ \vdots \\ u_2 \\ u_1 \\ u_0 \end{bmatrix} = x \begin{bmatrix} u_{N-1} \\ u_{N-2} \\ u_{N-3} \\ \vdots \\ u_2 \\ u_1 \\ u_0 \end{bmatrix}$$

- a) Show that the eigenvalues x are given by the zeros x_ν , $\nu = 1, \dots, N$ of $P_N(x)$, and that the corresponding eigenvectors have components $u_n = P_n(x_\nu)$, $n = 0, \dots, N-1$.
- b) Take the $x \rightarrow y$ limit of the Christoffel-Darboux formula from the preceding problem, and use it to show that the orthogonality and completeness relations for the eigenvectors can be written as

$$\sum_{n=0}^{N-1} P_n(x_\nu) P_n(x_\mu) = w_\nu^{-1} \delta_{\nu\mu},$$

$$\sum_{\nu=1}^N w_\nu P_n(x_\nu) P_m(x_\nu) = \delta_{nm}, \quad n, m \leq N-1,$$

where $w_\nu^{-1} = b_{N-1} P'_N(x_\nu) P_{N-1}(x_\nu)$.

- c) Use the original Christoffel-Darboux formula to show that, when the $P_n(x)$ are orthonormal with respect to the positive weight function $w(x)$, the normalization constants w_ν of this present problem coincide with the weights w_ν occurring in the Gauss quadrature rule. Conclude from this equality that the Gauss-quadrature weights are *positive*.

Exercise 2.15: Write the N -by- N tridiagonal matrix eigenvalue problem from the preceding exercise as $\mathbf{H}\mathbf{u} = x\mathbf{u}$, and set $d_N(x) = \det(x\mathbf{I} - \mathbf{H})$. Similarly define $d_n(x)$ to be the determinant of the n -by- n tridiagonal submatrix with $x - a_{n-1}, \dots, x - a_0$ along its principal diagonal. Laplace-develop the determinant $d_n(x)$ about its first row, and hence obtain the recurrence

$$d_{n+1}(x) = (x - a_n)d_n(x) - b_{n-1}^2 d_{n-1}(x).$$

Conclude that

$$\det(x\mathbf{I} - \mathbf{H}) = p_N(x),$$

where $p_n(x)$ is the monic orthogonal polynomial obeying

$$xp_n(x) = p_{n+1}(x) + a_n p_n(x) + b_{n-1}^2 p_{n-1}(x); \quad p_{-1}(x) = 0, \quad p_0(x) = 1.$$

Exercise 2.16: Again write the N -by- N tridiagonal matrix eigenvalue problem from the preceding exercises as $\mathbf{H}\mathbf{u} = x\mathbf{u}$.

- a) Show that the lowest and rightmost matrix element

$$\langle 0 | (x\mathbf{I} - \mathbf{H})^{-1} | 0 \rangle \equiv (x\mathbf{I} - \mathbf{H})_{00}^{-1}$$

of the *resolvent matrix* $(x\mathbf{I} - \mathbf{H})^{-1}$ is given by a continued fraction $G_{N-1,0}(x)$ where, for example,

$$G_{3,z}(x) = \frac{1}{x - a_0 - \frac{b_0^2}{x - a_1 - \frac{b_1^2}{x - a_2 - \frac{b_2^2}{x - a_3 + z}}}}.$$

b) Use induction on n to show that

$$G_{n,z}(x) = \frac{q_n(x)z + q_{n+1}(x)}{p_n(x)z + p_{n+1}(x)},$$

where $p_n(x)$, $q_n(x)$ are the monic polynomial functions of x defined by the recurrence relations

$$\begin{aligned} xp_n(x) &= p_{n+1}(x) + a_n p_n(x) + b_{n-1}^2 p_{n-1}(x), & p_{-1}(x) &= 0, & p_0(x) &= 1, \\ xq_n(x) &= q_{n+1}(x) + a_n q_n(x) + b_{n-1}^2 q_{n-1}(x), & q_0(x) &= 0, & q_1(x) &= 1. \end{aligned}$$

b) Conclude that

$$\langle 0 | (x\mathbf{I} - \mathbf{H})^{-1} | 0 \rangle = \frac{q_N(x)}{p_N(x)},$$

has a *pole* singularity when x approaches an eigenvalue x_ν . Show that the *residue* of the pole (the coefficient of $1/(x - x_\nu)$) is equal to the Gauss-quadrature weight w_ν for $w(x)$, the weight function (normalized so that $\int w dx = 1$) from which the coefficients a_n , b_n were derived.

Continued fractions were introduced by John Wallis in his *Arithmetica Infinitorum* (1656), as was the recursion formula for their evaluation. Today, when combined with the output of the next exercise, they provide the mathematical underpinning of the *Haydock recursion method* in the band theory of solids. Haydock's method computes $w(x) = \lim_{N \rightarrow \infty} \{\sum_\nu \delta(x - x_\nu) w_\nu\}$, and interprets it as the local density of states that is measured in scanning tunnelling microscopy.

Exercise 2.17: The Lanczos tridiagonalization algorithm. Let V be an N -dimensional complex vector space equipped with an inner product $\langle \cdot, \cdot \rangle$ and let $H : V \rightarrow V$ be a hermitian linear operator. Starting from a unit vector \mathbf{u}_0 , and taking $\mathbf{u}_{-1} = \mathbf{0}$, recursively generate the unit vectors \mathbf{u}_n and the numbers a_n , b_n and c_n by

$$H\mathbf{u}_n = b_n \mathbf{u}_{n+1} + a_n \mathbf{u}_n + c_{n-1} \mathbf{u}_{n-1},$$

where the coefficients

$$\begin{aligned} a_n &\equiv \langle \mathbf{u}_n, H\mathbf{u}_n \rangle, \\ c_{n-1} &\equiv \langle \mathbf{u}_{n-1}, H\mathbf{u}_n \rangle, \end{aligned}$$

ensure that \mathbf{u}_{n+1} is perpendicular to both \mathbf{u}_n and \mathbf{u}_{n-1} , and

$$b_n = \|H\mathbf{u}_n - a_n\mathbf{u}_n - c_{n-1}\mathbf{u}_{n-1}\|,$$

a positive real number, makes $\|\mathbf{u}_{n+1}\| = 1$.

- a) Use induction on n to show that \mathbf{u}_{n+1} , although only constructed to be perpendicular to the previous *two* vectors, is in fact (and in the absence of numerical rounding errors) perpendicular to *all* \mathbf{u}_m with $m < n$.
- b) Show that a_n, c_n are *real*, and that $c_{n-1} = b_{n-1}$.
- c) Conclude that $b_{N-1} = 0$, and (provided that no earlier b_n happens to vanish) that the \mathbf{u}_n , $n = 0, \dots, N-1$, constitute an orthonormal basis for V , in terms of which H is represented by the N -by- N real-symmetric tridiagonal matrix \mathbf{H} of the preceding exercises.

Because the eigenvalues of a tridiagonal matrix are given by the numerically easy-to-find zeros of the associated monic polynomial $p_N(x)$, the Lanczos algorithm provides a computationally efficient way of extracting the eigenvalues from a large sparse matrix. In theory, the entries in the tridiagonal \mathbf{H} can be computed while retaining only \mathbf{u}_n , \mathbf{u}_{n-1} and $H\mathbf{u}_n$ in memory at any one time. In practice, with finite precision computer arithmetic, orthogonality with the earlier \mathbf{u}_m is eventually lost, and spurious or duplicated eigenvalues appear. There exist, however, strategies for identifying and eliminating these fake eigenvalues.

The following two problems are “toy” versions of the *Lax pair* and *tau function* constructions that arise in the general theory of soliton equations. They provide useful practice in manipulating matrices and determinants.

Exercise 2.18: The monic orthogonal polynomials $p_i(x)$ have inner products

$$\langle p_i, p_j \rangle_w \equiv \int p_i(x) p_j(x) w(x) dx = h_i \delta_{ij},$$

and obey the recursion relation

$$xp_i(x) = p_{i+1}(x) + a_i p_i(x) + b_{i-1}^2 p_{i-1}(x); \quad p_{-1}(x) = 0, p_0(x) = 1.$$

Write the recursion relation as

$$\mathbf{L}\mathbf{p} = x\mathbf{p},$$

where

$$\mathbf{L} \equiv \begin{bmatrix} \ddots & \ddots & \ddots & \ddots & \vdots \\ \dots & 1 & a_2 & b_1^2 & 0 \\ \dots & 0 & 1 & a_1 & b_0^2 \\ \dots & 0 & 0 & 1 & a_0 \end{bmatrix}, \quad \mathbf{p} \equiv \begin{bmatrix} \vdots \\ p_2 \\ p_1 \\ p_0 \end{bmatrix}.$$

Suppose that

$$w(x) = \exp \left\{ - \sum_{n=1}^{\infty} t_n x^n \right\},$$

and consider how the $p_i(x)$ and the coefficients a_i and b_i^2 vary with the parameters t_n .

a) Show that

$$\frac{\partial \mathbf{p}}{\partial t_n} = \mathbf{M}^{(n)} \mathbf{p},$$

where $\mathbf{M}^{(n)}$ is some strictly upper triangular matrix - *i.e.* all entries on and below its principal diagonal are zero.

b) By differentiating $\mathbf{L}\mathbf{p} = x\mathbf{p}$ with respect to t_n show that

$$\frac{\partial \mathbf{L}}{\partial t_n} = [\mathbf{M}^{(n)}, \mathbf{L}].$$

c) Compute the matrix elements

$$\langle i | \mathbf{M}^{(n)} | j \rangle \equiv M_{ij}^{(n)} = \left\langle p_j, \frac{\partial p_i}{\partial t_n} \right\rangle_w$$

(note the interchange of the order of i and j in the $\langle \ , \ \rangle_w$ product!) by differentiating the orthogonality condition $\langle p_i, p_j \rangle_w = h_i \delta_{ij}$. Hence show that

$$\mathbf{M}^{(n)} = (\mathbf{L}^n)_+$$

where $(\mathbf{L}^n)_+$ denotes the strictly upper triangular projection of the n 'th power of \mathbf{L} — *i.e.* the matrix \mathbf{L}^n , but with its diagonal and lower triangular entries replaced by zero.

Thus

$$\frac{\partial \mathbf{L}}{\partial t_n} = [(\mathbf{L}^n)_+, \mathbf{L}]$$

describes a family of deformations of the semi-infinite matrix \mathbf{L} that, in some formal sense, preserve its eigenvalues x .

Exercise 2.19: Let the monic polynomials $p_n(x)$ be orthogonal with respect to the weight function

$$w(x) = \exp \left\{ - \sum_{n=1}^{\infty} t_n x^n \right\}.$$

Define the “tau-function” $\tau_n(t_1, t_2, t_3 \dots)$ of the parameters t_i to be the n -fold integral

$$\tau_n(t_1, t_2, \dots) = \iint \cdots \int dx_1 dx_2 \dots dx_n \Delta^2(x) \exp \left\{ - \sum_{\nu=1}^n \sum_{m=1}^{\infty} t_m x_{\nu}^m \right\}$$

where

$$\Delta(x) = \begin{vmatrix} x_1^{n-1} & x_1^{n-2} & \cdots & x_1 & 1 \\ x_2^{n-1} & x_2^{n-2} & \cdots & x_2 & 1 \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ x_n^{n-1} & x_n^{n-2} & \cdots & x_n & 1 \end{vmatrix} = \prod_{\nu < \mu} (x_{\nu} - x_{\mu})$$

is the n -by- n Vandermonde determinant.

a) Show that

$$\begin{vmatrix} x_1^{n-1} & x_1^{n-2} & \cdots & x_1 & 1 \\ x_2^{n-1} & x_2^{n-2} & \cdots & x_2 & 1 \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ x_n^{n-1} & x_n^{n-2} & \cdots & x_n & 1 \end{vmatrix} = \begin{vmatrix} p_{n-1}(x_1) & p_{n-2}(x_1) & \cdots & p_1(x_1) & p_0(x_1) \\ p_{n-1}(x_2) & p_{n-2}(x_2) & \cdots & p_1(x_2) & p_0(x_2) \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ p_{n-1}(x_n) & p_{n-2}(x_n) & \cdots & p_1(x_n) & p_0(x_n) \end{vmatrix}$$

b) Combine the identity from part a) with the orthogonality property of the $p_n(x)$ to show that

$$\begin{aligned} p_n(x) &= \frac{1}{\tau_n} \int dx_1 dx_2 \dots dx_n \Delta^2(x) \prod_{\mu=1}^n (x - x_{\mu}) \exp \left\{ - \sum_{\nu=1}^n \sum_{m=1}^{\infty} t_m x_{\nu}^m \right\} \\ &= x^n \frac{\tau_n(t'_1, t'_2, t'_3, \dots)}{\tau_n(t_1, t_2, t_3, \dots)} \end{aligned}$$

where

$$t'_m = t_m + \frac{1}{m x^m}.$$

Here are some problems on distributions:

Exercise 2.20: Let $f(x)$ be a continuous function. Observe that $f(x)\delta(x) = f(0)\delta(x)$. Deduce that

$$\frac{d}{dx}[f(x)\delta(x)] = f(0)\delta'(x).$$

If $f(x)$ were differentiable we might also have used the product rule to conclude that

$$\frac{d}{dx}[f(x)\delta(x)] = f'(x)\delta(x) + f(x)\delta'(x).$$

Show, by evaluating $f(0)\delta'(x)$ and $f'(x)\delta(x) + f(x)\delta'(x)$ on a test function $\varphi(x)$, that these two expressions for the derivative of $f(x)\delta(x)$ are equivalent.

Exercise 2.21: Let $\varphi(x)$ be a test function. Show that

$$\frac{d}{dt} \left\{ P \int_{-\infty}^{\infty} \frac{\varphi(x)}{(x-t)} dx \right\} = P \int_{-\infty}^{\infty} \frac{\varphi(x) - \varphi(t)}{(x-t)^2} dx.$$

Show further that the right-hand-side of this equation is equal to

$$- \left(\frac{d}{dx} P \left(\frac{1}{x-t} \right), \varphi \right) \equiv P \int_{-\infty}^{\infty} \frac{\varphi'(x)}{(x-t)} dx.$$

Exercise 2.22: Let $\theta(x)$ be the *step function* or *Heaviside distribution*

$$\theta(x) = \begin{cases} 1, & x > 0, \\ \text{undefined}, & x = 0, \\ 0, & x < 0. \end{cases}$$

By forming the weak derivative of both sides of the equation

$$\lim_{\varepsilon \rightarrow 0} \ln(x + i\varepsilon) = \ln|x| + i\pi\theta(-x),$$

show that

$$\lim_{\varepsilon \rightarrow 0} \left(\frac{1}{x + i\varepsilon} \right) = P \left(\frac{1}{x} \right) - i\pi\delta(x).$$

Exercise 2.23: Use induction on n to generalize exercise 2.21 and show that

$$\begin{aligned} \frac{d^n}{dt^n} \left\{ P \int_{-\infty}^{\infty} \frac{\varphi(x)}{(x-t)} dx \right\} &= P \int_{-\infty}^{\infty} \frac{n!}{(x-t)^{n+1}} \left[\varphi(x) - \sum_{m=0}^{n-1} \frac{1}{m!} (x-t)^m \varphi^{(m)}(t) \right] dx, \\ &= P \int_{-\infty}^{\infty} \frac{\varphi^{(n)}(x)}{x-t} dx. \end{aligned}$$

Exercise 2.24: Let the non-local functional $S[f]$ be defined by

$$S[f] = \frac{1}{4\pi} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \left\{ \frac{f(x) - f(x')}{x - x'} \right\}^2 dx dx'$$

Compute the functional derivative of $S[f]$ and verify that it is given by

$$\frac{\delta S}{\delta f(x)} = \frac{1}{\pi} \frac{d}{dx} \left\{ P \int_{-\infty}^{\infty} \frac{f(x')}{x - x'} dx' \right\}.$$

See exercise 6.8 for an occurrence of this functional.

Chapter 3

Linear Ordinary Differential Equations

In this chapter we will discuss linear ordinary differential equations. We will not describe tricks for solving any particular equation, but instead focus on those aspects the general theory that we will need later.

We will consider either *homogeneous equations*, $Ly = 0$ with

$$Ly \equiv p_0(x)y^{(n)} + p_1(x)y^{(n-1)} + \cdots + p_n(x)y, \quad (3.1)$$

or *inhomogeneous equations* $Ly = f$. In full,

$$p_0(x)y^{(n)} + p_1(x)y^{(n-1)} + \cdots + p_n(x)y = f(x). \quad (3.2)$$

We will begin with homogeneous equations.

3.1 Existence and Uniqueness of Solutions

The fundamental result in the theory of differential equations is the existence and uniqueness theorem for systems of first order equations.

3.1.1 Flows for first-order equations

Let x^1, \dots, x^n , be a system of coordinates in \mathbb{R}^n , and let $X^i(x^1, x^2, \dots, x^n, t)$, $i = 1, \dots, n$, be the components of a t -dependent vector field. Consider the

system of first-order differential equations

$$\begin{aligned}\frac{dx^1}{dt} &= X^1(x^1, x^2, \dots, x^n, t), \\ \frac{dx^2}{dt} &= X^2(x^1, x^2, \dots, x^n, t), \\ &\vdots \\ \frac{dx^n}{dt} &= X^n(x^1, x^2, \dots, x^n, t).\end{aligned}\tag{3.3}$$

For a sufficiently smooth vector field (X^1, X^2, \dots, X^n) there is a unique solution $x^i(t)$ for any initial condition $x^i(0) = x_0^i$. Rigorous proofs of this claim, including a statement of exactly what “sufficiently smooth” means, can be found in any standard book on differential equations. Here, we will simply assume the result. It is of course “physically” plausible. Regard the X^i as being the components of the velocity field in a fluid flow, and the solution $x^i(t)$ as the trajectory of a particle carried by the flow. An particle initially at $x^i(0) = x_0^i$ certainly goes somewhere, and unless something seriously pathological is happening, that “somewhere” will be unique.

Now introduce a single function $y(t)$, and set

$$\begin{aligned}x^1 &= y, \\ x^2 &= \dot{y}, \\ x^3 &= \ddot{y}, \\ &\vdots \\ x^n &= y^{(n-1)},\end{aligned}\tag{3.4}$$

and, given smooth functions $p_0(t), \dots, p_n(t)$ with $p_0(t)$ nowhere vanishing, look at the particular system of equations

$$\begin{aligned}\frac{dx^1}{dt} &= x^2, \\ \frac{dx^2}{dt} &= x^3, \\ &\vdots \\ \frac{dx^{n-1}}{dt} &= x^n, \\ \frac{dx^n}{dt} &= -\frac{1}{p_0} (p_1 x^n + p_2 x^{n-1} + \dots + p_n x^1).\end{aligned}\tag{3.5}$$

This system is equivalent to the single equation

$$p_0(t) \frac{d^n y}{dt^n} + p_1(t) \frac{d^{n-1} y}{dt^{n-1}} + \cdots + p_{n-1}(t) \frac{dy}{dt} + p_n(t) y(t) = 0. \quad (3.6)$$

Thus an n -th order ordinary differential equation (ODE) can be written as a first-order equation in n dimensions, and we can exploit the uniqueness result cited above. We conclude, provided p_0 never vanishes, that the differential equation $Ly = 0$ has a unique solution, $y(t)$, for each set of initial data $(y(0), \dot{y}(0), \ddot{y}(0), \dots, y^{(n-1)}(0))$. Thus,

- i) If $Ly = 0$ and $y(0) = 0, \dot{y}(0) = 0, \ddot{y}(0) = 0, \dots, y^{(n-1)}(0) = 0$, we deduce that $y \equiv 0$.
- ii) If $y_1(t)$ and $y_2(t)$ obey the same equation $Ly = 0$, and have the same initial data, then $y_1(t) = y_2(t)$.

3.1.2 Linear independence

In this section we will assume that p_0 does not vanish in the region of x we are interested in, and that all the p_i remain finite and differentiable sufficiently many times for our formulæ to make sense.

Consider an n -th order linear differential equation

$$p_0(x)y^{(n)} + p_1(x)y^{(n-1)} + \cdots + p_n(x)y = 0. \quad (3.7)$$

The set of solutions of this equation constitutes a *vector space* because if $y_1(x)$ and $y_2(x)$ are solutions, then so is any linear combination $\lambda y_1(x) + \mu y_2(x)$. We will show that the dimension of this vector space is n . To see that this is so, let $y_1(x)$ be a solution with initial data

$$\begin{aligned} y_1(0) &= 1, \\ y_1'(0) &= 0, \\ &\vdots \\ y_1^{(n-1)}(0) &= 0, \end{aligned} \quad (3.8)$$

let $y_2(x)$ be a solution with

$$\begin{aligned} y_2(0) &= 0, \\ y_2'(0) &= 1, \\ &\vdots \\ y_2^{(n-1)}(0) &= 0, \end{aligned} \quad (3.9)$$

and so on, up to $y_n(x)$, which has

$$\begin{aligned} y_n(0) &= 0, \\ y'_n(0) &= 0, \\ &\vdots \\ y_n^{(n-1)}(0) &= 1. \end{aligned} \tag{3.10}$$

We claim that the functions $y_i(x)$ are *linearly independent*. Suppose, to the contrary, that there are constants $\lambda_1, \dots, \lambda_n$ such that

$$0 = \lambda_1 y_1(x) + \lambda_2 y_2(x) + \dots + \lambda_n y_n(x). \tag{3.11}$$

Then

$$0 = \lambda_1 y_1(0) + \lambda_2 y_2(0) + \dots + \lambda_n y_n(0) \Rightarrow \lambda_1 = 0. \tag{3.12}$$

Differentiating once and setting $x = 0$ gives

$$0 = \lambda_1 y'_1(0) + \lambda_2 y'_2(0) + \dots + \lambda_n y'_n(0) \Rightarrow \lambda_2 = 0. \tag{3.13}$$

We continue in this manner all the way to

$$0 = \lambda_1 y_1^{(n-1)}(0) + \lambda_2 y_2^{(n-1)}(0) + \dots + \lambda_n y_n^{(n-1)}(0) \Rightarrow \lambda_n = 0. \tag{3.14}$$

All the λ_i are zero! There is therefore no non-trivial linear relation between the $y_i(x)$, and they are indeed linearly independent.

The solutions $y_i(x)$ also *span* the solution space, because the unique solution with initial data $y(0) = a_1$, $y'(0) = a_2$, \dots , $y^{(n-1)}(0) = a_n$ can be written in terms of them as

$$y(x) = a_1 y_1(x) + a_2 y_2(x) + \dots + a_n y_n(x). \tag{3.15}$$

Our chosen set of n solutions is therefore a *basis* for the solution space of the differential equation. The dimension of the solution space is therefore n , as claimed.

3.1.3 The Wronskian

If we manage to find a different set of n solutions, how will we know whether they are also linearly independent? The essential tool is the *Wronskian*:

$$W(y_1, \dots, y_n; x) \stackrel{\text{def}}{=} \begin{vmatrix} y_1 & y_2 & \dots & y_n \\ y'_1 & y'_2 & \dots & y'_n \\ \vdots & \vdots & \ddots & \vdots \\ y_1^{(n-1)} & y_2^{(n-1)} & \dots & y_n^{(n-1)} \end{vmatrix}. \tag{3.16}$$

Recall that the derivative of a determinant

$$D = \begin{vmatrix} a_{11} & a_{12} & \cdots & a_{1n} \\ a_{21} & a_{22} & \cdots & a_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ a_{n1} & a_{n2} & \cdots & a_{nn} \end{vmatrix} \quad (3.17)$$

may be evaluated by differentiating row-by-row:

$$\frac{dD}{dx} = \begin{vmatrix} a'_{11} & a'_{12} & \cdots & a'_{1n} \\ a_{21} & a_{22} & \cdots & a_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ a_{n1} & a_{n2} & \cdots & a_{nn} \end{vmatrix} + \begin{vmatrix} a_{11} & a_{12} & \cdots & a_{1n} \\ a'_{21} & a'_{22} & \cdots & a'_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ a_{n1} & a_{n2} & \cdots & a_{nn} \end{vmatrix} + \cdots + \begin{vmatrix} a_{11} & a_{12} & \cdots & a_{1n} \\ a_{21} & a_{22} & \cdots & a_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ a'_{n1} & a'_{n2} & \cdots & a'_{nn} \end{vmatrix}.$$

Applying this to the derivative of the Wronskian, we find

$$\frac{dW}{dx} = \begin{vmatrix} y_1 & y_2 & \cdots & y_n \\ y'_1 & y'_2 & \cdots & y'_n \\ \vdots & \vdots & \ddots & \vdots \\ y_1^{(n)} & y_2^{(n)} & \cdots & y_n^{(n)} \end{vmatrix}. \quad (3.18)$$

Only the term where the very last row is being differentiated survives. All the other row derivatives gives zero because they lead to a determinant with two identical rows. Now, if the y_i are all solutions of

$$p_0 y^{(n)} + p_1 y^{(n-1)} + \cdots + p_n y = 0, \quad (3.19)$$

we can substitute

$$y_i^{(n)} = -\frac{1}{p_0} \left(p_1 y_i^{(n-1)} + p_2 y_i^{(n-2)} + \cdots + p_n y_i \right), \quad (3.20)$$

use the row-by-row linearity of determinants,

$$\begin{vmatrix} \lambda a_{11} + \mu b_{11} & \lambda a_{12} + \mu b_{12} & \cdots & \lambda a_{1n} + \mu b_{1n} \\ c_{21} & c_{22} & \cdots & c_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ c_{n1} & c_{n2} & \cdots & c_{nn} \end{vmatrix} = \lambda \begin{vmatrix} a_{11} & a_{12} & \cdots & a_{1n} \\ c_{21} & c_{22} & \cdots & c_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ c_{n1} & c_{n2} & \cdots & c_{nn} \end{vmatrix} + \mu \begin{vmatrix} b_{11} & b_{12} & \cdots & b_{1n} \\ c_{21} & c_{22} & \cdots & c_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ c_{n1} & c_{n2} & \cdots & c_{nn} \end{vmatrix}, \quad (3.21)$$

and find, again because most terms have two identical rows, that only the terms with p_1 survive. The end result is

$$\frac{dW}{dx} = - \left(\frac{p_1}{p_0} \right) W. \quad (3.22)$$

Solving this first order equation gives

$$W(y_i; x) = W(y_i; x_0) \exp \left\{ - \int_{x_0}^x \left(\frac{p_1(\xi)}{p_0(\xi)} \right) d\xi \right\}. \quad (3.23)$$

Since the exponential function itself never vanishes, $W(x)$ either vanishes at all x , or never. This is *Liouville's theorem*, and (3.23) is called *Liouville's formula*.

Now suppose that y_1, \dots, y_n are a set of C^n functions of x , not necessarily solutions of an ODE. Suppose further that there are constants λ_i , not all zero, such that

$$\lambda_1 y_1(x) + \lambda_2 y_2(x) + \dots + \lambda_n y_n(x) \equiv 0, \quad (3.24)$$

(i.e. the functions are linearly dependent) then the set of equations

$$\begin{aligned} \lambda_1 y_1(x) + \lambda_2 y_2(x) + \dots + \lambda_n y_n(x) &= 0, \\ \lambda_1 y_1'(x) + \lambda_2 y_2'(x) + \dots + \lambda_n y_n'(x) &= 0, \\ &\vdots \\ \lambda_1 y_1^{(n-1)}(x) + \lambda_2 y_2^{(n-1)}(x) + \dots + \lambda_n y_n^{(n-1)}(x) &= 0, \end{aligned} \quad (3.25)$$

has a non-trivial solution $\lambda_1, \lambda_2, \dots, \lambda_n$, and so the determinant of the coefficients,

$$W = \begin{vmatrix} y_1 & y_2 & \dots & y_n \\ y_1' & y_2' & \dots & y_n' \\ \vdots & \vdots & \ddots & \vdots \\ y_1^{(n-1)} & y_2^{(n-1)} & \dots & y_n^{(n-1)} \end{vmatrix}, \quad (3.26)$$

must vanish. Thus

linear dependence $\Rightarrow W \equiv 0$.

There is a partial converse of this result: Suppose that y_1, \dots, y_n are solutions to an n -th order ODE and $W(y_i; x) = 0$ at $x = x_0$. Then there must exist a set of λ_i , not all zero, such that

$$Y(x) = \lambda_1 y_1(x) + \lambda_2 y_2(x) + \dots + \lambda_n y_n(x) \quad (3.27)$$

has $0 = Y(x_0) = Y'(x_0) = \dots = Y^{(n-1)}(x_0)$. This is because the system of linear equations determining the λ_i has the Wronskian as its determinant. Now the function $Y(x)$ is a solution of the ODE and has vanishing initial data. It is therefore identically zero. We conclude that

$$\boxed{\text{ODE and } W = 0 \Rightarrow \text{linear dependence.}}$$

If there is no OED, the Wronskian may vanish without the functions being linearly dependent. As an example, consider

$$\begin{aligned} y_1(x) &= \begin{cases} 0, & x \leq 0, \\ \exp\{-1/x^2\}, & x > 0. \end{cases} \\ y_2(x) &= \begin{cases} \exp\{-1/x^2\}, & x \leq 0, \\ 0, & x > 0. \end{cases} \end{aligned} \quad (3.28)$$

We have $W(y_1, y_2; x) \equiv 0$, but y_1, y_2 are not proportional to one another, and so not linearly dependent. (Note $y_{1,2}$ are smooth functions. In particular they have derivatives of all orders at $x = 0$.)

Given n linearly independent smooth functions y_i , can we always find an n -th order differential equation that has them as its solutions? The answer had better be “no”, or there would be a contradiction between the preceding theorem and the counterexample to its extension. If the functions *do* satisfy a common equation, however, we can use a Wronskian to construct it: Let

$$Ly = p_0(x)y^{(n)} + p_1(x)y^{(n-1)} + \dots + p_n(x)y \quad (3.29)$$

be the differential polynomial in $y(x)$ that results from expanding

$$D(y) = \begin{vmatrix} y^{(n)} & y^{(n-1)} & \dots & y \\ y_1^{(n)} & y_1^{(n-1)} & \dots & y_1 \\ \vdots & \vdots & \ddots & \vdots \\ y_n^{(n)} & y_n^{(n-1)} & \dots & y_n \end{vmatrix}. \quad (3.30)$$

Whenever y coincides with any of the y_i , the determinant will have two identical rows, and so $Ly = 0$. The y_i are indeed n solutions of $Ly = 0$. As we have noted, this construction cannot always work. To see what can go wrong, observe that it gives

$$p_0(x) = \begin{vmatrix} y_1^{(n-1)} & y_1^{(n-2)} & \dots & y_1 \\ y_2^{(n-1)} & y_2^{(n-2)} & \dots & y_2 \\ \vdots & \vdots & \ddots & \vdots \\ y_n^{(n-1)} & y_n^{(n-2)} & \dots & y_n \end{vmatrix} = W(y; x). \quad (3.31)$$

If this Wronskian is zero, then our construction fails to deliver an n -th order equation. Indeed, taking y_1 and y_2 to be the functions in the example above yields an equation in which all three coefficients p_0 , p_1 , p_2 are identically zero.

3.2 Normal Form

In elementary algebra a polynomial equation

$$a_0x^n + a_1x^{n-1} + \cdots + a_n = 0, \quad (3.32)$$

with $a_0 \neq 0$, is said to be in *normal form* if $a_1 = 0$. We can always put such an equation in normal form by defining a new variable \tilde{x} with $x = \tilde{x} - a_1(a_0)^{-1}$.

By analogy, an n -th order linear ODE with no $y^{(n-1)}$ term is also said to be in normal form. We can put an ODE in normal form by the substitution $y = w\tilde{y}$, for a suitable function $w(x)$. Let

$$p_0y^{(n)} + p_1y^{(n-1)} + \cdots + p_ny = 0. \quad (3.33)$$

Set $y = w\tilde{y}$. Using Leibniz' rule, we expand out

$$(w\tilde{y})^{(n)} = w\tilde{y}^{(n)} + nw'\tilde{y}^{(n-1)} + \frac{n(n-1)}{2!}w''\tilde{y}^{(n-2)} + \cdots + w^{(n)}\tilde{y}. \quad (3.34)$$

The differential equation becomes, therefore,

$$(wp_0)\tilde{y}^{(n)} + (p_1w + p_0nw')\tilde{y}^{(n-1)} + \cdots = 0. \quad (3.35)$$

We see that if we chose w to be a solution of

$$p_1w + p_0nw' = 0, \quad (3.36)$$

for example

$$w(x) = \exp \left\{ -\frac{1}{n} \int_0^x \left(\frac{p_1(\xi)}{p_0(\xi)} \right) d\xi \right\}, \quad (3.37)$$

then \tilde{y} obeys the equation

$$(wp_0)\tilde{y}^{(n)} + \tilde{p}_2\tilde{y}^{(n-2)} + \cdots = 0, \quad (3.38)$$

with no second-highest derivative.

Example: For a second order equation,

$$y'' + p_1 y' + p_2 y = 0, \quad (3.39)$$

we set $y(x) = v(x) \exp\{-\frac{1}{2} \int_0^x p_1(\xi) d\xi\}$ and find that v obeys

$$v'' + \Omega v = 0, \quad (3.40)$$

where

$$\Omega = p_2 - \frac{1}{2} p_1' - \frac{1}{4} p_1^2. \quad (3.41)$$

Reducing an equation to normal form gives us the best chance of solving it by inspection. For physicists, another advantage is that a second-order equation in normal form can be thought of as a Schrödinger equation,

$$-\frac{d^2 \psi}{dx^2} + (V(x) - E)\psi = 0, \quad (3.42)$$

and we can gain insight into the properties of the solution by bringing our physics intuition and experience to bear.

3.3 Inhomogeneous Equations

A linear *inhomogeneous* equation is one with a source term:

$$p_0(x)y^{(n)} + p_1(x)y^{(n-1)} + \cdots + p_n(x)y = f(x). \quad (3.43)$$

It is called “inhomogeneous” because the source term $f(x)$ does not contain y , and so is different from the rest. We will devote an entire chapter to the solution of such equations by the method of Green functions. Here, we simply review some elementary material.

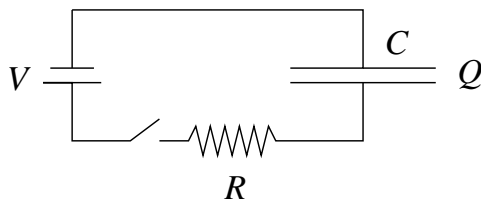
3.3.1 Particular integral and complementary function

One method of dealing with inhomogeneous problems, one that is especially effective when the equation has constant coefficients, is simply to try and guess a solution to (3.43). If you are successful, the guessed solution y_{PI} is then called a *particular integral*. We may add any solution y_{CF} of the homogeneous equation

$$p_0(x)y^{(n)} + p_1(x)y^{(n-1)} + \cdots + p_n(x)y = 0 \quad (3.44)$$

to y_{PI} and it will still be a solution of the inhomogeneous problem. We use this freedom to satisfy the boundary or initial conditions. The added solution, y_{CF} , is called the *complementary function*.

Example: Charging capacitor. The capacitor is initially uncharged, and the switch is closed at $t = 0$



The charge on the capacitor, Q , obeys

$$R \frac{dQ}{dt} + \frac{Q}{C} = V, \quad (3.45)$$

where R , C , V are constants. A particular integral is given by $Q(t) = CV$. The complementary-function solution of the homogeneous problem is

$$Q(t) = Q_0 e^{-t/RC}, \quad (3.46)$$

where Q_0 is constant. The solution satisfying the initial conditions is

$$Q(t) = CV (1 - e^{-t/RC}). \quad (3.47)$$

3.3.2 Variation of parameters

We now follow Lagrange, and solve

$$p_0(x)y^{(n)} + p_1(x)y^{(n-1)} + \cdots + p_n(x)y = f(x) \quad (3.48)$$

by writing

$$y = v_1 y_1 + v_2 y_2 + \cdots + v_n y_n \quad (3.49)$$

where the y_i are the n linearly independent solutions of the homogeneous equation and the v_i are functions of x that we have to determine. This method is called *variation of parameters*.

Now, differentiating gives

$$y' = v_1 y_1' + v_2 y_2' + \cdots + v_n y_n' + \{v_1' y_1 + v_2' y_2 + \cdots + v_n' y_n\}. \quad (3.50)$$

We will chose the v 's so as to make the terms in the braces vanish. Differentiate again:

$$y'' = v_1 y_1'' + v_2 y_2'' + \cdots + v_n y_n'' + \{v_1' y_1' + v_2' y_2' + \cdots + v_n' y_n'\}. \quad (3.51)$$

Again, we will chose the v 's to make the terms in the braces vanish. We proceed in this way until the very last step, at which we demand

$$\{v_1' y_1^{(n-1)} + v_2' y_2^{(n-1)} + \cdots + v_n' y_n^{(n-1)}\} = f(x)/p_0(x). \quad (3.52)$$

If you substitute the resulting y into the differential equation, you will see that the equation is satisfied.

We have imposed the following conditions on v_i' :

$$\begin{aligned} v_1' y_1 + v_2' y_2 + \cdots + v_n' y_n &= 0, \\ v_1' y_1' + v_2' y_2' + \cdots + v_n' y_n' &= 0, \\ &\vdots \\ v_1' y_1^{(n-1)} + v_2' y_2^{(n-1)} + \cdots + v_n' y_n^{(n-1)} &= f(x)/p_0(x). \end{aligned} \quad (3.53)$$

This system of linear equations will have a solution for v_1', \dots, v_n' , provided the Wronskian of the y_i is non-zero. This, however, is guaranteed by the assumed linear independence of the y_i . Having found the v_1', \dots, v_n' , we obtain the v_1, \dots, v_n themselves by a single integration.

Example: First-order linear equation. A simple and useful application of this method solves

$$\frac{dy}{dx} + P(x)y = f(x). \quad (3.54)$$

The solution to the homogeneous equation is

$$y_1 = e^{-\int_a^x P(s) ds}. \quad (3.55)$$

We therefore set

$$y = v(x) e^{-\int_a^x P(s) ds}, \quad (3.56)$$

and find that

$$v'(x) e^{-\int_a^x P(s) ds} = f(x). \quad (3.57)$$

We integrate once to find

$$v(x) = \int_b^x f(\xi) e^{\int_a^\xi P(s) ds} d\xi, \quad (3.58)$$

and so

$$y(x) = \int_b^x f(\xi) \left\{ e^{-\int_\xi^x P(s) ds} \right\} d\xi. \quad (3.59)$$

We select b to satisfy the initial condition.

3.4 Singular Points

So far in this chapter, we have been assuming, either explicitly or tacitly, that our coefficients $p_i(x)$ are smooth, and that $p_0(x)$ never vanishes. If $p_0(x)$ does become zero (or, more precisely, if one or more of the p_i/p_0 becomes singular) then bad things happen, and the location of the zero of p_0 is called a *singular point* of the differential equation. All other points are called *ordinary points*.

In physics application we often find singular points at the ends of the interval in which we wish to solve our differential equation. For example, the origin $r = 0$ is often a singular point when r is the radial coordinate in plane or spherical polars. The existence and uniqueness theorems that we have relied out throughout this chapter may fail at singular endpoints. Consider, for example, the equation

$$xy'' + y' = 0, \quad (3.60)$$

which is singular at $x = 0$. The two linearly independent solutions for $x > 0$ are $y_1(x) = 1$ and $y_2(x) = \ln x$. The general solution is therefore $A + B \ln x$, but no choice of A and B can satisfy the initial conditions $y(0) = a$, $y'(0) = b$ when b is non-zero. Because of these complications, we will delay a systematic study of singular endpoints until chapter 8.

3.4.1 Regular singular points

If, in the differential equation

$$p_0 y'' + p_1 y' + p_2 y = 0, \quad (3.61)$$

we have a point $x = a$ such that

$$p_0(x) = (x - a)^2 P(x), \quad p_1(x) = (x - a) Q(x), \quad p_2(x) = R(x), \quad (3.62)$$

where P and Q and R are analytic¹ and P and Q non-zero in a neighbourhood of a then the point $x = a$ is called a *regular singular point* of the equation.

¹A function is *analytic* at a point if it has a power-series expansion that converges to the function in a neighbourhood of the point.

All other singular points are said to be *irregular*. Close to a regular singular point a the equation looks like

$$P(a)(x-a)^2y'' + Q(a)(x-a)y' + R(a)y = 0. \quad (3.63)$$

The solutions of this reduced equation are

$$y_1 = (x-a)^{\lambda_1}, \quad y_2 = (x-a)^{\lambda_2}, \quad (3.64)$$

where $\lambda_{1,2}$ are the roots of the *indicial equation*

$$\lambda(\lambda-1)P(a) + \lambda Q(a) + R(a) = 0. \quad (3.65)$$

The solutions of the full equation are then

$$y_1 = (x-a)^{\lambda_1}f_1(x), \quad y_2 = (x-a)^{\lambda_2}f_2(x), \quad (3.66)$$

where $f_{1,2}$ have power series solutions convergent in a neighbourhood of a . An exception occurs when λ_1 and λ_2 coincide or differ by an integer, in which case the second solution is of the form

$$y_2 = (x-a)^{\lambda_1} \left(\ln(x-a)f_1(x) + f_2(x) \right), \quad (3.67)$$

where f_1 is the same power series that occurs in the first solution, and f_2 is a new power series. You will probably have seen these statements proved by the tedious procedure of setting

$$f_1(x) = (x-a)^\lambda (b_0 + b_1(x-a) + b_2(x-a)^2 + \cdots), \quad (3.68)$$

and obtaining a recurrence relation determining the b_i . Far more insight is obtained, however, by extending the equation and its solution to the complex plane, where the structure of the solution is related to its *monodromy properties*. If you are familiar with complex analytic methods, you might like to look at the discussion of monodromy in later chapters.

3.5 Exercises and Problems

Exercise 3.1: Reduction of Order. Sometimes additional information about the solutions of a differential equation enables us to reduce the order of the equation, and so solve it.

- a) Suppose that we know that $y_1 = u(x)$ is one solution to the equation

$$y'' + V(x)y = 0.$$

By trying $y = u(x)v(x)$ show that

$$y_2 = u(x) \int^x \frac{d\xi}{u^2(\xi)}$$

is also a solution of the differential equation. Is this new solution ever merely a constant multiple of the old solution, or must it be linearly independent? (Hint: evaluate the Wronskian $W(y_2, y_1)$.)

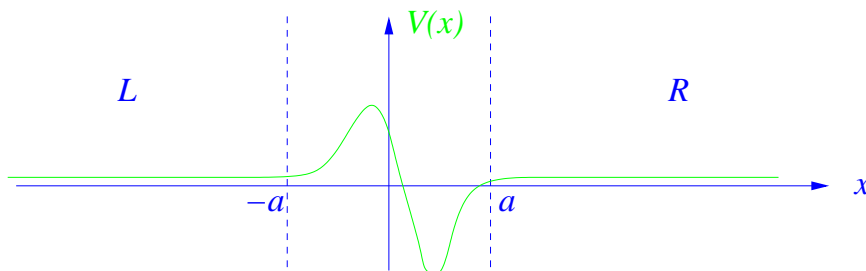
- b) Suppose that we are told that the product, $y_1 y_2$, of the two solutions to the equation $y'' + p_1 y' + p_2 y = 0$ is a constant. Show that this requires $2p_1 p_2 + p_2' = 0$.
- c) By using ideas from part b) or otherwise, find the general solution of the equation

$$(x+1)x^2 y'' + xy' - (x+1)^3 y = 0.$$

Exercise 3.2: One-dimensional scattering theory. Consider the one-dimensional Schrödinger equation

$$-\frac{d^2 \psi}{dx^2} + V(x)\psi = E\psi$$

where $V(x)$ is zero except in a finite interval $[-a, a]$ near the origin.



Let L denote the left asymptotic region, $-\infty < x < -a$, and similarly let R denote $\infty > x > a$. For $E = k^2$ and $k > 0$ there will be scattering solutions of the form

$$\psi_k(x) = \begin{cases} e^{ikx} + r_L(k)e^{-ikx}, & x \in L, \\ t_L(k)e^{ikx}, & x \in R, \end{cases}$$

describing waves incident on the potential $V(x)$ from the left. For $k < 0$ there will be solutions with waves incident from the right

$$\psi_k(x) = \begin{cases} t_R(k)e^{ikx}, & x \in L, \\ e^{ikx} + r_R(k)e^{-ikx}, & x \in R. \end{cases}$$

The wavefunctions in $[-a, a]$ will naturally be more complicated. Observe that $[\psi_k(x)]^*$ is also a solution of the Schrödinger equation.

By using properties of the Wronskian, show that:

- a) $|r_{L,R}|^2 + |t_{L,R}|^2 = 1$,
- b) $t_L(k) = t_R(-k)$.
- c) Deduce from parts a) and b) that $|r_L(k)| = |r_R(-k)|$.
- d) Take the specific example of $V(x) = \lambda\delta(x-b)$ with $|b| < a$. Compute the transmission and reflection coefficients and hence show that $r_L(k)$ and $r_R(-k)$ may differ by a phase.

Exercise 3.3: Suppose $\psi(x)$ obeys a Schrödinger equation

$$\left(-\frac{1}{2}\frac{d^2}{dx^2} + [V(x) - E]\right)\psi = 0.$$

- a) Make a smooth and invertible change of independent variable by setting $x = x(z)$ and find the second order differential equation in z obeyed by $\psi(z) \equiv \psi(x(z))$. Reduce this equation to normal form, and show that the resulting equation is

$$\left(-\frac{1}{2}\frac{d^2}{dz^2} + (x')^2[V(x(z)) - E] - \frac{1}{4}\{x, z\}\right)\tilde{\psi}(z) = 0,$$

where the primes denote differentiation with respect to z , and

$$\{x, z\} \stackrel{\text{def}}{=} \frac{x'''}{x'} - \frac{3}{2}\left(\frac{x''}{x'}\right)^2$$

is called the *Schwarzian* derivative of x with respect to z . Schwarzian derivatives play an important role in conformal field theory and string theory.

- b) Make a sequence of changes of variable $x \rightarrow z \rightarrow w$, and so establish *Cayley's identity*

$$\left(\frac{dz}{dw}\right)^2 \{x, z\} + \{z, w\} = \{x, w\}.$$

(Hint: If your proof takes more than a few lines, you are missing the point of the problem.)

Chapter 4

Linear Differential Operators

In this chapter we will begin to take a more sophisticated approach to differential equations. We will define, with some care, the notion of a linear differential operator, and explore the analogy between such operators and matrices. In particular, we will investigate what is required for a differential operator to have a complete set of eigenfunctions.

4.1 Formal *vs.* Concrete Operators

We will call the object

$$L = p_0(x)\frac{d^n}{dx^n} + p_1(x)\frac{d^{n-1}}{dx^{n-1}} + \cdots + p_n(x), \quad (4.1)$$

which we also write as

$$p_0(x)\partial_x^n + p_1(x)\partial_x^{n-1} + \cdots + p_n(x), \quad (4.2)$$

a *formal linear differential operator*. The word “formal” refers to the fact that we are not yet worrying about what sort of functions the operator is applied to.

4.1.1 The algebra of formal operators

Even though they are not acting on anything in particular, we can still form products of operators. For example if v and w are smooth functions of x we can define the operators $\partial_x + v(x)$ and $\partial_x + w(x)$ and find

$$(\partial_x + v)(\partial_x + w) = \partial_x^2 + w' + (w + v)\partial_x + vw, \quad (4.3)$$

or

$$(\partial_x + w)(\partial_x + v) = \partial_x^2 + v' + (w + v)\partial_x + vw, \quad (4.4)$$

We see from this example that the operator algebra is not usually commutative.

The algebra of formal operators has some deep applications. Consider, for example, the operators

$$L = -\partial_x^2 + q(x) \quad (4.5)$$

and

$$P = \partial_x^3 + a(x)\partial_x + \partial_x a(x). \quad (4.6)$$

In the last expression, the combination $\partial_x a(x)$ means “first multiply by $a(x)$, and then differentiate the result,” so we could also write

$$\partial_x a = a\partial_x + a'. \quad (4.7)$$

We can now form the commutator $[P, L] \equiv PL - LP$. After a little effort, we find

$$[P, L] = (3q' + 4a')\partial_x^2 + (3q'' + 4a'')\partial_x + q''' + 2aq' + a'''. \quad (4.8)$$

If we choose $a = -\frac{3}{4}q$, the commutator becomes a pure multiplication operator, with no differential part:

$$[P, L] = \frac{1}{4}q''' - \frac{3}{2}qq'. \quad (4.9)$$

The equation

$$\frac{dL}{dt} = [P, L], \quad (4.10)$$

or, equivalently,

$$\dot{q} = \frac{1}{4}q''' - \frac{3}{2}qq', \quad (4.11)$$

has a formal solution

$$L(t) = e^{tP}L(0)e^{-tP}, \quad (4.12)$$

showing that the time evolution of L is given by a similarity transformation, which (again formally) does not change its eigenvalues. The partial differential equation (4.11) is the famous Korteweg de Vries (KdV) equation, which has “soliton” solutions whose existence is intimately connected with the fact that it can be written as (4.10). The operators P and L are called a *Lax pair*, after Peter Lax who uncovered much of the structure.

4.1.2 Concrete operators

We want to explore the analogies between linear differential operators and matrices acting on a finite-dimensional vector space. Now the theory of matrix operators makes much use of inner products and orthogonality. Consequently the analogy is closest if we work with a function space equipped with these same notions. We therefore let our differential operators act on $L^2[a, b]$, the Hilbert space of square-integrable functions on $[a, b]$. A differential operator cannot act on all functions in the Hilbert space, however, because not all of them are differentiable. Even when we relax our notion of differentiability and permit weak derivatives, we must at least demand that the *domain* \mathcal{D} , the subset of functions on which we allow the operator to act, contain only functions that are sufficiently differentiable that the function resulting from applying the operator remains an element of $L^2[a, b]$. We will usually restrict the set of functions even further, by imposing boundary conditions at the endpoints of the interval. A *linear differential operator* is now defined as a formal linear differential operator, together with a specification of its domain \mathcal{D} .

The boundary conditions that we will impose will always be *linear* and *homogeneous*. This is so that the domain of definition is a linear space. In other words, if y_1 and y_2 obey the boundary conditions then so should $\lambda y_1 + \mu y_2$. Thus, for a second-order operator

$$L = p_0 \partial_x^2 + p_1 \partial_x + p_2 \quad (4.13)$$

on the interval $[a, b]$, we might impose

$$\begin{aligned} B_1[y] &= \alpha_{11}y(a) + \alpha_{12}y'(a) + \beta_{11}y(b) + \beta_{12}y'(b) = 0, \\ B_2[y] &= \alpha_{21}y(a) + \alpha_{22}y'(a) + \beta_{21}y(b) + \beta_{22}y'(b) = 0, \end{aligned} \quad (4.14)$$

but we will not, in defining the differential *operator*, impose *inhomogeneous* conditions, such as

$$\begin{aligned} B_1[y] &= \alpha_{11}y(a) + \alpha_{12}y'(a) + \beta_{11}y(b) + \beta_{12}y'(b) = A, \\ B_2[y] &= \alpha_{21}y(a) + \alpha_{22}y'(a) + \beta_{21}y(b) + \beta_{22}y'(b) = B, \end{aligned} \quad (4.15)$$

with non-zero A, B — even though we will solve differential *equations* with such boundary conditions.

Also, for an n -th order operator, we will not constrain derivatives of order higher than $n - 1$. This is reasonable¹: If we seek solutions of $Ly = f$ with L a second-order operator, for example, then the values of y'' at the endpoints are already determined in terms of y' and y by the differential equation. We cannot choose to impose some other value. By differentiating the equation enough times, we can similarly determine all higher endpoint derivatives in terms of y and y' . These two derivatives, therefore, are all we can fix by fiat.

The boundary and differentiability conditions that we impose make \mathcal{D} a subset of the entire Hilbert space. This subset will always be *dense*: any element of the Hilbert space can be obtained as a limit of functions in \mathcal{D} . In particular, there will never be a function in $L^2[a, b]$ that is orthogonal to all functions in \mathcal{D} .

4.2 The Adjoint Operator

One of the important properties of matrices, established in the appendix, is that a matrix that is *self-adjoint*, or *Hermitian*, may be *diagonalized*. In other words, the matrix has sufficiently many eigenvectors for them to form a basis for the space on which it acts. A similar property holds for self-adjoint differential operators, but we must be careful in our definition of self-adjointness.

Before reading this section, We suggest you review the material on adjoint operators on *finite*-dimensional spaces that appears in the appendix.

4.2.1 The formal adjoint

Given a formal differential operator

$$L = p_0(x) \frac{d^n}{dx^n} + p_1(x) \frac{d^{n-1}}{dx^{n-1}} + \cdots + p_n(x), \quad (4.16)$$

and a *weight function* $w(x)$, real and positive on the interval (a, b) , we can find another such operator L^\dagger , such that, for any sufficiently differentiable $u(x)$ and $v(x)$, we have

$$w(u^*Lv - v(L^\dagger u)^*) = \frac{d}{dx}Q[u, v], \quad (4.17)$$

¹There is a deeper reason which we will explain in chapter 9.

for some function Q , which depends bilinearly on u and v and their first $n-1$ derivatives. We call L^\dagger the *formal adjoint* of L with respect to the weight w . The equation (4.17) is called *Lagrange's identity*. The reason for the name “adjoint” is that if we define an inner product

$$\langle u, v \rangle_w = \int_a^b w u^* v \, dx, \quad (4.18)$$

and if the functions u and v have boundary conditions that make $Q[u, v]|_a^b = 0$, then

$$\langle u, Lv \rangle_w = \langle L^\dagger u, v \rangle_w, \quad (4.19)$$

which is the defining property of the adjoint operator on a vector space. The word “formal” means, as before, that we are not yet specifying the domain of the operator.

The method for finding the formal adjoint is straightforward: integrate by parts enough times to get all the derivatives off v and on to u .

Example: If

$$L = -i \frac{d}{dx} \quad (4.20)$$

then let us find the adjoint L^\dagger with respect to the weight $w \equiv 1$. We start from

$$u^*(Lv) = u^* \left(-i \frac{d}{dx} v \right),$$

and use the integration-by-parts technique once to get the derivative off v and onto u^* :

$$\begin{aligned} u^* \left(-i \frac{d}{dx} v \right) &= \left(i \frac{d}{dx} u^* \right) v - i \frac{d}{dx} (u^* v) \\ &= \left(-i \frac{d}{dx} u \right)^* v - i \frac{d}{dx} (u^* v) \\ &\equiv v (L^\dagger u)^* + \frac{d}{dx} Q[u, v]. \end{aligned} \quad (4.21)$$

We have ended up with the Lagrange identity

$$u^* \left(-i \frac{d}{dx} v \right) - v \left(-i \frac{d}{dx} u \right)^* = \frac{d}{dx} (-i u^* v), \quad (4.22)$$

and found that

$$L^\dagger = -i\frac{d}{dx}, \quad Q[u, v] = -iu^*v. \quad (4.23)$$

The operator $-id/dx$ (which you should recognize as the “momentum” operator from quantum mechanics) obeys $L = L^\dagger$, and is therefore, *formally self-adjoint*, or *Hermitian*.

Example: Let

$$L = p_0 \frac{d^2}{dx^2} + p_1 \frac{d}{dx} + p_2, \quad (4.24)$$

with the p_i all real. Again let us find the adjoint L^\dagger with respect to the inner product with $w \equiv 1$. Now, proceeding as above, but integrating by parts *twice*, we find

$$\begin{aligned} u^* [p_0 v'' + p_1 v' + p_2 v] - v [(p_0 u)'' - (p_1 u)' + p_2 u]^* \\ = \frac{d}{dx} [p_0 (u^{*'} v - v' u^*) + (p_1 - p_0') u^* v]. \end{aligned} \quad (4.25)$$

From this we read off that

$$\begin{aligned} L^\dagger &= \frac{d^2}{dx^2} p_0 - \frac{d}{dx} p_1 + p_2 \\ &= p_0 \frac{d^2}{dx^2} + (2p_0' - p_1) \frac{d}{dx} + (p_0'' - p_1' + p_2). \end{aligned} \quad (4.26)$$

What conditions do we need to impose on $p_{0,1,2}$ for this L to be formally self-adjoint with respect to the inner product with $w \equiv 1$? For $L = L^\dagger$ we need

$$\begin{aligned} p_0 &= p_0 \\ 2p_0' - p_1 &= p_1 \Rightarrow p_0' = p_1 \\ p_0'' - p_1' + p_2 &= p_2 \Rightarrow p_0'' = p_1'. \end{aligned} \quad (4.27)$$

We therefore require that $p_1 = p_0'$, and so

$$L = \frac{d}{dx} \left(p_0 \frac{d}{dx} \right) + p_2, \quad (4.28)$$

which is a *Sturm-Liouville* operator.

Example: Reduction to Sturm-Liouville form. Another way to make the operator

$$L = p_0 \frac{d^2}{dx^2} + p_1 \frac{d}{dx} + p_2, \quad (4.29)$$

self-adjoint is by a suitable choice of weight function w . Suppose that p_0 is positive on the interval (a, b) , and that p_0, p_1, p_2 are all real. Then we may define

$$w = \frac{1}{p_0} \exp \left\{ \int_a^x \left(\frac{p_1}{p_0} \right) dx' \right\} \quad (4.30)$$

and observe that it is positive on (a, b) , and that

$$Ly = \frac{1}{w} (wp_0 y')' + p_2 y. \quad (4.31)$$

Now

$$\langle u, Lv \rangle_w - \langle Lu, v \rangle_w = [wp_0(u^* v' - u^{*'} v)]_a^b, \quad (4.32)$$

where

$$\langle u, v \rangle_w = \int_a^b w u^* v dx. \quad (4.33)$$

Thus, provided p_0 does not vanish, there is always *some* inner product with respect to which a real second-order differential operator is formally self-adjoint.

Note that with

$$Ly = \frac{1}{w} (wp_0 y')' + p_2 y, \quad (4.34)$$

the eigenvalue equation

$$Ly = \lambda y \quad (4.35)$$

can be written

$$(wp_0 y')' + p_2 w y = \lambda w y. \quad (4.36)$$

When you come across a differential equation where, in the term containing the eigenvalue λ , the eigenfunction is being multiplied by some other function, you should immediately suspect that the operator will turn out to be self-adjoint with respect to the inner product having this other function as its weight.

Illustration (Bargmann-Fock space): This is a more exotic example of a formal adjoint. You may have met with it in quantum mechanics. Consider the space of polynomials $P(z)$ in the complex variable $z = x + iy$. Define an inner product by

$$\langle P, Q \rangle = \frac{1}{\pi} \int d^2 z e^{-z^* z} [P(z)]^* Q(z),$$

where $d^2z \equiv dx dy$ and the integration is over the entire x, y plane. With this inner product, we have

$$\langle z^n, z^m \rangle = n! \delta_{nm}.$$

If we define

$$\hat{a} = \frac{d}{dz},$$

then

$$\begin{aligned} \langle P, \hat{a} Q \rangle &= \frac{1}{\pi} \int d^2z e^{-z^*z} [P(z)]^* \frac{d}{dz} Q(z) \\ &= -\frac{1}{\pi} \int d^2z \left(\frac{d}{dz} e^{-z^*z} [P(z)]^* \right) Q(z) \\ &= \frac{1}{\pi} \int d^2z e^{-z^*z} z^* [P(z)]^* Q(z) \\ &= \frac{1}{\pi} \int d^2z e^{-z^*z} [zP(z)]^* Q(z) \\ &= \langle \hat{a}^\dagger P, \hat{Q} \rangle \end{aligned}$$

where $\hat{a}^\dagger = z$, *i.e.* the operation of multiplication by z . In this case, the adjoint is not even a differential operator².

Exercise 4.1: Consider the differential operator $\hat{L} = id/dx$. Find the formal adjoint of L with respect to the inner product $\langle u, v \rangle = \int w u^* v dx$, and find the corresponding surface term $Q[u, v]$.

²In deriving this result we have treated z and z^* as independent variables so that

$$\frac{d}{dz} e^{-z^*z} = -z^* e^{-z^*z},$$

and observed that, because $[P(z)]^*$ is a function of z^* only,

$$\frac{d}{dz} [P(z)]^* = 0.$$

If you are uneasy at regarding z, z^* as independent, you should confirm these formulae by expressing z and z^* in terms of x and y , and using

$$\frac{d}{dz} \equiv \frac{1}{2} \left(\frac{\partial}{\partial x} - i \frac{\partial}{\partial y} \right), \quad \frac{d}{dz^*} \equiv \frac{1}{2} \left(\frac{\partial}{\partial x} + i \frac{\partial}{\partial y} \right).$$

Exercise 4.2: Sturm-Liouville forms. By constructing appropriate weight functions $w(x)$ convert the following common operators into Sturm-Liouville form:

- a) $\hat{L} = (1 - x^2) d^2/dx^2 + [(\mu - \nu) - (\mu + \nu + 2)x] d/dx$.
- b) $\hat{L} = (1 - x^2) d^2/dx^2 - 3x d/dx$.
- c) $\hat{L} = d^2/dx^2 - 2x(1 - x^2)^{-1} d/dx - m^2(1 - x^2)^{-1}$.

4.2.2 A simple eigenvalue problem

A finite Hermitian matrix has a complete set of orthonormal eigenvectors. Does the same property hold for a Hermitian differential operator?

Consider the differential operator

$$T = -\partial_x^2, \quad \mathcal{D}(T) = \{y, Ty \in L^2[0, 1] : y(0) = y(1) = 0\}. \quad (4.37)$$

With the inner product

$$\langle y_1, y_2 \rangle = \int_0^1 y_1^* y_2 dx \quad (4.38)$$

we have

$$\langle y_1, Ty_2 \rangle - \langle Ty_1, y_2 \rangle = [y_1'^* y_2 - y_1^* y_2']_0^1 = 0. \quad (4.39)$$

The integrated-out part is zero because both y_1 and y_2 satisfy the boundary conditions. We see that

$$\langle y_1, Ty_2 \rangle = \langle Ty_1, y_2 \rangle \quad (4.40)$$

and so T is *Hermitian* or *symmetric*.

The eigenfunctions and eigenvalues of T are

$$\left. \begin{array}{l} y_n(x) = \sin n\pi x \\ \lambda_n = n^2\pi^2 \end{array} \right\} \quad n = 1, 2, \dots \quad (4.41)$$

We see that:

- i) the eigenvalues are *real*;
- ii) the eigenfunctions for different λ_n are *orthogonal*,

$$2 \int_0^1 \sin n\pi x \sin m\pi x dx = \delta_{nm}, \quad n = 1, 2, \dots \quad (4.42)$$

- iii) the normalized eigenfunctions $\varphi_n(x) = \sqrt{2} \sin n\pi x$ are *complete*: any function in $L^2[0, 1]$ has an (L^2) convergent expansion as

$$y(x) = \sum_{n=1}^{\infty} a_n \sqrt{2} \sin n\pi x \quad (4.43)$$

where

$$a_n = \int_0^1 y(x) \sqrt{2} \sin n\pi x \, dx. \quad (4.44)$$

This all looks very good — exactly the properties we expect for finite Hermitian matrices! Can we carry over all the results of finite matrix theory to these Hermitian operators? The answer sadly is *no*! Here is a counterexample:

Let

$$T = -i\partial_x, \quad \mathcal{D}(T) = \{y, Ty \in L^2[0, 1] : y(0) = y(1) = 0\}. \quad (4.45)$$

Again

$$\begin{aligned} \langle y_1, Ty_2 \rangle - \langle Ty_1, y_2 \rangle &= \int_0^1 dx \{y_1^* (-i\partial_x y_2) - (-i\partial_x y_1)^* y_2\} \\ &= -i[y_1^* y_2]_0^1 = 0. \end{aligned} \quad (4.46)$$

Once more, the integrated out part vanishes due to the boundary conditions satisfied by y_1 and y_2 , so T is nicely Hermitian. Unfortunately, T with these boundary conditions has *no* eigenfunctions at all — never mind a complete set! Any function satisfying $Ty = \lambda y$ will be proportional to $e^{i\lambda x}$, but an exponential function is never zero, and cannot satisfy the boundary conditions.

It seems clear that the boundary conditions are the problem. We need a better definition of “adjoint” than the formal one — one that pays more attention to boundary conditions. We will then be forced to distinguish between mere Hermiticity, or *symmetry*, and true self-adjointness.

Exercise 4.3: Another disconcerting example. Let $p = -i\partial_x$. Show that the following operator on the infinite real line is formally self-adjoint:

$$H = x^3 p + p x^3. \quad (4.47)$$

Now let

$$\psi_\lambda(x) = |x|^{-3/2} \exp \left\{ -\frac{\lambda}{4x^2} \right\}, \quad (4.48)$$

where λ is real and positive. Show that

$$H\psi_\lambda = -i\lambda\psi_\lambda, \quad (4.49)$$

so ψ_λ is an eigenfunction with a purely imaginary eigenvalue. Examine the usual proof that Hermitian operators have real eigenvalues, and identify at which point it breaks down. (*Hint:* H is formally self adjoint because it is of the form $T + T^\dagger$. Now ψ_λ is square-integrable, and so an element of $L^2(\mathbb{R})$. Is $T\psi_\lambda$ an element of $L^2(\mathbb{R})$?)

4.2.3 Adjoint boundary conditions

The usual definition of the adjoint operator in linear algebra is as follows: Given the operator $T : V \rightarrow V$ and an inner product $\langle \cdot, \cdot \rangle$, we look at $\langle u, Tv \rangle$, and ask if there is a w such that $\langle w, v \rangle = \langle u, Tv \rangle$ for all v . If there is, then u is in the domain of T^\dagger , and $T^\dagger u = w$.

For finite-dimensional vector spaces V there always is such a w , and so the domain of T^\dagger is the entire space. In an infinite dimensional Hilbert space, however, not all $\langle u, Tv \rangle$ can be written as $\langle w, v \rangle$ with w a finite-length element of L^2 . In particular δ -functions are not allowed — but these are exactly what we would need if we were to express the boundary values appearing in the integrated out part, $Q(u, v)$, as an inner-product integral. We must therefore ensure that u is such that $Q(u, v)$ vanishes, but then accept *any* u with this property into the domain of T^\dagger . What this means in practice is that we look at the integrated out term $Q(u, v)$ and see what is required of u to make $Q(u, v)$ zero for any v satisfying the boundary conditions appearing in $\mathcal{D}(T)$. These conditions on u are the *adjoint boundary conditions*, and define the domain of T^\dagger .

Example: Consider

$$T = -i\partial_x, \quad \mathcal{D}(T) = \{y, Ty \in L^2[0, 1] : y(1) = 0\}. \quad (4.50)$$

Now,

$$\begin{aligned} \int_0^1 dx u^*(-i\partial_x v) &= -i[u^*(1)v(1) - u^*(0)v(0)] + \int_0^1 dx (-i\partial_x u)^* v \\ &= -i[u^*(1)v(1) - u^*(0)v(0)] + \langle w, v \rangle, \end{aligned} \quad (4.51)$$

where $w = -i\partial_x u$. Since $v(x)$ is in the domain of T , we have $v(1) = 0$, and so the first term in the integrated out bit vanishes whatever value we take

for $u(1)$. On the other hand, $v(0)$ could be anything, so to be sure that the second term vanishes we must demand that $u(0) = 0$. This, then, is the adjoint boundary condition. It defines the domain of T^\dagger :

$$T^\dagger = -i\partial_x, \quad \mathcal{D}(T^\dagger) = \{y, Ty \in L^2[0, 1] : y(0) = 0\}. \quad (4.52)$$

For our problematic operator

$$T = -i\partial_x, \quad \mathcal{D}(T) = \{y, Ty \in L^2[0, 1] : y(0) = y(1) = 0\}, \quad (4.53)$$

we have

$$\begin{aligned} \int_0^1 dx u^*(-i\partial_x v) &= -i[u^*v]_0^1 + \int_0^1 dx (-i\partial_x u)^* v \\ &= 0 + \langle w, v \rangle, \end{aligned} \quad (4.54)$$

where again $w = -i\partial_x u$. This time *no* boundary conditions need be imposed on u to make the integrated out part vanish. Thus

$$T^\dagger = -i\partial_x, \quad \mathcal{D}(T^\dagger) = \{y, Ty \in L^2[0, 1]\}. \quad (4.55)$$

Although any of these operators “ $T = -i\partial_x$ ” is *formally* self-adjoint we have,

$$\mathcal{D}(T) \neq \mathcal{D}(T^\dagger), \quad (4.56)$$

so T and T^\dagger are not the same operator and none of them is *truly* self-adjoint.

Exercise 4.4: Consider the differential operator $M = d^4/dx^4$, Find the formal adjoint of M with respect to the inner product $\langle u, v \rangle = \int u^* v dx$, and find the corresponding surface term $Q[u, v]$. Find the adjoint boundary conditions defining the domain of M^\dagger for the case

$$\mathcal{D}(M) = \{y, y^{(4)} \in L^2[0, 1] : y(0) = y'''(0) = y(1) = y'''(1) = 0\}.$$

4.2.4 Self-adjoint boundary conditions

A *formally* self-adjoint operator T is *truly* self adjoint only if the domains of T^\dagger and T coincide. From now on, the unqualified phrase “self-adjoint” will always mean “truly self-adjoint”.

Self-adjointness is usually desirable in physics problems. It is therefore useful to investigate what boundary conditions lead to self-adjoint operators.

For example, what are the most general boundary conditions we can impose on $T = -i\partial_x$ if we require the resultant operator to be self-adjoint? Now,

$$\int_0^1 dx u^*(-i\partial_x v) - \int_0^1 dx (-i\partial_x u)^* v = -i(u^*(1)v(1) - u^*(0)v(0)). \quad (4.57)$$

Demanding that the right-hand side be zero gives us, after division by $u^*(0)v(1)$,

$$\frac{u^*(1)}{u^*(0)} = \frac{v(0)}{v(1)}. \quad (4.58)$$

We require this to be true for any u and v obeying the same boundary conditions. Since u and v are unrelated, both sides must equal a constant κ , and furthermore this constant must obey $\kappa^* = \kappa^{-1}$ in order that $u(1)/u(0)$ be equal to $v(1)/v(0)$. Thus, the boundary condition is

$$\frac{u(1)}{u(0)} = \frac{v(1)}{v(0)} = e^{i\theta} \quad (4.59)$$

for some real angle θ . The domain is therefore

$$\mathcal{D}(T) = \{y, Ty \in L^2[0, 1] : y(1) = e^{i\theta}y(0)\}. \quad (4.60)$$

These are *twisted periodic* boundary conditions.

With these generalized periodic boundary conditions, everything we expect of a self-adjoint operator actually works:

- i) The functions $u_n = e^{i(2\pi n + \theta)x}$, with $n = \dots, -2, -1, 0, 1, 2, \dots$ are eigenfunctions of T with eigenvalues $k_n \equiv 2\pi n + \theta$.
- ii) The eigenvalues are real.
- iii) The eigenfunctions form a complete orthonormal set.

Because self-adjoint operators possess a complete set of mutually orthogonal eigenfunctions, they are compatible with the interpretational postulates of quantum mechanics, where the square of the inner product of a state vector with an eigenstate gives the probability of measuring the associated eigenvalue. In quantum mechanics, self-adjoint operators are therefore called *observables*.

Example: The Sturm-Liouville equation. With

$$L = \frac{d}{dx}p(x)\frac{d}{dx} + q(x), \quad x \in [a, b], \quad (4.61)$$

we have

$$\langle u, Lv \rangle - \langle Lu, v \rangle = [p(u^*v' - u'^*v)]_a^b. \quad (4.62)$$

Let us seek to impose boundary conditions separately at the two ends. Thus, at $x = a$ we want

$$(u^*v' - u'^*v)|_a = 0, \quad (4.63)$$

or

$$\frac{u'^*(a)}{u^*(a)} = \frac{v'(a)}{v(a)}, \quad (4.64)$$

and similarly at b . If we want the boundary conditions imposed on v (which define the domain of L) to coincide with those for u (which define the domain of L^\dagger) then we must have

$$\frac{v'(a)}{v(a)} = \frac{u'(a)}{u(a)} = \tan \theta_a \quad (4.65)$$

for some real angle θ_a , and similar boundary conditions with a θ_b at b . We can also write these boundary conditions as

$$\begin{aligned} \alpha_a y(a) + \beta_a y'(a) &= 0, \\ \alpha_b y(b) + \beta_b y'(b) &= 0. \end{aligned} \quad (4.66)$$

Deficiency indices

There is a general theory of self-adjoint boundary conditions, due to Hermann Weyl and John von Neumann. We will not describe this theory in any detail, but simply give their recipe for counting the number of parameters in the most general self-adjoint boundary condition: To find this number you should first impose the strictest possible boundary conditions by setting to zero the boundary values of all the $y^{(n)}$ with n less than the order of the equation. Next count the number of square-integrable eigenfunctions of the resulting adjoint operator T^\dagger corresponding to eigenvalue $\pm i$. The numbers, n_+ and n_- , of these eigenfunctions are called the *deficiency indices*. If they are not equal then there is no possible way to make the operator self-adjoint. If they are equal, $n_+ = n_- = n$, then there is an n^2 real-parameter family of self-adjoint boundary conditions.

Example: The sad case of the “radial momentum operator.” We wish to define the operator $P_r = -i\partial_r$ on the half-line $0 < r < \infty$. We start with the

restrictive domain

$$P_r = -i\partial_r, \quad \mathcal{D}(T) = \{y, P_r y \in L^2[0, \infty] : y(0) = 0\}. \quad (4.67)$$

We then have

$$P_r^\dagger = -i\partial_r, \quad \mathcal{D}(P_r^\dagger) = \{y, P_r^\dagger y \in L^2[0, \infty]\} \quad (4.68)$$

with no boundary conditions. The equation $P_r^\dagger y = iy$ has a normalizable solution $y = e^{-r}$. The equation $P_r^\dagger y = -iy$ has no normalizable solution. The deficiency indices are therefore $n_+ = 1$, $n_- = 0$, and this operator cannot be rescued and made self adjoint.

Example: The Schrödinger operator. We now consider $-\partial_x^2$ on the half-line. Set

$$T = -\partial_x^2, \quad \mathcal{D}(T) = \{y, Ty \in L^2[0, \infty] : y(0) = y'(0) = 0\}. \quad (4.69)$$

We then have

$$T^\dagger = -\partial_x^2, \quad \mathcal{D}(T^\dagger) = \{y, T_r^\dagger y \in L^2[0, \infty]\}. \quad (4.70)$$

Again T^\dagger comes with *no* boundary conditions. The eigenvalue equation $T^\dagger y = iy$ has one normalizable solution $y(x) = e^{(i-1)x/\sqrt{2}}$, and the equation $T^\dagger y = -iy$ also has one normalizable solution $y(x) = e^{-(i+1)x/\sqrt{2}}$. The deficiency indices are therefore $n_+ = n_- = 1$. The Weyl-von Neumann theory now says that, by relaxing the restrictive conditions $y(0) = y'(0) = 0$, we can extend the domain of definition of the operator to find a one-parameter family of self-adjoint boundary conditions. These will be the conditions $y'(0)/y(0) = \tan \theta$ that we found above.

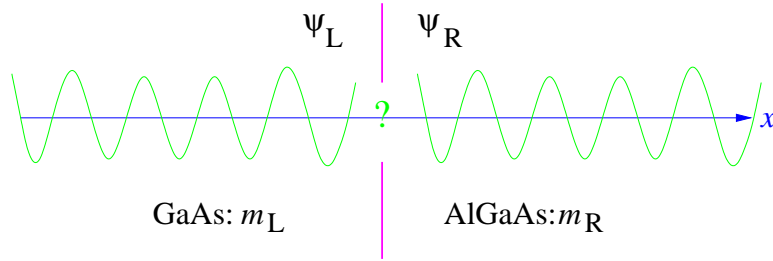
If we consider the operator $-\partial_x^2$ on the finite interval $[a, b]$, then both solutions of $(T^\dagger \pm i)y = 0$ are normalizable, and the deficiency indices will be $n_+ = n_- = 2$. There should therefore be $2^2 = 4$ real parameters in the self-adjoint boundary conditions. This is a larger class than those we found in (4.66), because it includes generalized boundary conditions of the form

$$\begin{aligned} B_1[y] &= \alpha_{11}y(a) + \alpha_{12}y'(a) + \beta_{11}y(b) + \beta_{12}y'(b) = 0, \\ B_2[y] &= \alpha_{21}y(a) + \alpha_{22}y'(a) + \beta_{21}y(b) + \beta_{22}y'(b) = 0 \end{aligned}$$

The next problem illustrates why we have spent so much time on identifying self-adjoint boundary conditions: the technique is important in practical physics problems.

Physics application: semiconductor heterojunction

A heterojunction is fabricated with two semiconductors, such as GaAs and $\text{Al}_x\text{Ga}_{1-x}\text{As}$, having different band-masses. We wish to describe the conduction electrons in the material by an effective Schrödinger equation containing these band masses. What matching condition should we impose on the wavefunction $\psi(x)$ at the interface between the two materials? A first guess is that the wavefunction must be continuous, but this is not correct because the “wavefunction” in an effective-mass band-theory Hamiltonian is not the actual wavefunction (which *is* continuous) but instead a slowly varying envelope function multiplying a Bloch wavefunction. The Bloch function is rapidly varying, fluctuating strongly on the scale of a single atom. Because the Bloch form of the solution is no longer valid at a discontinuity, the envelope function is not even defined in the neighbourhood of the interface, and certainly has no reason to be continuous. There must still be some linear relation between the ψ 's in the two materials, but finding it will involve a detailed calculation on the atomic scale. In the absence of these calculations, we must use general principles to constrain the form of the relation. What are these principles?



Heterojunction wavefunctions.

We know that, were we to do the atomic-scale calculation, the resulting connection between the right and left wavefunctions would:

- be linear,
- involve no more than $\psi(x)$ and its first derivative $\psi'(x)$,
- make the Hamiltonian into a self-adjoint operator.

We want to find the most general connection formula compatible with these principles. The first two are easy to satisfy. We therefore investigate what matching conditions are compatible with self-adjointness.

Suppose that the band masses are m_L and m_R , so that

$$\begin{aligned} H &= -\frac{1}{2m_L} \frac{d^2}{dx^2} + V_L(x), \quad x < 0, \\ &= -\frac{1}{2m_R} \frac{d^2}{dx^2} + V_R(x), \quad x > 0. \end{aligned} \quad (4.71)$$

Integrating by parts, and keeping the terms at the interface gives us

$$\langle \psi_1, H\psi_2 \rangle - \langle H\psi_1, \psi_2 \rangle = \frac{1}{2m_L} \{ \psi_{1L}^* \psi'_{2L} - \psi'_{1L}^* \psi_{2L} \} - \frac{1}{2m_R} \{ \psi_{1R}^* \psi'_{2R} - \psi'_{1R}^* \psi_{2R} \}. \quad (4.72)$$

Here, $\psi_{L,R}$ refers to the boundary values of ψ immediately to the left or right of the junction, respectively. Now we impose general linear homogeneous boundary conditions on ψ_2 :

$$\begin{pmatrix} \psi_{2L} \\ \psi'_{2L} \end{pmatrix} = \begin{pmatrix} a & b \\ c & d \end{pmatrix} \begin{pmatrix} \psi_{2R} \\ \psi'_{2R} \end{pmatrix}. \quad (4.73)$$

This relation involves four complex, and therefore eight real, parameters. Demanding that

$$\langle \psi_1, H\psi_2 \rangle = \langle H\psi_1, \psi_2 \rangle, \quad (4.74)$$

we find

$$\frac{1}{2m_L} \{ \psi_{1L}^* (c\psi_{2R} + d\psi'_{2R}) - \psi'_{1L}^* (a\psi_{2R} + b\psi'_{2R}) \} = \frac{1}{2m_R} \{ \psi_{1R}^* \psi'_{2R} - \psi'_{1R}^* \psi_{2R} \}, \quad (4.75)$$

and this must hold for arbitrary ψ_{2R} , ψ'_{2R} , so, picking off the coefficients of these expressions and complex conjugating, we find

$$\begin{pmatrix} \psi_{1R} \\ \psi'_{1R} \end{pmatrix} = \begin{pmatrix} m_R \\ m_L \end{pmatrix} \begin{pmatrix} a^* & -b^* \\ -c^* & d^* \end{pmatrix} \begin{pmatrix} \psi_{1L} \\ \psi'_{1L} \end{pmatrix}. \quad (4.76)$$

Because we wish the domain of H^\dagger to coincide with that of H , these must be same conditions that we imposed on ψ_2 . Thus we must have

$$\begin{pmatrix} a & b \\ c & d \end{pmatrix}^{-1} = \begin{pmatrix} m_R \\ m_L \end{pmatrix} \begin{pmatrix} a^* & -b^* \\ -c^* & d^* \end{pmatrix}. \quad (4.77)$$

Since

$$\begin{pmatrix} a & b \\ c & d \end{pmatrix}^{-1} = \frac{1}{ad - bc} \begin{pmatrix} a & -b \\ -c & d \end{pmatrix}, \quad (4.78)$$

we see that this requires

$$\begin{pmatrix} a & b \\ c & d \end{pmatrix} = e^{i\phi} \sqrt{\frac{m_L}{m_R}} \begin{pmatrix} A & B \\ C & D \end{pmatrix}, \quad (4.79)$$

where ϕ, A, B, C, D are real, and $AD - BC = 1$. Demanding self-adjointness has therefore cut the original eight real parameters down to four. These can be determined either by experiment or by performing the microscopic calculation³. Note that $4 = 2^2$, a perfect square, as required by the Weyl-Von Neumann theory.

Exercise 4.5: Consider the Schrödinger operator $\hat{H} = -\partial_x^2$ on the interval $[0, 1]$. Show that the most general self-adjoint boundary condition applicable to \hat{H} can be written as

$$\begin{bmatrix} \varphi(0) \\ \varphi'(0) \end{bmatrix} = e^{i\phi} \begin{bmatrix} a & b \\ c & d \end{bmatrix} \begin{bmatrix} \varphi(1) \\ \varphi'(1) \end{bmatrix},$$

where ϕ, a, b, c, d are real and $ac - bd = 1$. Consider \hat{H} as the quantum Hamiltonian of a particle on a ring constructed by attaching $x = 0$ to $x = 1$. Show that the self-adjoint boundary condition found above leads to unitary scattering at the point of join. Does the most general unitary point-scattering matrix correspond to the most general self-adjoint boundary condition?

4.3 Completeness of Eigenfunctions

Now that we have a clear understanding of what it means to be self-adjoint, we can reiterate the basic claim: an operator T that is self-adjoint with respect to an L^2 inner product possesses a complete set of mutually orthogonal eigenfunctions. The proof that the eigenfunctions are orthogonal is identical to that for finite matrices. We will sketch a proof of the completeness of the eigenfunctions of the Sturm-Liouville operator in the next section.

The set of eigenvalues is, with some mathematical cavils, called the *spectrum* of T . It is usually denoted by $\sigma(T)$. An eigenvalue is said to belong to the *point* spectrum when its associated eigenfunction is normalizable *i.e* is a *bona-fide* member of L^2 having a finite length. Usually (but not always) the eigenvalues of the point spectrum form a discrete set, and so the point spectrum is also known as the *discrete spectrum*. When the operator acts on

³T. Ando, S. Mori, Surface Science **113** (1982) 124.

functions on an infinite interval, the eigenfunctions may fail to be normalizable. The associated eigenvalues are then said to belong to the *continuous spectrum*. Sometimes, *e.g.* the hydrogen atom, the spectrum is partly discrete and partly continuous. There is also something called the *residual spectrum*, but this does not occur for self-adjoint operators.

4.3.1 Discrete spectrum

The simplest problems have a purely discrete spectrum. We have eigenfunctions $\phi_n(x)$ such that

$$T\phi_n(x) = \lambda_n\phi_n(x), \quad (4.80)$$

where n is an integer. After multiplication by suitable constants, the ϕ_n are orthonormal,

$$\int \phi_n^*(x)\phi_m(x') dx = \delta_{nm}, \quad (4.81)$$

and complete. We can express the *completeness condition* as the statement that

$$\sum_n \phi_n(x)\phi_n^*(x') = \delta(x - x'). \quad (4.82)$$

If we take this representation of the delta function and multiply it by $f(x')$ and integrate over x' , we find

$$f(x) = \sum_n \phi_n(x) \int \phi_n^*(x')f(x') dx'. \quad (4.83)$$

So,

$$f(x) = \sum_n a_n \phi_n(x) \quad (4.84)$$

with

$$a_n = \int \phi_n^*(x')f(x') dx'. \quad (4.85)$$

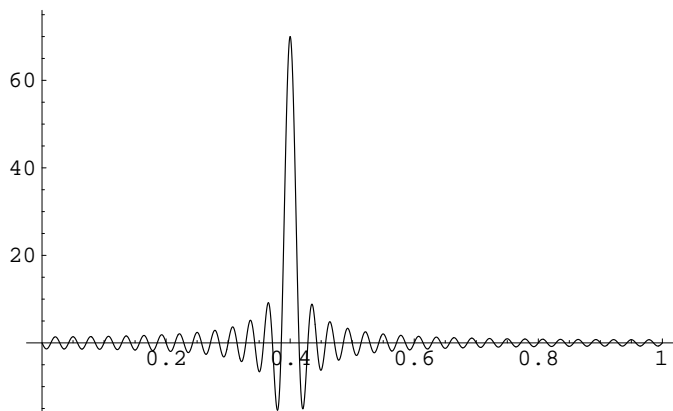
This means that if we can expand a delta function in terms of the $\phi_n(x)$, we can expand any (square integrable) function.

Note: The convergence of the series $\sum_n \phi_n(x)\phi_n^*(x')$ to $\delta(x - x')$ is neither pointwise nor in the L^2 sense. The sum tends to a limit only in the sense of a distribution — meaning that we must multiply the partial sums by a smooth test function and integrate over x before we have something that

actually converges in any meaningful manner. As an illustration consider our favourite orthonormal set: $\phi_n(x) = \sqrt{2}\sin(n\pi x)$ on the interval $[0, 1]$. A plot of the first m terms in the sum

$$\sum_{n=1}^{\infty} \sqrt{2}\sin(n\pi x)\sqrt{2}\sin(n\pi x') = \delta(x - x')$$

will show “wiggles” away from $x = x'$ whose amplitude does not decrease as m becomes large — although they become of higher and higher frequency. When multiplied by a smooth function and integrated, the contributions from adjacent positive and negative wiggle regions tend to cancel, and it is only after this integration that the sum tends to zero away from the spike at $x = x'$.



The sum $\sum_{n=1}^{70} 2\sin(n\pi x)\sin(n\pi x')$ for $x' = 0.4$. Take note of the very disparate scales on the horizontal and vertical axes.

Rayleigh-Ritz and completeness

For the Schrödinger eigenvalue problem

$$Ly = -y'' + q(x)y = \lambda y, \quad x \in [a, b], \quad (4.86)$$

the large eigenvalues are $\lambda_n \approx n^2\pi^2/(a - b)^2$. This is because the term qy eventually becomes negligible compared to λy , and then we can solve the problem with sines and cosines. We see that there is no upper limit to the magnitude of the eigenvalues. The eigenvalues of the Sturm-Liouville

problem

$$Ly = -(py')' + qy = \lambda y, \quad x \in [a, b], \quad (4.87)$$

are similarly unbounded. We will use this unboundedness of the spectrum to make an estimate of the rate of convergence of the eigenfunction expansion for functions in the domain of L , and extend this result to prove that the eigenfunctions form a complete set.

We know from chapter one that the Sturm-Liouville eigenvalues are the stationary values of $\langle y, Ly \rangle$ when the function y is constrained to have unit length, $\langle y, y \rangle = 1$. The lowest eigenvalue, λ_0 , is therefore given by

$$\lambda_0 = \inf_{y \in \mathcal{D}(L)} \frac{\langle y, Ly \rangle}{\langle y, y \rangle}. \quad (4.88)$$

As the *variational principle*, this formula provides a well-known method of obtaining approximate ground state energies in quantum mechanics. Part of its effectiveness comes from the stationary nature of $\langle y, Ly \rangle$ at the minimum: a crude approximation to y often gives a tolerably good approximation to λ_0 . In the wider world of eigenvalue problems, the variational principle is named after Rayleigh and Ritz⁴.

Suppose we have already found the first n normalized eigenfunctions y_0, y_1, \dots, y_{n-1} . Let the space spanned by these functions be V_n . Then an obvious extension of the variational principle gives

$$\lambda_n = \inf_{y \in V_n^\perp} \frac{\langle y, Ly \rangle}{\langle y, y \rangle}. \quad (4.89)$$

We now exploit this variational estimate to show that if we expand an arbitrary y in the domain of L in terms of the full set of eigenfunctions y_m ,

$$y = \sum_{m=0}^{\infty} a_m y_m, \quad (4.90)$$

where

$$a_m = \langle y_m, y \rangle, \quad (4.91)$$

⁴J. W. Strutt (later Lord Rayleigh), *In Finding the Correction for the Open End of an Organ-Pipe*. Phil. Trans. **161** (1870) 77; W. Ritz, *Über eine neue Methode zur Lösung gewisser Variationsprobleme der mathematischen Physik*. J. reine angew. Math. **135** (1908)

then the sum does indeed converge to y .

Let

$$h_n = y - \sum_{m=0}^{n-1} a_m y_m \quad (4.92)$$

be the residual error after the first n terms. By definition, $h_n \in V_n^\perp$. Let us assume that we have adjusted, by adding a constant to q if necessary, L so that all the λ_m are positive. This adjustment will not affect the y_m . We expand out

$$\langle h_n, Lh_n \rangle = \langle y, Ly \rangle - \sum_{m=0}^{n-1} \lambda_m |a_m|^2, \quad (4.93)$$

where we have made use of the orthonormality of the y_m . The subtracted sum is guaranteed positive, so

$$\langle h_n, Lh_n \rangle \leq \langle y, Ly \rangle. \quad (4.94)$$

Combining this inequality with Rayleigh-Ritz tells us that

$$\frac{\langle y, Ly \rangle}{\langle h_n, h_n \rangle} \geq \frac{\langle h_n, Lh_n \rangle}{\langle h_n, h_n \rangle} \geq \lambda_n. \quad (4.95)$$

In other words

$$\frac{\langle y, Ly \rangle}{\lambda_n} \geq \|y - \sum_{m=0}^{n-1} a_m y_m\|^2. \quad (4.96)$$

Since $\langle y, Ly \rangle$ is independent of n , and $\lambda_n \rightarrow \infty$, we have $\|y - \sum_{m=0}^{n-1} a_m y_m\|^2 \rightarrow 0$. Thus the eigenfunction expansion indeed converges to y , and does so faster than λ_n^{-1} goes to zero.

Our estimate of the rate of convergence applies only to the expansion of functions y for which $\langle y, Ly \rangle$ is defined — *i.e.* to functions $y \in \mathcal{D}(L)$. The domain $\mathcal{D}(L)$ is always a dense subset of the entire Hilbert space $L^2[a, b]$, however, and, since a dense subset of a dense subset is also dense in the larger space, we have shown that the linear span of the eigenfunctions is a dense subset of $L^2[a, b]$. Combining this observation with the alternative definition of completeness in 2.2.3, we see that the eigenfunctions do indeed form a complete orthonormal set. Any square integrable function therefore has a convergent expansion in terms of the y_m , but the rate of convergence may well be slower than that for functions $y \in \mathcal{D}(L)$.

Operator methods

Sometimes there are tricks for solving the eigenvalue problem.

Example: Quantum Harmonic Oscillator. Consider the operator

$$H = (-\partial_x + x)(\partial_x + x) + 1 = -\partial_x^2 + x^2. \quad (4.97)$$

This is in the form $Q^\dagger Q + 1$, where $Q = (\partial_x + x)$, and Q^\dagger is its formal adjoint. If we write these operators in the other order we have

$$QQ^\dagger = (\partial_x + x)(-\partial_x + x) = -\partial_x^2 + x^2 + 1 = H + 1. \quad (4.98)$$

Now, if ψ is an eigenfunction of $Q^\dagger Q$ with non-zero eigenvalue λ then $Q\psi$ is eigenfunction of QQ^\dagger with the same eigenvalue. This is because

$$Q^\dagger Q\psi = \lambda\psi \quad (4.99)$$

implies that

$$Q(Q^\dagger Q\psi) = \lambda Q\psi, \quad (4.100)$$

or

$$QQ^\dagger(Q\psi) = \lambda(Q\psi). \quad (4.101)$$

The only way that $Q\psi$ can fail to be an eigenfunction of QQ^\dagger is if it happens that $Q\psi = 0$, but this implies that $Q^\dagger Q\psi = 0$ and so the eigenvalue was zero. Conversely, if the eigenvalue *is* zero then

$$0 = \langle \psi, Q^\dagger Q\psi \rangle = \langle Q\psi, Q\psi \rangle, \quad (4.102)$$

and so $Q\psi = 0$. In this way, we see that $Q^\dagger Q$ and QQ^\dagger have exactly the same spectrum, with the possible exception of any zero eigenvalue.

Now notice that $Q^\dagger Q$ does have a zero eigenvalue because

$$\psi_0 = e^{-\frac{1}{2}x^2} \quad (4.103)$$

obeys $Q\psi_0 = 0$ and is normalizable. The operator QQ^\dagger , considered as an operator on $L^2[-\infty, \infty]$, does not have a zero eigenvalue because this would require $Q^\dagger\psi = 0$, and so

$$\psi = e^{+\frac{1}{2}x^2}, \quad (4.104)$$

which is not normalizable, and so not an element of $L^2[-\infty, \infty]$.

Since

$$H = Q^\dagger Q + 1 = QQ^\dagger - 1, \quad (4.105)$$

we see that ψ_0 is an eigenfunction of H with eigenvalue 1, and so an eigenfunction of QQ^\dagger with eigenvalue 2. Hence $Q^\dagger\psi_0$ is an eigenfunction of $Q^\dagger Q$ with eigenvalue 2 and so an eigenfunction H with eigenvalue 3. Proceeding in the way we find that

$$\psi_n = (Q^\dagger)^n \psi_0 \quad (4.106)$$

is an eigenfunction of H with eigenvalue $2n + 1$.

Since $Q^\dagger = -e^{\frac{1}{2}x^2} \partial_x e^{-\frac{1}{2}x^2}$, we can write

$$\psi_n(x) = H_n(x) e^{-\frac{1}{2}x^2}, \quad (4.107)$$

where

$$H_n(x) = (-1)^n e^{x^2} \frac{d^n}{dx^n} e^{-x^2} \quad (4.108)$$

are the *Hermite Polynomials*.

This is a useful technique for any second-order operator that can be factorized — and a surprising number of the equations for “special functions” can be. You will see it later, both in the exercises and in connection with Bessel functions.

Exercise 4.6: Show that we have found all the eigenfunctions and eigenvalues of $H = -\partial_x^2 + x^2$. Hint: Show that Q lowers the eigenvalue by 2 and use the fact that $Q^\dagger Q$ cannot have negative eigenvalues.

Exercise 4.7: Schrödinger equations of the form

$$-\frac{d^2\psi}{dx^2} - l(l+1)\operatorname{sech}^2 x \psi = E\psi$$

are known as *Pöschel-Teller equations*. By setting $u = l \tanh x$ and following the strategy of this problem one may relate solutions for l to those for $l-1$ and so find all bound states and scattering eigenfunctions for any integer l .

a) Suppose that we know that $\psi = \exp - \int^x u(x') dx'$ is a solution of

$$L\psi \equiv \left(-\frac{d^2}{dx^2} + W(x) \right) \psi = 0.$$

Show that L can be written as $L = M^\dagger M$ where

$$M = \left(\frac{d}{dx} + u(x) \right), \quad M^\dagger = \left(-\frac{d}{dx} + u(x) \right),$$

the adjoint being taken with respect to the product $\langle u, v \rangle = \int u^* v dx$.

- b) Now assume L is acting on functions on $[-\infty, \infty]$ and that we not have to worry about boundary conditions. Show that given an eigenfunction ψ_- obeying $M^\dagger M \psi_- = \lambda \psi_-$ we can multiply this equation on the left by M and so find a eigenfunction ψ_+ with the same eigenvalue for the differential operator

$$L' = MM^\dagger = \left(\frac{d}{dx} + u(x) \right) \left(-\frac{d}{dx} + u(x) \right)$$

and *vice-versa*. Show that this correspondence $\psi_- \leftrightarrow \psi_+$ will fail if, *and only if*, $\lambda = 0$.

- c) Apply the strategy from part b) in the case $u(x) = \tanh x$ and one of the two differential operators $M^\dagger M$, MM^\dagger is (up to an additive constant)

$$H = -\frac{d^2}{dx^2} - 2 \operatorname{sech}^2 x.$$

Show that H has eigenfunctions of the form $\psi_k = e^{ikx} P(\tanh x)$ and eigenvalue $E = k^2$ for any k in the range $-\infty < k < \infty$. The function $P(\tanh x)$ is a polynomial in $\tanh x$ which you should be able to find explicitly. By thinking about the exceptional case $\lambda = 0$, show that H has an eigenfunction $\psi_0(x)$, with eigenvalue $E = -1$, that tends rapidly to zero as $x \rightarrow \pm\infty$. Observe that there is no corresponding eigenfunction for the other operator of the pair.

4.3.2 Continuous spectrum

Rather than a give formal discussion, we will illustrate this subject with some examples drawn from quantum mechanics.

The simplest example is the free particle on the real line. We have

$$H = -\partial_x^2. \quad (4.109)$$

We eventually want to apply this to functions on the entire real line, but we will begin with the interval $[-L/2, L/2]$, and then take the limit $L \rightarrow \infty$

The operator H has formal eigenfunctions

$$\varphi_k(x) = e^{ikx}, \quad (4.110)$$

corresponding to eigenvalues $\lambda = k^2$. Suppose we impose periodic boundary conditions at $x = \pm L/2$:

$$\varphi_k(-L/2) = \varphi_k(+L/2). \quad (4.111)$$

This selects $k_n = 2\pi n/L$, where n is any positive, negative or zero integer, and allows us to find the normalized eigenfunctions

$$\chi_n(x) = \frac{1}{\sqrt{L}} e^{ik_n x}. \quad (4.112)$$

The completeness condition is

$$\sum_{n=-\infty}^{\infty} \frac{1}{L} e^{ik_n x} e^{-ik_n x'} = \delta(x - x'), \quad x, x' \in [-L/2, L/2]. \quad (4.113)$$

As L becomes large, the eigenvalues become so close that they can hardly be distinguished; hence the name *continuous spectrum*⁵, and the spectrum $\sigma(H)$ becomes the entire positive real line. In this limit, the sum on n becomes an integral

$$\sum_{n=-\infty}^{\infty} \left\{ \dots \right\} \rightarrow \int dn \left\{ \dots \right\} = \int dk \left(\frac{dn}{dk} \right) \left\{ \dots \right\}, \quad (4.114)$$

where

$$\frac{dn}{dk} = \frac{L}{2\pi} \quad (4.115)$$

is called the (momentum) density of states. If we divide this by L to get a density of states per unit length, we get an L independent “finite” quantity, the *local density of states*. We will often write

$$\frac{dn}{dk} = \rho(k). \quad (4.116)$$

If we express the density of states in terms of the eigenvalue λ then, by an abuse of notation, we have

$$\rho(\lambda) \equiv \frac{dn}{d\lambda} = \frac{L}{2\pi\sqrt{\lambda}}. \quad (4.117)$$

⁵When L is strictly infinite, $\varphi_k(x)$ is no longer normalizable. Mathematicians do not allow such un-normalizable functions to be considered as true eigenfunctions, and so a point in the continuous spectrum is not, to them, actually an eigenvalue. Instead, mathematicians say that a point λ lies in the continuous spectrum if for any $\epsilon > 0$ there exists an *approximate eigenfunction* φ_ϵ such that $\|\varphi_\epsilon\| = 1$, but $\|L\varphi_\epsilon - \lambda\varphi_\epsilon\| < \epsilon$. This is not a profitable definition for us. We will instead regard non-normalizable wavefunctions as being distributions.

Note that

$$\frac{dn}{d\lambda} = 2 \frac{dn}{dk} \frac{dk}{d\lambda}, \quad (4.118)$$

which looks a bit weird, but remember that *two* states, $\pm k_n$, correspond to the same λ and that the symbols

$$\frac{dn}{dk}, \quad \frac{dn}{d\lambda} \quad (4.119)$$

are ratios of measures, *i.e. Radon-Nykodym derivatives*, not ordinary derivatives.

In the $L \rightarrow \infty$ limit, the completeness condition becomes

$$\int_{-\infty}^{\infty} \frac{dk}{2\pi} e^{ik(x-x')} = \delta(x-x'), \quad (4.120)$$

and the length L has disappeared.

Suppose that we now apply boundary conditions $y = 0$ on $x = \pm L$. The normalized eigenfunctions are then

$$\chi_n = \sqrt{\frac{2}{L}} \sin k_n(x + L/2), \quad (4.121)$$

where $k_n = n\pi/L$. We see that the allowed k 's are twice as close together as they were with periodic boundary conditions, but now n is restricted to being a positive non-zero integer. The momentum density of states is therefore

$$\rho(k) = \frac{dn}{dk} = \frac{L}{\pi}, \quad (4.122)$$

which is twice as large as in the periodic case, but the eigenvalue density of states is

$$\rho(\lambda) = \frac{L}{2\pi\sqrt{\lambda}}, \quad (4.123)$$

which is exactly the same as before.

That the number of states per unit energy per unit volume does not depend on the boundary conditions at infinity makes physical sense: no local property of the sublunary realm should depend on what happens in the sphere of fixed stars. This point was not fully grasped by physicists,

however, until Rudolph Peierls⁶ explained that the quantum particle had to actually travel to the distant boundary and back before the precise nature of the boundary could be felt. This journey takes time T (depending on the particle's energy) and from the energy-time uncertainty principle, we can distinguish one boundary condition from another only by examining the spectrum with an energy resolution finer than \hbar/T . Neither the distance nor the nature of the boundary can affect the coarse details, such as the local density of states.

The dependence of the spectrum of a general differential operator on boundary conditions was investigated by Hermann Weyl. Weyl distinguished two classes of singular boundary points: *limit-circle*, where the spectrum depends on the choice of boundary conditions, and *limit-point*, where it does not. For the Schrödinger operator, the point at infinity, which is “singular” simply because it is at infinity, is in the limit-point class. We will discuss Weyl's theory of singular endpoints in chapter 8.

Phase-shifts

Consider the eigenvalue problem

$$\left(-\frac{d^2}{dr^2} + V(r)\right)\psi = E\psi \quad (4.124)$$

on the interval $[0, R]$, and with boundary conditions $\psi(0) = 0 = \psi(R)$. This problem arises when we solve the Schrödinger equation for a central potential in spherical polar coordinates, and assume that the wavefunction is a function of r only (*i.e.* S-wave, or $l = 0$). Again, we want the boundary at R to be infinitely far away, but we will start with R at a large but finite distance, and then take the $R \rightarrow \infty$ limit. Let us first deal with the simple case that $V(r) \equiv 0$; then the solutions are

$$\psi_k(r) \propto \sin kr, \quad (4.125)$$

with eigenvalue $E = k^2$, and with the allowed values of k being given by $k_n R = n\pi$. Since

$$\int_0^R \sin^2(k_n r) dr = \frac{R}{2}, \quad (4.126)$$

⁶Peierls was justifying why the phonon contribution to the specific heat of a crystal could be calculated by using periodic boundary conditions. Some sceptics thought that his calculation might be wrong by factors of two.

the normalized wavefunctions are

$$\psi_k = \sqrt{\frac{2}{R}} \sin kr, \quad (4.127)$$

and completeness reads

$$\sum_{n=1}^{\infty} \left(\frac{2}{R} \right) \sin(k_n r) \sin(k_n r') = \delta(r - r'). \quad (4.128)$$

As R becomes large, this sum goes over to an integral:

$$\begin{aligned} \sum_{n=1}^{\infty} \left(\frac{2}{R} \right) \sin(k_n r) \sin(k_n r') &\rightarrow \int_0^{\infty} dn \left(\frac{2}{R} \right) \sin(kr) \sin(kr'), \\ &= \int_0^{\infty} \frac{Rdk}{\pi} \left(\frac{2}{R} \right) \sin(kr) \sin(kr') \end{aligned} \quad (4.129)$$

Thus,

$$\left(\frac{2}{\pi} \right) \int_0^{\infty} dk \sin(kr) \sin(kr') = \delta(r - r'). \quad (4.130)$$

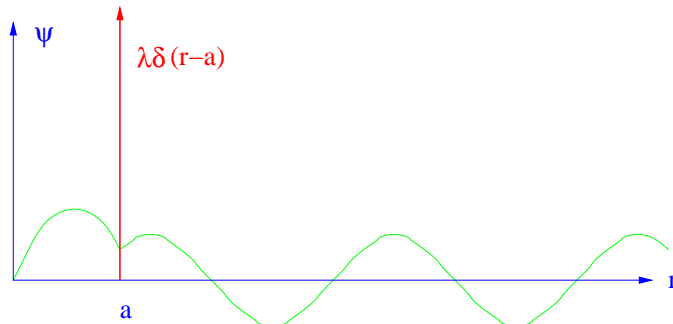
As before, the large distance, here R , no longer appears.

Now consider the more interesting problem which has the potential $V(r)$ included. We will assume, for simplicity, that there is an R_0 such that $V(r)$ is zero for $r > R_0$. In this case, we know that the solution for $r > R_0$ is of the form

$$\psi_k(r) = N_k \sin(kr + \eta(k)), \quad (4.131)$$

where the *phase shift* $\eta(k)$ is a functional of the potential V . The eigenvalue is still $E = k^2$.

Example: A delta-function shell. We take $V(r) = \lambda\delta(r - a)$.



Delta function shell potential.

A solution with eigenvalue $E = k^2$ and satisfying the boundary condition at $r = 0$ is

$$\psi(r) = \begin{cases} A \sin(kr), & r < a, \\ \sin(kr + \eta), & r > a. \end{cases} \quad (4.132)$$

The conditions to be satisfied at $r = a$ are:

- i) continuity, $\psi(a - \epsilon) = \psi(a + \epsilon) \equiv \psi(a)$, and
- ii) jump in slope, $-\psi'(a + \epsilon) + \psi'(a - \epsilon) + \lambda\psi(a) = 0$.

Therefore,

$$\frac{\psi'(a + \epsilon)}{\psi(a)} - \frac{\psi'(a - \epsilon)}{\psi(a)} = \lambda, \quad (4.133)$$

or

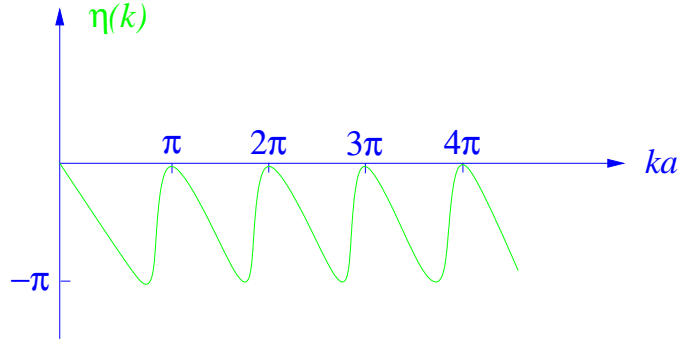
$$\frac{k \cos(ka + \eta)}{\sin(ka + \eta)} - \frac{k \cos(ka)}{\sin(ka)} = \lambda. \quad (4.134)$$

Thus,

$$\cot(ka + \eta) - \cot(ka) = \frac{\lambda}{k}, \quad (4.135)$$

and

$$\eta(k) = -ka + \cot^{-1} \left(\frac{\lambda}{k} + \cot ka \right). \quad (4.136)$$



Phase shift as a function of k .

The graph of $\eta(k)$ is shown in the figure. The allowed values of k are required by the boundary condition

$$\sin(kR + \eta(k)) = 0 \quad (4.137)$$

to satisfy

$$kR + \eta(k) = n\pi. \quad (4.138)$$

This is a transcendental equation for k , and so finding the individual solutions k_n is not simple. We can, however, write

$$n = \frac{1}{\pi} \left(kR + \eta(k) \right) \quad (4.139)$$

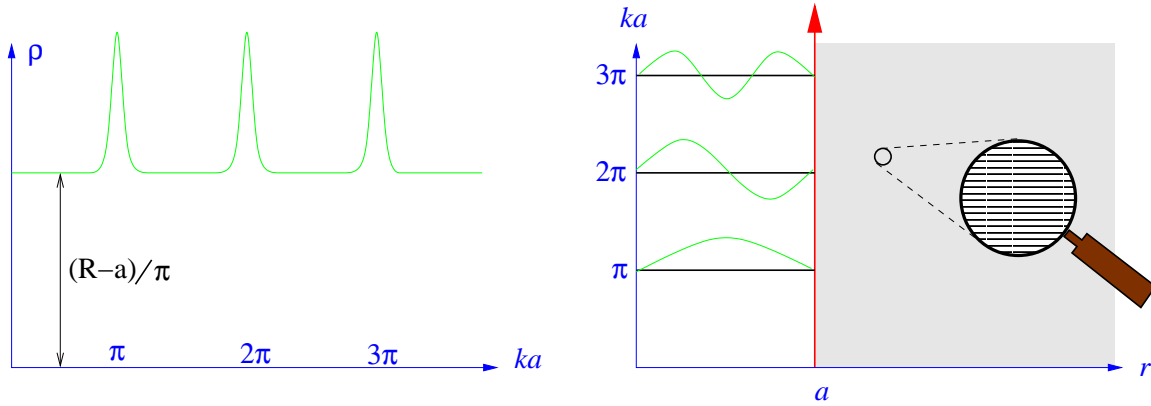
and observe that, when R becomes large, only an infinitesimal change in k is required to make n increment by unity. We may therefore regard n as a “continuous” variable which we can differentiate with respect to k to find

$$\frac{dn}{dk} = \frac{1}{\pi} \left\{ R + \frac{\partial \eta}{\partial k} \right\}. \quad (4.140)$$

The density of allowed k values is therefore

$$\rho(k) = \frac{1}{\pi} \left\{ R + \frac{\partial \eta}{\partial k} \right\}. \quad (4.141)$$

For our delta-shell example, a plot of $\rho(k)$ looks like



The density of states for a system with resonances. The extended states are so close in energy that we need an optical aid to resolve individual levels. The almost-bound resonance levels have to squeeze in between them.

which is understood as the resonant bound states at $ka = n\pi$ superposed on the background continuum density of states appropriate to a large box of length $(R - a)$. Each “spike” contains one extra state, so the average density

of states is that of a box of length R . We see that changing the potential does not create or destroy eigenstates, it just moves them around.

The spike is not exactly a delta function because of level repulsion between nearly degenerate eigenstates. The interloper elbows the nearby levels out of the way, and all the neighbours have to make do with a bit less room. The stronger the coupling between the states on either side of the delta-shell, the stronger is the inter-level repulsion, and the broader the resonance spike.

Normalization factor

We now evaluate

$$\int_0^R dr |\psi_k|^2 = N_k^{-2}, \quad (4.142)$$

so as to find the the normalized wavefunctions

$$\chi_k = N_k \psi_k. \quad (4.143)$$

Let $\psi_k(r)$ be a solution of

$$H\psi = \left(-\frac{d^2}{dr^2} + V(r) \right) \psi = k^2 \psi \quad (4.144)$$

satisfying the boundary condition $\psi_k(0) = 0$, but not necessarily the boundary condition at $r = R$. Such a solution exists for any k . We scale ψ_k by requiring that $\psi_k(r) = \sin(kr + \eta)$ for $r > R_0$. We now use Lagrange's identity to write

$$\begin{aligned} (k^2 - k'^2) \int_0^R dr \psi_k \psi_{k'} &= \int_0^R dr \{ (H\psi_k) \psi_{k'} - \psi_k (H\psi_{k'}) \} \\ &= [\psi_k \psi'_{k'} - \psi'_k \psi_{k'}]_0^R \\ &= \sin(kR + \eta) k' \cos(k'R + \eta) \\ &\quad - k \cos(kR + \eta) \sin(k'R + \eta). \end{aligned} \quad (4.145)$$

Here, we have used $\psi_{k,k'}(0) = 0$, so the integrated out part vanishes at the lower limit, and have used the explicit form of $\psi_{k,k'}$ at the upper limit.

Now differentiate with respect to k , and then set $k = k'$. We find

$$2k \int_0^R dr (\psi_k)^2 = -\frac{1}{2} \sin(2(kR + \eta)) + k \left\{ R + \frac{\partial \eta}{\partial k} \right\}. \quad (4.146)$$

In other words,

$$\int_0^R dr (\psi_k)^2 = \frac{1}{2} \left\{ R + \frac{\partial \eta}{\partial k} \right\} - \frac{1}{4k} \sin(2(kR + \eta)). \quad (4.147)$$

At this point, we impose the boundary condition at $r = R$. We therefore have $kR + \eta = n\pi$ and the last term on the right hand side vanishes. The final result for the normalization integral is therefore

$$\int_0^R dr |\psi_k|^2 = \frac{1}{2} \left\{ R + \frac{\partial \eta}{\partial k} \right\}. \quad (4.148)$$

Observe that the same expression occurs in both the density of states and the normalization integral.

The sum over the continuous spectrum in the completeness integral is therefore

$$\int_0^\infty dk \left(\frac{dn}{dk} \right) N_k^2 \psi_k(r) \psi_k(r') = \left(\frac{2}{\pi} \right) \int_0^\infty dk \psi_k(r) \psi_k(r'). \quad (4.149)$$

Both the density of states and the normalization factor have disappeared from the end result. This is a general feature of scattering problems: The completeness relation must give a delta function when evaluated far from the scatterer where the wavefunctions look like those of a free particle. So, provided we normalize ψ_k so that it reduces to a free particle wavefunction at large distance, the measure in the integral over k must also be the same as for the free particle.

Including any bound states in the discrete spectrum, the full statement of completeness is therefore

$$\sum_{\text{bound states}} \psi_n(r) \psi_n(r') + \left(\frac{2}{\pi} \right) \int_0^\infty dk \psi_k(r) \psi_k(r') = \delta(r - r'). \quad (4.150)$$

Example: We will exhibit a completeness relation for a problem on the entire real line. We have already met the Pöschel-Teller equation,

$$H\psi = \left(-\frac{d^2}{dx^2} - l(l+1) \operatorname{sech}^2 x \right) \psi = E\psi \quad (4.151)$$

in exercise 4.7. When l is an integer, the potential in this Schrödinger equation has the special property that it is reflectionless.

The simplest non-trivial example is $l = 1$. In this case, H has a single discrete bound state at $E_0 = -1$. The normalized eigenfunction is

$$\psi_0(x) = \frac{1}{\sqrt{2}} \operatorname{sech} x. \quad (4.152)$$

The rest of the spectrum consists of a continuum of unbound states with eigenvalues $E(k) = k^2$ and eigenfunctions

$$\psi_k(x) = \frac{1}{\sqrt{1+k^2}} e^{ikx} (-ik + \tanh x). \quad (4.153)$$

Here, k is any real number. The normalization of $\psi_k(x)$ has been chosen so that, at large $|x|$, where $\tanh x \rightarrow \pm 1$, we have

$$\psi_k^*(x) \psi_k(x') \rightarrow e^{-ik(x-x')}. \quad (4.154)$$

The measure in the completeness integral must therefore be $dk/2\pi$, the same as that for a free particle.

Let us compute the difference

$$\begin{aligned} I &= \delta(x-x') - \int_{-\infty}^{\infty} \frac{dk}{2\pi} \psi_k^*(x) \psi_k(x') \\ &= \int_{-\infty}^{\infty} \frac{dk}{2\pi} (e^{-ik(x-x')} - \psi_k^*(x) \psi_k(x')) \\ &= \int_{-\infty}^{\infty} \frac{dk}{2\pi} e^{-ik(x-x')} \frac{1 + ik(\tanh x - \tanh x') - \tanh x \tanh x'}{1 + k^2}. \end{aligned} \quad (4.155)$$

We use the standard result,

$$\int_{-\infty}^{\infty} \frac{dk}{2\pi} e^{-ik(x-x')} \frac{1}{1+k^2} = \frac{1}{2} e^{-|x-x'|}, \quad (4.156)$$

together with its x' derivative,

$$\int_{-\infty}^{\infty} \frac{dk}{2\pi} e^{-ik(x-x')} \frac{ik}{1+k^2} = \operatorname{sgn}(x-x') \frac{1}{2} e^{-|x-x'|}, \quad (4.157)$$

to find

$$I = \frac{1}{2} \left\{ 1 + \operatorname{sgn}(x-x')(\tanh x - \tanh x') - \tanh x \tanh x' \right\} e^{-|x-x'|}. \quad (4.158)$$

Assume, without loss of generality, that $x > x'$; then this reduces to

$$\begin{aligned} \frac{1}{2}(1 + \tanh x)(1 - \tanh x')e^{-(x-x')} &= \frac{1}{2}\operatorname{sech} x \operatorname{sech} x' \\ &= \psi_0(x)\psi_0(x'). \end{aligned} \quad (4.159)$$

Thus, the expected completeness condition

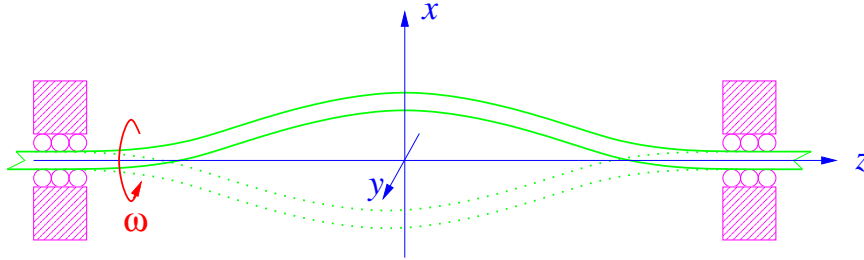
$$\psi_0(x)\psi_0(x') + \int_{-\infty}^{\infty} \frac{dk}{2\pi} \psi_k^*(x)\psi_k(x') = \delta(x - x'), \quad (4.160)$$

is confirmed.

4.4 Exercises and Problems

We begin with a practical engineering eigenvalue problem.

Exercise 4.8: Whirling drive shaft. A thin flexible drive shaft is supported by two bearings that impose the conditions $x' = y' = x = y = 0$ at $z = \pm L$. Here $x(z)$, $y(z)$ denote the transverse displacements of the shaft, and the primes denote derivatives with respect to z .



The $n = 1$ even-parity mode of a whirling shaft.

The shaft is driven at angular velocity ω . Experience shows that at certain critical frequencies ω_n the motion becomes unstable to *whirling* — a spontaneous vibration and deformation of the normally straight shaft. If the rotation frequency is raised above ω_n , the shaft becomes quiescent and straight again until we reach ω_{n+1} , at which frequency the pattern is repeated. Our task is to understand why this happens.

The kinetic energy of the whirling shaft is

$$E_k = \frac{1}{2} \int_{-L}^L \rho \{\dot{x}^2 + \dot{y}^2\} dz,$$

and the strain energy due to bending is

$$V[x, y] = \frac{1}{2} \int_{-L}^L \gamma \{ (x'')^2 + (y'')^2 \} dz.$$

- a) Write down the Lagrangian, and from it obtain the equations of motion for the shaft.
- b) Seek whirling-mode solutions of the equations of motion in the form

$$\begin{aligned} x(z, t) &= \psi(z) \cos \omega t, \\ y(z, t) &= \psi(z) \sin \omega t. \end{aligned}$$

Show that this quest requires the solution of the eigenvalue problem

$$\frac{\gamma}{\rho} \frac{d^4 \psi}{dz^4} = \omega_n^2 \psi, \quad \psi'(-L) = \psi(-L) = \psi'(L) = \psi(L) = 0.$$

- c) Show that the critical frequencies are given in terms of the solutions ξ_n to the transcendental equation

$$\tanh \xi_n = \pm \tan \xi_n, \quad (\star)$$

as

$$\omega_n = \sqrt{\frac{\gamma}{\rho}} \left(\frac{\xi_n}{L} \right)^2,$$

Show that the plus sign in \star applies to *odd* parity modes, where $\psi(z) = -\psi(-z)$, and the minus sign to *even* parity modes where $\psi(z) = \psi(-z)$.

Whirling, we conclude, occurs at the frequencies of the natural transverse vibration modes of the elastic shaft. These modes are excited by slight imbalances that have negligible effect except when the shaft is being rotated at the resonant frequency.

Insight into adjoint boundary conditions for an ODE can be obtained by thinking about how we would impose these boundary conditions in a numerical solution. The next exercise explores this.

Exercise 4.9: Discrete approximations and self-adjointness. Consider the second order inhomogeneous equation $Lu \equiv u'' = g(x)$ on the interval $0 \leq x \leq 1$. Here $g(x)$ is known and $u(x)$ is to be found. We wish to solve the problem on a computer, and so set up a discrete approximation to the ODE in the following way:

- replace the continuum of independent variables $0 \leq x \leq 1$ by the discrete lattice of points $0 \leq x_n \equiv (n - \frac{1}{2})/N \leq 1$. Here N is a positive integer and $n = 1, 2, \dots, N$;
- replace the functions $u(x)$ and $g(x)$ by the arrays of real variables $u_n \equiv u(x_n)$ and $g_n \equiv g(x_n)$;
- replace the continuum differential operator d^2/dx^2 by the difference operator \mathcal{D}^2 , defined by $\mathcal{D}^2 u_n \equiv u_{n+1} - 2u_n + u_{n-1}$.

Now do the following problems:

- Impose continuum Dirichlet boundary conditions $u(0) = u(1) = 0$. Decide what these correspond to in the discrete approximation, and write the resulting set of algebraic equations in matrix form. Show that the corresponding matrix is real and symmetric.
- Impose the periodic boundary conditions $u(0) = u(1)$ and $u'(0) = u'(1)$, and show that these require us to set $u_0 \equiv u_N$ and $u_{N+1} \equiv u_1$. Again write the system of algebraic equations in matrix form and show that the resulting matrix is real and symmetric.
- Consider the non-symmetric N -by- N matrix operator

$$D^2 u = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & \dots & 0 \\ 1 & -2 & 1 & 0 & 0 & \dots & 0 \\ 0 & 1 & -2 & 1 & 0 & \dots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots \\ 0 & \dots & 0 & 1 & -2 & 1 & 0 \\ 0 & \dots & 0 & 0 & 1 & -2 & 1 \\ 0 & \dots & 0 & 0 & 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} u_N \\ u_{N-1} \\ u_{N-2} \\ \vdots \\ u_3 \\ u_2 \\ u_1 \end{pmatrix}.$$

- What vectors span the null space of D^2 ?
- To what continuum boundary conditions for d^2/dx^2 does this matrix correspond?
- Consider the matrix $(D^2)^\dagger$. To what continuum boundary conditions does this matrix correspond? Are they the adjoint boundary conditions for the differential operator in part ii)?

Exercise 4.10: Consider the eigenvalue problem for the one-dimensional Dirac Hamiltonian on the half-line:

$$H\Psi \equiv \begin{pmatrix} -i\partial_x & m \\ m & i\partial_x \end{pmatrix} \begin{pmatrix} \psi_1 \\ \psi_2 \end{pmatrix} = E \begin{pmatrix} \psi_1 \\ \psi_2 \end{pmatrix}, \quad x > 0.$$

Show that the boundary condition

$$\frac{\psi_1(0)}{\psi_2(0)} = e^{i\theta},$$

where θ is a real number, makes H into a self-adjoint operator.

Here are three further problems involving the completeness of operators with a continuous spectrum:

Exercise 4.11: Missing State. In exercise 4.7 you will have found that the Schrödinger equation

$$\left(-\frac{d^2}{dx^2} - 2 \operatorname{sech}^2 x\right) \psi = E \psi$$

has eigensolutions

$$\psi_k(x) = e^{ikx}(-ik + \tanh x)$$

with eigenvalue $E = k^2$.

- For x large and positive $\psi_k(x) \approx A e^{ikx} e^{i\eta(k)}$, while for x large and negative $\psi_k(x) \approx A e^{ikx} e^{-i\eta(k)}$, the (complex) constant A being the same in both cases. Express the phase shift $\eta(k)$ as the inverse tangent of an algebraic expression in k .
- Impose periodic boundary conditions $\psi(-L/2) = \psi(+L/2)$ where $L \gg 1$. Find the allowed values of k and hence an explicit expression for the k -space density, $\rho(k) = \frac{dn}{dk}$, of the eigenstates.
- Compare your formula for $\rho(k)$ with the corresponding expression, $\rho_0(k) = L/2\pi$, for the eigenstate density of the zero-potential equation and compute the integral

$$\Delta N = \int_{-\infty}^{\infty} \{\rho(k) - \rho_0(k)\} dk.$$

- Deduce that one eigenfunction has gone missing from the continuum and become the localized bound state $\psi_0(x) = \frac{1}{\sqrt{2}} \operatorname{sech} x$.

Exercise 4.12: Continuum Completeness. Consider the differential operator

$$\hat{L} = -\frac{d^2}{dx^2}, \quad 0 \leq x < \infty$$

with self-adjoint boundary conditions $\psi(0)/\psi'(0) = \tan \theta$ for some fixed angle θ .

- Show that when $\tan \theta < 0$ there is a single normalizable negative-eigenvalue eigenfunction localized near the origin, but none when $\tan \theta > 0$.

- Show that there is a continuum of positive-eigenvalue eigenfunctions of the form $\psi_k(x) = \sin(kx + \eta(k))$ where the phase shift η is found from

$$e^{i\eta(k)} = \frac{1 + ik \tan \theta}{\sqrt{1 + k^2 \tan^2 \theta}}.$$

- Write down (no justification required) the appropriate completeness relation

$$\delta(x - x') = \int \frac{dn}{dk} N_k^2 \psi_k(x) \psi_k(x') dk + \sum_{\text{bound}} \psi_n(x) \psi_n(x')$$

with an explicit expression for the product (not the separate factors) of the density of states and the normalization constant N_k^2 , and with the correct limits on the integral over k .

- Confirm that the ψ_k continuum on its own, or together with the bound state when it exists, form a complete set. You will do this by evaluating the integral

$$I(x, x') = \frac{2}{\pi} \int_0^\infty \sin(kx + \eta(k)) \sin(kx' + \eta(k)) dk$$

and interpreting the result. You will need the following standard integral

$$\int_{-\infty}^\infty \frac{dk}{2\pi} e^{ikx} \frac{1}{1 + k^2 t^2} = \frac{1}{2|t|} e^{-|x|/|t|}.$$

Take care! You should monitor how the bound state contribution switches on and off as θ is varied. Keeping track of the modulus signs $|\dots|$ in the standard integral is essential for this.

Exercise 4.13: Levinson's Theorem and the Friedel sum rule. The interaction between an attractive impurity and (S -wave, and ignoring spin) electrons in a metal can be modelled by a one-dimensional Schrödinger equation

$$-\frac{d^2\chi}{dr^2} + V(r)\chi = k^2\chi.$$

Here r is the distance away from the impurity and $V(r)$ is the (spherically symmetric) impurity potential and $\chi(r) = \sqrt{4\pi r} \psi(r)$ where $\psi(r)$ is the three-dimensional wavefunction. The impurity attracts electrons to its vicinity. Let $\chi_k^0(r) = \sin(kr)$ denote the unperturbed wavefunction, and $\chi_k(r)$ denote the perturbed wavefunction that beyond the range of impurity potential becomes $\sin(kr + \eta(k))$.

- Show that the continuous-spectrum contribution to the change in the number of electrons within a sphere of radius R surrounding the impurity is given by

$$\frac{2}{\pi} \int_0^{k_f} \left(\int_0^R \{ |\chi_k(x)|^2 - |\chi_k^0(x)|^2 \} dr \right) dk = \frac{1}{\pi} [\eta(k_f) - \eta(0)] + \text{oscillations}.$$

Here k_f is the Fermi momentum, and “oscillations” refers to *Friedel oscillations* $\approx \cos(2(k_f R + \eta))$. You should write down an explicit expression for the Friedel oscillation term, and recognize it as the Fourier transform of a function $\propto k^{-1} \sin \eta(k)$.

- Appeal to the Riemann-Lebesgue lemma to argue that the Friedel density oscillations make no contribution to the accumulated electron number in the limit $R \rightarrow \infty$.

(Hint: You may want to look ahead to the next part of the problem in order to show that $k^{-1} \sin \eta(k)$ remains finite as $k \rightarrow 0$.)

The impurity-induced change in the number of unbound electrons in the interval $[0, R]$ is generically some fraction of an electron, and, in the case of an attractive potential, can be *negative* — the phase-shift being positive and decreasing steadily to zero as k increases to infinity. This should not be surprising. Each electron in the Fermi sea speeds up as it enters an attractive potential well, spends less time there, and so makes a smaller contribution to the average local density than it would in the absence of the potential. We would, however, surely expect an attractive potential to accumulate a net *positive* number of electrons.

- Show that a negative continuous-spectrum contribution to the accumulated electron number is more than compensated for by a positive number

$$N_{\text{bound}} = \int_0^\infty (\rho_0(k) - \rho(k)) dk = - \int_0^\infty \frac{1}{\pi} \frac{\partial \eta}{\partial k} dk = \frac{1}{\pi} \eta(0).$$

of electrons bound to the potential. After accounting for these bound electrons, show that the total number of electrons accumulated near the impurity is

$$Q_{\text{tot}} = \frac{1}{\pi} \eta(k_f).$$

This formula (together its higher angular momentum versions) is known as the *Friedel sum rule*. The relation between $\eta(0)$ and the number of bound states is called *Levinson's theorem*. A more rigorous derivation of this theorem would show that $\eta(0)$ may take the value $(n + 1/2)\pi$ when there is a non-normalizable zero-energy “half-bound” state. In this exceptional case the accumulated charge will depend on R .

Chapter 5

Green Functions

In this chapter we will study strategies for solving the inhomogeneous linear differential equation $Ly = f$. The tool we use is the *Green function*, which is an integral kernel representing the inverse operator L^{-1} . Apart from their use in solving inhomogeneous equations, Green functions play an important role in many areas of physics.

5.1 Inhomogeneous Linear equations

We wish to solve $Ly = f$ for y . Before we set about doing this, we should ask ourselves whether a solution *exists*, and, if it does, whether it is *unique*. The answers to these questions are summarized by the *Fredholm alternative*.

5.1.1 Fredholm alternative

The Fredholm alternative for operators on a finite-dimensional vector space is discussed in detail in the appendix on linear algebra. You will want to make sure that you have read and understood this material. Here, we merely restate the results.

Let V be finite-dimensional vector space, and A be a linear operator $A : V \rightarrow V$ on this space. Then

I. **Either**

i) $Ax = b$ has a *unique* solution,

or

ii) $Ax = 0$ has a non-trivial solution.

- II. If $Ax = 0$ has n linearly independent solutions, then so does $A^\dagger x = 0$.
- III. If alternative ii) holds, then $Ax = b$ has *no* solution unless b is perpendicular to all solutions of $A^\dagger x = 0$.

What is important for us in the present chapter is that this result continues to hold for linear differential operators L on a finite interval — provided that we define L^\dagger as in the previous chapter, *and provided the number of boundary conditions is equal to the order of the equation*.

If the number of boundary conditions is *not* equal to the order of the equation then the number of solutions to $Ly = 0$ and $L^\dagger y = 0$ will differ in general. It is still true, however, that $Ly = f$ has *no* solution unless f is perpendicular to all solutions of $L^\dagger y = 0$.

Example: Let

$$Ly = \frac{dy}{dx}, \quad y(0) = y(1) = 0. \quad (5.1)$$

Clearly $Ly = 0$ has only the trivial solution $y \equiv 0$. If a solution to $Ly = f$ exists, therefore, it will be unique.

We know that $L^\dagger = -\frac{dy}{dx}$, with *no* boundary conditions on the functions in its domain. The equation $L^\dagger y = 0$ therefore has the non-trivial solution $y = 1$. This means that there is no solution to $Ly = f$ unless

$$\langle 1, f \rangle = \int_0^1 f \, dx = 0. \quad (5.2)$$

If this condition is satisfied then

$$y(x) = \int_0^x f(x) \, dx \quad (5.3)$$

satisfies both the differential equation and the boundary conditions at $x = 0, 1$. If this condition is not satisfied, $y(x)$ is not a solution, because $y(1) \neq 0$.

Initially we will discuss only solutions of $Ly = f$ with homogeneous boundary conditions. After we have understood how to do this, we will extend our methods to deal with differential equations with inhomogeneous boundary conditions.

5.2 Constructing Green Functions

We wish to solve $Ly = f$, a differential equation with homogeneous boundary conditions, by finding an inverse operator L^{-1} , so that $y = L^{-1}f$. This inverse

operator L^{-1} will be represented by an integral kernel

$$(L^{-1})_{x,y} = G(x, y), \quad (5.4)$$

with the property

$$L_x G(x, y) = \delta(x - y). \quad (5.5)$$

Here, the subscript x on L indicates that L acts on the first argument of G . Then

$$y(x) = \int G(x, y) f(y) dy \quad (5.6)$$

will obey

$$L_x y = \int L_x G(x, y) f(y) dy = \int \delta(x - y) f(y) dy = f(x). \quad (5.7)$$

The problem is how to construct $G(x, y)$. There are three necessary ingredients:

- the function $\chi(x) \equiv G(x, y)$ must have some discontinuous behaviour at $x = y$ in order to generate the delta function;
- away from $x = y$, the function $\chi(x)$ must obey $L\chi = 0$;
- the function $\chi(x)$ must obey the homogeneous boundary conditions required of y at the ends of the interval.

The last ingredient ensures that the resulting solution, $y(x)$, obeys the boundary conditions. It also ensures that the range of the integral operator, G , coincides with the domain of L , a prerequisite if the product $LG = I$ is to make sense. The manner in which these ingredients are assembled to construct $G(x, y)$ is best explained through examples.

5.2.1 Sturm-Liouville equation

We want to find a function $G(x, x')$ such that $\chi(x) = G(x, x')$ obeys

$$L\chi = (p\chi')' + q\chi = \delta(x - x'), \quad (5.8)$$

The function $\chi(x)$ must also obey the homogeneous boundary conditions that are to be imposed on the solutions of $Ly = f$.

Now (5.8) tells us that $\chi(x)$ must be continuous at $x = x'$. For if not, the two differentiations applied to a jump function would give us the derivative of a delta function, and we want only a plain $\delta(x - x')$. If we write

$$G(x, x') = \begin{cases} Ay_L(x)y_R(x'), & x < x', \\ Ay_L(x')y_R(x), & x > x', \end{cases} \quad (5.9)$$

then $\chi(x) = G(x, x')$ is automatically continuous at $x = x'$. We take $y_L(x)$ to be a solution of $Ly = 0$, chosen to satisfy the boundary condition at the left hand end of the interval. Similarly y_R should solve $Ly = 0$ and satisfy the boundary condition at the right hand end. With these choices we satisfy (5.8) at all points away from $x = x'$.

To figure out how to satisfy the equation exactly *at* the location of the delta-function, we integrate (5.8) from $x' - \varepsilon$ to $x' + \varepsilon$ and find that

$$[p\chi']_{x'-\varepsilon}^{x'+\varepsilon} = 1 \quad (5.10)$$

This determines the constant A *via*

$$Ap(x') \left(y_L(x') y_R'(x') - y_L'(x') y_R(x') \right) = 1. \quad (5.11)$$

We recognize the Wronskian $W(y_L, y_R; x')$ on the left hand side of this equation. We therefore have

$$G(x, x') = \begin{cases} \frac{1}{Wp} y_L(x) y_R(x'), & x < x', \\ \frac{1}{Wp} y_L(x') y_R(x), & x > x'. \end{cases} \quad (5.12)$$

Now, for the Sturm-Liouville equation, the product pW is constant. This follows from Liouville's formula,

$$W(x) = W(0) \exp \left\{ - \int_0^x \left(\frac{p_1}{p_0} \right) dx' \right\}, \quad (5.13)$$

and from $p_1 = p'_0 = p'$ in the Sturm-Liouville equation. Thus

$$W(x) = W(0) \exp \left(- \ln(p(x)/p(0)) \right) = W(0) \frac{p(0)}{p(x)}. \quad (5.14)$$

The constancy of pW means that $G(x, x')$ is symmetric:

$$G(x, x') = G(x', x). \quad (5.15)$$

This is as it should be. The inverse of a symmetric matrix (and the real, self-adjoint, Sturm-Liouville operator is the function-space analogue of a real symmetric matrix) is itself symmetric.

The solution to

$$Ly = (p_0 y')' + qy = f(x) \quad (5.16)$$

is therefore

$$y(x) = \frac{1}{W_p} \left\{ y_L(x) \int_x^b y_R(x') f(x') dx' + y_R(x) \int_a^x y_L(x') f(x') dx' \right\}. \quad (5.17)$$

Take care to understand the ranges of integration in this formula. In the first integral $x' > x$ and we use $G(x, x') \propto y_L(x) y_R(x')$. In the second integral $x' < x$ and we use $G(x, x') \propto y_L(x') y_R(x)$. It is easy to get these the wrong way round.

Because we must divide by it in constructing $G(x, x')$, it is necessary that the Wronskian $W(y_L, y_R)$ not be zero. This is reasonable. If W were zero then $y_L \propto y_R$, and the single function y_R satisfies both $Ly_R = 0$ and the boundary conditions. This means that the differential operator L has y_R as a zero-mode, so there can be no unique solution to $Ly = f$.

Example: Solve

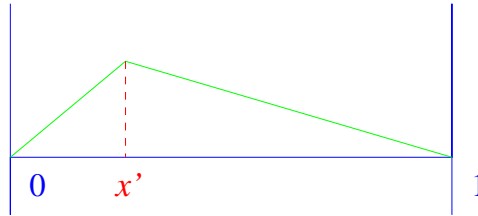
$$-\partial_x^2 y = f(x), \quad y(0) = y(1) = 0. \quad (5.18)$$

We have

$$\left. \begin{array}{l} y_L = x \\ y_R = 1 - x \end{array} \right\} \Rightarrow y'_L y_R - y_L y'_R \equiv 1. \quad (5.19)$$

We find that

$$G(x, x') = \begin{cases} x(1 - x'), & x < x', \\ x'(1 - x), & x > x', \end{cases} \quad (5.20)$$



The function $\chi(x) = G(x, x')$.

and

$$y(x) = (1 - x) \int_0^x x' f(x') dx' + x \int_x^1 (1 - x') f(x') dx'. \quad (5.21)$$

5.2.2 Initial-value problems

Initial value problems are those boundary-value problems where all boundary conditions are imposed at one end of the interval, instead of some conditions

at one end and some at the other. The same set of ingredients go into constructing the Green function, though.

Consider the problem

$$\frac{dy}{dt} - Q(t)y = F(t), \quad y(0) = 0. \quad (5.22)$$

We seek a Green function such that

$$L_t G(t, t') \equiv \left(\frac{d}{dt} - Q(t) \right) G(t, t') = \delta(t - t') \quad (5.23)$$

and $G(0, t') = 0$.

We need $\chi(t) = G(t, t')$ to satisfy $L_t \chi = 0$, except at $t = t'$ and need $G(0, t') = 0$. The unique solution of $L_t \chi = 0$ with $\chi(0) = 0$ is $\chi(t) \equiv 0$. This means that $G(t, 0) = 0$ for all $t < t'$. Near $t = t'$ we need

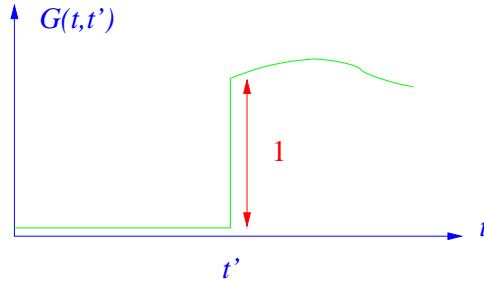
$$G(t' + \varepsilon, t') - G(t' - \varepsilon, t') = 1 \quad (5.24)$$

The unique solution is

$$G(t, t') = \theta(t - t') \exp \left\{ \int_{t'}^t Q(s) ds \right\}, \quad (5.25)$$

where $\theta(t - t')$ is the Heaviside step function

$$\theta(t) = \begin{cases} 0, & t < 0, \\ 1, & t > 0. \end{cases} \quad (5.26)$$



The Green function $G(t, t')$ for the first-order initial value problem .

Therefore

$$\begin{aligned}
 y(t) &= \int_0^\infty G(t, t') F(t') dt', \\
 &= \int_0^t \exp \left\{ \int_{t'}^t Q(s) ds \right\} F(t') dt' \\
 &= \exp \left\{ \int_0^t Q(s) ds \right\} \int_0^t \exp \left\{ - \int_0^{t'} Q(s) ds \right\} F(t') dt'. \quad (5.27)
 \end{aligned}$$

In chapter 3 we solved this problem by the method of variation of parameters.
Example: Forced, Damped, Harmonic Oscillator. An oscillator obeys the equation

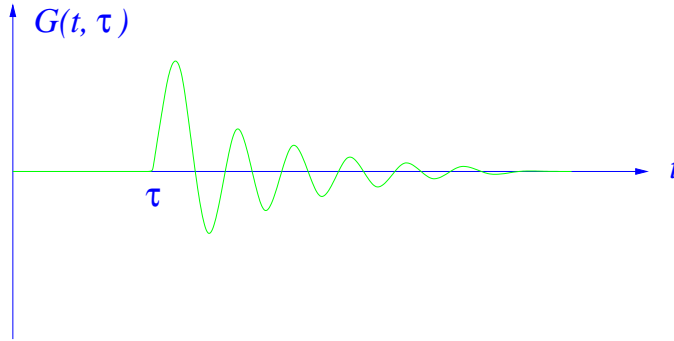
$$\ddot{x} + 2\gamma\dot{x} + (\Omega^2 + \gamma^2)x = F(t). \quad (5.28)$$

Here $\gamma > 0$ is the friction coefficient. Assuming that the oscillator is at rest at the origin at $t = 0$, we show that

$$x(t) = \left(\frac{1}{\Omega} \right) \int_0^t e^{-\gamma(t-\tau)} \sin \Omega(t-\tau) F(\tau) d\tau. \quad (5.29)$$

We seek a Green function $G(t, \tau)$ such that $\chi(t) = G(t, \tau)$ obeys $\chi(0) = \chi'(0) = 0$. Again, the unique solution of the differential equation with this initial data is $\chi(t) \equiv 0$. The Green function must be continuous at $t = \tau$, but its derivative must be discontinuous there, jumping from zero to unity to provide the delta function. Thereafter, it must satisfy the homogeneous equation. The unique function satisfying all these requirements is

$$G(t, \tau) = \theta(t - \tau) \frac{1}{\Omega} e^{-\gamma(t-\tau)} \sin \Omega(t - \tau). \quad (5.30)$$



The Green function $G(t, \tau)$ for the damped oscillator problem .

Both these initial-value Green functions $G(t, t')$ are identically zero when $t < t'$. This is because the Green function is the response of the system to a kick at time $t = t'$, and in physical problems, no effect comes before its cause. Such Green functions are said to be *causal*.

Physics application: friction without friction — The Caldeira-Leggett Model in Real Time.

This is an application of the initial-value problem Green function we found in the preceding example.

When studying the quantum mechanics of systems with friction, such as the viscously damped oscillator of the previous example, we need a tractable model of the dissipative process. Such a model was introduced by Caldeira and Leggett¹. They consider the Lagrangian

$$L = \frac{1}{2} \left(\dot{Q}^2 - (\Omega^2 - \Delta\Omega^2) Q^2 \right) - Q \sum_i f_i q^i + \sum_i \frac{1}{2} (\dot{q}_i^2 - \omega_i^2 q_i^2) \quad (5.31)$$

which describes a macroscopic variable $Q(t)$, linearly coupled to an *oscillator bath* of very many simple systems q_i representing the environment. The quantity

$$\Delta\Omega^2 \stackrel{\text{def}}{=} - \sum_i \left(\frac{f_i^2}{\omega_i^2} \right), \quad (5.32)$$

is a counter-term which is inserted cancel the frequency shift

$$\Omega^2 \rightarrow \Omega^2 - \sum_i \left(\frac{f_i^2}{\omega_i^2} \right), \quad (5.33)$$

caused by the coupling to the bath².

¹A. Caldeira, A. J. Leggett, Physical Review Letters **46** (1981) 211.

²The shift arises because a static Q displaces the bath oscillators so that $f_i q_i = -(f_i^2/\omega_i^2)Q$. Substituting these values for the $f_i q_i$ into the potential terms shows that, in the absence of ΔQ^2 , the effective potential seen by Q would be

$$\frac{1}{2} \Omega^2 Q^2 + \sum_i f_i q^i + \frac{1}{2} \omega_i^2 q_i^2 = \frac{1}{2} \left(\Omega^2 - \sum_i \left(\frac{f_i^2}{\omega_i^2} \right) \right) Q^2.$$

The equations of motion are

$$\begin{aligned}\ddot{Q} + (\Omega^2 - \Delta\Omega^2)Q + \sum_i f_i q_i &= 0, \\ \ddot{q}_i + \omega_i^2 q_i + f_i Q &= 0.\end{aligned}\tag{5.34}$$

Using our initial value Green function, we solve for the q_i in terms of $Q(t)$

$$f_i q_i = - \int_{-\infty}^t \left(\frac{f_i^2}{\omega_i} \right) \sin \omega_i(t - \tau) Q(\tau) d\tau.\tag{5.35}$$

The resulting motion of the q_i feeds back into the equation for Q to give

$$\ddot{Q} + (\Omega^2 - \Delta\Omega^2)Q + \int_{-\infty}^t F(t - \tau) Q(\tau) d\tau = 0,\tag{5.36}$$

where

$$F(t) = - \sum_i \left(\frac{f_i^2}{\omega_i} \right) \sin(\omega_i t)\tag{5.37}$$

is a *memory function*.

It is now convenient to introduce a *spectral function*

$$J(\omega) = \frac{\pi}{2} \sum_i \left(\frac{f_i^2}{\omega_i} \right) \delta(\omega - \omega_i),\tag{5.38}$$

in terms of which we can write

$$F(t) = -\frac{2}{\pi} \int_0^\infty J(\omega) \sin(\omega t) d\omega.\tag{5.39}$$

Although $J(\omega)$ is defined as a sum of delta function spikes, the oscillator bath contains a very large number of systems and this makes $J(\omega)$ effectively a smooth function. This is just as the density of a gas (a sum of delta functions at the location of the atoms) is macroscopically smooth. By taking different forms for $J(\omega)$ we can represent a wide range of environments. Caldeira and Leggett show that to obtain a friction force proportional to \dot{Q} we should make $J(\omega)$ proportional to the frequency ω . To see how this works, consider

$$J(\omega) = \eta \omega \left[\frac{\Lambda^2}{\Lambda^2 + \omega^2} \right],\tag{5.40}$$

where Λ is a high-frequency cutoff introduced to make the integrals over ω converge. With this choice

$$\frac{2}{\pi} \int_0^\infty J(\omega) \sin(\omega t) d\omega = \frac{2}{2\pi i} \int_{-\infty}^\infty \frac{\eta \omega \Lambda^2 e^{i\omega t}}{\Lambda^2 + \omega^2} d\omega = \text{sgn}(t) \eta \Lambda^2 e^{-\Lambda|t|}. \quad (5.41)$$

Therefore,

$$\begin{aligned} \int_{-\infty}^t F(t-\tau) Q(\tau) d\tau &= - \int_{-\infty}^t \eta \Lambda^2 e^{-\Lambda|t-\tau|} Q(\tau) d\tau \\ &= -\eta \Lambda Q(t) + \eta \dot{Q}(t) - \frac{\eta}{2\Lambda} \ddot{Q}(t) + \dots, \end{aligned} \quad (5.42)$$

where the second line results from expanding $Q(\tau)$ as Taylor series

$$Q(\tau) = Q(t) + (\tau - t) \dot{Q}(t) + \dots, \quad (5.43)$$

and integrating term-by-term. Now,

$$-\Delta \Omega^2 \equiv \sum_i \left(\frac{f_i^2}{\omega_i^2} \right) = \frac{2}{\pi} \int_0^\infty \frac{J(\omega)}{\omega} d\omega = \frac{2}{\pi} \int_0^\infty \frac{\eta \Lambda^2}{\Lambda^2 + \omega^2} d\omega = \eta \Lambda. \quad (5.44)$$

The $-\Delta \Omega^2 Q$ counterterm thus cancels the leading $-\eta \Lambda Q(t)$ in (5.42), which would otherwise represent a Λ -dependent frequency shift. After this cancellation we can safely let $\Lambda \rightarrow \infty$, and so ignore terms with negative powers of the cutoff. The only surviving term in (5.42) is then $\eta \dot{Q}$. This we substitute into (5.36), which becomes the equation for viscously damped motion:

$$\ddot{Q} + \eta \dot{Q} + \Omega^2 Q = 0. \quad (5.45)$$

The oscillators in the bath absorb energy but, unlike a pair of coupled oscillators which trade energy rhythmically back and forth, the incommensurate motion of the many q_i prevents them from cooperating for long enough to return any energy to $Q(t)$.

5.2.3 Modified Green function

When the equation $Ly = 0$ has a non trivial-solution, there can be no unique solution to $Ly = f$, but there still will be solutions provided f is orthogonal to all solutions of $L^\dagger y = 0$.

Example: Consider

$$Ly \equiv -\partial_x^2 y = f(x), \quad y'(0) = y'(1) = 0. \quad (5.46)$$

The equation $Ly = 0$ has one non-trivial solution, $y(x) = 1$. The operator L is self-adjoint, $L^\dagger = L$, and so there will be solutions to $Ly = f$ provided $\langle 1, f \rangle = \int_0^1 f dx = 0$.

We cannot define the the green function as a solution to

$$-\partial_x^2 G(x, x') = \delta(x - x'), \quad (5.47)$$

because $\int_0^1 \delta(x - x') dx = 1 \neq 0$, but we can seek a solution to

$$-\partial_x^2 G(x, x') = \delta(x - x') - 1 \quad (5.48)$$

as the right-hand integrates to zero.

A general solution to $-\partial_x^2 y = -1$ is

$$y = A + Bx + \frac{1}{2}x^2, \quad (5.49)$$

and the functions

$$\begin{aligned} y_L &= A + \frac{1}{2}x^2, \\ y_R &= C - x + \frac{1}{2}x^2, \end{aligned} \quad (5.50)$$

obey the boundary conditions at the left and right ends of the interval, respectively. Continuity at $x = x'$ demands that $A = C - x'$, and we are left with

$$G(x, x') = \begin{cases} C - x' + \frac{1}{2}x^2, & 0 < x < x' \\ C - x + \frac{1}{2}x^2, & x' < x < 1, \end{cases} \quad (5.51)$$

There is no freedom left to impose the condition

$$G'(x' - \varepsilon, x') - G'(x' + \varepsilon, x') = 1, \quad (5.52)$$

but it is *automatically satisfied*! Indeed,

$$\begin{aligned} G'(x' - \varepsilon, x') &= x' \\ G'(x' + \varepsilon, x') &= -1 + x'. \end{aligned} \quad (5.53)$$

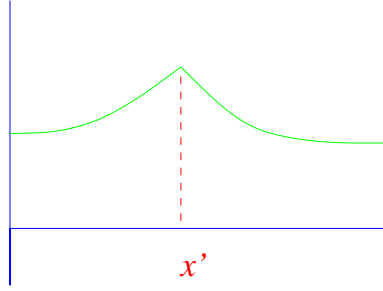
We may select a different value of C for each x' , and a convenient choice is

$$C = \frac{1}{2}x'^2 + \frac{1}{3} \quad (5.54)$$

which makes G symmetric:

$$G(x, x') = \begin{cases} \frac{1}{3} - x' + \frac{x^2 + x'^2}{2}, & 0 < x < x' \\ \frac{1}{3} - x + \frac{x^2 + x'^2}{2}, & x' < x < 1, \end{cases} \quad (5.55)$$

It also makes $\int_0^1 G(x, x') dx = 0$.



The modified Green function.

The solution to $Ly = f$ is

$$y(x) = \int_0^1 G(x, x') f(x') dx' + A, \quad (5.56)$$

where A is arbitrary.

5.3 Applications of Lagrange's Identity

5.3.1 Hermiticity of Green function

Earlier we noted the symmetry of the Green function for the Sturm-Liouville equation. We will now establish the corresponding result for general differential operators.

Let $G(x, x')$ obey $L_x G(x, x') = \delta(x - x')$ with homogeneous boundary conditions B , and let $G^\dagger(x, x')$ obey $L_x^\dagger G^\dagger(x, x') = \delta(x - x')$ with adjoint

boundary conditions B^\dagger . Then, from Lagrange's identity, we have

$$\begin{aligned}
 [Q(G, G^\dagger)]_a^b &= \int_a^b dx \left\{ \left(L_x^\dagger G^\dagger(x, x') \right)^* G(x, x'') - (G^\dagger(x, x'))^* L G(x, x'') \right\} \\
 &= \int_a^b dx \left\{ \delta(x - x') G(x, x'') - \left(G^\dagger(x, x') \right)^* \delta(x - x'') \right\} \\
 &= G(x', x'') - \left(G^\dagger(x'', x') \right)^*. \tag{5.57}
 \end{aligned}$$

Thus, provided $[Q(G, G^\dagger)]_a^b = 0$, which is indeed the case because the boundary conditions for L , L^\dagger are mutually adjoint, we have

$$G^\dagger(x', x) = \left(G(x, x') \right)^*, \tag{5.58}$$

and the Green functions, regarded as matrices with continuous rows and columns, are Hermitian conjugates of one another.

Example: Let

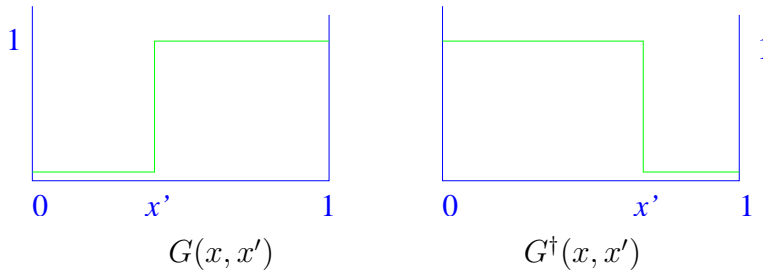
$$L = \frac{d}{dx}, \quad \mathcal{D}(L) = \{y, Ly \in L^2[0, 1] : y(0) = 0\}. \tag{5.59}$$

In this case $G(x, x') = \theta(x - x')$.

Now, we have

$$L^\dagger = -\frac{d}{dx}, \quad \mathcal{D}(L) = \{y, Ly \in L^2[0, 1] : y(1) = 0\} \tag{5.60}$$

and $G^\dagger(x, x') = \theta(x' - x)$.



5.3.2 Inhomogeneous boundary conditions

Our differential operators have been defined with linear *homogeneous* boundary conditions. We can, however, use them, and their Green-function inverses, to solve differential equations with *inhomogeneous* boundary conditions.

Suppose, for example, we wish to solve

$$-\partial_x^2 y = f(x), \quad y(0) = a, \quad y(1) = b. \quad (5.61)$$

We already know the Green function for the homogeneous boundary-condition problem with operator

$$L = -\partial_x^2, \quad \mathcal{D}(L) = \{y, Ly \in L^2[0, 1] : y(0) = 0, y(1) = 0\}. \quad (5.62)$$

It is

$$G(x, x') = \begin{cases} x(1 - x'), & x < x', \\ x'(1 - x), & x > x'. \end{cases} \quad (5.63)$$

Now we apply Lagrange's identity to $\chi(x) = G(x, x')$ and $y(x)$ to get

$$\int_0^1 dx \left\{ G(x, x') \left(-\partial_x^2 y(x) \right) - y(x) \left(-\partial_x^2 G(x, x') \right) \right\} = [G'(x, x')y(x) - G(x, x')y'(x)]_0^1. \quad (5.64)$$

Here, as usual, $G'(x, y) = \partial_x G(x, y)$. The integral is equal to

$$\int dx \{ G(x, x')f(x) - y(x)\delta(x - x') \} = \int G(x, x')f(x) dx - y(x'), \quad (5.65)$$

whilst the integrated-out bit is

$$-(1 - x')y(0) - 0 y'(0) - x'y(1) + 0 y'(1). \quad (5.66)$$

Therefore, we have

$$y(x') = \int G(x, x')f(x) dx + (1 - x')y(0) + x'y(1). \quad (5.67)$$

Here the term with $f(x)$ is the particular integral, whilst the remaining terms constitute the complementary function (obeying the differential equation without the source term) which serves to satisfy the boundary conditions. Observe that the arguments in $G(x, x')$ are not in the usual order, but, in the present example, this does not matter because G is symmetric.

When the operator L is not self-adjoint, we need to distinguish between L and L^\dagger , and G and G^\dagger . We then apply Lagrange's identity to the unknown function $u(x)$ and $\chi(x) = G^\dagger(x, y)$.

Example: We will use the Green-function method to solve the differential equation

$$\frac{du}{dx} = f(x), \quad x \in [0, 1], \quad u(0) = a. \quad (5.68)$$

You can, we hope, write down the answer to this problem directly, but it is interesting to see how the general strategy produces the answer. We first find the Green function $G(x, y)$ for the operator with the corresponding homogeneous boundary conditions. In the present case, this operator is

$$L = \partial_x, \quad \mathcal{D}(L) = \{u, Lu \in L^2[0, 1] : u(0) = 0\}, \quad (5.69)$$

and the appropriate Green function is $G(x, y) = \theta(x - y)$. From G we then read off the adjoint Green function as $G^\dagger(x, y) = (G(y, x))^*$. In the present example, we have $G^\dagger(x, y) = \theta(y - x)$. We now use Lagrange's identity in the form

$$\int_0^1 dx \left\{ (L_x^\dagger G^\dagger(x, y))^* u(x) - (G^\dagger(x, y))^* L_x u(x) \right\} = [Q(G^\dagger, u)]_0^1. \quad (5.70)$$

In all cases, the left hand side is equal to

$$\int_0^1 dx \left\{ \delta(x - y) u(x) - G^T(x, y) f(x) \right\}, \quad (5.71)$$

where T denotes transpose, $G^T(x, y) = G(y, x)$. The left hand side is therefore equal to

$$u(y) - \int_0^1 dx G(y, x) f(x). \quad (5.72)$$

The right hand side depends on the details of the problem. In the present case, the integrated out part is

$$[Q(G^\dagger, u)]_0^1 = -[G^T(x, y) u(x)]_0^1 = u(0). \quad (5.73)$$

At the last step we have used the specific form $G^T = \theta(y - x)$ to find that only the lower limit contributes. The end result is therefore the expected one:

$$u(y) = u(0) + \int_0^y f(x) dx. \quad (5.74)$$

Variations of this strategy enable us to solve any inhomogeneous boundary-value problem in terms of the Green function for the corresponding homogeneous boundary-value problem.

5.4 Eigenfunction Expansions

Self-adjoint operators possess a complete set of eigenfunctions, and we can expand the Green function in terms of these. Let

$$L\varphi_n = \lambda_n\varphi_n. \quad (5.75)$$

Let us further suppose that none of the λ_n are zero. Then the Green function has the eigenfunction expansion

$$G(x, x') = \sum_n \frac{\varphi_n(x)\varphi_n^*(x')}{\lambda_n}. \quad (5.76)$$

That this is so follows from

$$\begin{aligned} L_x \left(\sum_n \frac{\varphi_n(x)\varphi_n^*(x')}{\lambda_n} \right) &= \sum_n \frac{(L_x\varphi_n(x))\varphi_n^*(x')}{\lambda_n} \\ &= \sum_n \frac{\lambda_n\varphi_n(x)\varphi_n^*(x')}{\lambda_n} \\ &= \sum_n \varphi_n(x)\varphi_n^*(x') \\ &= \delta(x - x'). \end{aligned} \quad (5.77)$$

Example: : Consider our familiar exemplar

$$L = -\partial_x^2, \quad \mathcal{D}(L) = \{y, Ly \in L^2[0, 1] : y(0) = y(1) = 0\}, \quad (5.78)$$

for which

$$G(x, x') = \begin{cases} x(1 - x'), & x < x', \\ x'(1 - x), & x > x'. \end{cases} \quad (5.79)$$

Performing the Fourier series shows that

$$G(x, x') = \sum_{n=1}^{\infty} \left(\frac{2}{n^2\pi^2} \right) \sin(n\pi x) \sin(n\pi x'). \quad (5.80)$$

Modified Green function

If one or more of the eigenvalues is zero then the modified Green function is obtained by simply omitting the corresponding terms from the series.

$$G_{\text{mod}}(x, x') = \sum_{\lambda_n \neq 0} \frac{\varphi_n(x) \varphi_n^*(x')}{\lambda_n}. \quad (5.81)$$

Then

$$L_x G_{\text{mod}}(x, x') = \delta(x - x') - \sum_{\lambda_n = 0} \varphi_n(x) \varphi_n^*(x'). \quad (5.82)$$

We see that this G_{mod} is still hermitian, and, as a function of x , is orthogonal to the zero modes. These are the properties we elected in our earlier example.

5.5 Analytic Properties of Green Functions

In this section we will study some of the properties of Green functions considered as functions of a complex variable. Some of the formulæ are slightly easier to derive using contour integral methods, but these are not necessary and we will not use them here. The only complex-variable prerequisite is a familiarity with complex arithmetic and, in particular, knowledge of how to take the logarithm and the square root of a complex number.

5.5.1 Causality implies analyticity

If we have a causal Green function of the form $G(t - \tau)$ with the property $G(t - \tau) = 0$, for $t < \tau$, then if the integral defining its Fourier transform,

$$\tilde{G}(\omega) = \int_0^\infty e^{i\omega t} G(t) dt, \quad (5.83)$$

converges for real ω , it will converge even better when ω has a positive imaginary part. Consequently $\tilde{G}(\omega)$ will be a well-behaved function of the complex variable ω everywhere in the upper half of the complex plane. Indeed it will be *analytic* there, meaning that its Taylor series expansion about any point actually converges to the function. For example, the Green function for the damped oscillator

$$G(t) = \begin{cases} \frac{1}{\Omega} e^{-\gamma t} \sin(\Omega t), & t > 0, \\ 0, & t < 0, \end{cases} \quad (5.84)$$

has Fourier transform

$$\tilde{G}(\omega) = \frac{1}{\Omega^2 - (\omega + i\gamma)^2}, \quad (5.85)$$

which is always finite in the upper half-plane, although it has *pole* singularities at $\omega = -i\gamma \pm \Omega$ in the lower half-plane.

The only way that the Fourier transform \tilde{G} of a causal Green function can have a singularity in the upper half-plane is if G contains a exponential factor growing in time, in which case the system is *unstable* to perturbations (and the real-frequency Fourier transform does not exist). This observation is at the heart of the *Nyquist criterion* for the stability of linear electronic devices.

Inverting the Fourier transform, we have

$$G(t) = \theta(t) \frac{1}{\Omega} e^{-\gamma t} \sin(\Omega t) = \int_{-\infty}^{\infty} \frac{1}{\Omega^2 - (\omega + i\gamma)^2} e^{-i\omega t} \frac{d\omega}{2\pi}. \quad (5.86)$$

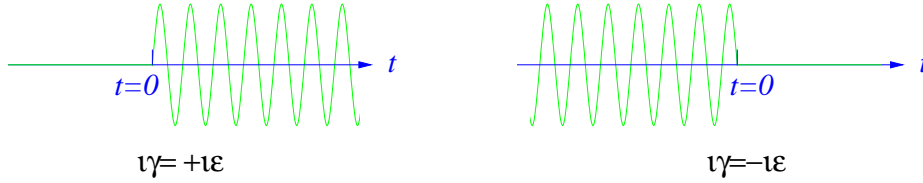
It is perhaps surprising that this integral is identically zero if $t < 0$, and non-zero if $t > 0$. This is one of the places where contour integral methods might cast some light, but because we have confidence in the Fourier inversion formula, we know that it must be correct.

Remember that in deriving (5.86) we have explicitly assumed that the damping coefficient γ is positive. It is important to realize that reversing the sign of γ on the right hand side of (5.86) does more than just change $e^{-\gamma t} \rightarrow e^{\gamma t}$ on the left-hand side. Naïvely setting $\gamma \rightarrow -\gamma$ on both sides of (5.86) gives an equation that cannot possibly be true. The right-hand side is the Fourier transform of a smooth function, and the Riemann-Lebesgue lemma tells us that such a Fourier transform must become zero when $|t| \rightarrow \infty$. The left-hand side, to the contrary, is a function whose oscillations grow without bound as t becomes large and positive.

To find the correct equation, observe that setting $\gamma \rightarrow -\gamma$ in the integral is equivalent to complex conjugation followed by a change of sign $t \rightarrow -t$. Performing the same two operations on the left-hand side of (5.86) leads to

$$-\theta(-t) \frac{1}{\Omega} e^{\gamma t} \sin(\Omega t) = \int_{-\infty}^{\infty} \frac{1}{\Omega^2 - (\omega - i\gamma)^2} e^{-i\omega t} \frac{d\omega}{2\pi}. \quad (5.87)$$

The new left-hand side represents an exponentially growing oscillation which is suddenly silenced by the kick at $t = 0$.



The effect on $G(t)$, the Green function of an undamped oscillator, of changing $i\gamma$ from $+i\varepsilon$ to $-i\varepsilon$.

The effect of taking the damping parameter γ from an infinitesimally small positive value ε to an infinitesimally small negative value $-\varepsilon$ is therefore to turn the *causal* Green function (no motion before it is started by the delta-function kick) of the *undamped* oscillator into an *anti-causal* Green function (no motion after it is stopped by the kick). Ultimately, this is because the differential operator corresponding to a harmonic oscillator with *initial*-value data is not self-adjoint, and its adjoint operator corresponds to a harmonic oscillator with *final*-value data.

This discontinuous dependence on an infinitesimal damping parameter is the subject of the next few sections.

Physics application: Caldeira-Leggett in frequency space

If we write the Caldeira-Leggett equations of motion (5.34) in Fourier frequency space by setting

$$Q(t) = \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} Q(\omega) e^{-i\omega t}, \quad (5.88)$$

and

$$q_i(t) = \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} q_i(\omega) e^{-i\omega t}, \quad (5.89)$$

we have (after including an external force F_{ext} to drive the system)

$$\begin{aligned} (-\omega^2 + (\Omega^2 - \Delta\Omega^2))Q(\omega) - \sum_i f_i q_i(\omega) &= F_{\text{ext}}(\omega), \\ (-\omega^2 + \omega_i^2)q_i(\omega) + f_i Q(\omega) &= 0. \end{aligned} \quad (5.90)$$

Eliminating the q_i , we obtain

$$\left(-\omega^2 + (\Omega^2 - \Delta\Omega^2)\right)Q(\omega) - \sum_i \frac{f_i^2}{\omega_i^2 - \omega^2} Q(\omega) = F_{\text{ext}}(\omega). \quad (5.91)$$

As before, sums over the index i are replaced by integrals over the spectral function

$$\sum_i \frac{f_i^2}{\omega_i^2 - \omega^2} \rightarrow \frac{2}{\pi} \int_0^\infty \frac{\omega' J(\omega')}{\omega'^2 - \omega^2} d\omega', \quad (5.92)$$

and

$$\Delta\Omega^2 \equiv \sum_i \left(\frac{f_i^2}{\omega_i^2} \right) \rightarrow \frac{2}{\pi} \int_0^\infty \frac{J(\omega')}{\omega'} d\omega'. \quad (5.93)$$

Then

$$Q(\omega) = \left(\frac{1}{\Omega^2 - \omega^2 + \Pi(\omega)} \right) F_{\text{ext}}(\omega), \quad (5.94)$$

where the *self-energy* $\Pi(\omega)$ is given by

$$\Pi(\omega) = \frac{2}{\pi} \int_0^\infty \left\{ \frac{J(\omega')}{\omega'} - \frac{\omega' J(\omega')}{\omega'^2 - \omega^2} \right\} d\omega' = -\omega^2 \frac{2}{\pi} \int_0^\infty \frac{J(\omega')}{\omega'(\omega'^2 - \omega^2)} d\omega'. \quad (5.95)$$

The expression

$$\mathcal{G}(\omega) \equiv \frac{1}{\Omega^2 - \omega^2 + \Pi(\omega)} \quad (5.96)$$

a typical *response function*. Analogous objects occur in all branches of physics.

For viscous damping we know that $J(\omega) = \eta\omega$. Let us evaluate the integral occurring in $\Pi(\omega)$ for this case:

$$I(\omega) = \int_0^\infty \frac{d\omega'}{\omega'^2 - \omega^2}. \quad (5.97)$$

We will assume that ω is positive. Now,

$$\frac{1}{\omega'^2 - \omega^2} = \frac{1}{2\omega} \left(\frac{1}{\omega' - \omega} - \frac{1}{\omega' + \omega} \right), \quad (5.98)$$

so

$$I = \left[\frac{1}{2\omega} \left(\ln(\omega' - \omega) - \ln(\omega' + \omega) \right) \right]_{\omega'=0}^\infty. \quad (5.99)$$

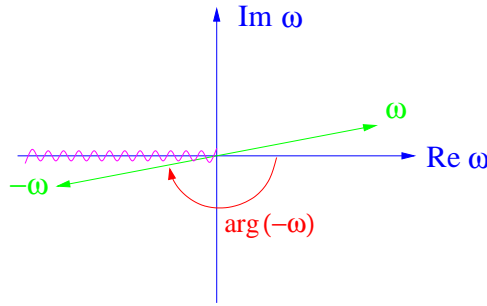
At the upper limit we have $\ln \left((\infty - \omega) / (\infty + \omega) \right) = \ln 1 = 0$. The lower limit contributes

$$-\frac{1}{2\omega} \left(\ln(-\omega) - \ln(\omega) \right). \quad (5.100)$$

To evaluate the logarithm of a negative quantity we must use

$$\ln \omega = \ln |\omega| + i \arg \omega, \quad (5.101)$$

where we will take $\arg \omega$ to lie in the range $-\pi < \arg \omega < \pi$.



When ω has a small positive imaginary part, $\arg(-\omega) \approx -\pi$.

To get an unambiguous answer, we need to give ω an infinitesimal imaginary part $\pm i\varepsilon$. Depending on the sign of this imaginary part, we find that

$$I(\omega \pm i\varepsilon) = \pm \frac{i\pi}{2\omega}, \quad (5.102)$$

so

$$\Pi(\omega \pm i\varepsilon) = \mp i\eta\omega. \quad (5.103)$$

Now the frequency-space version of

$$\ddot{Q}(t) + \eta\dot{Q} + \Omega^2 Q = F_{\text{ext}}(t) \quad (5.104)$$

is

$$(-\omega^2 - i\eta\omega + \Omega^2)Q(\omega) = F_{\text{ext}}(\omega), \quad (5.105)$$

so we must opt for the small shift in ω that leads to $\Pi(\omega) = -i\eta\omega$. This means that we must regard ω as having a *positive* infinitesimal imaginary part, $\omega \rightarrow \omega + i\varepsilon$. This imaginary part is a good and needful thing: it effects the replacement of the ill-defined singular integrals

$$I \stackrel{?}{=} \int_0^\infty \frac{1}{\omega_i^2 - \omega^2} e^{-i\omega t} d\omega, \quad (5.106)$$

which arise as we transform back to real time, with the unambiguous expressions

$$I_\varepsilon = \int_0^\infty \frac{1}{\omega_i^2 - (\omega + i\varepsilon)^2} e^{-i\omega t} d\omega. \quad (5.107)$$

The latter, we know, give rise to properly causal real-time Green functions.

5.5.2 Plemelj formulæ

The functions we are meeting can all be cast in the form

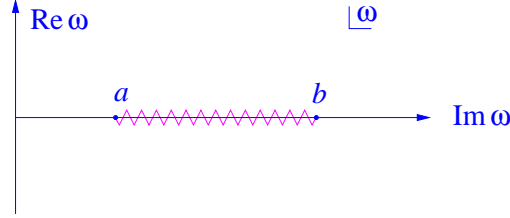
$$f(\omega) = \frac{1}{\pi} \int_a^b \frac{\rho(\omega')}{\omega' - \omega} d\omega'. \quad (5.108)$$

If ω lies in the integration range $[a, b]$, then we divide by zero as we integrate over $\omega' = \omega$. We ought to avoid doing this, but this interval is often exactly where we desire to evaluate f . As before, we evade the division by zero by giving ω an infinitesimally small imaginary part: $\omega \rightarrow \omega \pm i\varepsilon$. We can then apply the *Plemelj formulæ*, named for the Slovenian mathematician Josip Plemelj, which say that

$$\begin{aligned} \frac{1}{2} \left(f(\omega + i\varepsilon) - f(\omega - i\varepsilon) \right) &= i\rho(\omega), \\ \frac{1}{2} \left(f(\omega + i\varepsilon) + f(\omega - i\varepsilon) \right) &= \frac{1}{\pi} P \int_\Gamma \frac{\rho(\omega')}{\omega' - \omega} d\omega'. \end{aligned} \quad (5.109)$$

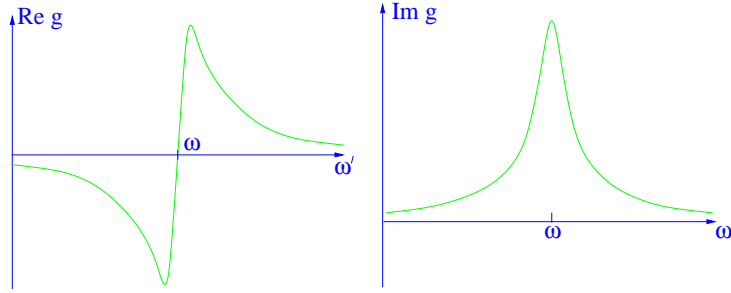
As explained in section 2.3.2, the “ P ” in front of the integral stands for *principal part*. Recall that it means that we are to delete an infinitesimal segment of the ω' integral lying symmetrically about the singular point $\omega' = \omega$.

The Plemelj formula mean that the otherwise smooth and analytic function $f(\omega)$ is discontinuous across the real axis between a and b . If the discontinuity $\rho(\omega)$ is itself an analytic function then the line joining the points a and b is a *branch cut*, and the endpoints of the integral are *branch-point* singularities of $f(\omega)$.



The analytic function $f(\omega)$ is discontinuous across the real axis between a and b .

The Plemelj formulae may be understood by considering the following figure:



Sketch of the real and imaginary parts of $g(\omega') = 1/(\omega' - (\omega + i\varepsilon))$.

The singular integrand is a product of $\rho(\omega')$ with

$$\frac{1}{\omega' - (\omega \pm i\varepsilon)} = \frac{\omega - \omega'}{(\omega' - \omega)^2 + \varepsilon^2} \pm \frac{i\varepsilon}{(\omega' - \omega)^2 + \varepsilon^2}. \quad (5.110)$$

The first term on the right is a symmetrically cut-off version $1/(\omega' - \omega)$ and provides the principal part integral. The the second term sharpens and tends to the delta function $\pm i\pi\delta(\omega' - \omega)$ as $\varepsilon \rightarrow 0$, and so gives $\pm i\pi\rho(\omega)$. Because of this explanation, the Plemelj equations are commonly encoded in physics papers via the “ $i\varepsilon$ ” cabbala

$$\frac{1}{\omega' - (\omega \pm i\varepsilon)} = P\left(\frac{1}{\omega' - \omega}\right) \pm i\pi\delta(\omega' - \omega). \quad (5.111)$$

If ρ is real, as it often is, then $f(\omega + i\eta) = \left(f(\omega - i\eta)\right)^*$. The discontinuity across the real axis is then purely imaginary, and

$$\frac{1}{2}\left(f(\omega + i\varepsilon) + f(\omega - i\varepsilon)\right) \quad (5.112)$$

is purely real. We therefore have

$$\operatorname{Re} f(\omega) = \frac{1}{\pi} P \int_a^b \frac{\operatorname{Im} f(\omega')}{\omega' - \omega} d\omega'. \quad (5.113)$$

This is typical of the relations linking the real and imaginary parts of causal response functions.

A practical illustration of such a relation is provided by the complex, frequency-dependent, *refractive index*, $n(\omega)$, of a medium. This is defined so that a travelling electromagnetic wave takes the form

$$\mathbf{E}(x, t) = \mathbf{E}_0 e^{in(\omega)kx - i\omega t}. \quad (5.114)$$

Here, $k = \omega/c$ is the *in vacuo* wavenumber. We can decompose n into its real and imaginary parts:

$$\begin{aligned} n(\omega) &= n_R + in_I \\ &= n_R(\omega) + \frac{i}{2k} \gamma(\omega), \end{aligned} \quad (5.115)$$

where γ is the extinction coefficient, defined so that the intensity falls off as $I = I_0 \exp(-\gamma x)$. A non-zero γ can arise from either energy absorption or scattering out of the forward direction. For the refractive index, we have the *Kramers-Kronig relation*

$$n_R(\omega) = 1 + \frac{c}{\pi} P \int_0^\infty \frac{\gamma(\omega')}{\omega'^2 - \omega^2} d\omega'. \quad (5.116)$$

Formulae like this will be rigorously derived later by the use of contour-integral methods.

5.5.3 Resolvent operator

Given a differential operator L , we define the *resolvent operator* to be $R_\lambda \equiv (L - \lambda I)^{-1}$. The resolvent is an analytic function of λ , except when λ lies in the spectrum of L .

We expand R_λ in terms of the eigenfunctions as

$$R_\lambda(x, x') = \sum_n \frac{\varphi_n(x) \varphi_n^*(x')}{\lambda_n - \lambda}. \quad (5.117)$$

When the spectrum is discrete, the resolvent has *poles* at the eigenvalues L . When the operator L has a continuous spectrum, the sum becomes an integral:

$$R_\lambda(x, x') = \int_{\mu \in \sigma(L)} \rho(\mu) \frac{\varphi_\mu(x) \varphi_\mu^*(x')}{\mu - \lambda} d\mu, \quad (5.118)$$

where $\rho(\mu)$ is the eigenvalue density of states. This is of the form that we saw in connection with the Plemelj formulæ. Consequently, when the spectrum comprises segments of the real axis, the resulting analytic function R_λ will be discontinuous across the real axis within them. The endpoints of the segments will branch point singularities of R_λ , and the segments themselves, considered as subsets of the complex plane, are the branch cuts.

The trace of the resolvent $\text{Tr } R_\lambda$ is defined by

$$\begin{aligned} \text{Tr } R_\lambda &= \int dx \{R_\lambda(x, x)\} \\ &= \int dx \left\{ \sum_n \frac{\varphi_n(x) \varphi_n^*(x)}{\lambda_n - \lambda} \right\} \\ &= \sum_n \frac{1}{\lambda_n - \lambda} \\ &\rightarrow \int \frac{\rho(\mu)}{\mu - \lambda} d\mu. \end{aligned} \quad (5.119)$$

Applying Plemelj to R_λ , we have

$$\text{Im} \left[\lim_{\varepsilon \rightarrow 0} \left\{ \text{Tr } R_{\lambda + i\varepsilon} \right\} \right] = \pi \rho(\lambda). \quad (5.120)$$

Here, we have used that fact that ρ is real, so

$$\text{Tr } R_{\lambda - i\varepsilon} = \left(\text{Tr } R_{\lambda + i\varepsilon} \right)^*. \quad (5.121)$$

The non-zero imaginary part therefore shows that R_λ is discontinuous across the real axis at points lying in the continuous spectrum.

Example: Consider

$$L = -\partial_x^2 + m^2, \quad \mathcal{D}(L) = \{y, Ly \in L^2[-\infty, \infty]\}. \quad (5.122)$$

As we know, this operator has a continuous spectrum, with eigenfunctions

$$\varphi_k = \frac{1}{\sqrt{L}} e^{ikx}. \quad (5.123)$$

Here, L is the (very large) length of the interval. The eigenvalues are $E = k^2 + m^2$, so the spectrum is all positive numbers greater than m^2 . The momentum density of states is

$$\rho(k) = \frac{L}{2\pi}. \quad (5.124)$$

The completeness relation is

$$\int_{-\infty}^{\infty} \frac{dk}{2\pi} e^{ik(x-x')} = \delta(x-x'), \quad (5.125)$$

which is just the Fourier integral formula for the delta function.

The Green function for L is

$$G(x-y) = \int_{-\infty}^{\infty} dk \left(\frac{dn}{dk} \right) \frac{\varphi_k(x) \varphi_k^*(y)}{k^2 + m^2} = \int_{-\infty}^{\infty} \frac{dk}{2\pi} \frac{e^{ik(x-y)}}{k^2 + m^2} = \frac{1}{2m} e^{-m|x-y|}. \quad (5.126)$$

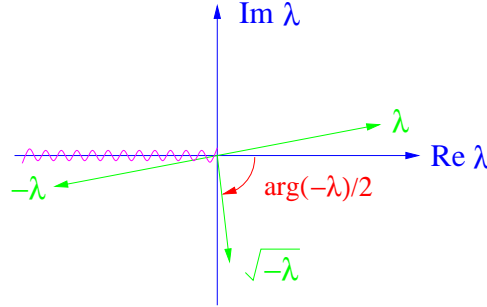
We can use the same calculation to look at the resolvent $R_\lambda = (-\partial_x^2 - \lambda)^{-1}$. Replacing m^2 by $-\lambda$, we have

$$R_\lambda(x, y) = \frac{1}{2\sqrt{-\lambda}} e^{-\sqrt{-\lambda}|x-y|}. \quad (5.127)$$

To appreciate this expression, we need to know how to evaluate \sqrt{z} where z is complex. We write $z = |z|e^{i\phi}$ where we require $-\pi < \phi < \pi$. We now define

$$\sqrt{z} = \sqrt{|z|} e^{i\phi/2}. \quad (5.128)$$

When we evaluate \sqrt{z} for z just below the negative real axis then this definition gives $-i\sqrt{|z|}$, and just above the axis we find $+i\sqrt{|z|}$. The discontinuity means that the negative real axis is a branch cut for the the square-root function. The $\sqrt{-\lambda}$'s appearing in R_λ therefore mean that the *positive* real axis will be a branch cut for R_λ . This branch cut therefore coincides with the spectrum of L , as promised earlier.



If $\text{Im } \lambda > 0$, and with the branch cut for \sqrt{z} in its usual place along the negative real axis, then $\sqrt{-\lambda}$ has negative imaginary part and positive real part.

If λ is positive and we shift $\lambda \rightarrow \lambda + i\varepsilon$ then

$$\frac{1}{2\sqrt{-\lambda}} e^{-\sqrt{-\lambda}|x-y|} \rightarrow \frac{i}{\sqrt{\lambda}} e^{-i\sqrt{\lambda}|x-y| - \varepsilon|x-y|/2\sqrt{\lambda}}. \quad (5.129)$$

Notice that this decays away as $|x-y| \rightarrow \infty$. The square root retains a positive real part when λ is shifted to $\lambda - i\varepsilon$, and so the decay is still present:

$$\frac{1}{2\sqrt{-\lambda}} e^{-\sqrt{-\lambda}|x-y|} \rightarrow -\frac{i}{\sqrt{\lambda}} e^{+i\sqrt{\lambda}|x-y| - \varepsilon|x-y|/2\sqrt{\lambda}}. \quad (5.130)$$

In each case, with λ either immediately above or immediately below the cut, the small imaginary part tempers the oscillatory behaviour of the Green function so that $\chi(x) = G(x, y)$ is square integrable and remains an element of $L^2[\mathbb{R}]$.

We now take the trace of R by setting $x = y$ and integrating:

$$\text{Tr } R_{\lambda+i\varepsilon} = i\pi \frac{L}{2\pi \sqrt{|\lambda|}}. \quad (5.131)$$

Thus,

$$\rho(\lambda) = \theta(\lambda) \frac{L}{2\pi \sqrt{|\lambda|}}, \quad (5.132)$$

which coincides with our direct calculation.

Example: Let

$$L = -i\partial_x, \quad \mathcal{D}(L) = \{y, Ly \in L^2[\mathbb{R}]\}. \quad (5.133)$$

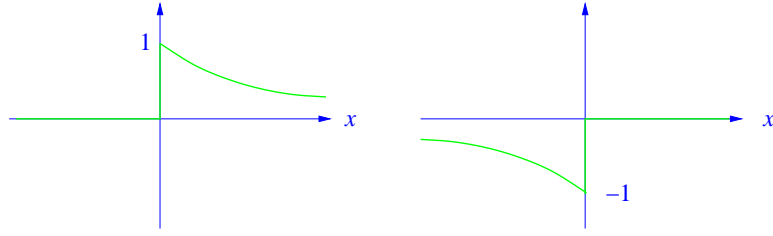
This has eigenfunctions e^{ikx} with eigenvalues k . The spectrum is therefore the entire real line. The local eigenvalue density of states is $1/2\pi$. The resolvent is therefore

$$(-i\partial_x - \lambda)_{x,x'}^{-1} = \frac{1}{2\pi} \int_{-\infty}^{\infty} e^{ik(x-x')} \frac{1}{k - \lambda} dk. \quad (5.134)$$

To evaluate this, first consider the Fourier transforms of

$$\begin{aligned} F_1(x) &= \theta(x)e^{-\kappa x}, \\ F_2(x) &= -\theta(-x)e^{\kappa x}, \end{aligned} \quad (5.135)$$

where κ is a positive real number.



The functions $F_1(x) = \theta(x)e^{-\kappa x}$ and $F_2(x) = -\theta(-x)e^{\kappa x}$.

We have

$$\int_{-\infty}^{\infty} \left\{ \theta(x)e^{-\kappa x} \right\} e^{-ikx} dx = \frac{1}{i} \frac{1}{k - i\kappa}, \quad (5.136)$$

$$\int_{-\infty}^{\infty} \left\{ -\theta(-x)e^{\kappa x} \right\} e^{-ikx} dx = \frac{1}{i} \frac{1}{k + i\kappa}. \quad (5.137)$$

Inverting the transforms gives

$$\begin{aligned} \theta(x)e^{-\kappa x} &= \frac{1}{2\pi i} \int_{-\infty}^{\infty} \frac{1}{k - i\kappa} e^{ikx} dk, \\ -\theta(-x)e^{\kappa x} &= \frac{1}{2\pi i} \int_{-\infty}^{\infty} \frac{1}{k + i\kappa} e^{ikx} dk. \end{aligned} \quad (5.138)$$

These are important formulæ in their own right, and you should take care to understand them. Now we apply them to evaluating the integral defining R_λ .

If we write $\lambda = \mu + i\nu$, we find

$$\frac{1}{2\pi} \int_{-\infty}^{\infty} e^{ik(x-x')} \frac{1}{k - \lambda} dk = \begin{cases} i\theta(x - x') e^{i\mu(x-x')} e^{-\nu(x-x')}, & \nu > 0, \\ -i\theta(x' - x) e^{i\mu(x-x')} e^{-\nu(x-x')}, & \nu < 0, \end{cases} \quad (5.139)$$

In each case, the resolvent is $\propto e^{i\lambda x}$ away from x' , and has jump of $+i$ at $x = x'$ so as to produce the delta function. It decays either to the right or to the left, depending on the sign of ν . The Heaviside factor ensures that it is multiplied by zero on the exponentially growing side of $e^{-\nu x}$, so as to satisfy the requirement of square integrability.

Taking the trace of this resolvent is a little problematic. We are to set $x = x'$ and integrate — but what value do we associate with $\theta(0)$? Remembering that Fourier transforms always give to the mean of the two values at a jump discontinuity, it seems reasonable to set $\theta(0) = \frac{1}{2}$. With this definition, we have

$$\text{Tr } R_\lambda = \begin{cases} \frac{i}{2}L, & \text{Im } \lambda > 0, \\ -\frac{i}{2}L, & \text{Im } \lambda < 0. \end{cases} \quad (5.140)$$

Our choice is therefore compatible with $\text{Tr } R_{\lambda+i\varepsilon} = \pi\rho = L/2\pi$. We have been lucky. The ambiguous expression $\theta(0)$ is not always safely evaluated as $1/2$.

5.6 Locality and the Gelfand-Dikii equation

The answers to many quantum physics problems can be expressed either as sums over wavefunctions or as expressions involving Green functions. One of the advantages writing the answer in terms of Green functions is that these typically depend only on the local properties of the differential operator whose inverse they are. This locality is in contrast to the individual wavefunctions and their eigenvalues, both of which are sensitive to the distant boundaries. Since physics is usually local, it follows that the Green function provides a more efficient route to the answer.

By the Green function being *local* we mean that its value for x, y near some point can be computed in terms of the coefficients in the differential operator evaluated near this point. To illustrate this claim, consider the Green function $G(x, y)$ for the Schrödinger operator $-\partial_x^2 + q(x) + \lambda$ on the entire real line. We will show that there is a not exactly obvious (but easy to obtain once you know the trick) local gradient expansion for the diagonal

elements $D(x) \equiv G(x, x)$. These elements are often all that is needed in physics. We begin by recalling that we can write

$$G(x, y) \propto u(x)v(y)$$

where $u(x)$, $v(x)$ are solutions of $(-\partial_x^2 + q(x) + \lambda)y = 0$ satisfying suitable boundary conditions to the right and left respectively. We set $D(x) = G(x, x)$ and differentiate three times with respect to x . We find

$$\begin{aligned} \partial_x^3 D(x) &= u^{(3)}v + 3u''v' + 3u'v'' + uv^{(3)} \\ &= (\partial_x(q + \lambda)u)v + 3(q + \lambda)\partial_x(uv) + (\partial_x(q + \lambda)v)u. \end{aligned}$$

Here, in passing from the first to second line, we have used the differential equation obeyed by u and v . We can re-express the second line as

$$(q\partial_x + \partial_x q - \frac{1}{2}\partial_x^3)D(x) = -2\lambda\partial_x D(x). \quad (5.141)$$

This relation is known as the *Gelfand-Dikii equation*. Using it we can find an expansion for the diagonal element $D(x)$ in terms of q and its derivatives. We begin by observing that for $q(x) \equiv 0$ we know that $D(x) = 1/(2\sqrt{\lambda})$. We therefore conjecture that we can expand

$$D(x) = \frac{1}{2\sqrt{\lambda}} \left(1 - \frac{b_1(x)}{2\lambda} + \frac{b_2(x)}{(2\lambda)^2} + \cdots + (-1)^n \frac{b_n(x)}{(2\lambda)^n} + \cdots \right).$$

If we insert this expansion into (5.141) we see that we get the recurrence relation

$$(q\partial_x + \partial_x q - \frac{1}{2}\partial_x^3)b_n = \partial_x b_{n+1}. \quad (5.142)$$

We can therefore find b_{n+1} from b_n by differentiation followed by a single integration. Remarkably, $\partial_x b_{n+1}$ is always the exact derivative of a polynomial in q and its derivatives. Further, the integration constants must be zero so that we recover the $q \equiv 0$ result. If we carry out this process, we find

$$\begin{aligned} b_1(x) &= q(x), \\ b_2(x) &= \frac{3q(x)^2}{2} - \frac{q''(x)}{2}, \\ b_3(x) &= \frac{5q(x)^3}{2} - \frac{5q'(x)^2}{4} - \frac{5q(x)q''(x)}{2} + \frac{q^{(4)}(x)}{4}, \\ b_4(x) &= \frac{35q(x)^4}{8} - \frac{35q(x)q'(x)^2}{4} - \frac{35q(x)^2q''(x)}{4} + \frac{21q''(x)^2}{8} \\ &\quad + \frac{7q'(x)q^{(3)}(x)}{2} + \frac{7q(x)q^{(4)}(x)}{4} - \frac{q^{(6)}(x)}{8}, \end{aligned} \quad (5.143)$$

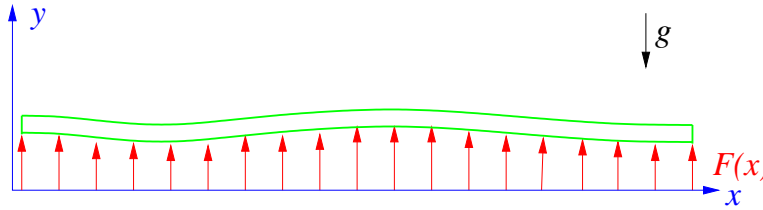
and so on. (Note how the terms in the expansion are graded: Each b_n is homogeneous in powers of q and its derivatives, provided we count two x derivatives as being worth one $q(x)$.) Keeping a few terms in this series expansion can provide an effective approximation for $G(x, x)$, but, in general, the series is not convergent, being only an *asymptotic expansion* for $D(x)$.

A similar strategy produces expansions for the diagonal element of the Green function of other one-dimensional differential operators. Such gradient expansions also exist in higher dimensions but the higher-dimensional *Seeley-coefficient* functions are not as easy to compute. Gradient expansions for the off-diagonal elements also exist, but, again, they are harder to obtain.

5.7 Exercises and problems

Here are some exercises that are intended to illustrate the material of this chapter:

Exercise 5.1: Fredholm Alternative. A heavy elastic bar with uniform mass m per unit length lies almost horizontally. It is supported by a distribution of upward forces $F(x)$.



The shape of the bar, $y(x)$, can be found by minimizing the energy

$$U[y] = \int_0^L \left\{ \frac{1}{2} \kappa (y'')^2 - (F(x) - mg)y \right\} dx.$$

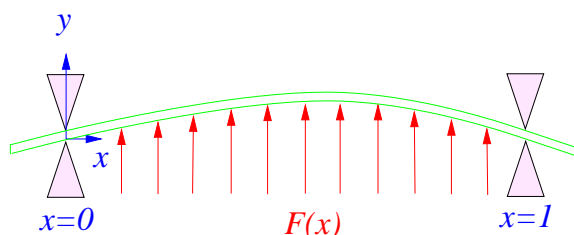
- Show that this minimization leads to the equation

$$\hat{L}y \equiv \kappa \frac{d^4 y}{dx^4} = F(x) - mg, \quad y'' = y''' = 0 \quad \text{at} \quad x = 0, L.$$

- Show that the boundary conditions are such that the operator \hat{L} is self-adjoint with respect to an inner product with weight function 1.

- Find the zero modes which span the null space of \hat{L} .
- If there are n linearly independent zero modes, then the codimension of the range of \hat{L} is also n . Using your explicit solutions from the previous part, find the conditions that must be obeyed by $F(x)$ for a solution of $\hat{L}y = F - mg$ to exist. What is the physical meaning of these conditions?
- The solution to the equation and boundary conditions is not unique. Is this non-uniqueness physically reasonable? Explain.

Exercise 5.2: Flexible rod again. A flexible rod is supported near its ends by means of knife edges that constrain its position, but not its slope or curvature. It is acted on by a force $F(x)$.



Simply supported rod.

The deflection of the rod is found by solving the the boundary value problem

$$\frac{d^4 y}{dx^4} = F(x), \quad y(0) = y(1) = 0, \quad y''(0) = y''(1) = 0.$$

We wish to find the Green function $G(x, y)$ that facilitates the solution of this problem.

- If the differential operator and domain (boundary conditions) above is denoted by L , what is the operator and domain for L^\dagger ? Is the problem self-adjoint?
- Are there any zero-modes? Does F have to satisfy any conditions for the solution to exist?
- Write down the conditions, if any, obeyed by $G(x, y)$ and its derivatives $\partial_x G(x, y)$, $\partial_{xx}^2 G(x, y)$, $\partial_{xxx}^3 G(x, y)$ at $x = 0$, $x = y$, and $x = 1$.
- Using the conditions above, find $G(x, y)$. (This requires some boring algebra — but if you start from the “jump condition” and work down, it can be completed in under a page)
- Is your Green function symmetric ($G(x, y) = G(y, x)$)? Is this in accord with the self-adjointness or not of the problem? (You can use this as a check of your algebra.)

- f) Write down the integral giving the general solution of the boundary value problem. Assume, if necessary, that $F(x)$ is in the range of the differential operator. Differentiate your answer and see if it does indeed satisfy the differential equation and boundary conditions.

Exercise 5.3: Hot ring. The equation governing the steady state heat flow on thin ring of unit circumference is

$$-y'' = f, \quad 0 < x < 1, \quad y(0) = y(1), \quad y'(0) = y'(1).$$

- a) This problem has a zero mode. Find the zero mode and the consequent condition on $f(x)$ for a solution to exist.
 b) Verify that a suitable modified Green function for the problem is

$$g(x, y) = \frac{1}{2}(x - y)^2 - \frac{1}{2}|x - y|.$$

You will need to verify that $g(x, y)$ satisfies both the differential equation and the boundary conditions.

Exercise 5.4: Seek a solution to the equation

$$-\frac{d^2y}{dx^2} = f(x), \quad x \in [0, 1]$$

with inhomogeneous boundary conditions $y'(0) = F_0$, $y'(1) = F_1$. Observe that the corresponding homogeneous boundary condition problem has a zero mode. Therefore the solution, if one exists, cannot be unique.

- a) Show that there can be no solution to the differential equation and inhomogeneous boundary condition unless $f(x)$ satisfies the condition

$$\int_0^1 f(x) dx = F_0 - F_1. \quad (\star)$$

- b) Let $G(x, \xi)$ denote the modified Green function (5.55)

$$G(x, \xi) = \begin{cases} \frac{1}{3} - \xi + \frac{x^2 + \xi^2}{2}, & 0 < x < \xi \\ \frac{1}{3} - x + \frac{x^2 + \xi^2}{2}, & \xi < x < 1, \end{cases}.$$

Use the Lagrange-identity method for inhomogeneous boundary conditions to deduce that if a solution exists then it necessarily obeys

$$y(x) = \int_0^1 y(\xi) d\xi + \int_0^1 G(\xi, x) f(\xi) d\xi + G(1, x) F_1 - G(0, x) F_0.$$

- c) By differentiating with respect to x , show that

$$y_{\text{tentative}}(x) = \int_0^1 G(\xi, x) f(\xi) d\xi + G(1, x)F_1 - G(0, x)F_0 + C,$$

where C is an arbitrary constant, obeys the boundary conditions.

- d) By differentiating a second time with respect to x , show that $y_{\text{tentative}}(x)$ is a solution of the differential equation if, and only if, the condition \star is satisfied.

Exercise 5.5: Lattice Green Functions . The $k \times k$ matrices

$$\mathbf{T}_1 = \begin{pmatrix} 2 & -1 & 0 & 0 & 0 & \dots & 0 \\ -1 & 2 & -1 & 0 & 0 & \dots & 0 \\ 0 & -1 & 2 & -1 & 0 & \dots & 0 \\ \vdots & \vdots & \ddots & \ddots & \ddots & \vdots & \vdots \\ 0 & \dots & 0 & -1 & 2 & -1 & 0 \\ 0 & \dots & 0 & 0 & -1 & 2 & -1 \\ 0 & \dots & 0 & 0 & 0 & -1 & 2 \end{pmatrix}, \quad \mathbf{T}_2 = \begin{pmatrix} 2 & -1 & 0 & 0 & 0 & \dots & 0 \\ -1 & 2 & -1 & 0 & 0 & \dots & 0 \\ 0 & -1 & 2 & -1 & 0 & \dots & 0 \\ \vdots & \vdots & \ddots & \ddots & \ddots & \vdots & \vdots \\ 0 & \dots & 0 & -1 & 2 & -1 & 0 \\ 0 & \dots & 0 & 0 & -1 & 2 & -1 \\ 0 & \dots & 0 & 0 & 0 & -1 & 1 \end{pmatrix}$$

represent two discrete lattice approximations to $-\partial_x^2$ on a finite interval.

- a) What are the boundary conditions defining the domains of the corresponding continuum differential operators? [They are either Dirichlet ($y = 0$) or Neumann ($y' = 0$) boundary conditions.] Make sure you explain your reasoning.
- b) Verify that

$$\begin{aligned} [\mathbf{T}_1^{-1}]_{ij} &= \min(i, j) - \frac{ij}{k+1}, \\ [\mathbf{T}_2^{-1}]_{ij} &= \min(i, j). \end{aligned}$$

- c) Find the continuum Green functions for the boundary value problems approximated by the matrix operators. Compare each of the matrix inverses with its corresponding continuum Green function. Are they similar?

Exercise 5.6: Eigenfunction expansion The resolvent (Green function) $G_\lambda(x, x') = (L - \lambda)_{xx'}^{-1}$ can be expanded as

$$(L - \lambda)_{xx'}^{-1} = \sum_{\lambda_n} \frac{\varphi_n(x)\varphi_n(x')}{\lambda_n - \lambda},$$

where $\varphi_n(x)$ is the normalized eigenfunction corresponding to the eigenvalue λ_n . The resolvent therefore has a *pole* whenever λ approaches λ_n . Consider the case

$$G_{\omega^2}(x, x') = \left(-\frac{d^2}{dx^2} - \omega^2 \right)_{xx'}^{-1},$$

with boundary conditions $y(0) = y(L) = 0$.

a) Show that

$$\begin{aligned} G_{\omega^2}(x, x') &= \frac{1}{\omega \sin \omega L} \sin \omega x \sin \omega(L - x'), & x < x', \\ &= \frac{1}{\omega \sin \omega L} \sin \omega(L - x) \sin \omega x', & x' < x \end{aligned}$$

- b) Confirm that G_{ω^2} becomes singular at exactly those values of ω^2 corresponding to eigenvalues ω_n^2 of $-\frac{d^2}{dx^2}$.
- c) Find the associated eigenfunctions $\varphi_n(x)$ and, by taking the limit of G_{ω^2} as $\omega^2 \rightarrow \omega_n^2$, confirm that the *residue* of the pole (the coefficient of $1/(\omega_n^2 - \omega^2)$) is precisely the product of the *normalized* eigenfunctions $\varphi_n(x)\varphi_n(x')$.

Chapter 6

Partial Differential Equations

Most differential equations of physics involve quantities depending on both space and time. Inevitably they involve partial derivatives, and so are partial differential equations (PDE's). Although PDE's are inherently more complicated than ODE's, many of the ideas from the previous chapters — in particular the notion of self adjointness and the resulting completeness of the eigenfunctions — carry over to the partial differential operators that occur in these equations.

6.1 Classification of PDE's

We will focus on second-order equations in two variables, such as the wave equation

$$\frac{\partial^2 \varphi}{\partial x^2} - \frac{1}{c^2} \frac{\partial^2 \varphi}{\partial t^2} = f(x, t), \quad (\text{Hyperbolic}) \quad (6.1)$$

Laplace or Poisson's equation

$$\frac{\partial^2 \varphi}{\partial x^2} + \frac{\partial^2 \varphi}{\partial y^2} = f(x, y), \quad (\text{Elliptic}) \quad (6.2)$$

or Fourier's heat equation

$$\frac{\partial^2 \varphi}{\partial x^2} - \kappa \frac{\partial \varphi}{\partial t} = f(x, t). \quad (\text{Parabolic}) \quad (6.3)$$

What do the names hyperbolic, elliptic and parabolic mean? In high-school co-ordinate geometry we learned that a real quadratic curve

$$ax^2 + 2bxy + cy^2 + fx + gy + h = 0 \quad (6.4)$$

represents a hyperbola, an ellipse or a parabola depending on whether the *discriminant*, $ac - b^2$, is less than zero, greater than zero, or equal to zero, these being the conditions for the matrix

$$\begin{bmatrix} a & b \\ b & c \end{bmatrix} \quad (6.5)$$

to have signature $(+, -)$, $(+, +)$ or $(+, 0)$.

By analogy, the equation

$$a(x, y) \frac{\partial^2 \varphi}{\partial x^2} + 2b(x, y) \frac{\partial^2 \varphi}{\partial x \partial y} + c(x, y) \frac{\partial^2 \varphi}{\partial y^2} + (\text{lower orders}) = 0, \quad (6.6)$$

is said to be hyperbolic, elliptic, or parabolic at a point (x, y) if

$$\begin{vmatrix} a(x, y) & b(x, y) \\ b(x, y) & c(x, y) \end{vmatrix} = (ac - b^2)|_{(x, y)}, \quad (6.7)$$

is less than, greater than, or equal to zero, respectively. This classification helps us understand what sort of initial or boundary data we need to specify the problem.

There are three broad classes of boundary conditions:

- a) **Dirichlet boundary conditions:** The value of the dependent variable is specified on the boundary.
- b) **Neumann boundary conditions:** The normal derivative of the dependent variable is specified on the boundary.
- c) **Cauchy boundary conditions:** Both the value and the normal derivative of the dependent variable are specified on the boundary.

Cauchy boundary conditions are analogous to the initial conditions for a second-order ordinary differential equation. These are given at one end of the interval only. The other two classes of boundary condition are higher-dimensional analogues of the conditions we impose on an ODE at both ends of the interval.

Each class of PDE's requires a different class of boundary conditions in order to have a unique, stable solution.

- 1) **Elliptic** equations require either Dirichlet or Neumann boundary conditions on a closed boundary surrounding the region of interest. Other boundary conditions are either insufficient to determine a unique solution, overly restrictive, or lead to instabilities.

- 2) **Hyperbolic** equations require Cauchy boundary conditions on a open surface. Other boundary conditions are either too restrictive for a solution to exist, or insufficient to determine a unique solution.
- 3) **Parabolic** equations require Dirichlet or Neumann boundary conditions on a open surface. Other boundary conditions are too restrictive.

6.2 Cauchy Data

Given a second-order ordinary differential equation

$$p_0 y'' + p_1 y' + p_2 y = f \quad (6.8)$$

with initial data $y(a)$, $y'(a)$ we can construct the solution incrementally. We take a step $\delta x = \varepsilon$ and use the initial slope to find $y(a + \varepsilon) = y(a) + \varepsilon y'(a)$. Next we find $y''(a)$ from the differential equation

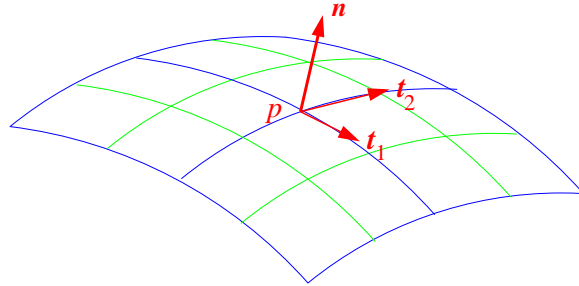
$$y''(a) = -\frac{1}{p_0}(p_1 y'(a) + p_2 y(a) - f(a)), \quad (6.9)$$

and use it to obtain $y'(a + \varepsilon) = y'(a) + \varepsilon y''(a)$. We now have initial data, $y(a + \varepsilon)$, $y'(a + \varepsilon)$, at the point $a + \varepsilon$, and can play the same game to proceed to $a + 2\varepsilon$, and onwards.

Suppose now that we have the analogous situation of a second order partial differential equation

$$a_{\mu\nu}(x) \frac{\partial^2 \varphi}{\partial x^\mu \partial x^\nu} + (\text{lower orders}) = 0. \quad (6.10)$$

in \mathbb{R}^n . We are also given initial data on a surface, Γ , of co-dimension one in \mathbb{R}^n .



The surface Γ on which we are given Cauchy Data.

At each point p on Γ we erect a basis $\mathbf{n}, \mathbf{t}_1, \mathbf{t}_2, \dots$ consisting of the normal to Γ and $n - 1$ tangent vectors. The information we have been given consists of the value of φ at every point p together with

$$\frac{\partial \varphi}{\partial n} \stackrel{\text{def}}{=} n^\mu \frac{\partial \varphi}{\partial x^\mu}, \quad (6.11)$$

the normal derivative of φ at p . We want to know if this *Cauchy data* is sufficient to find the second derivative in the normal direction, and so construct similar Cauchy data on the adjacent surface $\Gamma + \varepsilon \mathbf{n}$. If so, we can repeat the process and systematically propagate the solution forward through \mathbb{R}^n .

From the given data, we can construct

$$\begin{aligned} \frac{\partial^2 \varphi}{\partial n \partial t_i} &\stackrel{\text{def}}{=} n^\mu t_i^\nu \frac{\partial^2 \varphi}{\partial x^\mu \partial x^\nu}, \\ \frac{\partial^2 \varphi}{\partial t_i \partial t_j} &\stackrel{\text{def}}{=} t_i^\nu t_j^\nu \frac{\partial^2 \varphi}{\partial x^\mu \partial x^\nu}, \end{aligned} \quad (6.12)$$

but we do not yet have enough information to determine

$$\frac{\partial^2 \varphi}{\partial n \partial n} \stackrel{\text{def}}{=} n^\mu n^\nu \frac{\partial^2 \varphi}{\partial x^\mu \partial x^\nu}. \quad (6.13)$$

Can we fill the data gap by using the differential equation (6.10)? Suppose that

$$\frac{\partial^2 \varphi}{\partial x^\mu \partial x^\nu} = \phi_0^{\mu\nu} + n^\mu n^\nu \Phi \quad (6.14)$$

where $\phi_0^{\mu\nu}$ is a guess that is consistent with (6.12), and Φ is as yet unknown, and, because of the factor of $n^\mu n^\nu$, does not affect the derivatives (6.12). We plug into

$$a_{\mu\nu}(x_i) \frac{\partial^2 \varphi}{\partial x^\mu \partial x^\nu} + (\text{known lower orders}) = 0. \quad (6.15)$$

and get

$$a_{\mu\nu} n^\mu n^\nu \Phi + (\text{known}) = 0. \quad (6.16)$$

We can therefore find Φ provided that

$$a_{\mu\nu} n^\mu n^\nu \neq 0. \quad (6.17)$$

If this expression *is* zero, we are stuck. It is like having $p_0(x) = 0$ in an ordinary differential equation. On the other hand, knowing Φ tells us the

second normal derivative, and we can proceed to the adjacent surface where we play the same game once more.

Definition: A *characteristic surface* is a surface Σ such that $a_{\mu\nu}n^\mu n^\nu = 0$ at all points on Σ . We can therefore propagate our data forward, provided that the initial-data surface Γ is nowhere tangent to a characteristic surface. In two dimensions the characteristic surfaces become one-dimensional curves. An equation in two dimensions is hyperbolic, parabolic, or elliptic at a point (x, y) if it has two, one or zero characteristic curves through that point, respectively.

Characteristics are both a *curse* and *blessing*. They are a barrier to Cauchy data, but, as we will see in the next two subsections, are also the curves along which information is transmitted.

6.2.1 Characteristics and first-order equations

Suppose we have a linear first-order partial differential equation

$$a(x, y)\frac{\partial u}{\partial x} + b(x, y)\frac{\partial u}{\partial y} + c(x, y)u = f(x, y). \quad (6.18)$$

We can write this in vector notation as $(\mathbf{v} \cdot \nabla)u + cu = f$, where \mathbf{v} is the vector field $\mathbf{v} = (a, b)$. If we define the *flow* of the vector field to be the family of parametrized curves $x(t), y(t)$ satisfying

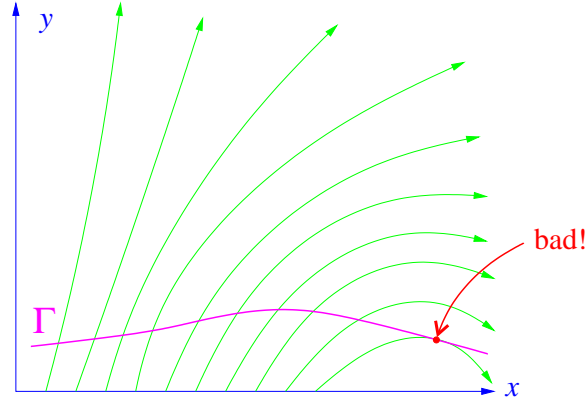
$$\frac{dx}{dt} = a(x, y), \quad \frac{dy}{dt} = b(x, y), \quad (6.19)$$

then the partial differential equation (6.18) reduces to an ordinary linear differential equation

$$\frac{du}{dt} + c(t)u(t) = f(t) \quad (6.20)$$

along each flow line. Here,

$$\begin{aligned} u(t) &\equiv u(x(t), y(t)), \\ c(t) &\equiv c(x(t), y(t)), \\ f(t) &\equiv f(x(t), y(t)). \end{aligned} \quad (6.21)$$



Initial data curve Γ , and flow-line characteristics.

Provided that $a(x, y)$ and $b(x, y)$ are never simultaneously zero, there will be one flow-line curve passing through each point in \mathbb{R}^2 . If we have been given the initial value of u on a curve Γ that is nowhere tangent to any of these flow lines then we can propagate this data forward along the flow by solving (6.20). On the other hand, if the curve Γ does become tangent to one of the flow lines at some point then the data will generally be inconsistent with (6.18) at that point, and no solution can exist. The flow lines therefore play a role analogous to the characteristics of a second-order partial differential equation, and are therefore also called characteristics. The trick of reducing the partial differential equation to a collection of ordinary differential equations along each of its flow lines is called the *method of characteristics*.

Exercise 6.1: Show that the general solution to the equation

$$\frac{\partial \varphi}{\partial x} - \frac{\partial \varphi}{\partial y} - (x - y)\varphi = 0$$

is

$$\varphi(x, y) = e^{-xy} f(x + y),$$

where f is an arbitrary function.

6.2.2 Second-order hyperbolic equations

Consider a second-order equation containing the operator

$$D = a(x, y) \frac{\partial^2}{\partial x^2} + 2b(x, y) \frac{\partial^2}{\partial x \partial y} + c(x, y) \frac{\partial^2}{\partial y^2} \quad (6.22)$$

We can always factorize

$$aX^2 + 2bXY + cY^2 = (\alpha X + \beta Y)(\gamma X + \delta Y), \quad (6.23)$$

and from this obtain

$$\begin{aligned} a \frac{\partial^2}{\partial x^2} + 2b \frac{\partial^2}{\partial x \partial y} + c \frac{\partial^2}{\partial y^2} &= \left(\alpha \frac{\partial}{\partial x} + \beta \frac{\partial}{\partial y} \right) \left(\gamma \frac{\partial}{\partial x} + \delta \frac{\partial}{\partial y} \right) + \text{lower}, \\ &= \left(\gamma \frac{\partial}{\partial x} + \delta \frac{\partial}{\partial y} \right) \left(\alpha \frac{\partial}{\partial x} + \beta \frac{\partial}{\partial y} \right) + \text{lower}. \end{aligned} \quad (6.24)$$

Here “lower” refers to terms containing only first order derivatives such as

$$\alpha \left(\frac{\partial \gamma}{\partial x} \right) \frac{\partial}{\partial x}, \quad \beta \left(\frac{\partial \delta}{\partial y} \right) \frac{\partial}{\partial y}, \quad \text{etc.}$$

A necessary condition, however, for the coefficients $\alpha, \beta, \gamma, \delta$ to be *real* is that

$$\begin{aligned} ac - b^2 &= \alpha\beta\gamma\delta - \frac{1}{4}(\alpha\delta + \beta\gamma)^2 \\ &= -\frac{1}{4}(\alpha\delta - \beta\gamma)^2 \leq 0. \end{aligned} \quad (6.25)$$

A factorization of the leading terms in the second-order operator D as the product of two real first-order differential operators therefore requires that D be *hyperbolic* or *parabolic*. It is easy to see that this is also a *sufficient* condition for such a real factorization. For the rest of this section we will assume that the equation is hyperbolic, and so

$$ac - b^2 = -\frac{1}{4}(\alpha\delta - \beta\gamma)^2 < 0. \quad (6.26)$$

With this condition, the two families of flow curves defined by

$$C_1 : \quad \frac{dx}{dt} = \alpha(x, y), \quad \frac{dy}{dt} = \beta(x, y), \quad (6.27)$$

and

$$C_2 : \quad \frac{dx}{dt} = \gamma(x, y), \quad \frac{dy}{dt} = \delta(x, y), \quad (6.28)$$

are distinct, and are the characteristics of D .

A hyperbolic second-order differential equation $Du = 0$ can therefore be written in either of two ways:

$$\left(\alpha \frac{\partial}{\partial x} + \beta \frac{\partial}{\partial y} \right) U_1 + F_1 = 0, \quad (6.29)$$

or

$$\left(\gamma \frac{\partial}{\partial x} + \delta \frac{\partial}{\partial y} \right) U_2 + F_2 = 0, \quad (6.30)$$

where

$$\begin{aligned} U_1 &= \gamma \frac{\partial u}{\partial x} + \delta \frac{\partial u}{\partial y}, \\ U_2 &= \alpha \frac{\partial u}{\partial x} + \beta \frac{\partial u}{\partial y}, \end{aligned} \quad (6.31)$$

and $F_{1,2}$ contain only $\partial u/\partial x$ and $\partial u/\partial y$. Given suitable Cauchy data, we can solve the two first-order partial differential equations by the method of characteristics described in the previous subsection, and so find $U_1(x, y)$ and $U_2(x, y)$. Because the hyperbolicity condition (6.26) guarantees that the determinant

$$\begin{vmatrix} \gamma & \delta \\ \alpha & \beta \end{vmatrix} = \gamma\beta - \alpha\delta$$

is not zero, we can solve (6.31) and so extract from $U_{1,2}$ the individual derivatives $\partial u/\partial x$ and $\partial u/\partial y$. From these derivatives and the initial values of u , we can determine $u(x, y)$.

6.3 Wave Equation

The wave equation provides the paradigm for hyperbolic equations that can be solved by the method of characteristics.

6.3.1 d'Alembert's Solution

Let $\varphi(x, t)$ obey the wave equation

$$\frac{\partial^2 \varphi}{\partial x^2} - \frac{1}{c^2} \frac{\partial^2 \varphi}{\partial t^2} = 0, \quad -\infty < x < \infty. \quad (6.32)$$

We will use the method of characteristics to propagate Cauchy data $\varphi(x, 0) = \varphi_0(x)$ and $\dot{\varphi}(x, 0) = v_0(x)$, given on the curve $\Gamma = \{x \in \mathbb{R}, t = 0\}$, forward in time.

We begin by factoring the wave equation as

$$0 = \left(\frac{\partial^2 \varphi}{\partial x^2} - \frac{1}{c^2} \frac{\partial^2 \varphi}{\partial t^2} \right) = \left(\frac{\partial}{\partial x} + \frac{1}{c} \frac{\partial}{\partial t} \right) \left(\frac{\partial \varphi}{\partial x} - \frac{1}{c} \frac{\partial \varphi}{\partial t} \right). \quad (6.33)$$

Thus,

$$\left(\frac{\partial}{\partial x} + \frac{1}{c} \frac{\partial}{\partial t} \right) (U - V) = 0, \quad (6.34)$$

where

$$U = \varphi' = \frac{\partial \varphi}{\partial x}, \quad V = \frac{1}{c} \dot{\varphi} = \frac{1}{c} \frac{\partial \varphi}{\partial t}. \quad (6.35)$$

The quantity $U - V$ is therefore constant along the characteristic curves

$$x - ct = \text{const.} \quad (6.36)$$

Writing the linear factors in the reverse order yields the equation

$$\left(\frac{\partial}{\partial x} - \frac{1}{c} \frac{\partial}{\partial t} \right) (U + V) = 0. \quad (6.37)$$

This implies that $U + V$ is constant along the characteristics

$$x + ct = \text{const.} \quad (6.38)$$

Putting these two facts together tells us that

$$\begin{aligned} V(x, t') &= \frac{1}{2} [V(x, t') + U(x, t')] + \frac{1}{2} [V(x, t') - U(x, t')] \\ &= \frac{1}{2} [V(x + ct', 0) + U(x + ct', 0)] + \frac{1}{2} [V(x - ct', 0) - U(x - ct', 0)]. \end{aligned} \quad (6.39)$$

The value of the variable V at the point (x, t') has therefore been computed in terms of the values of U and V on the initial curve Γ . After changing variables from t' to $\xi = x \pm ct'$ as appropriate, we can integrate up to find

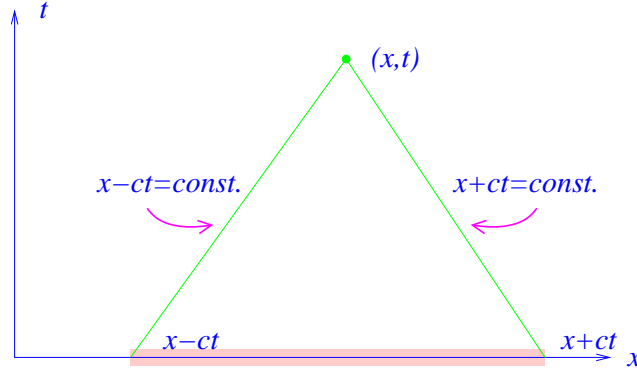
that

$$\begin{aligned}
 \varphi(x, t) &= \varphi(x, 0) + c \int_0^t V(x, t') dt' \\
 &= \varphi(x, 0) + \frac{1}{2} \int_x^{x+ct} \varphi'(\xi, 0) d\xi + \frac{1}{2} \int_x^{x-ct} \varphi'(\xi, 0) d\xi + \frac{1}{2c} \int_{x-ct}^{x+ct} \dot{\varphi}(\xi, 0) d\xi \\
 &= \frac{1}{2} \{ \varphi(x+ct, 0) + \varphi(x-ct, 0) \} + \frac{1}{2c} \int_{x-ct}^{x+ct} \dot{\varphi}(\xi, 0) d\xi,
 \end{aligned} \tag{6.40}$$

This result:

$$\varphi(x, t) = \frac{1}{2} \{ \varphi_0(x+ct) + \varphi_0(x-ct) \} + \frac{1}{2c} \int_{x-ct}^{x+ct} v_0(\xi) d\xi \tag{6.41}$$

is known as *d'Alembert's solution* of the wave equation.



Range of Cauchy data influencing $\varphi(x, t)$.

The value of φ at x, t , is determined by only a finite interval of the initial Cauchy data. In more generality, $\varphi(x, t)$ depends only on what happens in the past *light-cone* of the point, which is bounded by pair of characteristic curves.

An alternative derivation of d'Alembert's solution uses a method that applies most effectively to PDE's with constant coefficients. We first seek a *general solution* to the PDE involving two arbitrary functions. Begin with a change of variables. Let

$$\begin{aligned}
 \xi &= x + ct, \\
 \eta &= x - ct.
 \end{aligned} \tag{6.42}$$

be *light-cone co-ordinates*. In terms of them, we have

$$\begin{aligned}x &= \frac{1}{2}(\xi + \eta), \\t &= \frac{1}{2c}(\xi - \eta).\end{aligned}\tag{6.43}$$

Now,

$$\frac{\partial}{\partial \xi} = \frac{\partial x}{\partial \xi} \frac{\partial}{\partial x} + \frac{\partial t}{\partial \xi} \frac{\partial}{\partial t} = \frac{1}{2} \left(\frac{\partial}{\partial x} + \frac{1}{c} \frac{\partial}{\partial t} \right).\tag{6.44}$$

Similarly

$$\frac{\partial}{\partial \eta} = \frac{1}{2} \left(\frac{\partial}{\partial x} - \frac{1}{c} \frac{\partial}{\partial t} \right).\tag{6.45}$$

Thus

$$\left(\frac{\partial^2}{\partial x^2} - \frac{1}{c^2} \frac{\partial^2}{\partial t^2} \right) = \left(\frac{\partial}{\partial x} + \frac{1}{c} \frac{\partial}{\partial t} \right) \left(\frac{\partial}{\partial x} - \frac{1}{c} \frac{\partial}{\partial t} \right) = 4 \frac{\partial^2}{\partial \xi \partial \eta}.\tag{6.46}$$

The characteristics of the equation

$$4 \frac{\partial^2 \varphi}{\partial \xi \partial \eta} = 0\tag{6.47}$$

are $\xi = \text{const.}$ or $\eta = \text{const.}$ There are two characteristics curves through each point, so the equation is still hyperbolic.

With light-cone coordinates it is easy to see that a general solution to

$$\left(\frac{\partial^2}{\partial x^2} - \frac{1}{c^2} \frac{\partial^2}{\partial t^2} \right) \varphi = 4 \frac{\partial^2 \varphi}{\partial \xi \partial \eta} = 0\tag{6.48}$$

is

$$\varphi = f(\xi) + g(\eta) = f(x + ct) + g(x - ct).\tag{6.49}$$

We now exploit this solution to propagate the data $\varphi(x, 0) \equiv \varphi_0(x)$ and $\dot{\varphi}(x, 0) \equiv v_0(x)$. We do so by fitting the f and g in

$$\varphi(x, t) = f(x + ct) + g(x - ct).\tag{6.50}$$

We have

$$\begin{aligned}f(x) + g(x) &= \varphi_0(x), \\c(f'(x) - g'(x)) &= v_0(x),\end{aligned}\tag{6.51}$$

so

$$f(x) - g(x) = \frac{1}{c} \int_0^x v_0(\xi) d\xi + A. \quad (6.52)$$

Therefore

$$\begin{aligned} f(x) &= \frac{1}{2}\varphi_0(x) + \frac{1}{2c} \int_0^x v_0(\xi) d\xi + \frac{1}{2}A, \\ g(x) &= \frac{1}{2}\varphi_0(x) - \frac{1}{2c} \int_0^x v_0(\xi) d\xi - \frac{1}{2}A. \end{aligned} \quad (6.53)$$

Thus

$$\varphi(x, t) = \frac{1}{2} \{ \varphi_0(x + ct) + \varphi_0(x - ct) \} + \frac{1}{2c} \int_{x-ct}^{x+ct} v_0(\xi) d\xi. \quad (6.54)$$

Again we find d'Alembert's solution.

Exercise 6.2: Show that when the operator D in a constant-coefficient second-order PDE $D\varphi = 0$ is *reducible*, meaning that it can be factored into two distinct first-order factors $D = P_1 P_2$ where

$$P_i = \alpha_i \frac{\partial}{\partial x} + \beta_i \frac{\partial}{\partial y} + \gamma_i,$$

then the general solution to $D\varphi = 0$ can be written as $\varphi = \phi_1 + \phi_2$, where $P_1\phi_1 = 0$, $P_2\phi_2 = 0$. Hence, or otherwise, show that the general solution to the equation

$$\frac{\partial^2 \varphi}{\partial x \partial y} + 2 \frac{\partial^2 \varphi}{\partial y^2} - \frac{\partial \varphi}{\partial x} - 2 \frac{\partial \varphi}{\partial y} = 0$$

is

$$\varphi(x, y) = f(2x - y) + e^y g(x),$$

where f, g , are arbitrary functions.

Exercise 6.3: Show that when the constant-coefficient operator D is of the form

$$D = P^2 = \left(\alpha \frac{\partial}{\partial x} + \beta \frac{\partial}{\partial y} + \gamma \right)^2,$$

with $\alpha \neq 0$, then the general solution to $D\varphi = 0$ is given by $\varphi = \phi_1 + x\phi_2$, where $P\phi_{1,2} = 0$. (If $\alpha = 0$ and $\beta \neq 0$, then $\varphi = \phi_1 + y\phi_2$.)

6.3.2 Fourier's Solution

Starting from the same Cauchy data as d'Alembert, Joseph Fourier proposed a completely different approach to solving the wave equation. He sought a solution in the form

$$\varphi(x, t) = \int_{-\infty}^{\infty} \frac{dk}{2\pi} \{a(k)e^{ikx-i\omega_k t} + a^*(k)e^{-ikx+i\omega_k t}\}, \quad (6.55)$$

where $\omega_k \equiv c|k|$ is the *positive* root of $\omega^2 = c^2 k^2$. The terms being summed by the integral are all individually of the form $f(x - ct)$, or $f(x + ct)$, and so $\varphi(x, t)$ is indeed a solution of the wave equation. The positive-root convention means that positive k corresponds to right-going waves, and negative k to left-going waves.

We find the amplitudes $a(k)$ by fitting to the Fourier transforms of the initial data

$$\begin{aligned} \varphi(x, t=0) &= \int_{-\infty}^{\infty} \frac{dk}{2\pi} \Phi(k)e^{ikx}, \\ \dot{\varphi}(x, t=0) &= \int_{-\infty}^{\infty} \frac{dk}{2\pi} \chi(k)e^{ikx}, \end{aligned} \quad (6.56)$$

so

$$\begin{aligned} \Phi(k) &= a(k) + a^*(-k), \\ \chi(k) &= i\omega_k (a^*(-k) - a(k)). \end{aligned} \quad (6.57)$$

Solving, we find

$$\begin{aligned} a(k) &= \frac{1}{2} \left(\Phi(k) + \frac{i}{\omega_k} \chi(k) \right), \\ a^*(k) &= \frac{1}{2} \left(\Phi(-k) - \frac{i}{\omega_k} \chi(-k) \right). \end{aligned} \quad (6.58)$$

For some years after Fourier's trigonometric series solution was proposed, doubts persisted as to whether it was as general as that of d'Alembert. This was because many mathematicians of that era simply refused to believe that (almost) every function could be represented by a Fourier expansion. Fourier's solution is, however, completely equivalent to d'Alembert's.

6.3.3 Causal Green Function

We now add a source term:

$$\frac{1}{c^2} \frac{\partial^2 \varphi}{\partial t^2} - \frac{\partial^2 \varphi}{\partial x^2} = q(x, t). \quad (6.59)$$

We will solve this equation by finding a Green function such that

$$\left(\frac{1}{c^2} \frac{\partial^2}{\partial t^2} - \frac{\partial^2}{\partial x^2} \right) G(x, t; \xi, \tau) = \delta(x - \xi) \delta(t - \tau). \quad (6.60)$$

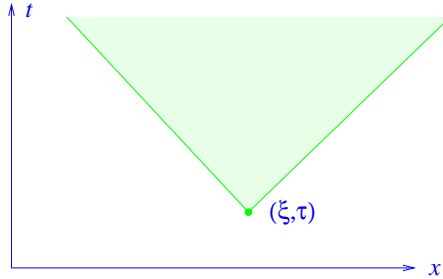
If the only waves in the system are those produced by the source, we should demand that the Green function be *causal*, in that $G(x, t; \xi, \tau) = 0$ if $t < \tau$.

To construct the causal Green function, we integrate the equation over an infinitesimal time interval from $\tau - \varepsilon$ to $\tau + \varepsilon$ and so find Cauchy data

$$\begin{aligned} G(x, \tau + \varepsilon; \xi, \tau) &= 0, \\ \frac{d}{dt} G(x, \tau + \varepsilon; \xi, \tau) &= c^2 \delta(x - \xi). \end{aligned} \quad (6.61)$$

We plug this into d'Alembert's solution to get

$$\begin{aligned} G(x, t; \xi, \tau) &= \theta(t - \tau) \frac{c}{2} \int_{x-c(t-\tau)}^{x+c(t-\tau)} \delta(\zeta - \xi) d\zeta \\ &= \frac{c}{2} \theta(t - \tau) \left\{ \theta(x - \xi + c(t - \tau)) - \theta(x - \xi - c(t - \tau)) \right\}. \end{aligned} \quad (6.62)$$

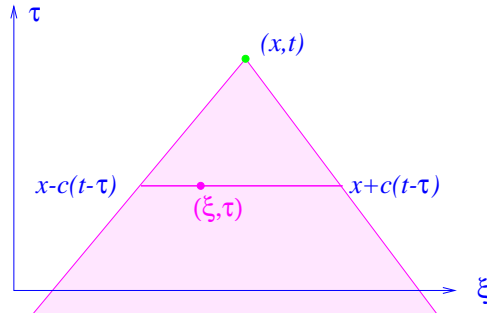


Support of $G(x, t; \xi, \tau)$ for fixed ξ, τ , or the “domain of influence”.

Using this we have

$$\begin{aligned}\varphi(x, t) &= \frac{c}{2} \int_{-\infty}^t d\tau \int_{x-c(t-\tau)}^{x+c(t-\tau)} q(\xi, \tau) d\xi \\ &= \frac{c}{2} \iint_{\Omega} q(\xi, \tau) d\tau d\xi\end{aligned}\tag{6.63}$$

where the domain of integration Ω is shown in the figure.



The region Ω , or the “domain of dependence”.

We can write the causal Green function in the form of Fourier’s solution of the wave equation. We claim that

$$G(x, t; \xi, \tau) = c^2 \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} \int_{-\infty}^{\infty} \frac{dk}{2\pi} \left\{ \frac{e^{ik(x-\xi)} e^{-i\omega(t-\tau)}}{c^2 k^2 - (\omega + i\varepsilon)^2} \right\}, \tag{6.64}$$

where the $i\varepsilon$ plays the same role in enforcing causality as it does for the harmonic oscillator in one dimension. This is only to be expected. If we decompose a vibrating string into normal modes, then each mode is an independent oscillator of with $\omega_k^2 = c^2 k^2$, and the Green function for the PDE is simply the sum of the ODE Green functions for each k mode. Using our previous results for the single-oscillator Green function to do the integral over ω , we find

$$G(x, t; 0, 0) = \theta(t) c^2 \int_{-\infty}^{\infty} \frac{dk}{2\pi} e^{ikx} \frac{1}{c|k|} \sin(|k|ct). \tag{6.65}$$

Despite the factor of $1/|k|$, there is no singularity at $k = 0$, so no $i\varepsilon$ is needed to make the integral over k well defined. We can do the k integral

by recognizing that the integrand is nothing but the Fourier representation, $\frac{1}{k} \sin ak$, of a square-wave pulse. We end up with

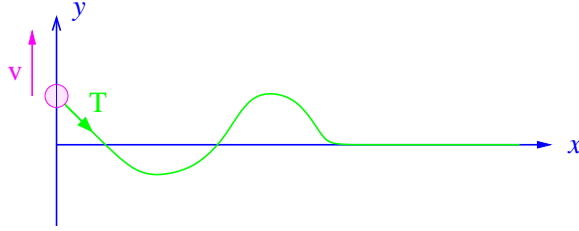
$$G(x, t; 0, 0) = \theta(t) \frac{c}{2} \{ \theta(x + ct) - \theta(x - ct) \}, \quad (6.66)$$

the same expression as from our direct construction. We can also write

$$G(x, t; 0, 0) = \frac{c}{2} \int_{-\infty}^{\infty} \frac{dk}{2\pi} \left(\frac{i}{|k|} \right) \{ e^{ikx - i|k|ct} - e^{-ikx + ic|k|t} \}, \quad t > 0, \quad (6.67)$$

which is in explicit Fourier-solution form with $a(k) = ic/2|k|$.

Illustration: Radiation Damping. A bead of mass M slides without friction on the y axis. It is attached to an infinite string which is initially undisturbed and lying along the x axis. The string has tension T , and a density such that the speed of waves on the string is c . Show that the wave energy emitted by the moving bead gives rise to an effective viscous damping force on it.



A bead connected to a string.

From the figure we see that $M\dot{v} = Ty'(0, t)$, and from the condition of no incoming waves we know that

$$y(x, t) = y(x - ct). \quad (6.68)$$

Thus $y'(0, t) = -\dot{y}(0, t)/c$. But the bead is attached to the string, so $v(t) = \dot{y}(0, t)$, and therefore

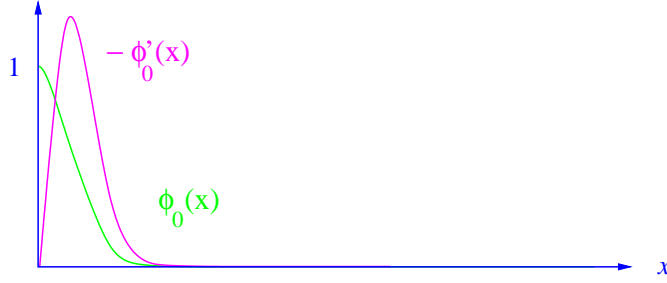
$$M\dot{v} = - \left(\frac{T}{c} \right) v. \quad (6.69)$$

The effective viscosity coefficient is thus $\eta = T/c$. Note that we need an infinitely long string for this formula to be true for all time. If the string has a finite length L , then, after a period of $2L/c$, energy will be reflected back to the bead and will complicate matters.

We can also derive the radiation damping from the Caldeira-Leggett analysis of chapter 5. Our bead-string contraption has Lagrangian

$$L = \frac{M}{2}[\dot{y}(0, t)]^2 - V[y(0, t)] + \int_0^L \left\{ \frac{\rho}{2}\dot{y}^2 - \frac{T}{2}y'^2 \right\} dx. \quad (6.70)$$

Here $V[y]$ is some potential energy for the bead. Introduce a function $\phi_0(x)$ such that $\phi_0(0) = 1$ and $\phi_0(x)$ decreases rapidly to zero as x increases.



The function $\phi_0(x)$ and its derivative.

We therefore have $-\phi'_0(x) \approx \delta(x)$. Expand $y(x, t)$ in terms of $\phi_0(x)$ and the normal modes of a string with fixed ends as

$$y(x, t) = y(0, t)\phi_0(x) + \sum_n q_n(t) \sqrt{\frac{2}{L\rho}} \sin k_n x. \quad (6.71)$$

Here $k_n L = n\pi$. Because $y(0, t)\phi_0(x)$ describes the motion of only an infinitesimal length of string, $y(0, t)$ makes a negligible contribution to the string kinetic energy, but it provides a linear coupling of the bead to the string normal modes, $q_n(t)$, through the $Ty'^2/2$ term. Plugging the expansion into L , and after about half a page of arithmetic, we end up with

$$L = \frac{M}{2}[\dot{y}(0)]^2 - V[y(0)] + y(0) \sum_n f_n q_n + \sum_n \left(\frac{1}{2} \dot{q}_n^2 - \omega_n^2 q_n^2 \right) - \frac{1}{2} \sum_n \left(\frac{f_n^2}{\omega_n^2} \right) y(0)^2, \quad (6.72)$$

where $\omega_n = ck_n$, and

$$f_n = T \sqrt{\frac{2}{L\rho}} k_n. \quad (6.73)$$

This is exactly the Caldeira-Leggett Lagrangian, including the frequency-shift counter-term. When L becomes large, the eigenvalue density of states

$$\rho(\omega) = \sum_n \delta(\omega - \omega_n) \quad (6.74)$$

becomes

$$\rho(\omega) = \frac{L}{\pi c}. \quad (6.75)$$

The Caldeira-Leggett spectral function

$$J(\omega) = \frac{\pi}{2} \sum_n \left(\frac{f_n^2}{\omega_n} \right) \delta(\omega - \omega_n), \quad (6.76)$$

is therefore

$$J(\omega) = \frac{\pi}{2} \cdot \frac{2T^2 k^2}{L\rho} \cdot \frac{1}{kc} \cdot \frac{L}{\pi c} = \left(\frac{T}{c} \right) \omega, \quad (6.77)$$

where we have used $c = \sqrt{T/\rho}$. Comparing with Caldeira-Leggett's $J(\omega) = \eta\omega$, we see that the effective viscosity is given by $\eta = T/c$, as before. The necessity of having an infinitely long string here translates into the requirement that we must have a *continuum* of oscillator modes. It is only after the sum over discrete modes ω_i is replaced by an integral over the continuum of ω 's that no energy is ever returned to the system being damped.

This formalism can be extended to other radiation damping problems. For example we may consider¹ the drag forces induced by the emission of radiation from accelerated charged particles. We end up with a deeper understanding of the traditional, but pathological, Abraham-Lorentz equation,

$$M(\dot{\mathbf{v}} - \tau \ddot{\mathbf{v}}) = \mathbf{F}_{\text{ext}}, \quad (6.78)$$

which is plagued by runaway solutions. (Here

$$\tau = \frac{2}{3} \frac{e^2}{c^3} \frac{1}{M} \left[\frac{1}{4\pi\epsilon_0} \right], \quad (6.79)$$

the factor in square brackets being needed for SI units. It is absent in Gaussian units.)

6.3.4 Odd vs. Even Dimensions

Consider the wave equation for sound in the three dimensions. We have a velocity potential ϕ which obeys the wave equation

$$\frac{\partial^2 \phi}{\partial x^2} + \frac{\partial^2 \phi}{\partial y^2} + \frac{\partial^2 \phi}{\partial z^2} - \frac{1}{c^2} \frac{\partial^2 \phi}{\partial t^2} = 0, \quad (6.80)$$

¹G. W. Ford, R. F. O'Connell, Phys. Lett. A **157** (1991) 217.

and from which the velocity, density, and pressure fluctuations can be extracted as

$$\begin{aligned} v_1 &= \nabla \phi, \\ \rho_1 &= -\frac{\rho_0}{c^2} \dot{\phi}, \\ P_1 &= c^2 \rho_1. \end{aligned} \quad (6.81)$$

In three dimensions, and considering only spherically symmetric waves, the wave equation becomes

$$\frac{\partial^2(r\phi)}{\partial r^2} - \frac{1}{c^2} \frac{\partial^2(r\phi)}{\partial t^2} = 0, \quad (6.82)$$

with solution

$$\phi(r, t) = \frac{1}{r} f\left(t - \frac{r}{c}\right) + \frac{1}{r} g\left(t + \frac{r}{c}\right). \quad (6.83)$$

Consider what happens if we put a point volume source at the origin (the sudden conversion of a negligible volume of solid explosive to a large volume of hot gas, for example). Let the rate at which volume is being intruded be \dot{q} . The gas velocity very close to the origin will be

$$v(r, t) = \frac{\dot{q}(t)}{4\pi r^2}. \quad (6.84)$$

Matching this to an outgoing wave gives

$$\frac{\dot{q}(t)}{4\pi r^2} = v_1(r, t) = \frac{\partial \phi}{\partial r} = -\frac{1}{r^2} f\left(t - \frac{r}{c}\right) - \frac{1}{rc} f'\left(t - \frac{r}{c}\right). \quad (6.85)$$

Close to the origin, in the *near field*, the term $\propto f/r^2$ will dominate, and so

$$-\frac{1}{4\pi} \dot{q}(t) = f(t). \quad (6.86)$$

Further away, in the *far field* or *radiation field*, only the second term will survive, and so

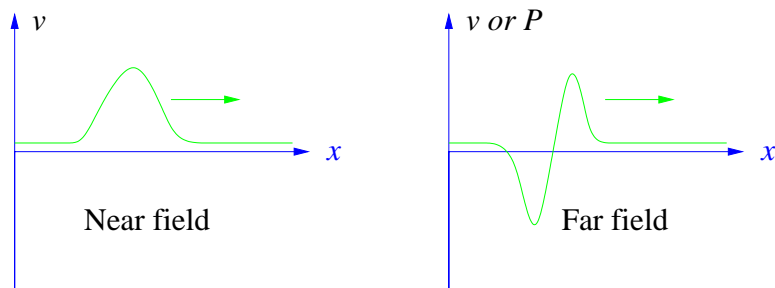
$$v_1 = \frac{\partial \phi}{\partial r} \approx -\frac{1}{rc} f'\left(t - \frac{r}{c}\right). \quad (6.87)$$

The far-field velocity-pulse profile v_1 is therefore the derivative of the near-field v_1 pulse profile.

The pressure pulse

$$P_1 = -\rho_0 \dot{\phi} = \frac{\rho_0}{4\pi r} \ddot{q} \left(t - \frac{r}{c} \right) \quad (6.88)$$

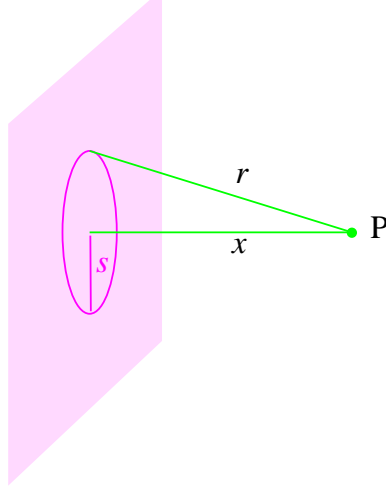
is also of this form. Thus, a sudden localized expansion of gas produces an outgoing pressure pulse which is first positive and then negative.



Three-dimensional blast wave.

This phenomenon can be seen in (old, we hope) news footage of bomb blasts in tropical regions. A spherical vapour condensation wave can be seen spreading out from the explosion. The condensation cloud is caused by the air cooling below the dew-point in the low-pressure region which tails the over-pressure blast.

Now consider what happens if we have a sheet of explosive, the simultaneous detonation of every part of which gives us a one-dimensional plane-wave pulse. We can obtain the plane wave by adding up the individual spherical waves from each point on the sheet.

*Sheet-source geometry.*

Using the notation defined in the figure, we have

$$\phi(x, t) = 2\pi \int_0^\infty \frac{1}{\sqrt{x^2 + s^2}} f\left(t - \frac{\sqrt{x^2 + s^2}}{c}\right) s ds \quad (6.89)$$

with $f(t) = -\dot{q}(t)/4\pi$, where now \dot{q} is the rate at which volume is being intruded per unit area of the sheet. We can write this as

$$\begin{aligned} & 2\pi \int_0^\infty f\left(t - \frac{\sqrt{x^2 + s^2}}{c}\right) d\sqrt{x^2 + s^2}, \\ &= 2\pi c \int_{-\infty}^{t-x/c} f(\tau) d\tau, \\ &= -\frac{c}{2} \int_{-\infty}^{t-x/c} \dot{q}(\tau) d\tau. \end{aligned} \quad (6.90)$$

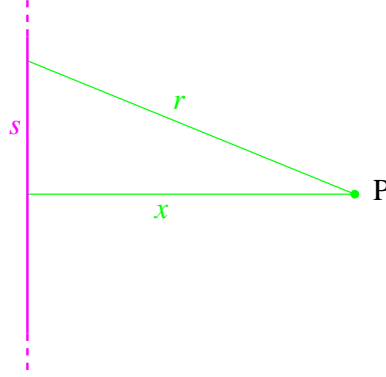
In the second line we have defined $\tau = t - \sqrt{x^2 + s^2}/c$, which, *inter alia*, interchanged the role of the upper and lower limits on the integral.

Thus, $v_1 = \phi'(x, t) = \frac{1}{2}\dot{q}(t - x/c)$. Since the near field motion produced by the intruding gas is $v_1(r) = \frac{1}{2}\dot{q}(t)$, the far-field displacement exactly reproduces the initial motion, suitably delayed of course. (The factor 1/2 is because half the intruded volume goes towards producing a pulse in the negative direction.)

In three dimensions, the far-field motion is the first derivative of the near-field motion. In one dimension, the far-field motion is exactly the same as the near-field motion. In two dimensions the far-field motion should therefore be the half-derivative of the near-field motion — but how do you half differentiate a function? An answer is suggested by the theory of Laplace transformations as

$$\left(\frac{d}{dt}\right)^{\frac{1}{2}} F(t) \stackrel{\text{def}}{=} \frac{1}{\sqrt{\pi}} \int_{-\infty}^t \frac{\dot{F}(\tau)}{\sqrt{t-\tau}} d\tau. \quad (6.91)$$

Let us now repeat the explosive sheet calculation for an exploding wire.



Line-source geometry.

Using

$$ds = d\left(\sqrt{r^2 - x^2}\right) = \frac{r \, dr}{\sqrt{r^2 - x^2}}, \quad (6.92)$$

and combining the contributions of the two parts of the wire that are the same distance from p , we can write

$$\begin{aligned} \phi(x, t) &= \int_x^\infty \frac{1}{r} f\left(t - \frac{r}{c}\right) \frac{2r \, dr}{\sqrt{r^2 - x^2}} \\ &= 2 \int_x^\infty f\left(t - \frac{r}{c}\right) \frac{dr}{\sqrt{r^2 - x^2}}, \end{aligned} \quad (6.93)$$

with $f(t) = -\dot{q}(t)/4\pi$, where now \dot{q} is the volume intruded per unit length. We may approximate $r^2 - x^2 \approx 2x(r - x)$ for the near parts of the wire where $r \approx x$, since these make the dominant contribution to the integral. We also

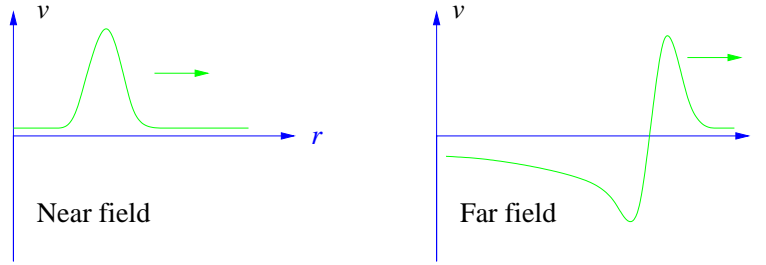
set $\tau = t - r/c$, and then have

$$\begin{aligned}\phi(x, t) &= \frac{2c}{\sqrt{2x}} \int_{-\infty}^{(t-x/c)} f(\tau) \frac{dr}{\sqrt{(ct-x)-c\tau}}, \\ &= -\frac{1}{2\pi} \sqrt{\frac{2c}{x}} \int_{-\infty}^{(t-x/c)} \dot{q}(\tau) \frac{d\tau}{\sqrt{(t-x/c)-\tau}}.\end{aligned}\quad (6.94)$$

The far-field velocity is the x gradient of this,

$$v_1(r, t) = \frac{1}{2\pi c} \sqrt{\frac{2c}{x}} \int_{-\infty}^{(t-x/c)} \ddot{q}(\tau) \frac{d\tau}{\sqrt{(t-x/c)-\tau}}, \quad (6.95)$$

and is therefore proportional to the 1/2-derivative of $\dot{q}(t - r/c)$.



In two dimensions the far-field pulse has a long tail.

The far-field pulse never completely dies away to zero, and this long tail means that one cannot use digital signalling in two dimensions.

Moral Tale: A couple of years ago one of our colleagues was performing numerical work on earthquake propagation. The source of his waves was a long deep linear fault, so he used the two-dimensional wave equation. Not wanting to be troubled by the actual creation of the wave pulse, he took as initial data an outgoing finite-width pulse. After a short propagation time his numerics always went crazy. He wasted several months in vain attempt to improve the stability of his code before it was pointed out him that what he was seeing was real. The lack of a long tail on his pulse meant that it could not have been created by a well-behaved line source. The numerical craziness was a consequence of the source striving to do the impossible. *Moral:* Always check that a solution actually exists before you waste your time trying to compute it.

Exercise 6.4: Use the calculus of improper integrals to show that, provided $F(-\infty) = 0$, we have

$$\frac{d}{dt} \left(\frac{1}{\sqrt{\pi}} \int_{-\infty}^t \frac{\dot{F}(\tau)}{\sqrt{t-\tau}} d\tau \right) = \frac{1}{\sqrt{\pi}} \int_{-\infty}^t \frac{\ddot{F}(\tau)}{\sqrt{t-\tau}} d\tau. \quad (6.96)$$

This means that

$$\frac{d}{dt} \left(\frac{d}{dt} \right)^{\frac{1}{2}} F(t) = \left(\frac{d}{dt} \right)^{\frac{1}{2}} \frac{d}{dt} F(t). \quad (6.97)$$

6.4 Heat Equation

Fourier's heat equation

$$\frac{\partial \phi}{\partial t} = \kappa \frac{\partial^2 \phi}{\partial x^2} \quad (6.98)$$

is the archetypal parabolic equation. It often comes with initial data $\phi(x, t = 0)$, but this is not Cauchy data, as the curve $t = \text{const.}$ is a characteristic.

The heat equation is also known as the *diffusion equation*.

6.4.1 Heat Kernel

If we Fourier transform the initial data

$$\phi(x, t = 0) = \int_{-\infty}^{\infty} \frac{dk}{2\pi} \tilde{\phi}(k) e^{ikx}, \quad (6.99)$$

and write

$$\phi(x, t) = \int_{-\infty}^{\infty} \frac{dk}{2\pi} \tilde{\phi}(k, t) e^{ikx}, \quad (6.100)$$

we can plug this into the heat equation and find that

$$\frac{\partial \tilde{\phi}}{\partial t} = -\kappa k^2 \tilde{\phi}. \quad (6.101)$$

Hence,

$$\begin{aligned} \phi(x, t) &= \int_{-\infty}^{\infty} \frac{dk}{2\pi} \tilde{\phi}(k, t) e^{ikx} \\ &= \int_{-\infty}^{\infty} \frac{dk}{2\pi} \tilde{\phi}(k, 0) e^{ikx - \kappa k^2 t}. \end{aligned} \quad (6.102)$$

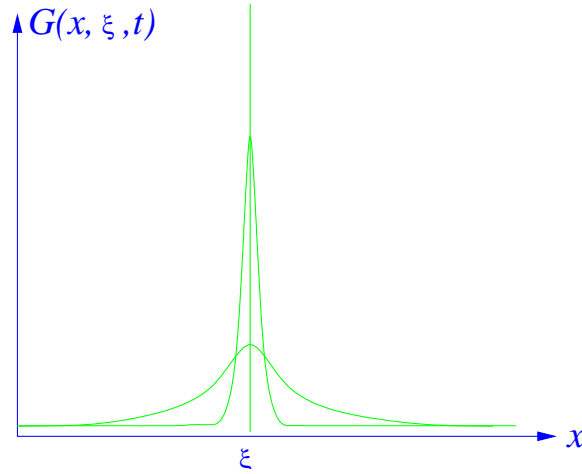
We may now express $\tilde{\phi}(k, 0)$ in terms of $\phi(x, 0)$ and rearrange the order of integration to get

$$\begin{aligned}\phi(x, t) &= \int_{-\infty}^{\infty} \frac{dk}{2\pi} \left(\int_{-\infty}^{\infty} \phi(\xi, 0) e^{ik\xi} d\xi \right) e^{ikx - \kappa k^2 t} \\ &= \int_{-\infty}^{\infty} \left(\int_{-\infty}^{\infty} \frac{dk}{2\pi} e^{ik(x-\xi) - \kappa k^2 t} \right) \phi(\xi, 0) d\xi \\ &= \int_{-\infty}^{\infty} G(x, \xi, t) \phi(\xi, 0) d\xi,\end{aligned}\tag{6.103}$$

where

$$G(x, \xi, t) = \int_{-\infty}^{\infty} \frac{dk}{2\pi} e^{ik(x-\xi) - \kappa k^2 t} = \frac{1}{\sqrt{4\pi\kappa t}} \exp \left\{ -\frac{1}{4\kappa t} (x - \xi)^2 \right\}.\tag{6.104}$$

Here, $G(x, \xi, t)$ is the *heat kernel*. It represents the spreading of a unit blob of heat.



The heat kernel at three successive times.

As the heat spreads, the area under the curve remains constant:

$$\int_{-\infty}^{\infty} \frac{1}{\sqrt{4\pi\kappa t}} \exp \left\{ -\frac{1}{4\kappa t} (x - \xi)^2 \right\} dx = 1.\tag{6.105}$$

The heat kernel possesses a *semigroup property*

$$G(x, \xi, t_1 + t_2) = \int_{-\infty}^{\infty} G(x, \eta, t_2) G(\eta, \xi, t_1) d\eta.\tag{6.106}$$

Exercise: Prove this.

6.4.2 Causal Green Function

Now we consider the inhomogeneous heat equation

$$\frac{\partial u}{\partial t} - \frac{\partial^2 u}{\partial x^2} = q(x, t), \quad (6.107)$$

with initial data $u(x, 0) = u_0(x)$. We define a Causal Green function by

$$\left(\frac{\partial}{\partial t} - \frac{\partial^2}{\partial x^2} \right) G(x, t; \xi, \tau) = \delta(x - \xi) \delta(t - \tau) \quad (6.108)$$

and the requirement that $G(x, t; \xi, \tau) = 0$ if $t < \tau$. Integrating the equation from $t = \tau - \varepsilon$ to $t = \tau + \varepsilon$ tells us that

$$G(x, \tau + \varepsilon; \xi, \tau) = \delta(x - \xi). \quad (6.109)$$

Taking this delta function as initial data $\phi(x, t = \tau)$ and inserting into (6.103) we read off

$$G(x, t; \xi, \tau) = \theta(t - \tau) \frac{1}{\sqrt{4\pi(t - \tau)}} \exp \left\{ -\frac{1}{4(t - \tau)} (x - \xi)^2 \right\}. \quad (6.110)$$

We apply this Green function to the solution of a problem involving both a heat source and initial data given at $t = 0$ on the entire real line. We exploit a variant of the Lagrange-identity method we used for solving one-dimensional ODE's with inhomogeneous boundary conditions. Let

$$D_{x,t} \equiv \frac{\partial}{\partial t} - \frac{\partial^2}{\partial x^2}, \quad (6.111)$$

and observe that its formal adjoint,

$$D_{x,t}^\dagger \equiv -\frac{\partial}{\partial t} - \frac{\partial^2}{\partial x^2}. \quad (6.112)$$

is a “backward” heat-equation operator. The corresponding “backward” Green function

$$G^\dagger(x, t; \xi, \tau) = \theta(\tau - t) \frac{1}{\sqrt{4\pi(\tau - t)}} \exp \left\{ -\frac{1}{4(\tau - t)} (x - \xi)^2 \right\} \quad (6.113)$$

obeys

$$D_{x,t}^\dagger G^\dagger(x, t; \xi, \tau) = \delta(x - \xi) \delta(t - \tau), \quad (6.114)$$

with adjoint boundary conditions. These make G^\dagger *anti-causal*, in that $G^\dagger(t - \tau)$ vanishes when $t > \tau$. Now we make use of the two-dimensional Lagrange identity

$$\begin{aligned} & \int_{-\infty}^{\infty} dx \int_0^T dt \left\{ u(x, t) D_{x,t}^\dagger G^\dagger(x, t; \xi, \tau) - \left(D_{x,t} u(x, t) \right) G^\dagger(x, t; \xi, \tau) \right\} \\ &= \int_{-\infty}^{\infty} dx \left\{ u(x, 0) G^\dagger(x, 0; \xi, \tau) \right\} - \int_{-\infty}^{\infty} dx \left\{ u(x, T) G^\dagger(x, T; \xi, \tau) \right\}. \end{aligned} \quad (6.115)$$

Assume that (ξ, τ) lies within the region of integration. Then the left hand side is equal to

$$u(\xi, \tau) - \int_{-\infty}^{\infty} dx \int_0^T dt \left\{ q(x, t) G^\dagger(x, t; \xi, \tau) \right\}. \quad (6.116)$$

On the right hand side, the second integral vanishes because G^\dagger is zero on $t = T$. Thus,

$$u(\xi, \tau) = \int_{-\infty}^{\infty} dx \int_0^T dt \left\{ q(x, t) G^\dagger(x, t; \xi, \tau) \right\} + \int_{-\infty}^{\infty} \left\{ u(x, 0) G^\dagger(x, 0; \xi, \tau) \right\} dx \quad (6.117)$$

Rewriting this by using

$$G^\dagger(x, t; \xi, \tau) = G(\xi, \tau; x, t), \quad (6.118)$$

and relabeling $x \leftrightarrow \xi$ and $t \leftrightarrow \tau$, we have

$$u(x, t) = \int_{-\infty}^{\infty} G(x, t; \xi, 0) u_0(\xi) d\xi + \int_{-\infty}^{\infty} \int_0^t G(x, t; \xi, \tau) q(\xi, \tau) d\xi d\tau. \quad (6.119)$$

Note how the effects of any heat source $q(x, t)$ active prior to the initial-data epoch at $t = 0$ have been subsumed into the evolution of the initial data.

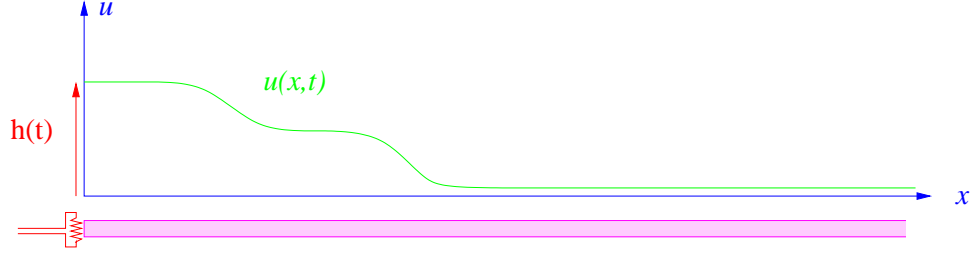
6.4.3 Duhamel's Principle

Often, the temperature of the spatial boundary of a region is specified in addition to the initial data. Dealing with this type of problem leads us to a new strategy.

Suppose we are required to solve

$$\frac{\partial u}{\partial t} = \kappa \frac{\partial^2 u}{\partial x^2} \quad (6.120)$$

for a semi-infinite rod $0 \leq x < \infty$. We are given a specified temperature, $u(0, t) = h(t)$, at the end $x = 0$, and for all other points $x > 0$ we are given an initial condition $u(x, 0) = 0$.



Semi-infinite rod heated at one end.

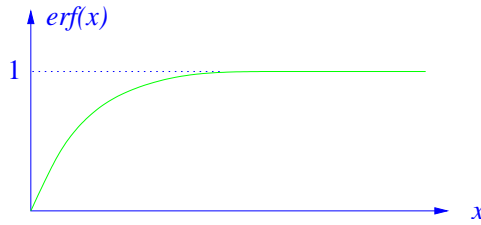
We begin by finding a solution $w(x, t)$ that satisfies the heat equation with $w(0, t) = 1$ and initial data $w(x, 0) = 0$, $x > 0$. This solution is constructed in the problems, and is

$$w = \theta(t) \left\{ 1 - \operatorname{erf} \left(\frac{x}{2\sqrt{t}} \right) \right\}. \quad (6.121)$$

Here $\operatorname{erf}(x)$ is the *error function*

$$\operatorname{erf}(x) = \frac{2}{\sqrt{\pi}} \int_0^x e^{-z^2} dz. \quad (6.122)$$

which obeys $\operatorname{erf}(0) = 0$ and $\operatorname{erf}(x) \rightarrow 1$ as $x \rightarrow \infty$.



Error function.

If we were given

$$h(t) = h_0 \theta(t - t_0), \quad (6.123)$$

then the desired solution would be

$$u(x, t) = h_0 w(x, t - t_0). \quad (6.124)$$

For a sum

$$h(t) = \sum_n h_n \theta(t - t_n), \quad (6.125)$$

the principle of superposition (*i.e.* the linearity of the problem) tell us that the solution is the corresponding sum

$$u(x, t) = \sum_n h_n w(x, t - t_n). \quad (6.126)$$

We therefore decompose $h(t)$ into a sum of step functions

$$\begin{aligned} h(t) &= h(0) + \int_0^t \dot{h}(\tau) d\tau \\ &= h(0) + \int_0^\infty \theta(t - \tau) \dot{h}(\tau) d\tau. \end{aligned} \quad (6.127)$$

It is should now be clear that

$$\begin{aligned} u(x, t) &= \int_0^t w(x, t - \tau) \dot{h}(\tau) d\tau + h(0)w(x, t) \\ &= - \int_0^t \left(\frac{\partial}{\partial \tau} w(x, t - \tau) \right) h(\tau) d\tau \\ &= \int_0^t \left(\frac{\partial}{\partial t} w(x, t - \tau) \right) h(\tau) d\tau. \end{aligned} \quad (6.128)$$

This is called *Duhamel's solution*, and the trick of expressing the data as a sum of Heaviside step functions is called Duhamel's principle.

We do not need to be as clever as Duhamel. We could have obtained this result by using the method of images to find a suitable causal Green function for the half line, and then using the same Lagrange-identity method as before.

6.5 Laplace's Equation

The topic of *potential theory*, as problems involving the Laplacian are known, is quite extensive. Here we will only explore the foothills.

Poisson's equation, $-\nabla^2 \chi = f(\mathbf{r})$, $\mathbf{r} \in \Omega$, and the Laplace equation to which it reduces when $f(\mathbf{r}) \equiv 0$, come with various boundary conditions, of

which the commonest are

$$\begin{aligned} \chi &= \rho(x) & \text{on} & \partial\Omega, & (\text{Dirichlet}) \\ (\mathbf{n} \cdot \nabla)\chi &= q(x) & \text{on} & \partial\Omega. & (\text{Neumann}) \end{aligned} \quad (6.129)$$

A function for which $\nabla^2\chi = 0$ in some region Ω is said to be *harmonic* there.

Uniqueness and Existence of Solutions

A function harmonic in a bounded subset Ω of \mathbb{R}^3 is uniquely determined by its values on the boundary of Ω . To see that this is so, suppose that φ_1 and φ_2 both satisfy $\nabla^2\varphi = 0$ in Ω , and take the same values on the boundary. Then $\chi = \varphi_1 - \varphi_2$ obeys $\nabla^2\chi = 0$ in Ω , and is zero on the boundary. Integrating by parts we find that

$$\int_{\Omega} |\nabla\chi|^2 d^n x = \int_{\partial\Omega} \chi(\mathbf{n} \cdot \nabla)\chi dS = 0. \quad (6.130)$$

Here dS is the element of area on the boundary and \mathbf{n} the outward-directed normal. Now, because the second derivatives exist, the partial derivatives entering into $\nabla\chi$ must be continuous, and so the vanishing of integral of $|\nabla\chi|^2$ tells us that $\nabla\chi$ is zero everywhere in Ω . This means that χ is constant — and because it is zero on the boundary it is zero everywhere.

An almost identical argument show that if φ_1 and φ_2 both satisfy $\nabla^2\varphi = 0$ in Ω and have the same values of $(\mathbf{n} \cdot \nabla)\varphi$ on the boundary then $\varphi_1 = \varphi_2 + \text{const.}$ We have therefore shown that, if it exists, the solutions of the Dirichlet boundary value problem is unique, and the solution of the Neumann problem is unique up to the addition of an arbitrary constant.

In the Neumann case, with boundary condition $(\mathbf{n} \cdot \nabla)\varphi = q$, the integral

$$\int_{\Omega} \nabla^2\varphi d^n x = \int_{\partial\Omega} (\mathbf{n} \cdot \nabla)\varphi dS = \int_{\partial\Omega} q dS = 0 \quad (6.131)$$

shows that boundary data $q(x)$ must satisfy $\int_{\partial\Omega} q dS = 0$, if a solution to $\nabla^2\varphi = 0$ is to exist. This is an example the Fredholm alternative that relates the existence of a non-trivial null space to constraints on the source terms. For the inhomogeneous equation $\nabla^2\varphi = f$, the condition is $\int_{\partial\Omega} q dS = \int_{\Omega} f d^n x$.

Given that we have satisfied any Fredholm constraint, do solutions to the Dirichlet and Neumann problem always exist? That solutions should exist is

suggested by physics: the Dirichlet problem corresponds to an electrostatic problem with specified boundary potentials and the Neumann problem corresponds to finding the electric potential due to specified boundary charges. The Fredholm constraint is then the Gauss'-law condition that the total electric charge within a hollow conductor must be zero. Surely solutions always exist to these physics problems? In the Dirichlet case we can even make a mathematically plausible argument for existence: We observe that the boundary-value problem is solved by the φ that minimizes the functional

$$J[\varphi] = \int_{\Omega} |\nabla \varphi|^2 d^n x \quad (6.132)$$

over the set of twice-differentiable functions taking the given boundary values. Since J is positive, and hence bounded below, it seems intuitively obvious that there must be some function φ for which J is a minimum. The appeal of this *Dirichlet principle* argument led even Riemann astray. The fallacy was exposed by Weierstrass who provided counterexamples. The problem reveals itself in three or more dimensions when the boundary of Ω has a sharp re-entrant spike that is held at a different potential from the rest of the boundary. One can then find a sequence of trial functions for which J becomes arbitrarily small, but the sequence of functions has no limit consistent with the boundary data. The physics argument also fails: if we tried to create a physical realization of this situation, the electric field would become infinite near the spike, and the charge would leak off and thwart our attempts to establish the potential difference. For reasonably smooth boundaries, however, a minimizing function does exist. In two dimensions, and provided the boundary is connected, a solution exists even when the boundary is very jagged.

Here is a simple illustration of how a functional minimization problem can fail to provide a satisfactory solution: Suppose we are required to find a continuous function $y(x)$ that minimizes

$$J[y] = \int_0^1 y^2 dx$$

subject to the conditions $y(0) = 0$, $y(1) = 1$. Since $J[y]$ is bounded below by zero it seems plausible that such a y exists. We try the functions $y_n = x^n$, $n = 1, 2, \dots$, all of which satisfy the boundary data. We find

$$J[y_n] = \frac{1}{2n+1},$$

and this can be made arbitrarily small provided we take n large enough. Thus the infimum of J must be zero. If, however, there were a continuous y such that $J[y]$ actually took the value zero, then the continuity of y ensures that y must be zero — but $y(x) = 0$ is inconsistent with the boundary data.

Exercise 6.5: Helmholtz decomposition

- a) Cite the conditions for the existence of a solution to the Neumann problem to show that if Ω is a three-dimensional region and \mathbf{u} is a smooth vector field defined in Ω , then there exist a unique solenoidal (*i.e.* having zero divergence) vector field \mathbf{v} with $\mathbf{v} \cdot \mathbf{n} = 0$ on the boundary of Ω , and a unique scalar field ϕ such that

$$\mathbf{u} = \mathbf{v} + \nabla\phi.$$

Here \mathbf{n} is the normal to the (assumed smooth) bounding surface of Ω .

- b) In many cases (but not always) we can write $\mathbf{v} = \text{curl } \mathbf{w}$. Show that if we *can* do this, then \mathbf{w} is not unique, but we can always make it unique by demanding it to obey the conditions $\text{div } \mathbf{w} = 0$ and $\mathbf{w} \cdot \mathbf{n} = 0$. (In general $\mathbf{u} = \nabla\phi + \text{curl } \mathbf{w} + \mathbf{h}$ where \mathbf{h} obeys $\nabla^2 \mathbf{h} = 0$ and suitable boundary conditions. See exercise 6.14 for a discussion.)
- c) Use the Helmholtz decomposition of part a) with $\mathbf{u} \rightarrow (\mathbf{v} \cdot \nabla)\mathbf{v}$ to show that in the Euler equation

$$\frac{\partial \mathbf{v}}{\partial t} + (\mathbf{v} \cdot \nabla)\mathbf{v} = -\nabla P, \quad \mathbf{v} \cdot \mathbf{n} = 0 \text{ on } \partial\Omega$$

governing the motion of an incompressible ($\text{div } \mathbf{v} = 0$) fluid the instantaneous flow field $\mathbf{v}(x, y, z, t)$ uniquely determines $\dot{\mathbf{v}}$, and hence the time evolution of the flow. (This observation provides the basis of practical numerical algorithms for incompressible flow.)

6.5.1 Separation of Variables

Cartesian Coordinates

When the region of interest is a square or a rectangle, we can solve Laplace boundary problems by separating the Laplace operator in cartesian co-ordinates. Let

$$\frac{\partial^2 \varphi}{\partial x^2} + \frac{\partial^2 \varphi}{\partial y^2} = 0, \tag{6.133}$$

and write

$$\varphi = X(x)Y(y), \tag{6.134}$$

so that

$$\frac{1}{X} \frac{\partial^2 X}{\partial x^2} + \frac{1}{Y} \frac{\partial^2 Y}{\partial y^2} = 0. \quad (6.135)$$

Since the first term is a function of x only, and the second of y only, both must be constants and the sum of these constants must be zero. Therefore

$$\begin{aligned} \frac{1}{X} \frac{\partial^2 X}{\partial x^2} &= -k^2, \\ \frac{1}{Y} \frac{\partial^2 Y}{\partial y^2} &= k^2, \end{aligned} \quad (6.136)$$

or, equivalently

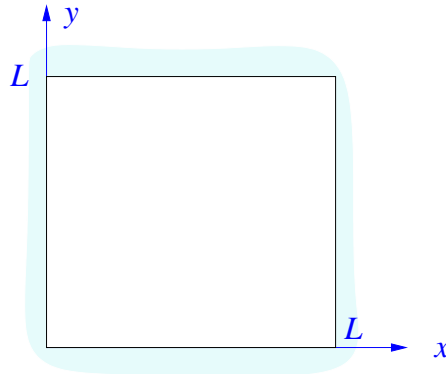
$$\begin{aligned} \frac{\partial^2 X}{\partial x^2} + k^2 X &= 0, \\ \frac{\partial^2 Y}{\partial y^2} - k^2 Y &= 0. \end{aligned} \quad (6.137)$$

The number that we have, for later convenience, written as k^2 is called a *separation constant*. The solutions are $X = e^{\pm ikx}$ and $Y = e^{\pm ky}$. Thus

$$\varphi = e^{\pm ikx} e^{\pm ky}, \quad (6.138)$$

or a sum of such terms where the allowed k 's are determined by the boundary conditions.

How do we know that the separated form $X(x)Y(y)$ captures all possible solutions? We can be confident that we have them all if we can use the separated solutions to solve boundary-value problems with arbitrary boundary data.



Square region.

We can use our separated solutions to construct the unique harmonic function taking given values on the sides a square of side L . To see how to do this, consider the four families of functions

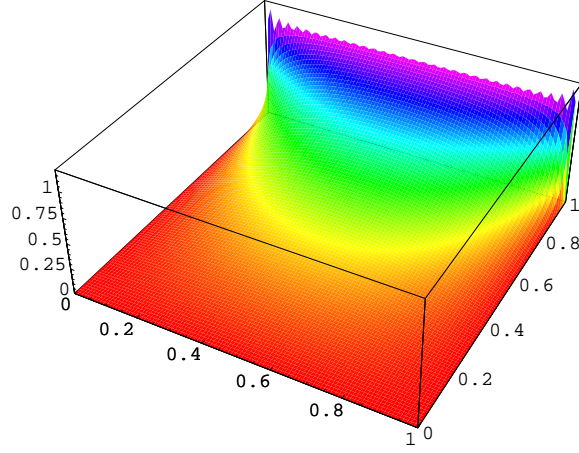
$$\begin{aligned}
 \varphi_{1,n} &= \sqrt{\frac{2}{L \sinh n\pi}} \sin \frac{n\pi x}{L} \sinh \frac{n\pi y}{L}, \\
 \varphi_{2,n} &= \sqrt{\frac{2}{L \sinh n\pi}} \sinh \frac{n\pi x}{L} \sin \frac{n\pi y}{L}, \\
 \varphi_{3,n} &= \sqrt{\frac{2}{L \sinh n\pi}} \sin \frac{n\pi x}{L} \sinh \frac{n\pi(L-y)}{L}, \\
 \varphi_{4,n} &= \sqrt{\frac{2}{L \sinh n\pi}} \sinh \frac{n\pi(L-x)}{L} \sin \frac{n\pi y}{L}.
 \end{aligned} \tag{6.139}$$

Each of these comprises solutions to $\nabla^2 \varphi = 0$. The family $\varphi_{1,n}(x, y)$ has been constructed so that every member is zero on three sides of the square, but on the side $y = L$ it becomes $\varphi_{1,n}(x, L) = \sqrt{2/L} \sin(n\pi x/L)$. The $\varphi_{1,n}(x, L)$ therefore constitute an complete orthonormal set in terms of which we can expand the boundary data on the side $y = L$. Similarly, the other other families are non-zero on only one side, and are complete there. Thus, any boundary data can be expanded in terms of these four function sets, and the solution to the boundary value problem will be a sum

$$\varphi(x, y) = \sum_{m=1}^4 \sum_{n=1}^{\infty} a_{m,n} \varphi_{m,n}(x, y). \tag{6.140}$$

The solution to $\nabla^2 \varphi = 0$ in the unit square with $\varphi = 1$ on the side $y = 1$ and zero on the other sides is, for example,

$$\varphi(x, y) = \sum_{n=0}^{\infty} \frac{4}{(2n+1)\pi} \frac{1}{\sinh(2n+1)\pi} \sin((2n+1)\pi x) \sinh((2n+1)\pi y) \tag{6.141}$$



Plot of first thirty terms in (6.141).

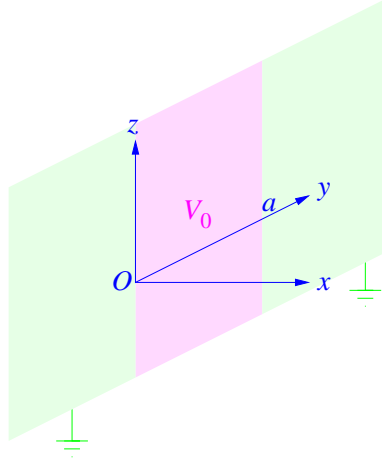
For cubes, and higher dimensional hypercubes, we can use similar boundary expansions. For the unit cube in three dimensions we would use

$$\varphi_{1,nm}(x, y, z) = \frac{1}{\sinh(\pi\sqrt{n^2 + m^2})} \sin(n\pi x) \sin(m\pi y) \sinh(\pi z\sqrt{n^2 + m^2}),$$

to expand the data on the face $z = 1$, together with five other solution families, one for each of the other five faces of the cube.

If some of the boundaries are at infinity, we may need only need some of these functions.

Example: We have three conducting sheets, each infinite in the z direction. The central one has width a , and is held at voltage V_0 . The outer two extend to infinity also in the y direction, and are grounded. The resulting potential should tend to zero as $|x|, |y| \rightarrow \infty$.



Conducting sheets.

The voltage in the $x = 0$ plane is

$$\varphi(0, y, z) = \int_{-\infty}^{\infty} \frac{dk}{2\pi} a(k) e^{-iky}, \quad (6.142)$$

where

$$a(k) = V_0 \int_{-a/2}^{a/2} e^{iky} dy = \frac{2V_0}{k} \sin(ka/2). \quad (6.143)$$

Then, taking into account the boundary condition at large x , the solution to $\nabla^2 \varphi = 0$ is

$$\varphi(x, y, z) = \int_{-\infty}^{\infty} \frac{dk}{2\pi} a(k) e^{-iky} e^{-|k||x|}. \quad (6.144)$$

The evaluation of this integral, and finding the charge distribution on the sheets, is left as an exercise.

The Cauchy Problem is Ill-posed

Although the Laplace equation has no characteristics, the Cauchy data problem is *ill-posed*, meaning that the solution is not a continuous function of the data. To see this, suppose we are given $\nabla^2 \varphi = 0$ with Cauchy data on $y = 0$:

$$\begin{aligned} \varphi(x, 0) &= 0, \\ \left. \frac{\partial \varphi}{\partial y} \right|_{y=0} &= \varepsilon \sin kx. \end{aligned} \quad (6.145)$$

Then

$$\varphi(x, y) = \frac{\varepsilon}{k} \sin(kx) \sinh(ky). \quad (6.146)$$

Provided k is large enough — even if ε is tiny — the exponential growth of the hyperbolic sine will make this arbitrarily large. Any infinitesimal uncertainty in the high frequency part of the initial data will be vastly amplified, and the solution, although formally correct, is useless in practice.

Polar coordinates

We can use the separation of variables method in polar coordinates. Here,

$$\nabla^2 \chi = \frac{\partial^2 \chi}{\partial r^2} + \frac{1}{r} \frac{\partial \chi}{\partial r} + \frac{1}{r^2} \frac{\partial^2 \chi}{\partial \theta^2}. \quad (6.147)$$

Set

$$\chi(r, \theta) = R(r)\Theta(\theta). \quad (6.148)$$

Then $\nabla^2 \chi = 0$ implies

$$\begin{aligned} 0 &= \frac{r^2}{R} \left(\frac{\partial^2 R}{\partial r^2} + \frac{1}{r} \frac{\partial R}{\partial r} \right) + \frac{1}{\Theta} \frac{\partial^2 \Theta}{\partial \theta^2} \\ &= \quad m^2 \quad - \quad m^2, \end{aligned} \quad (6.149)$$

where in the second line we have written the separation constant as m^2 . Therefore,

$$\frac{d^2 \Theta}{d\theta^2} + m^2 \Theta = 0, \quad (6.150)$$

implying that $\Theta = e^{im\theta}$, where m must be an integer if Θ is to be single-valued, and

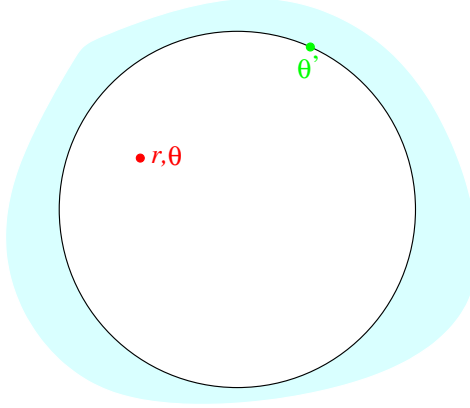
$$r^2 \frac{d^2 R}{dr^2} + r \frac{dR}{dr} - m^2 R = 0, \quad (6.151)$$

whose solutions are $R = r^{\pm m}$ when $m \neq 0$, and 1 or $\ln r$ when $m = 0$. The general solution is therefore a sum of these

$$\chi = A_0 + B_0 \ln r + \sum_{m \neq 0} (A_m r^{|m|} + B_m r^{-|m|}) e^{im\theta}. \quad (6.152)$$

The singular terms, $\ln r$ and $r^{-|m|}$, are not solutions at the origin, and should be omitted when that point is part of the region where $\nabla^2 \chi = 0$.

Example: Dirichlet problem in the interior of the unit circle. Solve $\nabla^2 \chi = 0$ in $\Omega = \{\mathbf{r} \in \mathbb{R}^2 : |\mathbf{r}| < 1\}$ with $\chi = f(\theta)$ on $\partial\Omega \equiv \{|\mathbf{r}| = 1\}$.



Dirichlet problem in the unit circle.

We expand

$$\chi(r, \theta) = \sum_{m=-\infty}^{\infty} A_m r^{|m|} e^{im\theta}, \quad (6.153)$$

and read off the coefficients from the boundary data as

$$A_m = \frac{1}{2\pi} \int_0^{2\pi} e^{-im\theta'} f(\theta') d\theta'. \quad (6.154)$$

Thus,

$$\chi = \frac{1}{2\pi} \int_0^{2\pi} \left[\sum_{m=-\infty}^{\infty} r^{|m|} e^{im(\theta-\theta')} \right] f(\theta') d\theta'. \quad (6.155)$$

We can sum the geometric series

$$\begin{aligned} \sum_{m=-\infty}^{\infty} r^{|m|} e^{im(\theta-\theta')} &= \left(\frac{1}{1 - re^{i(\theta-\theta')}} + \frac{re^{-i(\theta-\theta')}}{1 - re^{-i(\theta-\theta')}} \right) \\ &= \frac{1 - r^2}{1 - 2r \cos(\theta - \theta') + r^2}. \end{aligned} \quad (6.156)$$

Therefore,

$$\chi(r, \theta) = \frac{1}{2\pi} \int_0^{2\pi} \left(\frac{1 - r^2}{1 - 2r \cos(\theta - \theta') + r^2} \right) f(\theta') d\theta'. \quad (6.157)$$

This expression is known as the *Poisson kernel formula*. Observe how the integrand sharpens towards a delta function as r approaches unity, and so makes the value of $\chi(r, \theta)$ given by the integral consistent with the boundary data.

If we set $r = 0$ in the Poisson formula, we find

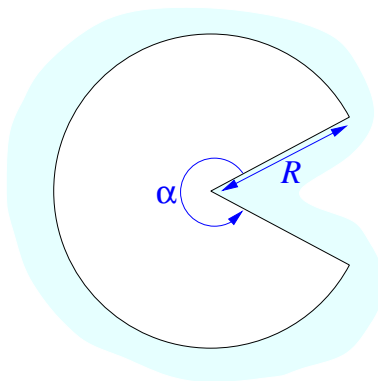
$$\chi(0, \theta) = \frac{1}{2\pi} \int_0^{2\pi} f(\theta') d\theta'. \quad (6.158)$$

We deduce that if $\nabla^2 \chi = 0$ in some domain then the value of χ at a point in the domain is the average of its values on any circle centred on the chosen point and lying wholly in the domain.

This average-value property means that χ can have no local maxima or minima within Ω . The same result holds in \mathbb{R}^n , and a formal theorem to this effect can be proved:

Theorem (The mean-value theorem for harmonic functions): If χ is harmonic ($\nabla^2 \chi = 0$) within the bounded (open, connected) domain $\Omega \in \mathbb{R}^n$, and is continuous on its closure $\overline{\Omega}$, and if $m \leq \chi \leq M$ on $\partial\Omega$, then $m < \chi < M$ in Ω — unless, that is, $m = M$, when χ is constant.

Pie-shaped regions



A pie-shaped region of opening angle α .

Electrostatics problems involving regions with corners can often be understood by solving Laplace's equation within a pie-shaped region.

Suppose we have a pie-shaped region of opening angle α and radius R . If the boundary value of the potential is zero on the wedge and non-zero on

the boundary arc, we can seek solutions as a sum of r, θ separated terms

$$\varphi(r, \theta) = \sum_{n=1}^{\infty} a_n r^{n\pi/\alpha} \sin\left(\frac{n\pi\theta}{\alpha}\right). \quad (6.159)$$

Here the trigonometric function is not 2π periodic, but instead has been constructed so as to make φ vanish at $\theta = 0$ and $\theta = \alpha$. These solutions show that close to the edge of a conducting wedge of external opening angle α , the surface charge density σ usually varies as $\sigma(r) \propto r^{\alpha/\pi-1}$.

If we have non-zero boundary data on the edge of the wedge at $\theta = \alpha$, but have $\varphi = 0$ on the edge at $\theta = 0$ and on the curved arc $r = R$, then the solutions can be expressed as a continuous sum of r, θ separated terms

$$\begin{aligned} \varphi(r, \theta) &= \frac{1}{2i} \int_0^{\infty} a(\nu) \left(\left(\frac{r}{R}\right)^{i\nu} - \left(\frac{r}{R}\right)^{-i\nu} \right) \frac{\sinh(\nu\theta)}{\sinh(\nu\alpha)} d\nu, \\ &= \int_0^{\infty} a(\nu) \sin[\nu \ln(r/R)] \frac{\sinh(\nu\theta)}{\sinh(\nu\alpha)} d\nu. \end{aligned} \quad (6.160)$$

The Mellin sine transformation can be used to computing the coefficient function $a(\nu)$. This transformation lets us write

$$f(r) = \frac{2}{\pi} \int_0^{\infty} F(\nu) \sin(\nu \ln r) d\nu, \quad 0 < r < 1, \quad (6.161)$$

where

$$F(\nu) = \int_0^1 \sin(\nu \ln r) f(r) \frac{dr}{r}. \quad (6.162)$$

The Mellin sine transformation is a disguised version of the Fourier sine transform of functions on $[0, \infty)$. We simply map the positive x axis onto the interval $(0, 1]$ by the change of variables $x = -\ln r$.

Despite its complexity when expressed in terms of these formulae, the simple solution $\varphi(r, \theta) = a\theta$ is often the physically relevant one when the two sides of the wedge are held at different potentials and the potential is allowed to vary on the curved arc.

Example: Consider a pie-shaped region of opening angle π and radius $R = \infty$. This region can be considered to be the upper half-plane. Suppose that we are told that the positive x axis is held at potential $+1/2$ and the negative x axis is at potential $-1/2$, and are required to find the potential for positive

y . If we separate Laplace's equation in cartesian co-ordinates and match to the boundary data on the x -axes, we end up with

$$\varphi_{xy}(x, y) = \frac{1}{\pi} \int_0^\infty \frac{1}{k} e^{-ky} \sin(kx) dk.$$

On the other hand, the function

$$\varphi_{r\theta}(r, \theta) = \frac{1}{\pi}(\pi/2 - \theta)$$

satisfies both Laplace's equation and the boundary data. At this point we ought to worry that we do not have enough data to determine the solution uniquely — nothing was said in the statement of the problem about the behavior of φ on the boundary arc at infinity — but a little effort shows that

$$\begin{aligned} \frac{1}{\pi} \int_0^\infty \frac{1}{k} e^{-ky} \sin(kx) dk &= \frac{1}{\pi} \tan^{-1} \left(\frac{x}{y} \right), \quad y > 0, \\ &= \frac{1}{\pi}(\pi/2 - \theta), \end{aligned} \tag{6.163}$$

and so the two expressions for $\varphi(x, y)$ are equal.

6.5.2 Eigenfunction Expansions

Elliptic operators are the natural analogues of the one-dimensional linear differential operators we studied in earlier chapters.

The operator $L = -\nabla^2$ is formally self-adjoint with respect to the inner product

$$\langle \phi, \chi \rangle = \iint \phi^* \chi \, dx dy. \tag{6.164}$$

This property follows from Green's identity

$$\iint_\Omega \{ \phi^* (-\nabla^2 \chi) - (-\nabla^2 \phi)^* \chi \} \, dx dy = \int_{\partial\Omega} \{ \phi^* (-\nabla \chi) - (-\nabla \phi)^* \chi \} \cdot \mathbf{n} \, ds \tag{6.165}$$

where $\partial\Omega$ is the boundary of the region Ω and \mathbf{n} is the outward normal on the boundary.

The method of separation of variables also allows us to solve eigenvalue problems involving the Laplace operator. For example, the Dirichlet eigenvalue problem requires us to find the eigenfunctions and eigenvalues of the operator

$$L = -\nabla^2, \quad \mathcal{D}(L) = \{\phi \in L^2[\Omega] : \phi = 0, \text{ on } \partial\Omega\}. \quad (6.166)$$

Suppose Ω is the rectangle $0 \leq x \leq L_x$, $0 \leq y \leq L_y$. The normalized eigenfunctions are

$$\phi_{n,m}(x, y) = \sqrt{\frac{4}{L_x L_y}} \sin\left(\frac{n\pi x}{L_x}\right) \sin\left(\frac{m\pi y}{L_y}\right), \quad (6.167)$$

with eigenvalues

$$\lambda_{n,m} = \left(\frac{n^2\pi^2}{L_x^2}\right) + \left(\frac{m^2\pi^2}{L_y^2}\right). \quad (6.168)$$

The eigenfunctions are orthonormal,

$$\int \phi_{n,m} \phi_{n',m'} dx dy = \delta_{nn'} \delta_{mm'}, \quad (6.169)$$

and complete. Thus, any function in $L^2[\Omega]$ can be expanded as

$$f(x, y) = \sum_{m,n=1}^{\infty} A_{nm} \phi_{n,m}(x, y), \quad (6.170)$$

where

$$A_{nm} = \iint \phi_{n,m}(x, y) f(x, y) dx dy. \quad (6.171)$$

We can find a complete set of eigenfunctions in product form whenever we can separate the Laplace operator in a system of co-ordinates ξ_i such that the boundary becomes $\xi_i = \text{const.}$ Completeness in the multidimensional space is then guaranteed by the completeness of the eigenfunctions of each one-dimensional differential operator. For other than rectangular co-ordinates, however, the separated eigenfunctions are not elementary functions.

The Laplacian has a complete set of Dirichlet eigenfunctions in any region, but in general these eigenfunctions cannot be written as separated products of one-dimensional functions.

6.5.3 Green Functions

Once we know the eigenfunctions φ_n and eigenvalues λ_n for $-\nabla^2$ in a region Ω , we can write down the Green function as

$$g(\mathbf{r}, \mathbf{r}') = \sum_n \frac{1}{\lambda_n} \varphi_n(\mathbf{r}) \varphi_n^*(\mathbf{r}').$$

For example, the Green function for the Laplacian in the entire \mathbb{R}^n is given by the sum over eigenfunctions

$$g(\mathbf{r}, \mathbf{r}') = \int \frac{d^n k}{(2\pi)^n} \frac{e^{i\mathbf{k} \cdot (\mathbf{r} - \mathbf{r}')}}{k^2}. \quad (6.172)$$

Thus

$$-\nabla_{\mathbf{r}}^2 g(\mathbf{r}, \mathbf{r}') = \int \frac{d^n k}{(2\pi)^n} e^{i\mathbf{k} \cdot (\mathbf{r} - \mathbf{r}')} = \delta^n(\mathbf{r} - \mathbf{r}'). \quad (6.173)$$

We can evaluate the integral for any n by using *Schwinger's trick* to turn the integrand into a Gaussian:

$$\begin{aligned} g(\mathbf{r}, \mathbf{r}') &= \int_0^\infty ds \int \frac{d^n k}{(2\pi)^n} e^{i\mathbf{k} \cdot (\mathbf{r} - \mathbf{r}')} e^{-sk^2} \\ &= \int_0^\infty ds \left(\sqrt{\frac{\pi}{s}} \right)^n \frac{1}{(2\pi)^n} e^{-\frac{1}{4s} |\mathbf{r} - \mathbf{r}'|^2} \\ &= \frac{1}{2^n \pi^{n/2}} \int_0^\infty dt t^{\frac{n}{2}-2} e^{-t |\mathbf{r} - \mathbf{r}'|^2 / 4} \\ &= \frac{1}{2^n \pi^{n/2}} \Gamma\left(\frac{n}{2} - 1\right) \left(\frac{|\mathbf{r} - \mathbf{r}'|^2}{4} \right)^{1-n/2} \\ &= \frac{1}{(n-2)S_{n-1}} \left(\frac{1}{|\mathbf{r} - \mathbf{r}'|} \right)^{n-2} \end{aligned} \quad (6.174)$$

Here, $\Gamma(x)$ is Euler's gamma function:

$$\Gamma(x) = \int_0^\infty dt t^{x-1} e^{-t}, \quad (6.175)$$

and

$$S_{n-1} = \frac{2\pi^{n/2}}{\Gamma(n/2)} \quad (6.176)$$

is the surface area of the n -dimensional unit ball.

For three dimensions we find

$$g(\mathbf{r}, \mathbf{r}') = \frac{1}{4\pi} \frac{1}{|\mathbf{r} - \mathbf{r}'|}, \quad n = 3. \quad (6.177)$$

In two dimensions the Fourier integral is divergent for small k . We may control this divergence by using *dimensional regularization*. We treat n as being a continuous variable and use

$$\Gamma(x) = \frac{1}{x} \Gamma(x+1) \quad (6.178)$$

together with

$$a^x = e^{a \ln x} = 1 + a \ln x + \cdots \quad (6.179)$$

to to examine the behaviour of $g(\mathbf{r}, \mathbf{r}')$ near $n = 2$:

$$\begin{aligned} g(\mathbf{r}, \mathbf{r}') &= \frac{1}{4\pi} \frac{\Gamma(n/2)}{(n/2-1)} (1 - (n/2-1) \ln(\pi|\mathbf{r} - \mathbf{r}'|^2) + O[(n-2)^2]) \\ &= \frac{1}{4\pi} \left(\frac{1}{n/2-1} - 2 \ln|\mathbf{r} - \mathbf{r}'| - \ln \pi - \gamma + \cdots \right). \end{aligned} \quad (6.180)$$

Here $\gamma = -\Gamma'(1) = .57721 \dots$ is the *Euler-Mascheroni constant*. Although the pole $1/(n-2)$ blows up at $n = 2$, it is independent of position. We simply absorb it, and the $-\ln \pi - \gamma$, into an undetermined additive constant. Once we have done this, the limit $n \rightarrow 2$ can be taken and we find

$$g(\mathbf{r}, \mathbf{r}') = -\frac{1}{2\pi} \ln|\mathbf{r} - \mathbf{r}'| + \text{const.}, \quad n = 2. \quad (6.181)$$

The constant does not affect the Green-function property, so we can chose any convenient value for it.

Although we have managed to sweep the small- k divergence of the Fourier integral under a rug, the hidden infinity still has the capacity to cause problems. The Green function in \mathbb{R}^3 allows us to to solve for $\varphi(\mathbf{r})$ in the equation

$$-\nabla^2 \varphi = q(\mathbf{r}),$$

with the boundary condition $\varphi(\mathbf{r}) \rightarrow 0$ as $|\mathbf{r}| \rightarrow \infty$, as

$$\varphi(\mathbf{r}) = \int g(\mathbf{r}, \mathbf{r}') q(\mathbf{r}') d^3r.$$

In two dimensions, however we try to adjust the arbitrary constant in (6.181), the divergence of the logarithm at infinity means that there can be no solution to the corresponding boundary-value problem unless $\int q(\mathbf{r}) d^3r = 0$. This is not a Fredholm-alternative constraint because once the constraint is satisfied the solution is unique. The two-dimensional problem is therefore pathological from the viewpoint of Fredholm theory. This pathology is of the same character as the non-existence of solutions to the three-dimensional Dirichlet boundary-value problem with boundary spikes.

Exercise 6.6: Evaluate our formula for the \mathbb{R}^n Laplace Green function,

$$g(\mathbf{r}, \mathbf{r}') = \frac{1}{(n-2)S_{n-1}|\mathbf{r} - \mathbf{r}'|^{n-2}}$$

with $S_{n-1} = 2\pi^{n/2}/\Gamma(n/2)$, for the case $n = 1$. Show that the resulting expression for $g(x, x')$ is not divergent, and obeys

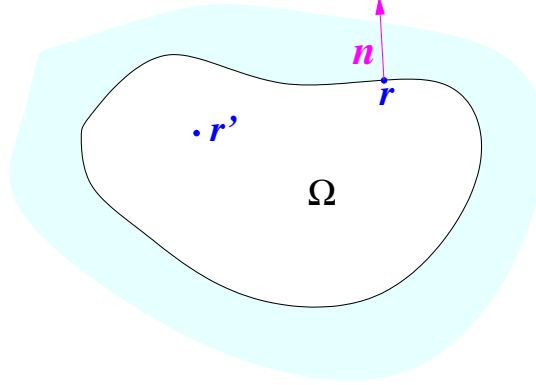
$$-\frac{d^2}{dx^2}g(x, x') = \delta(x - x').$$

Our formula therefore makes sense as a Green function — even though the original integral (6.172) is linearly divergent at $k = 0$! We will have to defer an explanation of this miracle until we discuss *analytic continuation* in the context of complex analysis.

(Hint: recall that $\Gamma(1/2) = \sqrt{\pi}$)

6.5.4 Boundary-value problems

We now look at how the Green function can be used to solve the interior Dirichlet boundary-value problem in regions where the method of separation of variables is not available. Suppose Ω to be a finite region with a smooth boundary $\partial\Omega$.



Interior Dirichlet problem.

We wish to solve $-\nabla^2 \varphi = q(\mathbf{r})$ for $\mathbf{r} \in \Omega$ and with $\varphi(\mathbf{r}) = f(\mathbf{r})$ for $\mathbf{r} \in \partial\Omega$.

Suppose we have found a Green function that obeys

$$-\nabla_{\mathbf{r}}^2 g(\mathbf{r}, \mathbf{r}') = \delta^n(\mathbf{r} - \mathbf{r}'), \quad \mathbf{r}, \mathbf{r}' \in \Omega, \quad g(\mathbf{r}, \mathbf{r}') = 0, \quad \mathbf{r} \in \partial\Omega. \quad (6.182)$$

We first show that $g(\mathbf{r}, \mathbf{r}') = g(\mathbf{r}', \mathbf{r})$ by the same methods we used for one-dimensional self-adjoint operators. Next we follow the strategy that we used for one-dimensional inhomogeneous differential equations: we use Lagrange's identity (in this context called Green's theorem) to write

$$\begin{aligned} \int_{\Omega} d^n r \{g(\mathbf{r}, \mathbf{r}') \nabla_{\mathbf{r}}^2 \varphi(\mathbf{r}) - \varphi(\mathbf{r}) \nabla_{\mathbf{r}}^2 g(\mathbf{r}, \mathbf{r}')\} \\ = \int_{\partial\Omega} d\mathbf{S}_{\mathbf{r}} \cdot \{g(\mathbf{r}, \mathbf{r}') \nabla_{\mathbf{r}} \varphi(\mathbf{r}) - \varphi(\mathbf{r}) \nabla_{\mathbf{r}} g(\mathbf{r}, \mathbf{r}')\}, \end{aligned} \quad (6.183)$$

where $d\mathbf{S}_{\mathbf{r}} = \mathbf{n} dS_{\mathbf{r}}$, with \mathbf{n} the outward normal to $\partial\Omega$ at the point \mathbf{r} . The left hand side is

$$\begin{aligned} \text{L.H.S.} &= \int_{\Omega} d^n r \{-g(\mathbf{r}, \mathbf{r}') q(\mathbf{r}) + \varphi(\mathbf{r}) \delta^n(\mathbf{r} - \mathbf{r}')\}, \\ &= - \int_{\Omega} d^n r g(\mathbf{r}, \mathbf{r}') q(\mathbf{r}) + \varphi(\mathbf{r}'), \\ &= - \int_{\Omega} d^n r g(\mathbf{r}', \mathbf{r}) q(\mathbf{r}) + \varphi(\mathbf{r}'). \end{aligned} \quad (6.184)$$

On the right hand side, the boundary condition on $g(\mathbf{r}, \mathbf{r}')$ makes the first term zero, so

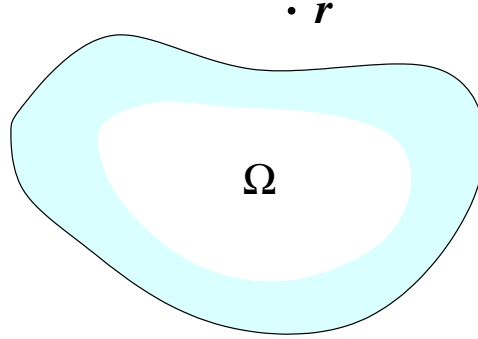
$$\text{R.H.S} = - \int_{\partial\Omega} dS_{\mathbf{r}} f(\mathbf{r}) (\mathbf{n} \cdot \nabla_{\mathbf{r}}) g(\mathbf{r}, \mathbf{r}'). \quad (6.185)$$

Therefore,

$$\varphi(\mathbf{r}') = \int_{\Omega} g(\mathbf{r}', \mathbf{r}) q(\mathbf{r}) d^n r - \int_{\partial\Omega} f(\mathbf{r})(\mathbf{n} \cdot \nabla_{\mathbf{r}}) g(\mathbf{r}, \mathbf{r}') dS_{\mathbf{r}}. \quad (6.186)$$

In the language of chapter 3, the first term is a particular integral and the second (the boundary integral term) is the complementary function.

Exercise 6.7: Show that the limit of $\varphi(\mathbf{r}')$ as \mathbf{r}' approaches the boundary is indeed $f(\mathbf{r}')$. (Hint: When \mathbf{r}, \mathbf{r}' are very close to it, assume that the boundary can be approximated by a straight line segment, and so $g(\mathbf{r}, \mathbf{r}')$ can be found by the method of images.)



Exterior Dirichlet problem.

A similar method works for the exterior Dirichlet problem. In this case we seek a Green function obeying

$$-\nabla_{\mathbf{r}}^2 g(\mathbf{r}, \mathbf{r}') = \delta^n(\mathbf{r} - \mathbf{r}'), \quad \mathbf{r}, \mathbf{r}' \in \mathbb{R}^n \setminus \Omega \quad g(\mathbf{r}, \mathbf{r}') = 0, \quad \mathbf{r} \in \partial\Omega. \quad (6.187)$$

(The notation $\mathbb{R}^n \setminus \Omega$ means the region outside Ω .) We also impose a further boundary condition by requiring $g(\mathbf{r}, \mathbf{r}')$, and hence $\varphi(\mathbf{r})$, to tend to zero as $|\mathbf{r}| \rightarrow \infty$. The final formula for $\varphi(\mathbf{r})$ is the same except for the region of integration and the sign of the boundary term.

The hard part of both the interior and exterior problems is to find the Green function for the given domain.

Exercise 6.8: Suppose that $\varphi(x, y)$ is harmonic in the half-plane $y > 0$, tends to zero as $y \rightarrow \infty$, and takes the values $f(x)$ on the boundary $y = 0$. Show that

$$\varphi(x, y) = \frac{1}{\pi} \int_{-\infty}^{\infty} \frac{y}{(x - x')^2 + y^2} f(x') dx', \quad y > 0.$$

Deduce that the “energy” functional

$$S[f] \stackrel{\text{def}}{=} \frac{1}{2} \int_{y>0} |\nabla \varphi|^2 dx dy \equiv -\frac{1}{2} \int_{-\infty}^{\infty} f(x) \left. \frac{\partial \varphi}{\partial y} \right|_{y=0} dx$$

can be expressed as

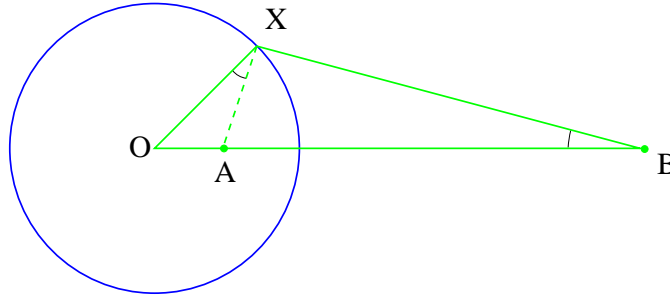
$$S[f] = \frac{1}{4\pi} \iint_{-\infty}^{\infty} \left\{ \frac{f(x) - f(x')}{x - x'} \right\}^2 dx' dx.$$

The non-local functional $S[f]$ appears in the quantum version of the Caldeira-Leggett model. See also exercise 2.24.

Method of Images

When $\partial\Omega$ is a sphere or a circle we can find the Dirichlet Green functions for the region Ω by using the *method of images*.

Consider a circle of radius R .



Points inverse with respect to a circle.

Given B outside the circle, and a point X on the circle, we construct A inside and on the line OB, so that $\angle OBX = \angle OXA$. We now observe that $\triangle XOA$ is similar to $\triangle BOX$, and so

$$\frac{OA}{OX} = \frac{OX}{OB}. \quad (6.188)$$

Thus, $OA \times OB = (OX)^2 \equiv R^2$. The points A and B are therefore *mutually inverse* with respect to the circle. In particular, the point A does not depend on which point X was chosen.

Now let $AX = r_i$, $BX = r_0$ and $OB = B$. Then, using similarity again, we have

$$\frac{AX}{OX} = \frac{BX}{OB}, \quad (6.189)$$

or

$$\frac{R}{r_i} = \frac{B}{r_0}, \quad (6.190)$$

and so

$$\frac{1}{r_i} \left(\frac{R}{B} \right) - \frac{1}{r_0} = 0. \quad (6.191)$$

Interpreting the figure as a slice through the centre of a sphere of radius R , we see that if we put a unit charge at B, then the insertion of an *image charge* of magnitude $q = -R/B$ at A serves to keep the entire surface of the sphere at zero potential.

Thus, in three dimensions, and with Ω the region exterior to the sphere, the Dirichlet Green function is

$$g_\Omega(\mathbf{r}, \mathbf{r}_B) = \frac{1}{4\pi} \left(\frac{1}{|\mathbf{r} - \mathbf{r}_B|} - \left(\frac{R}{|\mathbf{r}_B|} \right) \frac{1}{|\mathbf{r} - \mathbf{r}_A|} \right). \quad (6.192)$$

In two dimensions, we find similarly that

$$g_\Omega(\mathbf{r}, \mathbf{r}_B) = -\frac{1}{2\pi} \left(\ln |\mathbf{r} - \mathbf{r}_B| - \ln |\mathbf{r} - \mathbf{r}_A| - \ln (|\mathbf{r}_B|/R) \right), \quad (6.193)$$

has $g_\Omega(\mathbf{r}, \mathbf{r}_B) = 0$ for \mathbf{r} on the circle. Thus, this is the Dirichlet Green function for Ω , the region exterior to the circle.

We can use the same method to construct the interior Green functions for the sphere and circle.

6.5.5 Kirchhoff *vs.* Huygens

Even if we do not have a Green function tailored for the specific region in which we are interested, we can still use the whole-space Green function to convert the differential equation into an *integral equation*, and so make progress. An example of this technique is provided by Kirchhoff's partial justification of Huygens' construction.

The Green function $G(\mathbf{r}, \mathbf{r}')$ for the elliptic Helmholtz equation

$$(-\nabla^2 + \kappa^2)G(\mathbf{r}, \mathbf{r}') = \delta^3(\mathbf{r} - \mathbf{r}') \quad (6.194)$$

in \mathbb{R}^3 is given by

$$\int \frac{d^3k}{(2\pi)^3} \frac{e^{i\mathbf{k} \cdot (\mathbf{r} - \mathbf{r}')}}{k^2 + \kappa^2} = \frac{1}{4\pi|\mathbf{r} - \mathbf{r}'|} e^{-\kappa|\mathbf{r} - \mathbf{r}'|}. \quad (6.195)$$

Exercise 6.9: Perform the k integration and confirm this.

For solutions of the wave equation with $e^{-i\omega t}$ time dependence, we want a Green function such that

$$\left[-\nabla^2 - \left(\frac{\omega^2}{c^2} \right) \right] G(\mathbf{r}, \mathbf{r}') = \delta^3(\mathbf{r} - \mathbf{r}'), \quad (6.196)$$

and so we have to take κ^2 negative. We therefore have two possible Green functions

$$G_{\pm}(\mathbf{r}, \mathbf{r}') = \frac{1}{4\pi|\mathbf{r} - \mathbf{r}'|} e^{\pm ik|\mathbf{r} - \mathbf{r}'|}, \quad (6.197)$$

where $k = |\omega|/c$. These correspond to taking the real part of κ^2 negative, but giving it an infinitesimal imaginary part, as we did when discussing resolvent operators in chapter 5. If we want outgoing waves, we must take $G \equiv G_+$.

Now suppose we want to solve

$$(\nabla^2 + k^2)\psi = 0 \quad (6.198)$$

in an arbitrary region Ω . As before, we use Green's theorem to write

$$\begin{aligned} & \int_{\Omega} \{G(\mathbf{r}, \mathbf{r}')(\nabla_{\mathbf{r}}^2 + k^2)\psi(\mathbf{r}) - \psi(\mathbf{r})(\nabla_{\mathbf{r}}^2 + k^2)G(\mathbf{r}, \mathbf{r}')\} d^3x \\ &= \int_{\partial\Omega} \{G(\mathbf{r}, \mathbf{r}')\nabla_{\mathbf{r}}\psi(\mathbf{r}) - \psi(\mathbf{r})\nabla_{\mathbf{r}}G(\mathbf{r}, \mathbf{r}')\} \cdot d\mathbf{S}_{\mathbf{r}} \end{aligned} \quad (6.199)$$

where $d\mathbf{S}_{\mathbf{r}} = \mathbf{n} dS_{\mathbf{r}}$, with \mathbf{n} the outward normal to $\partial\Omega$ at the point \mathbf{r} . The left hand side is

$$\int_{\Omega} \psi(\mathbf{r})\delta^3(\mathbf{r} - \mathbf{r}') d^3x = \begin{cases} \psi(\mathbf{r}'), & \mathbf{r}' \in \Omega \\ 0, & \mathbf{r}' \notin \Omega \end{cases} \quad (6.200)$$

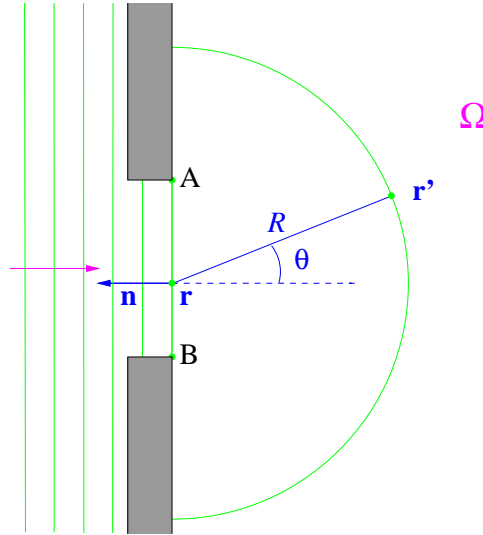
and so

$$\psi(\mathbf{r}') = \int_{\partial\Omega} \{G(\mathbf{r}, \mathbf{r}')(\mathbf{n} \cdot \nabla_{\mathbf{r}})\psi(\mathbf{r}) - \psi(\mathbf{r})(\mathbf{n} \cdot \nabla_{\mathbf{r}})G(\mathbf{r}, \mathbf{r}')\} dS_{\mathbf{r}}, \quad \mathbf{r}' \in \Omega. \quad (6.201)$$

This must *not* be thought of as solution to the wave equation in terms of an integral over the boundary, analogous to the solution (6.186) of the Dirichlet problem that we found in the last section. Here, unlike that earlier case, $G(\mathbf{r}, \mathbf{r}')$ knows nothing of the boundary $\partial\Omega$, and so both terms in the surface

integral contribute to ψ . We therefore have a formula for $\psi(\mathbf{r})$ in the interior in terms of both Dirichlet *and* Neumann data on the boundary $\partial\Omega$, and giving *both* over-prescribes the problem. If we take arbitrary values for ψ and $(\mathbf{n} \cdot \nabla)\psi$ on the boundary, and plug them into (6.201) so as to compute $\psi(\mathbf{r})$ within Ω then there is no reason for the resulting $\psi(\mathbf{r})$ to reproduce, as \mathbf{r} approaches the boundary, the values ψ and $(\mathbf{n} \cdot \nabla)\psi$ appearing in the integral. If we demand that the output $\psi(\mathbf{r})$ *does* reproduce the input boundary data, then this is equivalent to demanding that the boundary data come from a solution of the differential equation in a region encompassing Ω .

The mathematical inconsistency of assuming arbitrary boundary data notwithstanding, this is exactly what we do when we follow Kirchhoff and use (6.201) to provide a justification of Huygens' construction as used in optics. Consider the problem of a plane wave, $\psi = e^{ikx}$, incident on a screen from the left and passing through the aperture labelled AB in the following figure.



Huygens' construction.

We take the region Ω to be everything to the right of the obstacle. The Kirchhoff approximation consists of assuming that the values of ψ and $(\mathbf{n} \cdot \nabla)\psi$ on the surface AB are e^{ikx} and $-ike^{ikx}$, the same as they would be if the obstacle were not there, and that they are identically zero on all other parts of the boundary. In other words, we completely ignore any scattering by the material in which the aperture resides. We can then use our formula

to estimate ψ in the region to the right of the aperture. If we further set

$$\nabla_{\mathbf{r}} G(\mathbf{r}, \mathbf{r}') \approx ik \frac{(\mathbf{r} - \mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|^2} e^{ik|\mathbf{r} - \mathbf{r}'|}, \quad (6.202)$$

which is a good approximation provided we are more than a few wavelengths away from the aperture, we find

$$\psi(\mathbf{r}') \approx \frac{k}{4\pi i} \int_{\text{aperture}} \frac{e^{ik|\mathbf{r} - \mathbf{r}'|}}{|\mathbf{r} - \mathbf{r}'|^2} (1 + \cos \theta) dS_{\mathbf{r}}. \quad (6.203)$$

Thus, each part of the wavefront on the surface AB acts as a source for the diffracted wave in Ω .

This result, although still an approximation, provides two substantial improvements to the naïve form of Huygens' construction as presented in elementary courses:

- i) There is factor of $(1 + \cos \theta)$ which suppresses backward propagating waves. The traditional exposition of Huygens construction takes no notice of which way the wave is going, and so provides no explanation as to why a wavefront does not act a source for a backward wave.
- ii) There is a factor of $i^{-1} = e^{-i\pi/2}$ which corrects a 90° error in the phase made by the naïve Huygens construction. For two-dimensional slit geometry we must use the more complicated two-dimensional Green function (it is a Bessel function), and this provides an $e^{-i\pi/4}$ factor which corrects for the 45° phase error that is manifest in the Cornu spiral of Fresnel diffraction.

For this reason the Kirchhoff approximation is widely used.

Exercise 6.10: Use the method of images to construct i) the Dirichlet, and ii) the Neumann, Green function for the region Ω , consisting of everything to the right of the screen. Use your Green functions to write the solution to the diffraction problem in this region a) in terms of the values of ψ on the aperture surface AB, b) in terms of the values of $(\mathbf{n} \cdot \nabla)\psi$ on the aperture surface. In each case, assume that the boundary data are identically zero on the dark side of the screen. Your expressions should coincide with the *Rayleigh-Sommerfeld diffraction integrals* of the first and second kind, respectively². Explore the differences between the predictions of these two formulæ and that of Kirchhoff for case of the diffraction of a plane wave incident on the aperture from the left.

²M. Born and E. Wolf *Principles of Optics* 7th (expanded) edition, section 8.11.

6.6 Exercises and problems

Exercise 6.11: Critical Mass. An infinite slab of fissile material has thickness L . The neutron density $n(x)$ in the material obeys the equation

$$\frac{\partial n}{\partial t} = D \frac{\partial^2 n}{\partial x^2} + \lambda n + \mu,$$

where $n(x, t)$ is zero at the surface of the slab at $x = 0, L$. Here D is the neutron diffusion constant, the term λn describes the creation of new neutrons by induced fission, and the constant μ is the rate of production per unit volume of neutrons by spontaneous fission.

- a) Expand $n(x, t)$ as a series

$$n(x, t) = \sum_m a_m(t) \varphi_m(x)$$

where the $\varphi_m(x)$ are a complete set of functions you think suitable for solving the problem.

- b) Find an explicit expression for the coefficients $a_m(t)$ in terms of their initial values $a_m(0)$.
 c) Determine the critical thickness, L_{crit} , above which the slab will explode.
 d) Assuming that $L < L_{\text{crit}}$, find the equilibrium distribution $n_{\text{eq}}(x)$ of neutrons in the slab. (You may either sum your series expansion to get an explicit closed-form answer, or use another (Green function?) method.)

Exercise 6.12: Semi-infinite Rod. Consider the heat equation

$$\frac{\partial \theta}{\partial t} = D \nabla^2 \theta, \quad 0 < x < \infty$$

with the temperature $\theta(x, t)$ obeying the initial condition $\theta(x, 0) = \theta_0$ for $0 < x < \infty$, and the boundary condition $\theta(0, t) = 0$.

- a) Show that the boundary condition at $x = 0$ may be satisfied at all times by introducing a suitable mirror image of the initial data in the region $-\infty < x < 0$, and then applying the heat kernel for the entire real line to this extended initial data. Show that the resulting solution of the semi-infinite rod problem can be expressed in terms of the *error function*

$$\text{erf}(x) = \frac{2}{\sqrt{\pi}} \int_0^x e^{-\xi^2} d\xi,$$

as

$$\theta(x, t) = \theta_0 \text{erf} \left(\frac{x}{\sqrt{4t}} \right).$$

- b) Solve the same problem by using a Fourier integral expansion in terms of $\sin kx$ on the half-line $0 < x < \infty$ and obtaining the time evolution of the Fourier coefficients. Invert the transform and show that your answer reduces to that of part a). (Hint: replace the initial condition by $\theta(x, 0) = \theta_0 e^{-\epsilon x}$, so that the Fourier transform converges, and then take the limit $\epsilon \rightarrow 0$ at the end of your calculation.)

Exercise 6.13: Seasonal Heat Waves. Suppose that the measured temperature of the air above the arctic permafrost is expressed as a Fourier series

$$\theta(t) = \theta_0 + \sum_{n=1}^{\infty} \theta_n \cos n\omega t,$$

where $T = 2\pi/\omega$ is one year. Solve the heat equation for the soil temperature

$$\frac{\partial \theta}{\partial t} = \kappa \frac{\partial^2 \theta}{\partial z^2}, \quad 0 < z < \infty$$

with this boundary condition, and find the temperature $\theta(z, t)$ at a depth z below the surface as a function of time. Observe that the sub-surface temperature fluctuates with the same period as that of the air, but with a phase lag that depends on the depth. Also observe that the longest period temperature fluctuations penetrate the deepest into the ground. (Hint: for each Fourier component, write θ as $\text{Re}[A_n(z) \exp in\omega t]$ where A_n is a complex function of z .)

The next problem is an illustration of a Dirichlet principle.

Exercise 6.14: Helmholtz-Hodge decomposition. Given a three-dimensional region Ω with smooth boundary $\partial\Omega$, introduce the real Hilbert space $L^2_{\text{vec}}(\Omega)$ of finite-norm vector fields, with inner product

$$\langle \mathbf{u}, \mathbf{v} \rangle = \int_{\Omega} \mathbf{u} \cdot \mathbf{v} \, d^3x.$$

Consider the spaces $\mathcal{L} = \{\mathbf{v} : \mathbf{v} = \nabla \phi\}$ and $\mathcal{T} = \{\mathbf{v} : \mathbf{v} = \text{curl } \mathbf{w}\}$ consisting of vector fields in $L^2_{\text{vec}}(\Omega)$ that can be written as gradients and curls, respectively. (Strictly speaking, we should consider the completions of these spaces.)

- a) Show that if we demand that either (or both) of ϕ and the tangential component of \mathbf{w} vanish on $\partial\Omega$, then these two spaces are mutually orthogonal with respect to the $L^2_{\text{vec}}(\Omega)$ inner product.

Let $\mathbf{u} \in L^2_{\text{vec}}(\Omega)$. We will try to express \mathbf{u} as the sum of a gradient and a curl by seeking to make the distance functional

$$\begin{aligned} F_{\mathbf{u}}[\phi, \mathbf{w}] &= \|\mathbf{u} - \nabla\phi - \text{curl } \mathbf{w}\|^2 \\ &\equiv \int_{\Omega} |\mathbf{u} - \nabla\phi - \text{curl } \mathbf{w}|^2 d^3x \end{aligned}$$

equal to zero.

- b) Show that if we find a \mathbf{w} and ϕ that minimize $F_{\mathbf{u}}[\phi, \mathbf{w}]$, then the residual vector field

$$\mathbf{h} = \mathbf{u} - \nabla\phi - \text{curl } \mathbf{w}$$

obeys $\text{curl } \mathbf{h} = 0$ and $\text{div } \mathbf{h} = 0$, together with boundary conditions determined by the constraints imposed on ϕ and \mathbf{w} :

- i) If ϕ is unconstrained on $\partial\Omega$, but the tangential boundary component of \mathbf{w} is required to vanish, then the component of \mathbf{h} normal to the boundary must be zero.
 - ii) If $\phi = 0$ on $\partial\Omega$, but the tangential boundary component of \mathbf{w} is unconstrained, then the tangential boundary component of \mathbf{h} must be zero.
 - iii) If $\phi = 0$ on $\partial\Omega$ and also the tangential boundary component of \mathbf{w} is required to vanish, then \mathbf{h} need satisfy no boundary condition.
- c) Assuming that we can find suitable minimizing ϕ and \mathbf{w} , deduce that under each of the three boundary conditions of the previous part, we have a *unique* $L^2_{\text{vec}}(\Omega)$ orthogonal *Helmholtz-Hodge decomposition*

$$\mathbf{u} = \nabla\phi + \text{curl } \mathbf{w} + \mathbf{h}.$$

Observe that the residual vector field \mathbf{h} is *harmonic* — *i.e.* it satisfies the equation $\nabla^2 \mathbf{h} = 0$, where

$$\nabla^2 \mathbf{h} \stackrel{\text{def}}{=} \text{grad div } \mathbf{h} - \text{curl curl } \mathbf{h}$$

is the *vector Laplacian* acting on \mathbf{h} .

If \mathbf{u} is sufficiently smooth, we will be able to find ϕ and \mathbf{w} that minimize the distance $\|\mathbf{u} - \nabla\phi - \text{curl } \mathbf{w}\|$ and satisfy the boundary conditions. Whether or not \mathbf{h} is needed in the decomposition is another matter. It depends both on how we constrain ϕ and \mathbf{w} , and on the topology of Ω . At issue is whether or not the boundary conditions imposed on \mathbf{h} are sufficient to force it to be zero. If Ω is the interior of a torus, for example, then \mathbf{h} can be non-zero whenever its tangential component is unconstrained.

The Helmholtz-Hodge decomposition is closely related to the vector-field eigenvalue problems commonly met with in electromagnetism or elasticity. The next few exercises lead up to this connection.

Exercise 6.15: Self-adjointness and the Vector Laplacian. Consider the vector Laplacian (defined in the previous problem) as a linear operator on the Hilbert space $L^2_{\text{vec}}(\Omega)$.

a) Show that

$$\int_{\Omega} d^3x \{ \mathbf{u} \cdot (\nabla^2 \mathbf{v}) - \mathbf{v} \cdot (\nabla^2 \mathbf{u}) \} = \int_{\partial\Omega} \{ (\mathbf{n} \cdot \mathbf{u}) \operatorname{div} \mathbf{v} - (\mathbf{n} \cdot \mathbf{v}) \operatorname{div} \mathbf{u} - \mathbf{u} \cdot (\mathbf{n} \times \operatorname{curl} \mathbf{v}) + \mathbf{v} \cdot (\mathbf{n} \times \operatorname{curl} \mathbf{u}) \} dS$$

b) Deduce from the identity in part a) that the domain of ∇^2 coincides with the domain of $(\nabla^2)^\dagger$, and hence the vector Laplacian defines a truly self-adjoint operator with a complete set of mutually orthogonal eigenfunctions, when we take as boundary conditions one of the following:

- o) Dirichlet-Dirichlet: $\mathbf{n} \cdot \mathbf{u} = 0$ and $\mathbf{n} \times \mathbf{u} = 0$ on $\partial\Omega$,
- i) Dirichlet-Neumann: $\mathbf{n} \cdot \mathbf{u} = 0$ and $\mathbf{n} \times \operatorname{curl} \mathbf{u} = 0$ on $\partial\Omega$,
- ii) Neumann-Dirichlet: $\operatorname{div} \mathbf{u} = 0$ and $\mathbf{n} \times \mathbf{u} = 0$ on $\partial\Omega$,
- iii) Neumann-Neumann: $\operatorname{div} \mathbf{u} = 0$ and $\mathbf{n} \times \operatorname{curl} \mathbf{u} = 0$ on $\partial\Omega$.

c) Show that the more general *mixed* (or *Robin*) boundary conditions

$$\begin{aligned} \alpha(\mathbf{n} \cdot \mathbf{u}) + \beta \operatorname{div} \mathbf{u} &= 0, \\ \lambda(\mathbf{n} \times \mathbf{u}) + \mu(\mathbf{n} \times \operatorname{curl} \mathbf{u}) &= 0, \end{aligned}$$

where α, β, μ, ν can be position dependent, also give rise to a truly self-adjoint operator.

Exercise 6.16: Cavity electrodynamics and the Hodge-Weyl decomposition. Each of the self-adjoint boundary conditions in the previous problem gives rise to a complete set of mutually orthogonal vector eigenfunctions obeying

$$-\nabla^2 \mathbf{u}_n = k_n^2 \mathbf{u}_n.$$

For these eigenfunctions to describe the normal modes of the electric field \mathbf{E} and the magnetic field \mathbf{B} ($= \mathbf{H}$) within a cavity bounded by a perfect conductor, we need to additionally impose the Maxwell equations $\operatorname{div} \mathbf{B} = \operatorname{div} \mathbf{E} = 0$ everywhere within Ω , and to satisfy the perfect-conductor boundary conditions $\mathbf{n} \times \mathbf{E} = \mathbf{n} \cdot \mathbf{B} = 0$.

- a) For each eigenfunction \mathbf{u}_n corresponding to a non-zero eigenvalue k_n^2 , define

$$\mathbf{v}_n = \frac{1}{k_n^2} \text{curl}(\text{curl } \mathbf{u}_n), \quad \mathbf{w}_n = -\frac{1}{k_n^2} \text{grad}(\text{div } \mathbf{u}_n),$$

so that $\mathbf{u}_n = \mathbf{v}_n + \mathbf{w}_n$. Show that \mathbf{v}_n and \mathbf{w}_n are, if non-zero, each eigenfunctions of $-\nabla^2$ with eigenvalue k_n^2 . The vector eigenfunctions that are not in the null-space of ∇^2 can therefore be decomposed into their *transverse* (the \mathbf{v}_n , which obey $\text{div } \mathbf{v}_n = 0$) and *longitudinal* (the \mathbf{w}_n , which obey $\text{curl } \mathbf{w}_n = 0$) parts. However, it is not immediately clear what boundary conditions the \mathbf{v}_n and \mathbf{w}_n separately obey.

- b) The boundary-value problems of relevance to electromagnetism are the cases

$$\begin{aligned} \text{i):} \quad & \begin{cases} -\nabla^2 \mathbf{h}_n = k_n^2 \mathbf{h}_n, & \text{within } \Omega \\ \mathbf{n} \cdot \mathbf{h}_n = 0, \quad \mathbf{n} \times \text{curl } \mathbf{h}_n = 0 & \text{on } \partial\Omega, \end{cases} \\ \text{ii):} \quad & \begin{cases} -\nabla^2 \mathbf{e}_n = k_n^2 \mathbf{e}_n, & \text{within } \Omega \\ \text{div } \mathbf{e}_n = 0, \quad \mathbf{n} \times \mathbf{e}_n = 0, & \text{on } \partial\Omega. \end{cases} \\ \text{iii):} \quad & \begin{cases} -\nabla^2 \mathbf{b}_n = k_n^2 \mathbf{b}_n, & \text{within } \Omega \\ \text{div } \mathbf{b}_n = 0, \quad \mathbf{n} \times \text{curl } \mathbf{b}_n = 0, & \text{on } \partial\Omega, \end{cases} \end{aligned}$$

These are respectively the Dirichlet-Neumann, Neumann-Dirichlet, and Neumann-Neumann boundary conditions from the previous problem.

Show that the divergence-free transverse eigenfunctions

$$\mathbf{H}_n = \frac{1}{k_n^2} \text{curl}(\text{curl } \mathbf{h}_n), \quad \mathbf{E}_n = \frac{1}{k_n^2} \text{curl}(\text{curl } \mathbf{e}_n), \quad \mathbf{B}_n = \frac{1}{k_n^2} \text{curl}(\text{curl } \mathbf{b}_n),$$

obey $\mathbf{n} \cdot \mathbf{H}_n = \mathbf{n} \cdot \mathbf{E}_n = \mathbf{n} \times \text{curl } \mathbf{B}_n = 0$, and that from these and the eigenvalue equations we can deduce that $\mathbf{n} \times \text{curl } \mathbf{H}_n = \mathbf{n} \cdot \mathbf{B}_n = \mathbf{n} \cdot \text{curl } \mathbf{E}_n = 0$. The perfect-conductor boundary conditions are therefore satisfied.

Simultaneously show that the corresponding longitudinal eigenfunctions

$$\boldsymbol{\eta}_n = \frac{1}{k_n^2} \text{grad}(\text{div } \mathbf{h}_n), \quad \boldsymbol{\epsilon}_n = \frac{1}{k_n^2} \text{grad}(\text{div } \mathbf{e}_n), \quad \boldsymbol{\beta}_n = \frac{1}{k_n^2} \text{grad}(\text{div } \mathbf{b}_n)$$

obey $\mathbf{n} \cdot \boldsymbol{\eta}_n = \mathbf{n} \times \boldsymbol{\epsilon}_n = \mathbf{n} \times \boldsymbol{\beta}_n = 0$.

- c) By considering the counterexample provided by a rectangular box, show that the Dirichlet-Dirichlet boundary condition is not compatible with a longitudinal+transverse decomposition. (A purely transverse wave incident on such a boundary will, on reflection, acquire a longitudinal component.)

d) Show that

$$0 = \int_{\Omega} \boldsymbol{\eta}_n \cdot \mathbf{H}_m d^3x = \int_{\Omega} \boldsymbol{\epsilon}_n \cdot \mathbf{E}_m d^3x = \int_{\Omega} \boldsymbol{\beta}_n \cdot \mathbf{B}_m d^3x,$$

but that the \mathbf{v}_n and \mathbf{w}_n obtained from the Dirichlet-Dirichlet boundary condition \mathbf{u}_n 's are not in general orthogonal to each other. Use the continuity of the $L^2_{\text{vec}}(\Omega)$ inner product

$$\mathbf{x}_n \rightarrow \mathbf{x} \quad \Rightarrow \quad \langle \mathbf{x}_n, \mathbf{y} \rangle \rightarrow \langle \mathbf{x}, \mathbf{y} \rangle$$

to show that this individual-eigenfunction orthogonality is retained by limits of sums of the eigenfunctions. Deduce that, for each of the boundary conditions i)-iii) (but *not* for the Dirichlet-Dirichlet case), we have the *Hodge-Weyl* decomposition of $L^2_{\text{vec}}(\Omega)$ as the orthogonal direct sum

$$L^2_{\text{vec}}(\Omega) = \mathcal{L} \oplus \mathcal{T} \oplus \mathcal{N}$$

where \mathcal{L} , \mathcal{T} are respectively the spaces of functions representable as infinite sums of the longitudinal and transverse eigenfunctions, and \mathcal{N} is the finite-dimensional space of harmonic (nullspace) eigenfunctions.

Complete sets of vector eigenfunctions for the interior of a rectangular box, and for each of the four sets of boundary conditions we have considered, can be found in Morse and Feshbach §13.1.

Exercise 6.17: Hodge-Weyl and Helmholtz-Hodge. In this exercise we consider the problem of exactly what classes of vector-valued functions can be expanded out in terms of the various families of eigenfunctions of the previous problem. It is tempting (but wrong) to think that we are restricted to expanding functions that obey the same boundary conditions as the eigenfunctions themselves. Thus, we might erroneously expect that the \mathbf{E}_n are good only for expanding functions whose divergence vanishes and have vanishing tangential boundary components, or that the $\boldsymbol{\eta}_n$ can expand out only curl-free vector fields with vanishing normal boundary component. That this supposition can be false was exposed in section 2.2.3 where we showed that functions that are zero at the endpoints of an interval can be used to expand out functions that are not zero there. The key point is that each of our four families of \mathbf{u}_n constitute a *complete orthonormal set* in $L^2_{\text{vec}}(\Omega)$, and can therefore expand *any* vector field. As a consequence, the infinite sum $\sum a_n \mathbf{B}_n \in \mathcal{T}$ can, for example, represent any vector-valued function $\mathbf{u} \in L^2_{\text{vec}}(\Omega)$ provided only that \mathbf{u} possesses no component lying either in the subspace \mathcal{L} of the longitudinal eigenfunctions $\boldsymbol{\beta}_n$, or in the nullspace \mathcal{N} .

- a) Let $\mathcal{T} = \langle \mathbf{E}_n \rangle$ be space of functions representable as infinite sums of the \mathbf{E}_n . Show that

$$\langle \mathbf{E}_n \rangle^\perp = \{ \mathbf{u} : \text{curl } \mathbf{u} = 0 \text{ within } \Omega, \mathbf{n} \times \mathbf{u} = 0 \text{ on } \partial\Omega \}.$$

Find the corresponding perpendicular spaces for each of the other eight orthogonal decomposition spaces.

- b) Exploit your list of perpendicularity conditions from part a) to show that

$$\begin{aligned} \langle \boldsymbol{\eta}_n \rangle &= \{ \mathbf{u} : \text{curl } \mathbf{u} = 0 \text{ within } \Omega, \text{ no condition on } \partial\Omega \} \\ \langle \mathbf{H}_n \rangle &= \{ \mathbf{u} : \text{div } \mathbf{u} = 0 \text{ within } \Omega, \mathbf{n} \cdot \mathbf{u} = 0 \text{ on } \partial\Omega \} \\ \langle \boldsymbol{\epsilon}_n \rangle &= \{ \mathbf{u} : \text{curl } \mathbf{u} = 0 \text{ within } \Omega, \mathbf{n} \times \mathbf{u} = 0 \text{ on } \partial\Omega \} \\ \langle \mathbf{E}_n \rangle &= \{ \mathbf{u} : \text{div } \mathbf{u} = 0 \text{ within } \Omega, \text{ no condition on } \partial\Omega \} \\ \langle \boldsymbol{\beta}_n \rangle &= \{ \mathbf{u} : \text{curl } \mathbf{u} = 0 \text{ within } \Omega, \mathbf{n} \times \mathbf{u} = 0 \text{ on } \partial\Omega \} \\ \langle \mathbf{B}_n \rangle &= \{ \mathbf{u} : \text{div } \mathbf{u} = 0 \text{ within } \Omega, \mathbf{n} \cdot \mathbf{u} = 0 \text{ on } \partial\Omega \} \end{aligned}$$

- c) Conclude from the previous part, that any vector field $\mathbf{u} \in L^2_{\text{vec}}(\Omega)$ can be uniquely decomposed as the $L^2_{\text{vec}}(\Omega)$ orthogonal sum

$$\mathbf{u} = \nabla\phi + \text{curl } \mathbf{w} + \mathbf{h},$$

where $\nabla\phi \in \mathcal{L}$, $\text{curl } \mathbf{w} \in \mathcal{T}$, and $\mathbf{h} \in \mathcal{N}$, under each of the following sets of conditions:

- i) The scalar ϕ is unrestricted, but \mathbf{w} obeys $\mathbf{n} \times \mathbf{w} = 0$ on $\partial\Omega$, and the harmonic \mathbf{h} obeys $\mathbf{n} \cdot \mathbf{h} = 0$ on $\partial\Omega$. (The condition on \mathbf{w} makes $\text{curl } \mathbf{w}$ have vanishing normal boundary component.)
 - ii) The scalar ϕ is zero on $\partial\Omega$, while \mathbf{w} is unrestricted on $\partial\Omega$. The harmonic \mathbf{h} obeys $\mathbf{n} \times \mathbf{h} = 0$ on $\partial\Omega$. (The condition on ϕ makes $\nabla\phi$ have zero tangential boundary component.)
 - iii) The scalar ϕ is zero on $\partial\Omega$, the vector \mathbf{w} obeys $\mathbf{n} \times \mathbf{w} = 0$ on $\partial\Omega$, while the harmonic \mathbf{h} requires no boundary condition. (The conditions on ϕ and \mathbf{w} make $\nabla\phi$ have zero tangential boundary component and $\text{curl } \mathbf{w}$ have vanishing normal boundary component.)
- d) As an illustration of the practical distinctions between the decompositions in part c), take Ω to be the unit cube in \mathbb{R}^3 , and $\mathbf{u} = (1, 0, 0)$ a constant vector field. Show that with conditions i) we have $\mathbf{u} \in \mathcal{L}$, but for ii) we have $\mathbf{u} \in \mathcal{T}$, and for iii) we have $\mathbf{u} \in \mathcal{N}$.

We see that the Hodge-Weyl decompositions of the eigenspaces correspond one-to-one with to the Helmholtz-Hodge decompositions of problem 6.14.

Chapter 7

The Mathematics of Real Waves

Waves are found everywhere in the physical world, but we often need more than the simple wave equation to understand them. The principal complications are non-linearity and dispersion. In this chapter we will digress a little from our monotonous catalogue of linear problems, and describe the mathematics lying behind some commonly observed, but still fascinating, phenomena.

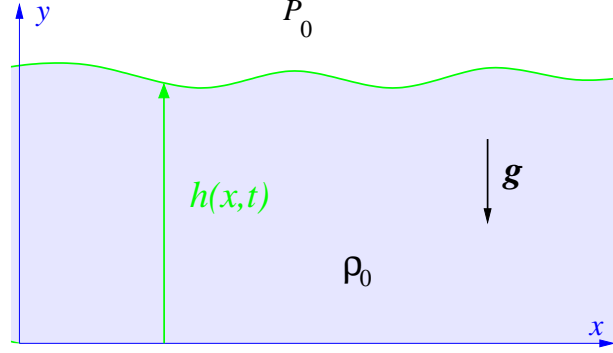
7.1 Dispersive waves

In this section we will investigate the effects of *dispersion*, the dependence of the speed of propagation on the frequency of the wave. We will see that dispersion has a profound effect on the behaviour of a wave-packet.

7.1.1 Ocean Waves

The most commonly seen dispersive waves are those on the surface of water. Although often used to illustrate wave motion in class demonstrations, these waves are not as simple as they seem.

In chapter one we derived the equations governing the motion of water with a free surface. Now we will solve these equations. Recall that we described the flow by introducing a velocity potential ϕ such that, $\mathbf{v} = \nabla\phi$, and a variable $h(x, t)$ which is the depth of the water at abscissa x .



Water with a free surface.

Again looking back to chapter one, we see that the fluid motion is determined by imposing

$$\nabla^2 \phi = 0 \quad (7.1)$$

everywhere in the bulk of the fluid, together with boundary conditions

$$\frac{\partial \phi}{\partial y} = 0, \quad \text{on } y = 0, \quad (7.2)$$

$$\frac{\partial \phi}{\partial t} + \frac{1}{2}(\nabla \phi)^2 + gy = 0, \quad \text{on the free surface } y = h, \quad (7.3)$$

$$\frac{\partial h}{\partial t} - \frac{\partial \phi}{\partial y} + \frac{\partial h}{\partial x} \frac{\partial \phi}{\partial x} = 0, \quad \text{on the free surface } y = h. \quad (7.4)$$

Recall the physical interpretation of these equations: The vanishing of the Laplacian of the velocity potential simply means that the bulk flow is incompressible

$$\nabla \cdot \mathbf{v} \equiv \nabla^2 \phi = 0. \quad (7.5)$$

The first two of the boundary conditions are also easy to interpret: The first says that no water escapes through the lower boundary at $y = 0$. The second, a form of Bernoulli's equation, asserts that the free surface is everywhere at constant (atmospheric) pressure. The remaining boundary condition is more obscure. It states that a fluid particle initially on the surface stays on the surface. Remember that we set $f(x, y, t) = h(x, t) - y$, so the water surface is given by $f(x, y, t) = 0$. If the surface particles are carried with the flow then the convective derivative of f ,

$$\frac{df}{dt} \equiv \frac{\partial f}{\partial t} + (\mathbf{v} \cdot \nabla)f, \quad (7.6)$$

should vanish on the free surface. Using $\mathbf{v} = \nabla\phi$ and the definition of f , this reduces to

$$\frac{\partial h}{\partial t} + \frac{\partial \phi}{\partial x} \frac{\partial h}{\partial x} - \frac{\partial \phi}{\partial y} = 0, \quad (7.7)$$

which is indeed the last boundary condition.

Using our knowledge of solutions of Laplace's equation, we can immediately write down a wave-like solution satisfying the boundary condition at $y = 0$

$$\phi(x, y, t) = a \cosh(ky) \cos(kx - \omega t). \quad (7.8)$$

The tricky part is satisfying the remaining two boundary conditions. The difficulty is that they are non-linear, and so couple modes with different wave-numbers. We will circumvent the difficulty by restricting ourselves to small amplitude waves, for which the boundary conditions can be linearized. Suppressing all terms that contain a product of two or more small quantities, we are left with

$$\frac{\partial \phi}{\partial t} + gh = 0, \quad (7.9)$$

$$\frac{\partial h}{\partial t} - \frac{\partial \phi}{\partial y} = 0. \quad (7.10)$$

Because of the linearization, these equations should be applied at $y = h_0$, the equilibrium surface of the fluid. It is convenient to eliminate h to get

$$\frac{\partial^2 \phi}{\partial t^2} + g \frac{\partial \phi}{\partial y} = 0, \quad \text{on } y = h_0. \quad (7.11)$$

Enforcing this condition on ϕ leads to the *dispersion equation*

$$\omega^2 = gk \tanh kh_0, \quad (7.12)$$

relating the frequency to the wave-number.

Two limiting cases are of interest:

- i) *Long waves on shallow water:* Here $kh_0 \ll 1$, and, in this limit,

$$\omega = k\sqrt{gh_0}.$$

- ii) *Waves on deep water:* Here, $kh_0 \gg 1$, leading to $\omega = \sqrt{gk}$.

For deep water, the velocity potential becomes

$$\phi(x, y, t) = ae^{k(y-h_0)} \cos(kx - \omega t). \quad (7.13)$$

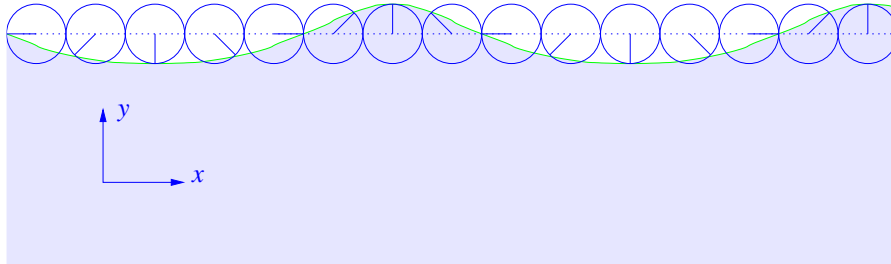
We see that the disturbance due to the surface wave dies away exponentially, and becomes very small only a few wavelengths below the surface.

Remember that the velocity of the fluid is $\mathbf{v} = \nabla\phi$. To follow the motion of individual particles of fluid we must solve the equations

$$\begin{aligned} \frac{dx}{dt} &= v_x = -ake^{k(y-h_0)} \sin(kx - \omega t), \\ \frac{dy}{dt} &= v_y = ake^{k(y-h_0)} \cos(kx - \omega t). \end{aligned} \quad (7.14)$$

This is a system of non-linear differential equations, but to find the small amplitude motion of particles at the surface we may, to a first approximation, set $x = x_0$, $y = h_0$ on the right-hand side. The orbits of the surface particles are therefore approximately

$$\begin{aligned} x(t) &= x_0 - \frac{ak}{\omega} \cos(kx_0 - \omega t), \\ y(t) &= y_0 - \frac{ak}{\omega} \sin(kx_0 - \omega t). \end{aligned} \quad (7.15)$$



Surface waves on deep water.

For right-moving waves, the particle orbits are clockwise circles. At the wave-crest the particles move in the direction of the wave propagation; in the troughs they move in the opposite direction. The figure shows that this results in a characteristic up-down asymmetry in the wave profile.

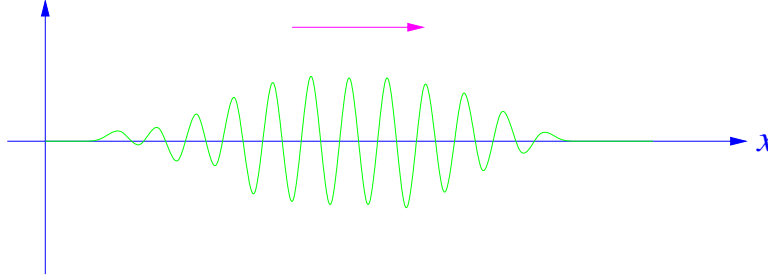
When the effect of the bottom becomes significant, the circular orbits deform into ellipses. For shallow water waves, the motion is principally back and forth with motion in the y direction almost negligible.

7.1.2 Group Velocity

The most important effect of dispersion is that the *group velocity* of the waves — the speed at which a wave-packet travels — differs from the *phase velocity* — the speed at which individual wave-crests move. The group velocity is also the speed at which the *energy* associated with the waves travels.

Suppose that we have waves with dispersion equation $\omega = \omega(k)$. A right-going wave-packet of finite extent, and with initial profile $\varphi(x)$, can be Fourier analyzed to give

$$\varphi(x) = \int_{-\infty}^{\infty} \frac{dk}{2\pi} A(k) e^{ikx}. \quad (7.16)$$



A right-going wavepacket.

At later times this will evolve to

$$\varphi(x, t) = \int_{-\infty}^{\infty} \frac{dk}{2\pi} A(k) e^{ikx - i\omega(k)t}. \quad (7.17)$$

Let us suppose for the moment that $A(k)$ is non-zero only for a narrow band of wavenumbers around k_0 , and that, restricted to this narrow band, we can approximate the full $\omega(k)$ dispersion equation by

$$\omega(k) \approx \omega_0 + U(k - k_0). \quad (7.18)$$

Thus

$$\varphi(x, t) = \int_{-\infty}^{\infty} \frac{dk}{2\pi} A(k) e^{ik(x-Ut) - i(\omega_0 - Uk_0)t}. \quad (7.19)$$

Comparing this with the Fourier expression for the initial profile, we find that

$$\varphi(x, t) = e^{-i(\omega_0 - Uk_0)t} \varphi(x - Ut). \quad (7.20)$$

The pulse envelope therefore travels at speed U . This velocity

$$U \equiv \frac{\partial \omega}{\partial k} \quad (7.21)$$

is the *group velocity*. The individual wave crests, on the other hand, move at the *phase velocity* $\omega(k)/k$.

When the initial pulse contains a broad range of frequencies we can still explore its evolution. We make use of a powerful tool for estimating the behavior of integrals that contain a large parameter. In this case the parameter is the time t . We begin by writing the Fourier representation of the wave as

$$\varphi(x, t) = \int_{-\infty}^{\infty} \frac{dk}{2\pi} A(k) e^{it\psi(k)} \quad (7.22)$$

where

$$\psi(k) = k \left(\frac{x}{t} \right) - \omega(k). \quad (7.23)$$

Now look at the behaviour of this integral as t becomes large, but while we keep the ratio x/t fixed. Since t is very large, any variation of ψ with k will make the integrand a very rapidly oscillating function of k . Cancellation between adjacent intervals with opposite phase will cause the net contribution from such a region of the k integration to be very small. The principal contribution will come from the neighbourhood of *stationary phase* points, *i.e.* points where

$$0 = \frac{d\psi}{dk} = \frac{x}{t} - \frac{\partial \omega}{\partial k}. \quad (7.24)$$

This means that, at points in space where $x/t = U$, we will only get contributions from the Fourier components with wave-number satisfying

$$U = \frac{\partial \omega}{\partial k}. \quad (7.25)$$

The initial packet will therefore spread out, with those components of the wave having wave-number k travelling at speed

$$v_{\text{group}} = \frac{\partial \omega}{\partial k}. \quad (7.26)$$

This is the same expression for the group velocity that we obtained in the narrow-band case. Again this speed of propagation should be contrasted with that of the wave-crests, which travel at

$$v_{\text{phase}} = \frac{\omega}{k}. \quad (7.27)$$

The “stationary phase” argument may seem a little hand-waving, but it can be developed into a systematic approximation scheme. We will do this in later chapters.

Example: Water Waves. The dispersion equation for waves on deep water is $\omega = \sqrt{gk}$. The phase velocity is therefore

$$v_{\text{phase}} = \sqrt{\frac{g}{k}}, \quad (7.28)$$

whilst the group velocity is

$$v_{\text{group}} = \frac{1}{2} \sqrt{\frac{g}{k}} = \frac{1}{2} v_{\text{phase}}. \quad (7.29)$$

This difference is easily demonstrated by tossing a stone into a pool and observing how individual wave-crests overtake the circular wave packet and die out at the leading edge, while new crests and troughs come into being at the rear and make their way to the front.

This result can be extended to three dimensions with

$$v_{\text{group}}^i = \frac{\partial \omega}{\partial k_i} \quad (7.30)$$

Example: de Broglie Waves. The plane-wave solutions of the time-dependent Schrödinger equation

$$i \frac{\partial \psi}{\partial t} = -\frac{1}{2m} \nabla^2 \psi, \quad (7.31)$$

are

$$\psi = e^{i\mathbf{k} \cdot \mathbf{r} - i\omega t}, \quad (7.32)$$

with

$$\omega(k) = \frac{1}{2m} \mathbf{k}^2. \quad (7.33)$$

The group velocity is therefore

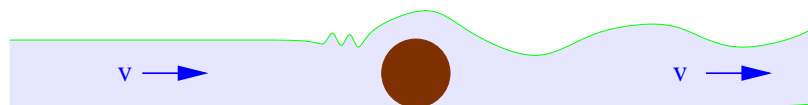
$$\mathbf{v}_{\text{group}} = \frac{1}{m} \mathbf{k}, \quad (7.34)$$

which is the classical velocity of the particle.

7.1.3 Wakes

There are many circumstances when waves are excited by object moving at a constant velocity through a background medium, or by a stationary object immersed in a steady flow. The resulting *wakes* carry off energy, and therefore create *wave drag*. Wakes are involved, for example, in sonic booms, Čerenkov radiation, the Landau criterion for superfluidity, and Landau damping of plasma oscillations. Here, we will consider some simple water-wave analogues of these effects. The common principle for all wakes is that the resulting wave pattern is time independent when observed from the object exciting it.

Example: Obstacle in a Stream. Consider a log lying submerged in a rapidly flowing stream.



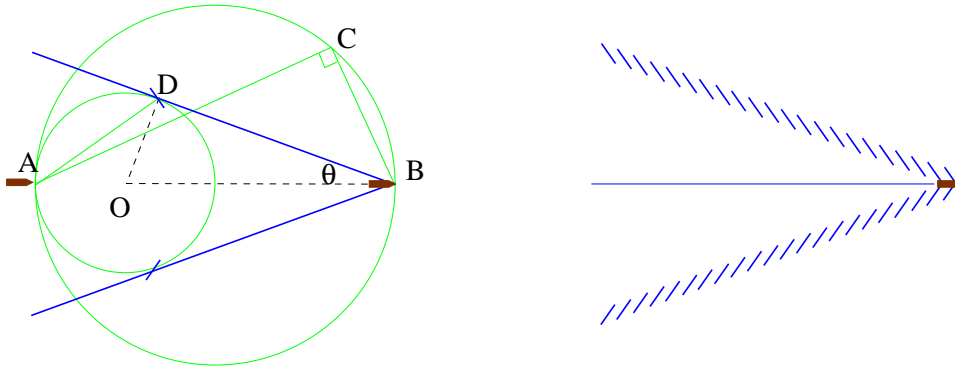
Log in a stream.

The obstacle disturbs the water and generates a train of waves. If the log lies athwart the stream, the problem is essentially one-dimensional and easy to analyse. The essential point is that the distance of the wavecrests from the log does not change with time, and therefore the wavelength of the disturbance the log creates is selected by the condition that the *phase velocity* of the wave, coincide with the velocity of the mean flow¹. The group velocity does come into play, however. If the group velocity of the waves is *less* than the phase velocity, the energy being deposited in the wave-train by the disturbance will be swept downstream, and the wake will lie *behind* the obstacle. If the group velocity is *higher* than the phase velocity, and this is the case with very short wavelength ripples on water where surface tension is more important than gravity, the energy will propagate against the flow, and so the ripples appear *upstream* of the obstacle.

¹In his book *Waves in Fluids*, M. J. Lighthill quotes Robert Frost on this phenomenon:

The black stream, catching on a sunken rock,
Flung backward on itself in one white wave,
And the white water rode the black forever,
Not gaining but not losing.

Example: Kelvin Ship Waves. A more subtle problem is the pattern of waves left behind by a ship on deep water. The shape of the pattern is determined by the group velocity for deep-water waves being one-half that of the phase velocity.



Kelvin's ship-wave construction.

In order that the wave pattern be time independent, the waves emitted in the direction AC must have phase velocity such that their crests travel from A to C while the ship goes from A to B. The crest of the wave emitted from the bow of the ship in the direction AC will therefore lie along the line BC — or at least there would be a wave crest on this line if the emitted wave energy travelled at the phase velocity. The angle at C must be a right angle because the direction of propagation is perpendicular to the wave-crests. Euclid, by virtue of his angle-in-a-semicircle theorem, now tells us that the locus of all possible points C (for all directions of wave emission) is the larger circle. Because, however, the wave energy only travels at one-half the phase velocity, the waves going in the direction AC actually have significant amplitude only on the smaller circle, which has half the radius of the larger. The wake therefore lies on, and within, the Kelvin wedge, whose boundary lies at an angle θ to the ship's path. This angle is determined by the ratio $OD/OB=1/3$ to be

$$\theta = \sin^{-1}(1/3) = 19.5^\circ. \quad (7.35)$$

Remarkably, this angle, and hence the width of the wake, is independent of the speed of the ship.

The waves actually on the edge of the wedge are usually the most prominent, and they will have crests perpendicular to the line AD. This orientation is indicated on the left hand figure, and reproduced as the predicted pattern

of wavecrests on the right. The prediction should be compared with the wave systems in the image below.



Large-scale Kelvin wakes. (Image source: US Navy)



Small-scale Kelvin wake. (Photograph by Fabrice Neyret)

7.1.4 Hamilton's Theory of Rays

We have seen that wave packets travel at a frequency-dependent group velocity. We can extend this result to study the motion of waves in weakly inhomogeneous media, and so derive an analogy between the “geometric optics” limit of wave motion and classical dynamics.

Consider a packet composed of a roughly uniform train of waves spread out over a region that is substantially longer and wider than their mean wavelength. The essential feature of such a wave train is that at any particular point of space and time, \mathbf{x} and t , it has a definite phase $\Theta(\mathbf{x}, t)$. Once we know this phase, we can define the local frequency ω and wave-vector \mathbf{k} by

$$\omega = - \left(\frac{\partial \Theta}{\partial t} \right)_x, \quad k_i = \left(\frac{\partial \Theta}{\partial x_i} \right)_t. \quad (7.36)$$

These definitions are motivated by the idea that

$$\Theta(\mathbf{x}, t) \sim \mathbf{k} \cdot \mathbf{x} - \omega t, \quad (7.37)$$

at least locally.

We wish to understand how \mathbf{k} changes as the wave propagates through a slowly varying medium. We introduce the inhomogeneity by assuming that the dispersion equation $\omega = \omega(\mathbf{k})$, which is initially derived for a uniform medium, can be extended to $\omega = \omega(\mathbf{k}, \mathbf{x})$, where the \mathbf{x} dependence arises, for example, as a result of a position-dependent refractive index. This assumption is only an approximation, but it is a good approximation when the distance over which the medium changes is much larger than the distance between wavecrests.

Applying the equality of mixed partials to the definitions of \mathbf{k} and ω gives us

$$\left(\frac{\partial \omega}{\partial x_i} \right)_t = - \left(\frac{\partial k_i}{\partial t} \right)_x, \quad \left(\frac{\partial k_i}{\partial x_j} \right)_{x_i} = \left(\frac{\partial k_j}{\partial x_i} \right)_{x_j}. \quad (7.38)$$

The subscripts indicate what is being left fixed when we differentiate. We must be careful about this, because we want to use the dispersion equation to express ω as a function of \mathbf{k} and \mathbf{x} , and the wave-vector \mathbf{k} will itself be a function of \mathbf{x} and t .

Taking this dependence into account, we write

$$\left(\frac{\partial \omega}{\partial x_i} \right)_t = \left(\frac{\partial \omega}{\partial x_i} \right)_{\mathbf{k}} + \left(\frac{\partial \omega}{\partial k_j} \right)_{\mathbf{x}} \left(\frac{\partial k_j}{\partial x_i} \right)_t. \quad (7.39)$$

We now use (7.38) to rewrite this as

$$\left(\frac{\partial k_i}{\partial t}\right)_{\mathbf{x}} + \left(\frac{\partial \omega}{\partial k_j}\right)_{\mathbf{x}} \left(\frac{\partial k_i}{\partial x_j}\right)_t = - \left(\frac{\partial \omega}{\partial x_i}\right)_{\mathbf{k}}. \quad (7.40)$$

Interpreting the left hand side as a convective derivative

$$\frac{dk_i}{dt} = \left(\frac{\partial k_i}{\partial t}\right)_{\mathbf{x}} + (\mathbf{v}_g \cdot \nabla) k_i,$$

we read off that

$$\frac{dk_i}{dt} = - \left(\frac{\partial \omega}{\partial x_i}\right)_{\mathbf{k}} \quad (7.41)$$

provided we are moving at velocity

$$\frac{dx_i}{dt} = (\mathbf{v}_g)_i = \left(\frac{\partial \omega}{\partial k_i}\right)_{\mathbf{x}}. \quad (7.42)$$

Since this is the group velocity, the packet of waves is actually travelling at this speed. The last two equations therefore tell us how the orientation and wavelength of the wave train evolve if we ride along with the packet as it is refracted by the inhomogeneity.

The formulæ

$$\begin{aligned} \dot{\mathbf{k}} &= - \frac{\partial \omega}{\partial \mathbf{x}}, \\ \dot{\mathbf{x}} &= \frac{\partial \omega}{\partial \mathbf{k}}, \end{aligned} \quad (7.43)$$

are *Hamilton's ray equations*. These Hamilton equations are identical in form to Hamilton's equations for classical mechanics

$$\begin{aligned} \dot{\mathbf{p}} &= - \frac{\partial H}{\partial \mathbf{x}}, \\ \dot{\mathbf{x}} &= \frac{\partial H}{\partial \mathbf{p}}, \end{aligned} \quad (7.44)$$

except that \mathbf{k} is playing the role of the canonical momentum, \mathbf{p} , and $\omega(\mathbf{k}, \mathbf{x})$ replaces the Hamiltonian, $H(\mathbf{p}, \mathbf{x})$. This formal equivalence of geometric optics and classical mechanics was mystery in Hamilton's time. Today we understand that classical mechanics is nothing but the geometric optics limit of wave mechanics.

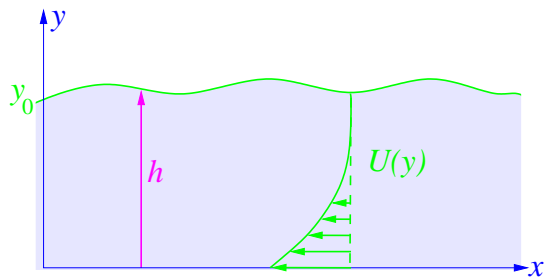
7.2 Making Waves

Many waves occurring in nature are generated by the energy of some steady flow being stolen away to drive an oscillatory motion. Familiar examples include the music of a flute and the waves raised on the surface of water by the wind. The latter process is quite subtle and was not understood until the work of J. W. Miles in 1957. Miles showed that in order to excite waves the wind speed has to vary with the height above the water, and that waves of a given wavelength take energy only from the wind at that height where the windspeed matches the phase velocity of the wave. The resulting resonant energy transfer turns out to have analogues in many branches of science. In this section we will exhibit this phenomenon in the simpler situation where the varying flow is that of the water itself.

7.2.1 Rayleigh's Equation

Consider water flowing in a shallow channel where friction forces keep the water in contact the stream-bed from moving. We will show that the resulting shear flow is unstable to the formation of waves on the water surface. The consequences of this instability are most often seen in a thin sheet of water running down the face of a dam. The sheet starts off flowing smoothly, but, as the water descends, waves form and break, and the water reaches the bottom in irregular pulses called *roll waves*.

It is easiest to describe what is happening from the vantage of a reference frame that rides along with the surface water. In this frame the velocity profile of the flow will be as shown in the figure.



The velocity profile $U(y)$ in a frame at which the surface is at rest.

Since the flow is incompressible but not irrotational, we will describe the

motion by using a stream function Ψ , in terms of which the fluid velocity is given by

$$\begin{aligned} v_x &= -\partial_y \Psi, \\ v_y &= \partial_x \Psi. \end{aligned} \quad (7.45)$$

This parameterization automatically satisfies $\nabla \cdot \mathbf{v} = 0$, while the (z component of) the vorticity becomes

$$\Omega \equiv \partial_x v_y - \partial_y v_x = \nabla^2 \Psi. \quad (7.46)$$

We will consider a stream function of the form²

$$\Psi(x, y, t) = \psi_0(y) + \psi(y)e^{ikx - i\omega t}, \quad (7.47)$$

where ψ_0 obeys $-\partial_y \psi_0 = v_x = U(y)$, and describes the horizontal mean flow. The term containing $\psi(y)$ represents a small-amplitude wave disturbance superposed on the mean flow. We will investigate whether this disturbance grows or decreases with time.

Euler's equation can be written as,

$$\dot{\mathbf{v}} + \mathbf{v} \times \Omega = -\nabla \left(P + \frac{v^2}{2} + gy \right) = 0. \quad (7.48)$$

Taking the curl of this, and taking into account the two dimensional character of the problem, we find that

$$\partial_t \Omega + (\mathbf{v} \cdot \nabla) \Omega = 0. \quad (7.49)$$

This, a general property of two-dimensional incompressible motion, says that vorticity is convected with the flow. We now express (7.49) in terms of Ψ , when it becomes

$$\nabla^2 \dot{\Psi} + (\mathbf{v} \cdot \nabla) \nabla^2 \Psi = 0. \quad (7.50)$$

Substituting the expression (7.47) into (7.50), and keeping only terms of first order in ψ , gives

$$-i\omega \left(\frac{d^2}{dy^2} - k^2 \right) \psi + iUk \left(\frac{d^2}{dy^2} - k^2 \right) \psi + ik\psi \partial_y (-\partial_y U) = 0,$$

²The physical stream function is, of course, the real part of this expression.

or

$$\left(\frac{d^2}{dy^2} - k^2\right)\psi - \left(\frac{\partial^2 U}{\partial y^2}\right) \frac{1}{(U - \omega/k)}\psi = 0. \quad (7.51)$$

This is *Rayleigh's equation*³. If only the first term were present, it would have solutions $\psi \propto e^{\pm ky}$, and we would have recovered the results of section 7.1.1. The second term is significant, however. It will diverge if there is a point y_c such that $U(y_c) = \omega/k$. In other words, if there is a depth at which the flow speed coincides with the phase velocity of the wave disturbance, thus allowing a resonant interaction between the wave and flow. An actual infinity in (7.51) will be evaded, though, because ω will gain a small imaginary part $\omega \rightarrow \omega_R + i\gamma$. A positive imaginary part means that the wave amplitude is growing exponentially with time. A negative imaginary part means that the wave is being damped. With γ included, we then have

$$\begin{aligned} \frac{1}{(U - \omega/k)} &\approx \frac{U - \omega_R/k}{(U - \omega_R/k)^2 + \gamma^2} + i\pi \operatorname{sgn}\left(\frac{\gamma}{k}\right) \delta(U(y) - \omega_R/k) \\ &= \frac{U - \omega_R/k}{(U - \omega_R/k)^2 + \gamma^2} + i\pi \operatorname{sgn}\left(\frac{\gamma}{k}\right) \left|\frac{\partial U}{\partial y}\right|_{y_c}^{-1} \delta(y - y_c). \end{aligned} \quad (7.52)$$

To specify the problem fully we need to impose boundary conditions on $\psi(y)$. On the lower surface we can set $\psi(0) = 0$, as this will keep the fluid at rest there. On the upper surface $y = h$ we apply Euler's equation

$$\dot{\mathbf{v}} + \mathbf{v} \times \boldsymbol{\Omega} = -\nabla \left(P + \frac{v^2}{2} + gh \right) = 0. \quad (7.53)$$

We observe that P is constant, being atmospheric pressure, and the $v^2/2$ can be neglected as it is of second order in the disturbance. Then, considering the x component, we have

$$-\nabla_x gh = -g \partial_x \int^t v_y dt = -g \left(\frac{k^2}{i\omega} \right) \psi \quad (7.54)$$

on the free surface. To lowest order we can apply the boundary condition on the equilibrium free surface $y = y_0$. The boundary condition is therefore

$$\frac{1}{\psi} \frac{d\psi}{dy} + \frac{k}{\omega} \frac{\partial U}{\partial y} = g \frac{k^2}{\omega^2}, \quad y = y_0. \quad (7.55)$$

³Lord Rayleigh. *On the stability or instability of certain fluid motions*. Proc. Lond. Math. Soc. Vol. 11 (1880)

We usually have $\partial U/\partial y = 0$ near the surface, so this simplifies to

$$\frac{1}{\psi} \frac{d\psi}{dy} = g \frac{k^2}{\omega^2}. \quad (7.56)$$

That this is sensible can be confirmed by considering the case of waves on still, deep water, where $\psi(y) = e^{|k|y}$. The boundary condition then reduces to $|k| = gk^2/\omega^2$, or $\omega^2 = g|k|$, which is the correct dispersion equation for such waves.

We find the corresponding dispersion equation for waves on shallow flowing water by computing

$$\left. \frac{1}{\psi} \frac{d\psi}{dy} \right|_{y_0}, \quad (7.57)$$

from Rayleigh's equation (7.51). Multiplying by ψ^* and integrating gives

$$0 = \int_0^{y_0} dy \left\{ \psi^* \left(\frac{d^2}{dy^2} - k^2 \right) \psi + k \left(\frac{\partial^2 U}{\partial y^2} \right) \frac{1}{(\omega - Uk)} |\psi|^2 \right\}. \quad (7.58)$$

An integration by parts then gives

$$\left[\psi^* \frac{d\psi}{dy} \right]_0^{y_0} = \int_0^{y_0} dy \left\{ \left| \frac{d\psi}{dy} \right|^2 + k^2 |\psi|^2 + \left(\frac{\partial^2 U}{\partial y^2} \right) \frac{1}{(U - \omega/k)} |\psi|^2 \right\}. \quad (7.59)$$

The lower limit makes no contribution, since ψ^* is zero there. On using (7.52) and taking the imaginary part, we find

$$\text{Im} \left(\psi^* \frac{d\psi}{dy} \right)_{y_0} = \text{sgn} \left(\frac{\gamma}{k} \right) \pi \left(\frac{\partial^2 U}{\partial y^2} \right)_{y_c} \left| \frac{\partial U}{\partial y} \right|_{y_c}^{-1} |\psi(y_c)|, \quad (7.60)$$

or

$$\text{Im} \left(\frac{1}{\psi} \frac{d\psi}{dy} \right)_{y_0} = \text{sgn} \left(\frac{\gamma}{k} \right) \pi \left(\frac{\partial^2 U}{\partial y^2} \right)_{y_c} \left| \frac{\partial U}{\partial y} \right|_{y_c}^{-1} \frac{|\psi(y_c)|^2}{|\psi(y_0)|^2}. \quad (7.61)$$

This equation is most useful if the interaction with the flow does not substantially perturb $\psi(y)$ away from the still-water result $\psi(y) = \sinh(|k|y)$, and assuming this is so provides a reasonable first approximation.

If we insert (7.61) into (7.56), where we approximate,

$$g \left(\frac{k^2}{\omega^2} \right) \approx g \left(\frac{k^2}{\omega_R^2} \right) - 2ig \left(\frac{k^2}{\omega_R^3} \right) \gamma,$$

we find

$$\begin{aligned}\gamma &= \frac{\omega_R^3}{2gk^2} \text{Im} \left(\frac{1}{\psi} \frac{d\psi}{dy} \right)_{y_0} \\ &= \text{sgn} \left(\frac{\gamma}{k} \right) \pi \frac{\omega_R^3}{2gk^2} \left(\frac{\partial^2 U}{\partial y^2} \right)_{y_c} \left| \frac{\partial U}{\partial y} \right|_{y_c}^{-1} \frac{|\psi(y_c)|^2}{|\psi(y_0)|^2}.\end{aligned}\quad (7.62)$$

We see that either sign of γ is allowed by our analysis. Thus the resonant interaction between the shear flow and wave appears to lead to either exponential growth or damping of the wave. This is inevitable because our inviscid fluid contains no mechanism for dissipation, and its motion is necessarily time-reversal invariant. Nonetheless, as in our discussion of “friction without friction” in section 5.2.2, only one sign of γ is actually observed. This sign is determined by the initial conditions, but a rigorous explanation of how this works mathematically is not easy, and is the subject of many papers. These show that the correct sign is given by

$$\gamma = -\pi \frac{\omega_R^3}{2gk^2} \left(\frac{\partial^2 U}{\partial y^2} \right)_{y_c} \left| \frac{\partial U}{\partial y} \right|_{y_c}^{-1} \frac{|\psi(y_c)|^2}{|\psi(y_0)|^2}.\quad (7.63)$$

Since our velocity profile has $\partial^2 U / \partial y^2 < 0$, this means that the waves grow in amplitude.

We can also establish the correct sign for γ by computing the change of momentum in the background flow due to the wave⁴. The crucial element is whether, in the neighbourhood of the critical depth, more fluid is overtaking the wave than lagging behind it. This is exactly what the quantity $\partial^2 U / \partial y^2$ measures.

7.3 Non-linear Waves

Non-linear effects become important when some dimensionless measure of the amplitude of the disturbance, say $\Delta P / P$ for a sound wave, or $\Delta h / \lambda$ for a water wave, is no longer $\ll 1$.

⁴G. E. Vekstein *Landau resonance mechanism for plasma and wind-generated water waves*. American Journal of Physics, vol.66 (1998) pages 886-92.

7.3.1 Sound in Air

The simplest non-linear wave system is one-dimensional sound propagation in a gas. This problem was studied by Riemann.

The one dimensional motion of a fluid is determined by the mass conservation equation

$$\partial_t \rho + \partial_x(\rho v) = 0, \quad (7.64)$$

and Euler's equation of motion

$$\rho(\partial_t v + v \partial_x v) = -\partial_x P. \quad (7.65)$$

In a fluid with equation of state $P = P(\rho)$, the speed of sound, c , is given by

$$c^2 = \frac{dP}{d\rho}. \quad (7.66)$$

It will in general depend on P , the speed of propagation being usually higher when the pressure is higher.

Riemann was able to simplify these equations by defining a new thermodynamic variable $\pi(P)$ as

$$\pi = \int_{P_0}^P \frac{1}{\rho c} dP, \quad (7.67)$$

where P_0 is the equilibrium pressure of the undisturbed air. The quantity π obeys

$$\frac{d\pi}{dP} = \frac{1}{\rho c}. \quad (7.68)$$

In terms of π , Euler's equation divided by ρ becomes

$$\partial_t v + v \partial_x v + c \partial_x \pi = 0, \quad (7.69)$$

whilst the equation of mass conservation divided by ρ/c becomes

$$\partial_t \pi + v \partial_x \pi + c \partial_x v = 0. \quad (7.70)$$

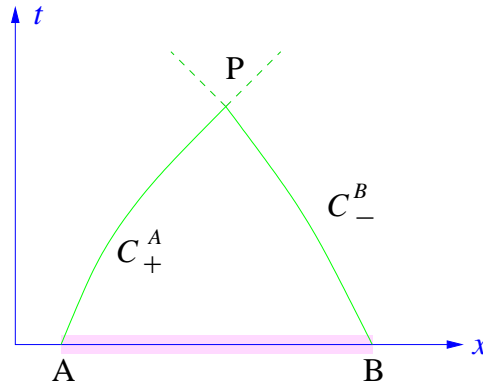
Adding and subtracting, we get *Riemann's equations*

$$\begin{aligned} \partial_t(v + \pi) + (v + c)\partial_x(v + \pi) &= 0, \\ \partial_t(v - \pi) + (v - c)\partial_x(v - \pi) &= 0. \end{aligned} \quad (7.71)$$

These assert that the *Riemann invariants* $v \pm \pi$ are constant along the *characteristic curves*

$$\frac{dx}{dt} = v \pm c. \quad (7.72)$$

This tell us that signals travel at the speed $v \pm c$. In other words, they travel, with respect to the fluid, at the local speed of sound c . Using the Riemann equations, we can propagate initial data $v(x, t = 0)$, $\pi(x, t = 0)$ into the future by using the method of characteristics.



Non-linear characteristic curves.

In the figure, the value of $v + \pi$ is constant along the characteristic curve C_+^A which is the solution of

$$\frac{dx}{dt} = v + c \quad (7.73)$$

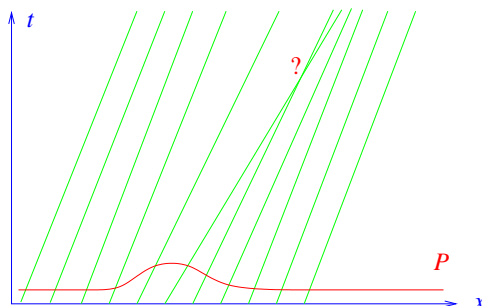
passing through A, while the value of $v - \pi$ is constant along C_-^B which is the solution of

$$\frac{dx}{dt} = v - c \quad (7.74)$$

passing through B. Thus the values of π and v at the point P can be found if we know the initial values of $v + \pi$ at the point A and $v - \pi$ at the point B. Having found v and π at P we can invert $\pi(P)$ to find the pressure P , and hence c , and so continue the characteristics into the future, as indicated by the dotted lines. We need, of course, to know v and c at every point along the characteristics C_+^A and C_-^B in order to construct them, and this requires us to treat every point as a “P”. The values of the dynamical quantities at P therefore depend on the initial data at all points lying between A and B. This is the *domain of dependence* of P

A sound wave caused by a localized excess of pressure will eventually break up into two distinct pulses, one going forwards and one going backwards. Once these pulses are sufficiently separated that they no longer interact with one another they are *simple waves*. Consider a forward-going pulse propagating into undisturbed air. The backward characteristics are coming from the undisturbed region where both π and v are zero. Clearly $\pi - v$ is zero everywhere on these characteristics, and so $\pi = v$. Now $\pi + v = 2v = 2\pi$ is constant the forward characteristics, and so π and v are individually constant along them. Since π is constant, so is c . With v also being constant, this means that $c + v$ is constant. In other words, for a simple wave, *the characteristics are straight lines*.

This simple-wave simplification contains within it the seeds of its own destruction. Suppose we have a positive pressure pulse in a fluid whose speed of sound increases with the pressure.



Simple wave characteristics.

The figure shows that the straight-line characteristics travel faster in the high pressure region, and eventually catch up with and intersect the slower-moving characteristics. When this happens the dynamical variables will become multivalued. How do we deal with this?

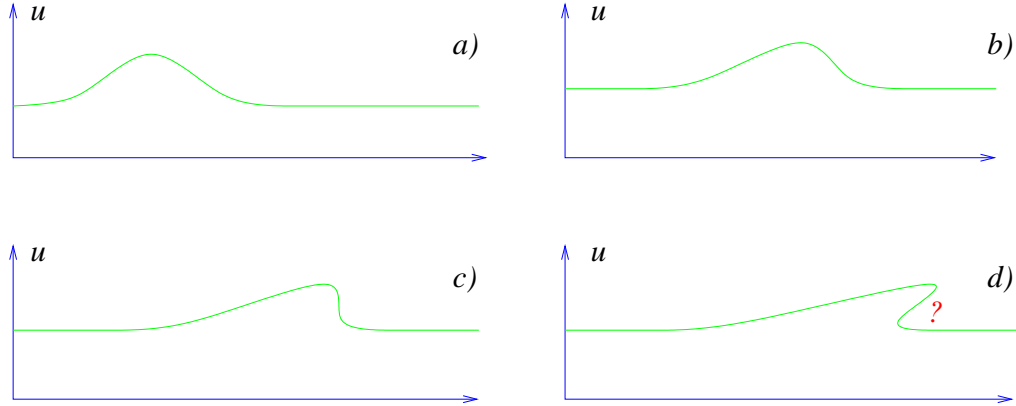
7.3.2 Shocks

Let us untangle the multivaluedness by drawing another set of pictures. Suppose u obeys the non-linear “half” wave equation

$$(\partial_t + u\partial_x)u = 0. \quad (7.75)$$

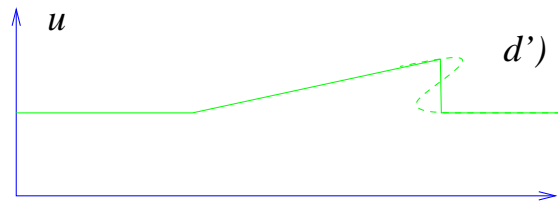
The velocity of propagation of the wave is therefore u itself, so the parts of the wave with large u will overtake those with smaller u , and the wave will

“break”.



A breaking non-linear wave.

Physics does not permit such multivalued solutions, and what usually happens is that the assumptions underlying the model which gave rise to the nonlinear equation will no longer be valid. New terms should be included in the equation which prevent the solution becoming multivalued, and instead a steep “shock” will form.



Formation of a shock.

Examples of an equation with such additional terms are Burgers' equation

$$(\partial_t + u\partial_x)u = \nu\partial_{xx}^2 u, \quad (7.76)$$

and the Korteweg de-Vries (KdV) equation (4.11), which, by a suitable rescaling of x and t , we can write as

$$(\partial_t + u\partial_x)u = \delta\partial_{xxx}^3 u. \quad (7.77)$$

Burgers' equation, for example, can be thought of as including the effects of thermal conductivity, which was not included in the derivation of Riemann's

equations. In both these modified equations, the right hand side is negligible when u is slowly varying, but it completely changes the character of the solution when the waves steepen and try to break.

Although these extra terms are essential for the stabilization of the shock, once we know that such a discontinuous solution has formed, we can find many of its properties — for example the propagation velocity — from general principles, without needing their detailed form. All we need is to know what conservation laws are applicable.

Multiplying $(\partial_t + u\partial_x)u = 0$ by u^{n-1} , we deduce that

$$\partial_t \left\{ \frac{1}{n} u^n \right\} + \partial_x \left\{ \frac{1}{n+1} u^{n+1} \right\} = 0, \quad (7.78)$$

and this implies that

$$Q_n = \int_{-\infty}^{\infty} u^n dx \quad (7.79)$$

is time independent. There are infinitely many of these conservation laws, one for each n . Suppose that the n -th conservation law continues to hold even in the presence of the shock, and that the discontinuity is at $X(t)$. Then

$$\frac{d}{dt} \left\{ \int_{-\infty}^{X(t)} u^n dx + \int_{X(t)}^{\infty} u^n dx \right\} = 0. \quad (7.80)$$

This is equal to

$$u_-^n(X)\dot{X} - u_+^n(X)\dot{X} + \int_{-\infty}^{X(t)} \partial_t u^n dx + \int_{X(t)}^{\infty} \partial_t u^n dx = 0, \quad (7.81)$$

where $u_-^n(X) \equiv u^n(X-\epsilon)$ and $u_+^n(X) \equiv u^n(X+\epsilon)$. Now, using $(\partial_t + u\partial_x)u = 0$ in the regions away from the shock, where it is reliable, we can write this as

$$\begin{aligned} (u_+^n - u_-^n)\dot{X} &= -\frac{n}{n+1} \int_{-\infty}^{X(t)} \partial_x u^n dx - \frac{n}{n+1} \int_{X(t)}^{\infty} \partial_x u^n dx \\ &= \left(\frac{n}{n+1} \right) (u_+^{n+1} - u_-^{n+1}). \end{aligned} \quad (7.82)$$

The velocity at which the shock moves is therefore

$$\dot{X} = \left(\frac{n}{n+1} \right) \frac{(u_+^{n+1} - u_-^{n+1})}{(u_+^n - u_-^n)}. \quad (7.83)$$

Since the shock can only move at one velocity, only one of the infinitely many conservation laws can continue to hold in the modified theory!

Example: Burgers' equation. From

$$(\partial_t + u\partial_x)u = \nu\partial_{xx}^2 u, \quad (7.84)$$

we deduce that

$$\partial_t u + \partial_x \left\{ \frac{1}{2}u^2 - \nu\partial_x u \right\} = 0, \quad (7.85)$$

so that $Q_1 = \int u dx$ is conserved, but further investigation shows that no other conservation law survives. The shock speed is therefore

$$\dot{X} = \frac{1}{2} \frac{(u_+^2 - u_-^2)}{(u_+ - u_-)} = \frac{1}{2}(u_+ + u_-). \quad (7.86)$$

Example: KdV equation. From

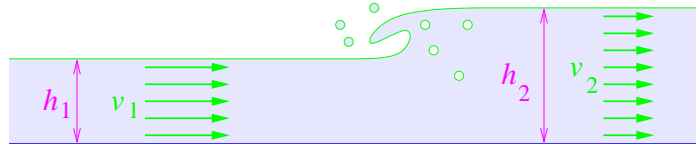
$$(\partial_t + u\partial_x)u = \delta\partial_{xxx}^3 u, \quad (7.87)$$

we deduce that

$$\begin{aligned} \partial_t u + \partial_x \left\{ \frac{1}{2}u^2 - \delta\partial_{xx}^2 u \right\} &= 0, \\ \partial_t \left\{ \frac{1}{2}u^2 \right\} + \partial_x \left\{ \frac{1}{3}u^3 - \delta u\partial_{xx}^2 u + \frac{1}{2}\delta(\partial_x u)^2 \right\} &= 0 \\ &\vdots \end{aligned}$$

where the dots refer to an infinite sequence of (not exactly obvious) conservation laws. Since more than one conservation law survives, the KdV equation cannot have shock-like solutions. Instead, the steepening wave breaks up into a sequence of *solitons*. A movie of this phenomenon can be seen on the course home-page.

Example: Hydraulic Jump, or Bore



A Hydraulic Jump.

A stationary hydraulic jump is a place in a stream where the fluid abruptly increases in depth from h_1 to h_2 , and simultaneously slows down from supercritical (faster than wave-speed) flow to subcritical (slower than wave-speed) flow. Such jumps are commonly seen near weirs, and white-water rapids⁵. A circular hydraulic jump is easily created in your kitchen sink. The moving equivalent is the *tidal bore*. A link to pictures of hydraulic jumps and bores is provided on the course web-site.

The equations governing uniform (meaning that v is independent of the depth) flow in channels are mass conservation

$$\partial_t h + \partial_x \{hv\} = 0, \quad (7.88)$$

and Euler's equation

$$\partial_t v + v \partial_x v = -\partial_x \{gh\}. \quad (7.89)$$

We could manipulate these into the Riemann form, and work from there, but it is more direct to combine them to derive the momentum conservation law

$$\partial_t \{hv\} + \partial_x \left\{ hv^2 + \frac{1}{2}gh^2 \right\} = 0. \quad (7.90)$$

From Euler's equation, assuming steady flow, $\dot{v} = 0$, we can also deduce Bernoulli's equation

$$\frac{1}{2}v^2 + gh = \text{const.}, \quad (7.91)$$

which is an energy conservation law. At the jump, mass and momentum must be conserved:

$$\begin{aligned} h_1 v_1 &= h_2 v_2, \\ h_1 v_1^2 + \frac{1}{2}gh_1^2 &= h_2 v_2^2 + \frac{1}{2}gh_2^2, \end{aligned} \quad (7.92)$$

and v_2 may be eliminated to find

$$v_1^2 = \frac{1}{2}g \left(\frac{h_2}{h_1} \right) (h_1 + h_2). \quad (7.93)$$

A change of frame reveals that v_1 is the speed at which a wall of water of height $h = (h_2 - h_1)$ would propagate into stationary water of depth h_1 .

⁵The breaking crest of Frost's "white wave" is probably as much as an example of a hydraulic jump as of a smooth downstream wake.

Bernoulli's equation is inconsistent with the two equations we have used, and so

$$\frac{1}{2}v_1^2 + gh_1 \neq \frac{1}{2}v_2^2 + gh_2. \quad (7.94)$$

This means that energy is being dissipated: for strong jumps, the fluid downstream is turbulent. For weaker jumps, the energy is radiated away in a train of waves – the so-called “undular bore”.

Example: Shock Wave in Air: At a shock wave in air we have conservation of mass

$$\rho_1 v_1 = \rho_2 v_2, \quad (7.95)$$

momentum

$$\rho_1 v_1^2 + P_1 = \rho_2 v_2^2 + P_2. \quad (7.96)$$

In this case, however, Bernoulli's equation *does* hold⁶, so

$$\frac{1}{2}v_1^2 + h_1 = \frac{1}{2}v_2^2 + h_2. \quad (7.97)$$

Here, h is the specific enthalpy ($E + PV$ per unit mass). Entropy, though, is not conserved, so we cannot use $PV^\gamma = \text{const.}$ across the shock. From mass and momentum conservation alone we find

$$v_1^2 = \left(\frac{\rho_2}{\rho_1} \right) \frac{P_2 - P_1}{\rho_2 - \rho_1}. \quad (7.98)$$

For an ideal gas with $c_p/c_v = \gamma$, we can use energy conservation to eliminate the densities, and find

$$v_1 = c_0 \sqrt{1 + \frac{\gamma + 1}{2\gamma} \frac{P_2 - P_1}{P_1}}. \quad (7.99)$$

Here, c_0 is the speed of sound in the undisturbed gas.

⁶Recall that enthalpy is conserved in a *throttling process*, even in the presence of dissipation. Bernoulli's equation for a gas is the generalization of this thermodynamic result to include the kinetic energy of the gas. The difference between the shock wave in air, where Bernoulli holds, and the hydraulic jump, where it does not, is that the enthalpy of the gas keeps track of the lost mechanical energy, which has been absorbed by the internal degrees of freedom. The Bernoulli equation for channel flow keeps track only of the mechanical energy of the mean flow.

7.3.3 Weak Solutions

We want to make mathematically precise the sense in which a function u with a discontinuity can be a solution to the differential equation

$$\partial_t \left\{ \frac{1}{n} u^n \right\} + \partial_x \left\{ \frac{1}{n+1} u^{n+1} \right\} = 0, \quad (7.100)$$

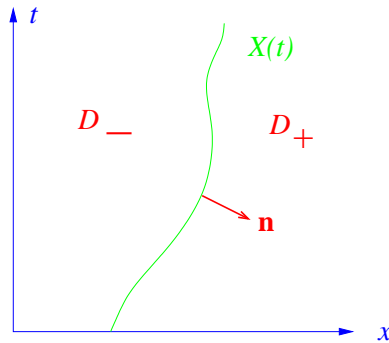
even though the equation is surely meaningless if the functions to which the derivatives are being applied are not in fact differentiable.

We could play around with distributions like the Heaviside step function or the Dirac delta, but this is unsafe for non-linear equations, because the product of two distributions is generally not meaningful. What we do is introduce a new concept. We say that u is a *weak solution* to (7.100) if

$$\int_{\mathbb{R}^2} dx dt \left\{ u^n \partial_t \varphi + \frac{n}{n+1} u^{n+1} \partial_x \varphi \right\} = 0, \quad (7.101)$$

for all test functions φ in some suitable space \mathcal{T} . This equation has formally been obtained from (7.100) by multiplying it by $\varphi(x, t)$, integrating over all space-time, and then integrating by parts to move the derivatives off u , and onto the smooth function φ . If u is assumed smooth then all these manipulations are legitimate and the new equation (7.101) contains no new information. A conventional solution to (7.100) is therefore also a weak solution. The new formulation (7.101), however, admits solutions in which u has shocks.

Let us see what is required of a weak solution if we assume that u is everywhere smooth except for a single jump from $u_-(t)$ to $u_+(t)$ at the point $X(t)$.



A weak solution.

We therefore have

$$0 = \int_{D_-} dx dt \left\{ u^n \partial_t \varphi + \frac{n}{n+1} u^{n+1} \partial_x \varphi \right\} + \int_{D_+} dx dt \left\{ u^n \partial_t \varphi + \frac{n}{n+1} u^{n+1} \partial_x \varphi \right\}. \quad (7.102)$$

Let

$$\mathbf{n} = \left(\frac{1}{\sqrt{1 + |\dot{X}|^2}}, \frac{-\dot{X}}{\sqrt{1 + |\dot{X}|^2}} \right) \quad (7.103)$$

be the unit outward normal to D_- , then, using the divergence theorem, we have

$$\begin{aligned} \int_{D_-} dx dt \left\{ u^n \partial_t \varphi + \frac{n}{n+1} u^{n+1} \partial_x \varphi \right\} &= \int_{D_-} dx dt \left\{ -\varphi \left(\partial_t u^n + \frac{n}{n+1} \partial_x u^{n+1} \right) \right\} \\ &\quad + \int_{\partial D_-} dt \left\{ \varphi \left(-\dot{X}(t) u_-^n + \frac{n}{n+1} u_-^{n+1} \right) \right\} \end{aligned} \quad (7.104)$$

Here we have written the integration measure over the boundary as

$$ds = \sqrt{1 + |\dot{X}|^2} dt. \quad (7.105)$$

Performing the same manoeuvre for D_+ , and observing that φ can be any smooth function, we deduce that

- i) $\partial_t u^n + \frac{n}{n+1} \partial_x u^{n+1} = 0$ within D_{\pm} .
- ii) $\dot{X}(u_+^n - u_-^n) = \frac{n}{n+1}(u_+^{n+1} - u_-^{n+1})$ on $X(t)$.

The reasoning here is identical to that in chapter one, where we considered variations at endpoints to obtain natural boundary conditions. We therefore end up with the same equations for the motion of the shock as before.

The notion of weak solutions is widely used in applied mathematics, and it is the principal ingredient of the *finite element* method of numerical analysis in continuum dynamics.

7.4 Solitons

A localized disturbance in a dispersive medium soon falls apart, since its various frequency components travel at differing speeds. At the same time,

non-linear effects will distort the wave profile. In some systems, however, these effects of dispersion and non-linearity can compensate each other and give rise to *solitons*, stable solitary waves which propagate for long distances without changing their form. Not all equations possessing wave-like solutions also possess solitary wave solutions. The best known example of equations that do, are:

- 1) The Korteweg-de-Vries (KdV) equation, which in the form

$$\frac{\partial u}{\partial t} + u \frac{\partial u}{\partial x} = -\frac{\partial^3 u}{\partial x^3}, \quad (7.106)$$

has a solitary wave solution

$$u = 2\alpha^2 \text{sech}^2(\alpha x - \alpha^3 t) \quad (7.107)$$

which travels at speed α^2 . The larger the amplitude, therefore, the faster the solitary wave travels. This equation applies to steep waves in shallow water.

- 2) The non-linear Schrödinger (NLS) equation with attractive interactions

$$i \frac{\partial \psi}{\partial t} = -\frac{1}{2m} \frac{\partial^2 \psi}{\partial x^2} - \lambda |\psi|^2 \psi, \quad (7.108)$$

where $\lambda > 0$. It has solitary-wave solution

$$\psi = e^{ikx - i\omega t} \sqrt{\frac{\alpha}{m\lambda}} \text{sech} \sqrt{\alpha}(x - Ut), \quad (7.109)$$

where

$$k = mU, \quad \omega = \frac{1}{2}mU^2 - \frac{\alpha}{2m}. \quad (7.110)$$

In this case, the speed is independent of the amplitude, and the moving solution can be obtained from a stationary one by means of a Galilean boost. The nonlinear equation for the stationary wavepacket may be solved by observing that

$$(-\partial_x^2 - 2\text{sech}^2 x)\psi_0 = -\psi_0 \quad (7.111)$$

where $\psi_0(x) = \text{sech } x$. This is the bound-state of the Pöschl-Teller equation that we have met several times in the homework. The non-linear Schrödinger equation describes many systems, including the dynamics of tornadoes, where the solitons manifest as the knot-like kinks sometimes seen winding their way up thin funnel clouds⁷.

⁷H.Hasimoto, J. Fluid Mech. **51** (1972) 477.

3) The sine-Gordon (SG) equation is

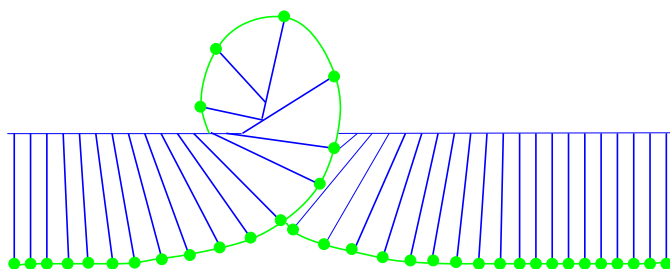
$$\frac{\partial^2 \varphi}{\partial t^2} - \frac{\partial^2 \varphi}{\partial x^2} + \frac{m^2}{\beta} \sin \beta \varphi = 0. \quad (7.112)$$

This has solitary-wave solutions

$$\varphi = \frac{4}{\beta} \tan^{-1} \left\{ e^{\pm m\gamma(x-Ut)} \right\}, \quad (7.113)$$

where $\gamma = (1 - U^2)^{-\frac{1}{2}}$ and $|U| < 1$. Again, the velocity is not related to the amplitude, and the moving soliton can be obtained by boosting a stationary soliton. The boost is now a Lorentz transformation, and so we only get subluminal solitons, whose width is Lorentz contracted by the usual relativistic factor of γ . The sine-Gordon equation describes, for example, the evolution of light pulses whose frequency is in resonance with an atomic transition in the propagation medium⁸.

In the case of the sine-Gordon soliton, the origin of the solitary wave is particularly easy to understand, as it can be realized as a “twist” in a chain of coupled pendulums. The handedness of the twist determines whether we take the $+$ or $-$ sign in the solution given above.



A sine-Gordon solitary wave as a twist in a ribbon of coupled pendulums.

The existence of solitary-wave solutions is interesting in its own right. It was the fortuitous observation of such a wave by John Scott Russell on the Union Canal, near Hermiston in England, that founded the subject⁹.

⁸See G. L. Lamb, Rev. Mod. Phys. **43**(1971) 99, for a nice review.

⁹“I was observing the motion of a boat which was rapidly drawn along a narrow channel by a pair of horses, when the boat suddenly stopped - not so the mass of water in the channel which it had put in motion; it accumulated round the prow of the vessel in a state of violent agitation, then suddenly leaving it behind, rolled forward with great velocity,

Even more remarkable was Scott Russell's subsequent discovery (made in a specially constructed trough in his garden) of what is now called the *soliton property*: two colliding solitary waves interact in a complicated manner yet emerge from the encounter with their form unchanged, having suffered no more than a slight time delay. Each of the three equations given above has exact *multi-soliton* solutions which show this phenomenon.

After languishing for more than a century, soliton theory has grown to be a huge subject. It is, for example, studied by electrical engineers who use soliton pulses in fibre-optic communications. No other type of signal can propagate through thousands of kilometers of undersea cable without degradation. Solitons, or “quantum lumps” are also important in particle physics. The nucleon can be thought of as a knotted soliton (in this case called a “skyrmion”) in the pion field, and gauge-field monopole solitons appear in many string and field theories. The soliton equations themselves are aristocrats among partial differential equations, with ties into almost every other branch of mathematics.

Physics Illustration: Solitons in Optical Fibres. We wish to transmit picosecond pulses of light with a carrier frequency ω_0 . Suppose that the dispersive properties of the fibre are such that the associated wavenumber for frequencies near ω_0 can be expanded as

$$k = \Delta k + k_0 + \beta_1(\omega - \omega_0) + \frac{1}{2}\beta_2(\omega - \omega_0)^2 + \cdots \quad (7.114)$$

Here, β_1 is the reciprocal of the group velocity, and β_2 is a parameter called the *group velocity dispersion* (GVD). The term Δk parameterizes the change in refractive index due to non-linear effects. It is proportional to the square of the electric field. Let us write the electric field as

$$E(x, t) = A(x, t)e^{ik_0z - \omega_0t}, \quad (7.115)$$

assuming the form of a large solitary elevation, a rounded, smooth and well-defined heap of water, which continued its course along the channel apparently without change of form or diminution of speed. I followed it on horseback, and overtook it still rolling on at a rate of some eight or nine miles an hour, preserving its original figure some thirty feet long and a foot to a foot and a half in height. Its height gradually diminished, and after a chase of one or two miles I lost it in the windings of the channel. Such, in the month of August 1834, was my first chance interview with that singular and beautiful phenomenon which I have called the Wave of Translation.” —John Scott Russell, 1844

where $A(x, t)$ is a slowly varying envelope function. When we transform from Fourier variables to space and time we have

$$(\omega - \omega_0) \rightarrow i \frac{\partial}{\partial t}, \quad (k - k_0) \rightarrow -i \frac{\partial}{\partial z}, \quad (7.116)$$

and so the equation determining A becomes

$$-i \frac{\partial A}{\partial z} = i \beta_1 \frac{\partial A}{\partial t} - \frac{\beta_2}{2} \frac{\partial^2 A}{\partial t^2} + \Delta k A. \quad (7.117)$$

If we set $\Delta k = \gamma |A|^2$, where γ is normally positive, we have

$$i \left(\frac{\partial A}{\partial z} + \beta_1 \frac{\partial A}{\partial t} \right) = \frac{\beta_2}{2} \frac{\partial^2 A}{\partial t^2} - \gamma |A|^2 A. \quad (7.118)$$

We may get rid of the first-order time derivative by transforming to a frame moving at the group velocity. We do this by setting

$$\begin{aligned} \tau &= t - \beta_1 z, \\ \zeta &= z \end{aligned} \quad (7.119)$$

and using the chain rule, as we did for the Galilean transformation in homework set 0. The equation for A ends up being

$$i \frac{\partial A}{\partial \zeta} = \frac{\beta_2}{2} \frac{\partial^2 A}{\partial \tau^2} - \gamma |A|^2 A. \quad (7.120)$$

This looks like our non-linear Schrödinger equation, but with the role of space and time interchanged! Also, the coefficient of the second derivative has the wrong sign so, to make it coincide with the Schrödinger equation we studied earlier, we must have $\beta_2 < 0$. When this condition holds, we are said to be in the “anomalous dispersion” regime — although this is rather a misnomer since it is the *group refractive index*, $N_g = c/v_{\text{group}}$, that is decreasing with frequency, not the ordinary refractive index. For pure SiO_2 glass, β_2 is negative for wavelengths greater than $1.27 \mu\text{m}$. We therefore have anomalous dispersion in the technologically important region near $1.55 \mu\text{m}$, where the glass is most transparent. In the anomalous dispersion regime we have solitons with

$$A(\zeta, \tau) = e^{i\alpha|\beta_2|\zeta/2} \sqrt{\frac{\beta_2\alpha}{\gamma}} \text{sech } \sqrt{\alpha}(\tau), \quad (7.121)$$

leading to

$$E(z, t) = \sqrt{\frac{\beta_2 \alpha}{\gamma}} \operatorname{sech} \sqrt{\alpha}(t - \beta_1 z) e^{i\alpha|\beta_2|z/2} e^{ik_0 z - i\omega_0 t}. \quad (7.122)$$

This equation describes a pulse propagating at β_1^{-1} , which is the group velocity.

Exercise 7.1: Find the expression for the sine-Gordon soliton, by first showing that the static sine-Gordon equation

$$-\frac{\partial^2 \varphi}{\partial x^2} + \frac{m^2}{\beta} \sin \beta \varphi = 0$$

implies that

$$\frac{1}{2} \varphi'^2 + \frac{m^2}{\beta^2} \cos \beta \varphi = \text{const.},$$

and solving this equation (for a suitable choice of the constant) by separation of variables. Next, show that if $f(x)$ is solution of the static equation, then $f(\gamma(x - Ut))$, $\gamma = (1 - U^2)^{-1/2}$, $|U| < 1$ is a solution of the time-dependent equation.

Exercise 7.2: Lax pair for the non-linear Schrödinger equation. Let L be the matrix differential operator

$$L = \begin{bmatrix} i\partial_x & \chi^* \\ \chi & i\partial_x \end{bmatrix},$$

and let P the matrix

$$P = \begin{bmatrix} i|\chi|^2 & \chi'^* \\ -\chi' & -i|\chi|^2 \end{bmatrix}.$$

Show that the equation

$$\dot{L} = [L, P]$$

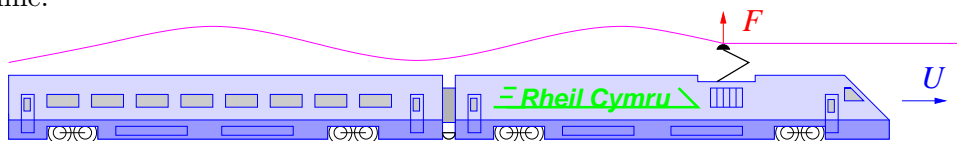
is equivalent to the non-linear Schrödinger equation

$$i\dot{\chi} = -\chi'' - 2|\chi|^2 \chi.$$

7.5 Exercises and Problems

Here are some further problems on non-linear and dispersive waves:

Exercise 7.3: Pantograph Drag. A high-speed train picks up its electrical power via a pantograph from an overhead line. The locomotive travels at speed U and the pantograph exerts a constant vertical force F on the power line.



A high-speed train.

We make the usual small amplitude approximations and assume (not unrealistically) that the line is supported in such a way that its vertical displacement obeys an inhomogeneous Klein-Gordon equation

$$\rho \ddot{y} - Ty'' + \rho \Omega^2 y = F \delta(x - Ut),$$

with $c = \sqrt{T/\rho}$, the velocity of propagation of short-wavelength transverse waves on the overhead cable.

- Assume that $U < c$ and solve for the steady state displacement of the cable about the pickup point. (Hint: the disturbance is time-independent when viewed from the train.)
- Now assume that $U > c$. Again find an expression for the displacement of the cable. (The same hint applies, but the physically appropriate boundary conditions are very different!)
- By equating the rate at which wave-energy

$$E = \int \left\{ \frac{1}{2} \rho \dot{y}^2 + \frac{1}{2} T y'^2 + \frac{1}{2} \rho \Omega^2 y^2 \right\} dx$$

is being created to rate at the which the locomotive is doing work, calculate the wave-drag on the train. In particular, show that there is no drag at all until U exceeds c . (Hint: While the front end of the wake is moving at speed U , the trailing end of the wake is moving forward at the *group velocity* of the wave-train.)

- By carefully considering the force the pantograph exerts on the overhead cable, again calculate the induced drag. You should get the same answer as in part c) (Hint: The tension in the cable is the same before and

after the train has passed, but the direction in which the tension acts is different. The force F is therefore not *exactly* vertical, but has a small forward component. Don't forget that the resultant of the forces is accelerating the cable.)

This problem of wake formation and drag is related both to Čerenkov radiation and to the Landau criterion for superfluidity.

Exercise 7.4: Inertial waves. A rotating tank of incompressible ($\rho \equiv 1$) fluid can host waves whose restoring force is provided by angular momentum conservation. Suppose the fluid velocity at the point \mathbf{r} is given by

$$\mathbf{v}(\mathbf{r}, t) = \mathbf{u}(\mathbf{r}, t) + \boldsymbol{\Omega} \times \mathbf{r},$$

where \mathbf{u} is a perturbation imposed on the rigid rotation of the fluid at angular velocity $\boldsymbol{\Omega}$.

- a) Show that when viewed from a co-ordinate frame rotating with the fluid we have

$$\frac{\partial \mathbf{u}}{\partial t} = \left(\frac{\partial \mathbf{u}}{\partial t} - \boldsymbol{\Omega} \times \mathbf{u} + ((\boldsymbol{\Omega} \times \mathbf{r}) \cdot \nabla) \mathbf{u} \right)_{\text{lab}}.$$

Deduce that the lab-frame Euler equation

$$\frac{\partial \mathbf{v}}{\partial t} + (\mathbf{v} \cdot \nabla) \mathbf{v} = -\nabla P,$$

becomes, in the rotating frame,

$$\frac{\partial \mathbf{u}}{\partial t} + 2(\boldsymbol{\Omega} \times \mathbf{u}) + (\mathbf{u} \cdot \nabla) \mathbf{u} = -\nabla \left(P - \frac{1}{2} |\boldsymbol{\Omega} \times \mathbf{r}|^2 \right).$$

We see that in the non-inertial rotating frame the fluid experiences a $-2(\boldsymbol{\Omega} \times \mathbf{u})$ Coriolis and a $\nabla |\boldsymbol{\Omega} \times \mathbf{r}|^2/2$ centrifugal force. By linearizing the rotating-frame Euler equation, show that for small \mathbf{u} we have

$$\frac{\partial \boldsymbol{\omega}}{\partial t} - 2(\boldsymbol{\Omega} \cdot \nabla) \mathbf{u} = 0, \quad (\star)$$

where $\boldsymbol{\omega} = \text{curl } \mathbf{u}$.

- b) Take $\boldsymbol{\Omega}$ to be directed along the z axis. Seek plane-wave solutions to \star in the form

$$\mathbf{u}(\mathbf{r}, t) = \mathbf{u}_0 e^{i(\mathbf{k} \cdot \mathbf{r} - \omega t)}$$

where \mathbf{u}_0 is a constant, and show that the dispersion equation for these small amplitude *inertial waves* is

$$\omega = 2\Omega \sqrt{\frac{k_z^2}{k_x^2 + k_y^2 + k_z^2}}.$$

Deduce that the group velocity is directed *perpendicular* to \mathbf{k} — *i.e.* at right-angles to the phase velocity. Conclude also that any slow flow that is steady (time independent) when viewed from the rotating frame is necessarily independent of the co-ordinate z . (This is the origin of the phenomenon of *Taylor columns*, which are columns of stagnant fluid lying above and below any obstacle immersed in such a flow.)

Exercise 7.5: Non-linear Waves. In this problem we will explore the Riemann invariants for a fluid with $P = \lambda^2 \rho^3 / 3$. This is the equation of state of one-dimensional non-interacting Fermi gas.

- a) From the continuity equation

$$\partial_t \rho + \partial_x \rho v = 0,$$

and Euler's equation of motion

$$\rho(\partial_t v + v \partial_x v) = -\partial_x P,$$

deduce that

$$\begin{aligned} \left(\frac{\partial}{\partial t} + (\lambda \rho + v) \frac{\partial}{\partial x} \right) (\lambda \rho + v) &= 0, \\ \left(\frac{\partial}{\partial t} + (-\lambda \rho + v) \frac{\partial}{\partial x} \right) (-\lambda \rho + v) &= 0. \end{aligned}$$

In what limit do these equations become equivalent to the wave equation for one-dimensional sound? What is the sound speed in this case?

- b) Show that the Riemann invariants $v \pm \lambda \rho$ are constant on suitably defined characteristic curves. What is the local speed of propagation of the waves moving to the right or left?
- c) The fluid starts from rest, $v = 0$, but with a region where the density is higher than elsewhere. Show that the Riemann equations will inevitably break down at some later time due to the formation of shock waves.

Exercise 7.6: Burgers Shocks. As simple mathematical model for the formation and decay of a shock wave consider *Burgers' Equation*:

$$\partial_t u + u \partial_x u = \nu \partial_x^2 u.$$

Note its similarity to the Riemann equations of the previous exercise. The additional term on the right-hand side introduces dissipation and prevents the solution becoming multi-valued.

- a) Show that if $\nu = 0$ any solution of Burgers' equation having a region where u decreases to the right will always eventually become multivalued.
- b) Show that the *Hopf-Cole* transformation, $u = -2\nu \partial_x \ln \psi$, leads to ψ obeying a heat diffusion equation

$$\partial_t \psi = \nu \partial_x^2 \psi.$$

- c) Show that

$$\psi(x, t) = Ae^{\nu a^2 t - ax} + Be^{\nu b^2 t - bx}$$

is a solution of the heat equation, and so deduce that Burgers' equation has a shock-wave-like solution which travels to the right at speed $C = \nu(a + b) = \frac{1}{2}(u_L + u_R)$, the mean of the wave speeds to the left and right of the shock. Show that the width of the shock is $\approx 4\nu/|u_L - u_R|$.

Chapter 8

Special Functions I

In solving Laplace's equation by the method of separation of variables we come across the most important of the *special functions* of mathematical physics. These functions have been studied for many years, and books such as the Bateman manuscript project¹ summarize the results. Any serious student theoretical physics needs to be familiar with this material, and should at least read the standard text: *A Course of Modern Analysis* by E. T. Whittaker and G. N. Watson (Cambridge University Press). Although it was originally published in 1902, nothing has superseded this book in its accessibility and usefulness.

In this chapter we will focus only on the properties that *all* physics students should know *by heart*.

8.1 Curvilinear Co-ordinates

Laplace's equation can be separated in a number of coordinate systems. These are all *orthogonal* systems in that the local coordinate axes cross at right angles.

¹The Bateman manuscript project contains the formulæ collected by Harry Bateman, who was professor of Mathematics, Theoretical Physics, and Aeronautics at the California Institute of Technology. After his death in 1946, several dozen shoe boxes full of file cards were found in his garage. These proved to be the index to a mountain of paper containing his detailed notes. A subset of the material was eventually published as the three volume series *Higher Transcendental Functions*, and the two volume *Tables of Integral Transformations*, A. Erdélyi *et al.* eds.

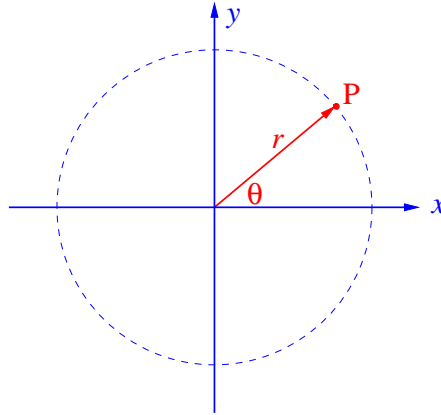
To any system of orthogonal curvilinear coordinates is associated a *metric* of the form

$$ds^2 = h_1^2(dx^1)^2 + h_2^2(dx^2)^2 + h_3^2(dx^3)^2. \quad (8.1)$$

This expression tells us the distance $\sqrt{ds^2}$ between the adjacent points $(x^1 + dx^1, x^2 + dx^2, x^3 + dx^3)$ and (x^1, x^2, x^3) . In general, the h_i will depend on the co-ordinates x^i .

The most commonly used orthogonal curvilinear co-ordinate systems are plane polars, spherical polars, and cylindrical polars. The Laplacian also separates in plane elliptic, or three-dimensional ellipsoidal coordinates and their degenerate limits, such as parabolic cylindrical co-ordinates — but these are not so often encountered, and for their properties we refer the reader to comprehensive treatises such as Morse and Feshbach's *Methods of Theoretical Physics*.

Plane Polar Co-ordinates

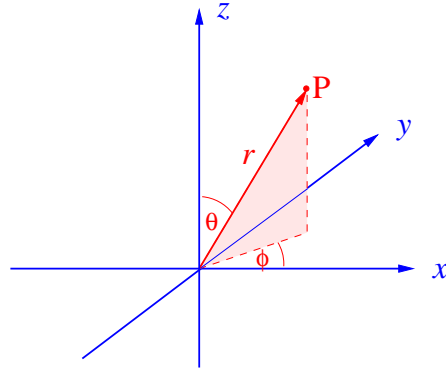


Plane polar co-ordinates.

Plane polar co-ordinates have metric

$$ds^2 = dr^2 + r^2 d\theta^2, \quad (8.2)$$

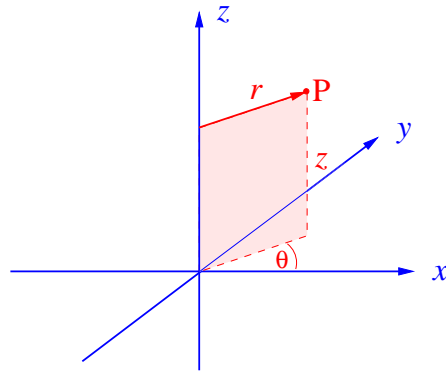
so $h_r = 1$, $h_\theta = r$.

Spherical Polar Co-ordinates*Spherical co-ordinates.*

This system has metric

$$ds^2 = dr^2 + r^2 d\theta^2 + r^2 \sin^2 \theta d\phi^2, \quad (8.3)$$

so $h_r = 1$, $h_\theta = r$, $h_\phi = r \sin \theta$,

Cylindrical Polar Co-ordinates*Cylindrical co-ordinates.*

These have metric

$$ds^2 = dr^2 + r^2 d\theta^2 + dz^2, \quad (8.4)$$

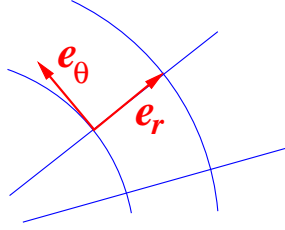
so $h_r = 1$, $h_\theta = r$, $h_z = 1$.

8.1.1 Div, Grad and Curl in Curvilinear Co-ordinates

It is very useful to know how to write the curvilinear co-ordinate expressions for the common operations of the vector calculus. Knowing these, we can then write down the expression for the Laplace operator.

The gradient operator

We begin with the gradient operator. This is a vector quantity, and to express it we need to understand how to associate a set of basis vectors with our co-ordinate system. The simplest thing to do is to take unit vectors \mathbf{e}_i tangential to the local co-ordinate axes. Because the coordinate system is orthogonal, these unit vectors will then constitute an orthonormal system.



Unit basis vectors in plane polar co-ordinates.

The vector corresponding to an infinitesimal co-ordinate displacement dx^i is then given by

$$d\mathbf{r} = h_1 dx^1 \mathbf{e}_1 + h_2 dx^2 \mathbf{e}_2 + h_3 dx^3 \mathbf{e}_3. \quad (8.5)$$

Using the orthonormality of the basis vectors, we find that

$$ds^2 \equiv |d\mathbf{r}|^2 = h_1^2 (dx^1)^2 + h_2^2 (dx^2)^2 + h_3^2 (dx^3)^2, \quad (8.6)$$

as before.

In the unit-vector basis, the gradient vector is

$$\text{grad } \phi \equiv \nabla \phi = \frac{1}{h_1} \left(\frac{\partial \phi}{\partial x_1} \right) \mathbf{e}_1 + \frac{1}{h_2} \left(\frac{\partial \phi}{\partial x_2} \right) \mathbf{e}_2 + \frac{1}{h_3} \left(\frac{\partial \phi}{\partial x_3} \right) \mathbf{e}_3, \quad (8.7)$$

so that

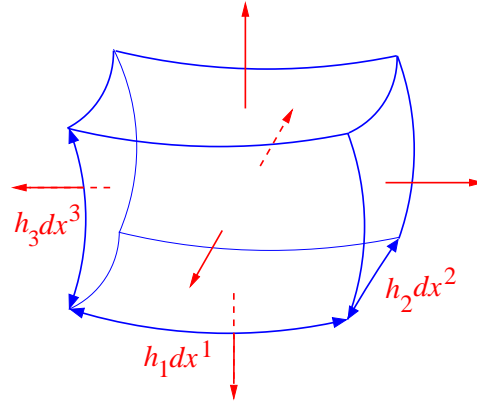
$$(\text{grad } \phi) \cdot d\mathbf{r} = \frac{\partial \phi}{\partial x^1} dx^1 + \frac{\partial \phi}{\partial x^2} dx^2 + \frac{\partial \phi}{\partial x^3} dx^3, \quad (8.8)$$

which is the change in the value ϕ due the displacement.

The numbers $(h_1 dx^1, h_2 dx^2, h_3 dx^3)$ are often called the *physical components* of the displacement $d\mathbf{r}$, to distinguish them from the numbers (dx^1, dx^2, dx^3) which are the *co-ordinate components* of $d\mathbf{r}$. The physical components of a displacement vector all have the dimensions of length. The co-ordinate components may have different dimensions and units for each component. In plane polar co-ordinates, for example, the units will be meters and radians. This distinction extends to the gradient itself: the co-ordinate components of an electric field expressed in polar co-ordinates will have units of volts per meter and volts per radian for the radial and angular components, respectively. The factor $1/h_\theta = r^{-1}$ serves to convert the latter to volts per meter.

The divergence

The divergence of a vector field \mathbf{A} is defined to be the flux of \mathbf{A} out of an infinitesimal region, divided by volume of the region.



Flux out of an infinitesimal volume with sides of length $h_1 dx^1, h_2 dx^2, h_3 dx^3$. In the figure, the flux out of the two end faces is

$$dx^2 dx^3 \left[A_1 h_2 h_3|_{(x^1+dx^1, x^2, x^3)} - A_1 h_2 h_3|_{(x^1, x^2, x^3)} \right] \approx dx^1 dx^2 dx^3 \frac{\partial(A_1 h_2 h_3)}{\partial x^1}. \quad (8.9)$$

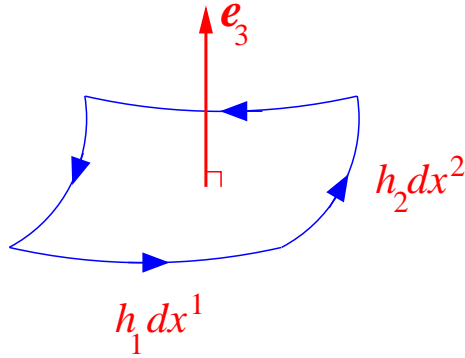
Adding the contributions from the other two pairs of faces, and dividing by the volume, $h_1 h_2 h_3 dx^1 dx^2 dx^3$, gives

$$\text{div } \mathbf{A} = \frac{1}{h_1 h_2 h_3} \left\{ \frac{\partial}{\partial x^1} (h_2 h_3 A_1) + \frac{\partial}{\partial x^2} (h_1 h_3 A_2) + \frac{\partial}{\partial x^3} (h_1 h_2 A_3) \right\}. \quad (8.10)$$

Note that in curvilinear coordinates $\text{div } \mathbf{A}$ is no longer simply $\nabla \cdot \mathbf{A}$, although one often writes it as such.

The curl

The curl of a vector field \mathbf{A} is a vector whose component in the direction of the normal to an infinitesimal area element, is line integral of \mathbf{A} round the infinitesimal area, divided by the area.



Line integral round infinitesimal area with sides of length $h_1 dx^1$, $h_2 dx^2$, and normal \mathbf{e}_3 .

The third component is, for example,

$$(\text{curl } \mathbf{A})_3 = \frac{1}{h_1 h_2} \left(\frac{\partial h_2 A_2}{\partial x^1} - \frac{\partial h_1 A_1}{\partial x^2} \right). \quad (8.11)$$

The other two components are found by cyclically permuting $1 \rightarrow 2 \rightarrow 3 \rightarrow 1$ in this formula. The curl is thus no longer equal to $\nabla \times \mathbf{A}$, although it is common to write it as if it were.

Note that the factors of h_i are disposed so that the vector identities

$$\text{curl grad } \varphi = 0, \quad (8.12)$$

and

$$\text{div curl } \mathbf{A} = 0, \quad (8.13)$$

continue to hold for any scalar field φ , and any vector field \mathbf{A} .

8.1.2 The Laplacian in Curvilinear Co-ordinates

The Laplacian acting on scalars, is “div grad”, and is therefore

$$\nabla^2 \varphi = \frac{1}{h_1 h_2 h_3} \left\{ \frac{\partial}{\partial x_1} \left(\frac{h_2 h_3}{h_1} \frac{\partial \varphi}{\partial x_1} \right) + \frac{\partial}{\partial x_2} \left(\frac{h_1 h_3}{h_2} \frac{\partial \varphi}{\partial x_2} \right) + \frac{\partial}{\partial x_3} \left(\frac{h_1 h_2}{h_3} \frac{\partial \varphi}{\partial x_3} \right) \right\}. \quad (8.14)$$

This formula is worth committing to memory.

When the Laplacian is to act on a *vector field*, we must use the *vector Laplacian*

$$\nabla^2 \mathbf{A} = \text{grad div } \mathbf{A} - \text{curl curl } \mathbf{A}. \quad (8.15)$$

In curvilinear co-ordinates this is no longer equivalent to the Laplacian acting on each component of \mathbf{A} , treating it as if it were a scalar. The expression (8.15) is the appropriate generalization of the vector Laplacian to curvilinear co-ordinates because it is defined in terms of the co-ordinate independent operators div, grad, and curl, and reduces to the Laplacian on the individual components when the co-ordinate system is Cartesian.

In spherical polars the Laplace operator acting on the scalar field φ is

$$\begin{aligned} \nabla^2 \varphi &= \frac{1}{r^2} \frac{\partial}{\partial r} \left(r^2 \frac{\partial \varphi}{\partial r} \right) + \frac{1}{r^2 \sin \theta} \frac{\partial}{\partial \theta} \left(\sin \theta \frac{\partial \varphi}{\partial \theta} \right) + \frac{1}{r^2 \sin^2 \theta} \frac{\partial^2 \varphi}{\partial \phi^2} \\ &= \frac{1}{r} \frac{\partial^2 (r\varphi)}{\partial r^2} + \frac{1}{r^2} \left\{ \frac{1}{\sin \theta} \frac{\partial}{\partial \theta} \left(\sin \theta \frac{\partial \varphi}{\partial \theta} \right) + \frac{1}{\sin^2 \theta} \frac{\partial^2 \varphi}{\partial \phi^2} \right\} \\ &= \frac{1}{r} \frac{\partial^2 (r\varphi)}{\partial r^2} - \frac{\hat{L}^2}{r^2} \varphi, \end{aligned} \quad (8.16)$$

where

$$\hat{L}^2 = -\frac{1}{\sin \theta} \frac{\partial}{\partial \theta} \sin \theta \frac{\partial}{\partial \theta} - \frac{1}{\sin^2 \theta} \frac{\partial^2}{\partial \phi^2}, \quad (8.17)$$

is (after multiplication by \hbar^2) the operator representing the square of the angular momentum in quantum mechanics.

In cylindrical polars the Laplacian is

$$\nabla^2 = \frac{1}{r} \frac{\partial}{\partial r} r \frac{\partial}{\partial r} + \frac{1}{r^2} \frac{\partial^2}{\partial \theta^2} + \frac{\partial^2}{\partial z^2}. \quad (8.18)$$

8.2 Spherical Harmonics

We saw that Laplace's equation in spherical polars is

$$0 = \frac{1}{r} \frac{\partial^2(r\varphi)}{\partial r^2} - \frac{\hat{L}^2}{r^2} \varphi. \quad (8.19)$$

To solve this by the method of separation of variables, we factorize

$$\varphi = R(r)Y(\theta, \phi), \quad (8.20)$$

so that

$$\frac{1}{Rr} \frac{d^2(rR)}{dr^2} - \frac{1}{r^2} \left(\frac{1}{Y} \hat{L}^2 Y \right) = 0. \quad (8.21)$$

Taking the separation constant to be $l(l+1)$, we have

$$r \frac{d^2(rR)}{dr^2} - l(l+1)(rR) = 0, \quad (8.22)$$

and

$$\hat{L}^2 Y = l(l+1)Y. \quad (8.23)$$

The solution for R is r^l or r^{-l-1} . The equation for Y can be further decomposed by setting $Y = \Theta(\theta)\Phi(\phi)$. Looking back at the definition of \hat{L}^2 , we see that we can take

$$\Phi(\phi) = e^{im\phi} \quad (8.24)$$

with m an integer to ensure single valuedness. The equation for Θ is then

$$\frac{1}{\sin \theta} \frac{d}{d\theta} \left(\sin \theta \frac{d\Theta}{d\theta} \right) - \frac{m^2}{\sin^2 \theta} \Theta = -l(l+1)\Theta. \quad (8.25)$$

It is convenient to set $x = \cos \theta$; then

$$\left(\frac{d}{dx} (1-x^2) \frac{d}{dx} + l(l+1) - \frac{m^2}{1-x^2} \right) \Theta = 0. \quad (8.26)$$

8.2.1 Legendre Polynomials

We first look at the axially symmetric case where $m = 0$. We are left with

$$\left(\frac{d}{dx} (1-x^2) \frac{d}{dx} + l(l+1) \right) \Theta = 0. \quad (8.27)$$

This is *Legendre's equation*. We can think of it as an eigenvalue problem

$$-\left(\frac{d}{dx}(1-x^2)\frac{d}{dx}\right)\Theta(x) = l(l+1)\Theta(x), \quad (8.28)$$

on the interval $-1 \leq x \leq 1$, this being the range of $\cos \theta$ for real θ . Legendre's equation is of Sturm-Liouville form, but with regular singular points at $x = \pm 1$. Because the endpoints of the interval are singular, we cannot impose as boundary conditions that Θ , Θ' , or some linear combination of these, be zero there. We do need some boundary conditions, however, so as to have a self-adjoint operator and hence a complete set of eigenfunctions.

Given one or more singular endpoints, a possible route to a well-defined eigenvalue problem is to demand solutions that are square-integrable, and so normalizable. This works for the harmonic-oscillator Schrödinger equation, for example, where, as we will describe in detail later in the chapter, the oscillator equation's singular endpoints at $x = \pm\infty$ are in Weyl's *limit-point* class. For Legendre's equation with $l = 0$, the two independent solutions are $\Theta(x) = 1$ and $\Theta(x) = \ln(1+x) - \ln(1-x)$. Both of these solutions have finite $L^2[-1, 1]$ norms, and this square integrability persists for all values of l . Thus, requiring normalizability is not enough to select a unique boundary condition. The two singular endpoints are both in Weyl's *limit-circle* class, and each endpoint possesses a family of boundary conditions that lead to self-adjoint operators. We therefore make the more restrictive demand that the allowed eigenfunctions be *finite* at the endpoints. Because the north and south pole of the sphere are not special points, this is a physically reasonable condition. If we start with a finite $\Theta(x)$ at one end of the interval and demand that the solution remain finite at the other end, we obtain a discrete spectrum of eigenvalues. When l is an integer, then one of the solutions, $P_l(x)$, becomes a polynomial, and so is finite at $x = \pm 1$. The second solution, $Q_l(x)$, is divergent at both ends, and so is not an allowed solution. When l is not an integer, neither solution is finite. The eigenvalues are therefore $l(l+1)$ with l zero or a positive integer. Despite its unfamiliar form, the "finite" boundary condition makes the Legendre operator self-adjoint, and the *Legendre polynomials* $P_l(x)$ form a complete orthogonal set for $L^2[-1, 1]$.

Proving orthogonality is easy: we follow the usual strategy for Sturm-Liouville equations with non-singular boundary conditions to deduce that

$$[l(l+1) - m(m+1)] \int_{-1}^1 P_l(x)P_m(x) dx = [(P_l P'_m - P'_l P_m)(1-x^2)]_{-1}^1. \quad (8.29)$$

Since the P_l 's remain finite at ± 1 , the right hand side is zero because of the $(1 - x^2)$ factor, and so $\int_{-1}^1 P_l(x)P_m(x) dx$ is zero if $l \neq m$. (Note that this differs from the usual argument, where it is the vanishing of the eigenfunction or its derivative that makes the integrated-out term zero.)

Because they are orthogonal polynomials, the $P_l(x)$ can be obtained by applying the Gram-Schmidt procedure to the sequence $1, x, x^2, \dots$ to obtain polynomials orthogonal with respect to the $w \equiv 1$ inner product, and then fixing the normalization constant. The result of this process can be expressed in closed form as

$$P_l(x) = \frac{1}{2^l l!} \frac{d^l}{dx^l} (x^2 - 1)^l. \quad (8.30)$$

This is called *Rodriguez' formula*. It should be clear that this formula outputs a polynomial of degree l . The coefficient $1/2^l l!$ comes from the traditional normalization for the Legendre polynomials that makes $P_l(1) = 1$. This convention does not lead to an orthonormal set. Instead, we have

$$\int_{-1}^1 P_l(x)P_m(x) dx = \frac{2}{2l+1} \delta_{lm}. \quad (8.31)$$

It is easy to show that this integral is zero if $l > m$ —simply integrate by parts l times so as to take the l derivatives off $(x^2 - 1)^l$ and onto $(x^2 - 1)^m$, which they kill. We will evaluate the $l = m$ integral in the next section.

We now show that the $P_l(x)$ given by Rodriguez formula are indeed solutions of Legendre's equation: Let $v = (x^2 - 1)^l$, then

$$(1 - x^2)v' + 2lxv = 0. \quad (8.32)$$

We differentiate this $l + 1$ times using Leibniz theorem

$$\begin{aligned} [uv]^{(n)} &= \sum_{m=0}^n \binom{n}{m} u^{(m)} v^{(n-m)} \\ &= uv^{(n)} + nu'v^{(n-1)} + \frac{1}{2}n(n-1)u''v^{(n-2)} + \dots \end{aligned} \quad (8.33)$$

We find that

$$\begin{aligned} [(1 - x^2)v']^{(l+1)} &= (1 - x^2)v^{(l+2)} - (l+1)2xv^{(l+1)} - l(l+1)v^{(l)}, \\ [2xnv]^{(l+1)} &= 2xlv^{(l+1)} + 2l(l+1)v^{(l)}. \end{aligned} \quad (8.34)$$

Putting these two terms together we obtain

$$\left((1-x^2) \frac{d^2}{dx^2} - 2x \frac{d}{dx} + l(l+1) \right) \frac{d^l}{dx^l} (x^2-1)^l = 0, \quad (8.35)$$

which is Legendre's equation.

The $P_l(x)$ have alternating parity

$$P_l(-x) = (-1)^l P_l(x), \quad (8.36)$$

and the first few are

$$\begin{aligned} P_0(x) &= 1, \\ P_1(x) &= x, \\ P_2(x) &= \frac{1}{2}(3x^2 - 1), \\ P_3(x) &= \frac{1}{2}(5x^3 - 3x), \\ P_4(x) &= \frac{1}{8}(35x^4 - 30x^2 + 3). \end{aligned}$$

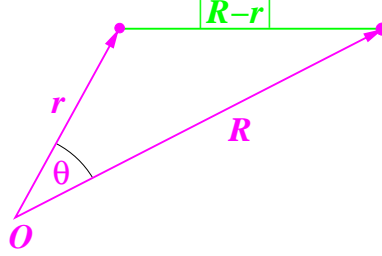
8.2.2 Axisymmetric potential problems

The essential property of the $P_l(x)$ is that the general axisymmetric solution of $\nabla^2 \varphi = 0$ can be expanded in terms of them as

$$\varphi(r, \theta) = \sum_{l=0}^{\infty} (A_l r^l + B_l r^{-l-1}) P_l(\cos \theta). \quad (8.37)$$

You should memorize this formula. You should also know by heart the explicit expressions for the first four $P_l(x)$, and the factor of $2/(2l+1)$ in the orthogonality formula.

Example: Point charge. Put a unit charge at the point \mathbf{R} , and find an expansion for the potential as a Legendre polynomial series in a neighbourhood of the origin.



Geometry for generating function.

Let start by assuming that $|\mathbf{r}| < |\mathbf{R}|$. We know that in this region the point charge potential $1/|\mathbf{r} - \mathbf{R}|$ is a solution of Laplace's equation, and so we can expand

$$\frac{1}{|\mathbf{r} - \mathbf{R}|} \equiv \frac{1}{\sqrt{r^2 + R^2 - 2rR \cos \theta}} = \sum_{l=0}^{\infty} A_l r^l P_l(\cos \theta). \quad (8.38)$$

We knew that the coefficients B_l were zero because φ is finite when $r = 0$. We can find the coefficients A_l by setting $\theta = 0$ and Taylor expanding

$$\frac{1}{|\mathbf{r} - \mathbf{R}|} = \frac{1}{R - r} = \frac{1}{R} \left(1 + \left(\frac{r}{R} \right) + \left(\frac{r}{R} \right)^2 + \cdots \right), \quad r < R. \quad (8.39)$$

By comparing the two series and noting that $P_l(1) = 1$, we find that $A_l = R^{-l-1}$. Thus

$$\frac{1}{\sqrt{r^2 + R^2 - 2rR \cos \theta}} = \frac{1}{R} \sum_{l=0}^{\infty} \left(\frac{r}{R} \right)^l P_l(\cos \theta), \quad r < R. \quad (8.40)$$

This last expression is the *generating function formula* for Legendre polynomials. It is also a useful formula to have in your long-term memory.

If $|\mathbf{r}| > |\mathbf{R}|$, then we must take

$$\frac{1}{|\mathbf{r} - \mathbf{R}|} \equiv \frac{1}{\sqrt{r^2 + R^2 - 2rR \cos \theta}} = \sum_{l=0}^{\infty} B_l r^{-l-1} P_l(\cos \theta), \quad (8.41)$$

because we know that φ tends to zero when $r = \infty$. We now set $\theta = 0$ and compare with

$$\frac{1}{|\mathbf{r} - \mathbf{R}|} = \frac{1}{r - R} = \frac{1}{r} \left(1 + \left(\frac{R}{r} \right) + \left(\frac{R}{r} \right)^2 + \cdots \right), \quad R < r, \quad (8.42)$$

to get

$$\frac{1}{\sqrt{r^2 + R^2 - 2rR \cos \theta}} = \frac{1}{r} \sum_{l=0}^{\infty} \left(\frac{R}{r}\right)^l P_l(\cos \theta), \quad R < r. \quad (8.43)$$

Observe that we made no use of the normalization integral

$$\int_{-1}^1 \{P_l(x)\}^2 dx = 2/(2l+1) \quad (8.44)$$

in deriving the the generating function expansion for the Legendre polynomials. The following exercise shows that this expansion, taken together with their previously established orthogonality property, can be used to establish 8.44.

Exercise 8.1: Use the generating function for Legendre polynomials $P_l(x)$ to show that

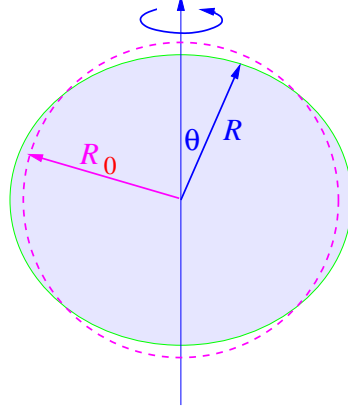
$$\sum_{l=0}^{\infty} z^{2l} \left(\int_{-1}^1 \{P_l(x)\}^2 dx \right) = \int_{-1}^1 \frac{1}{1 - 2xz + z^2} dx = -\frac{1}{z} \ln \left(\frac{1-z}{1+z} \right), \quad |z| < 1.$$

By Taylor expanding the logarithm, and comparing the coefficients of z^{2l} , evaluate $\int_{-1}^1 \{P_l(x)\}^2 dx$.

Example: A planet is spinning on its axis and so its shape deviates slightly from a perfect sphere. The position of its surface is given by

$$R(\theta, \phi) = R_0 + \eta P_2(\cos \theta). \quad (8.45)$$

Observe that, to first order in η , this deformation does not alter the volume of the body. Assuming that the planet has a uniform density ρ_0 , compute the external gravitational potential of the planet.

*Deformed planet.*

The gravitational potential obeys Poisson's equation

$$\nabla^2 \phi = 4\pi G \rho(\mathbf{x}), \quad (8.46)$$

where G is Newton's gravitational constant. We expand ϕ as a power series in η

$$\phi(r, \theta) = \phi_0(r, \theta) + \eta \phi_1(r, \theta) + \dots \quad (8.47)$$

We also decompose the gravitating mass into a uniform undeformed sphere, which gives the external potential

$$\phi_{0,\text{ext}}(r, \theta) = - \left(\frac{4}{3} \pi R_0^3 \rho_0 \right) \frac{G}{r}, \quad r > R_0, \quad (8.48)$$

and a thin spherical shell of areal mass-density

$$\sigma(\theta) = \rho_0 \eta P_2(\cos \theta). \quad (8.49)$$

The thin shell gives rise to the potential

$$\phi_{1,\text{int}}(r, \theta) = A r^2 P_2(\cos \theta), \quad r < R_0, \quad (8.50)$$

and

$$\phi_{1,\text{ext}}(r, \theta) = B \frac{1}{r^3} P_2(\cos \theta), \quad r > R_0. \quad (8.51)$$

At the shell we must have $\phi_{1,\text{int}} = \phi_{1,\text{ext}}$ and

$$\frac{\partial \phi_{1,\text{ext}}}{\partial r} - \frac{\partial \phi_{1,\text{int}}}{\partial r} = 4\pi G \sigma(\theta). \quad (8.52)$$

Thus $A = BR_0^{-5}$, and

$$B = -\frac{4}{5}\pi G\eta\rho_0 R_0^4. \quad (8.53)$$

Putting this together, we have

$$\phi(r, \theta) = -\left(\frac{4}{3}\pi G\rho_0 R_0^3\right)\frac{1}{r} - \frac{4}{5}(\pi G\eta\rho_0 R_0^4)\frac{P_2(\cos\theta)}{r^3} + O(\eta^2), \quad r > R_0. \quad (8.54)$$

8.2.3 General spherical harmonics

When we do not have axisymmetry, we need the full set of spherical harmonics. These involve solutions of

$$\left(\frac{d}{dx}(1-x^2)\frac{d}{dx} + l(l+1) - \frac{m^2}{1-x^2}\right)\Phi = 0, \quad (8.55)$$

which is the *associated Legendre* equation. This looks like another complicated equation with singular endpoints, but its bounded solutions can be obtained by differentiating Legendre polynomials. On substituting $y = (1-x^2)^{m/2}z(x)$ into (8.55), and comparing the resulting equation for $z(x)$ with the m -th derivative of Legendre's equation, we find that

$$P_l^m(x) \stackrel{\text{def}}{=} (-1)^m (1-x^2)^{m/2} \frac{d^m}{dx^m} P_l(x) \quad (8.56)$$

is a solution of (8.55) that remains finite ($m = 0$) or goes to zero ($m > 0$) at the endpoints $x = \pm 1$. Since $P_l(x)$ is a polynomial of degree l , we must have $P_l^m(x) = 0$ if $m > l$. For each l , the allowed values of m in this formula are therefore $0, 1, \dots, l$. Our definition (8.56) of the $P_l^m(x)$ can be extended to negative integer m by interpreting $d^{-|m|}/dx^{-|m|}$ as an instruction to integrate the Legendre polynomial m times, instead of differentiating it, but the resulting $P_l^{-|m|}(x)$ are proportional to $P_l^m(x)$, so nothing new is gained by this conceit.

The *spherical harmonics* are the normalized product of these *associated Legendre functions* with the corresponding $e^{im\phi}$:

$$Y_l^m(\theta, \phi) \propto P_l^{|m|}(\cos\theta)e^{im\phi}, \quad -l \leq m \leq l. \quad (8.57)$$

The first few are

$$l = 0 \quad Y_0^0 = \frac{1}{\sqrt{4\pi}} \quad (8.58)$$

$$l = 1 \quad \begin{cases} Y_1^1 &= -\sqrt{\frac{3}{8\pi}} \sin \theta e^{i\phi}, \\ Y_1^0 &= \sqrt{\frac{3}{4\pi}} \cos \theta, \\ Y_1^{-1} &= \sqrt{\frac{3}{8\pi}} \sin \theta e^{-i\phi}. \end{cases} \quad (8.59)$$

$$l = 2 \quad \begin{cases} Y_2^2 &= \frac{1}{4} \sqrt{\frac{15}{2\pi}} \sin^2 \theta e^{2i\phi}, \\ Y_2^1 &= -\sqrt{\frac{15}{8\pi}} \sin \theta \cos \theta e^{i\phi}, \\ Y_2^0 &= \sqrt{\frac{5}{4\pi}} \left(\frac{3}{2} \cos^2 \theta - \frac{1}{2} \right), \\ Y_2^{-1} &= \sqrt{\frac{15}{8\pi}} \sin \theta \cos \theta e^{-i\phi}, \\ Y_2^{-2} &= \frac{1}{4} \sqrt{\frac{15}{2\pi}} \sin^2 \theta e^{-2i\phi}. \end{cases} \quad (8.60)$$

When $m = 0$, the spherical harmonics are independent of the azimuthal angle ϕ , and so must be proportional to the Legendre polynomials. The exact relation is

$$Y_l^0(\theta, \phi) = \sqrt{\frac{2l+1}{4\pi}} P_l(\cos \theta). \quad (8.61)$$

If we use a unit vector \mathbf{n} to denote a point on the unit sphere, we have the symmetry properties

$$[Y_l^m(\mathbf{n})]^* = (-1)^m Y_l^{-m}(\mathbf{n}), \quad Y_l^m(-\mathbf{n}) = (-1)^l Y_l^m(\mathbf{n}). \quad (8.62)$$

These identities are useful when we wish to know how quantum mechanical wavefunctions transform under time reversal or parity.

Exercise 8.2: Show that

$$\begin{aligned} \begin{pmatrix} Y_1^1 \\ Y_1^0 \\ Y_1^{-1} \end{pmatrix} &\propto \begin{pmatrix} x + iy, \\ z, \\ x - iy \end{pmatrix} \\ \begin{pmatrix} Y_2^2 \\ Y_2^1 \\ Y_2^0 \\ Y_2^{-1} \\ Y_2^{-2} \end{pmatrix} &\propto \begin{pmatrix} (x + iy)^2, \\ (x + iy)z, \\ x^2 + y^2 - 2z^2, \\ (x - iy)z, \\ (x - iy)^2, \end{pmatrix} \end{aligned}$$

where $x^2 + y^2 + z^2 = 1$ are the usual Cartesian co-ordinates, restricted to the unit sphere.

The spherical harmonics form a complete set of orthonormal functions on the unit sphere:

$$\int_0^{2\pi} d\phi \int_0^\pi d(\cos \theta) [Y_l^m(\theta, \phi)]^* Y_{l'}^{m'}(\theta, \phi) = \delta_{ll'} \delta_{mm'}, \quad (8.63)$$

and

$$\sum_{l=0}^{\infty} \sum_{m=-l}^l [Y_l^m(\theta', \phi')]^* Y_l^m(\theta, \phi) = \delta(\phi - \phi') \delta(\cos \theta' - \cos \theta). \quad (8.64)$$

In terms of them, the general solution to $\nabla^2 \varphi = 0$ is

$$\varphi(r, \theta, \phi) = \sum_{l=0}^{\infty} \sum_{m=-l}^l (A_{lm} r^l + B_{lm} r^{-l-1}) Y_l^m(\theta, \phi). \quad (8.65)$$

This is definitely a formula to remember.

There is an addition theorem

$$P_l(\cos \gamma) = \frac{4\pi}{2l+1} \sum_{m=-l}^l [Y_l^m(\theta', \phi')]^* Y_l^m(\theta, \phi), \quad (8.66)$$

where γ is the angle between the directions (θ, ϕ) and (θ', ϕ') , and is found from

$$\cos \gamma = \cos \theta \cos \theta' + \sin \theta \sin \theta' \cos(\phi - \phi'). \quad (8.67)$$

The addition theorem is established by first showing that the right-hand side is rotationally invariant, and then setting the direction (θ', ϕ') to point along the z axis. Addition theorems of this sort are useful because they allow one to replace a simple function of an entangled variable by a sum of functions of unentangled variables. For example, the point-charge potential can be disentangled as

$$\frac{1}{|\mathbf{r} - \mathbf{r}'|} = \sum_{l=0}^{\infty} \sum_{m=-l}^l \frac{4\pi}{2l+1} \left(\frac{r_{<}^l}{r_{>}^{l+1}} \right) [Y_l^m(\theta', \phi')]^* Y_l^m(\theta, \phi) \quad (8.68)$$

where $r_{<}$ is the smaller of $|\mathbf{r}|$ or $|\mathbf{r}'|$, and $r_{>}$ is the greater and (θ, ϕ) , (θ', ϕ') specify the direction of \mathbf{r} , \mathbf{r}' respectively. This expansion is derived by combining the generating function for the Legendre polynomials with the addition formula. It is useful for defining and evaluating multipole expansions.

8.3 Bessel Functions

In cylindrical polars, Laplace's equation is

$$0 = \nabla^2 \varphi = \frac{1}{r} \frac{\partial}{\partial r} r \frac{\partial \varphi}{\partial r} + \frac{1}{r^2} \frac{\partial^2 \varphi}{\partial \theta^2} + \frac{\partial^2 \varphi}{\partial z^2}. \quad (8.69)$$

If we set $\varphi = R(r)e^{im\phi}e^{\pm kx}$ we find that $R(r)$ obeys

$$\frac{d^2 R}{dr^2} + \frac{1}{r} \frac{dR}{dr} + \left(k^2 - \frac{m^2}{r^2} \right) R = 0. \quad (8.70)$$

Now

$$\frac{d^2 y}{dx^2} + \frac{1}{x} \frac{dy}{dx} + \left(1 - \frac{\nu^2}{x^2} \right) y = 0 \quad (8.71)$$

is *Bessel's equation* and its solutions are *Bessel functions* of order ν . The solutions for R will therefore be Bessel functions of order m , but with x replaced by kr .

8.3.1 Cylindrical Bessel Functions

We now set about solving Bessel's equation,

$$\frac{d^2 y}{dx^2} + \frac{1}{x} \frac{dy}{dx} + \left(1 - \frac{\nu^2}{x^2} \right) y(x) = 0. \quad (8.72)$$

This has a regular singular point at the origin, and an irregular singular point at infinity. We seek a series solution of the form

$$y = x^\lambda (1 + a_1 x + a_2 x^2 + \cdots), \quad (8.73)$$

and find from the indicial equation that $\lambda = \pm \nu$. Setting $\lambda = \nu$ and inserting the series into the equation, we find, with a conventional choice for normalization, that

$$y = J_\nu(x) \stackrel{\text{def}}{=} \left(\frac{x}{2} \right)^\nu \sum_{n=0}^{\infty} \frac{(-1)^n}{n!(n+\nu)!} \left(\frac{x}{2} \right)^{2n}. \quad (8.74)$$

Here $(n+\nu)! \equiv \Gamma(n+\nu+1)$. The function $J_\nu(x)$ is known as a cylindrical Bessel function

If ν is an integer we find that $J_{-n}(x) = (-1)^n J_n(x)$, so we have only found one of the two independent solutions. Because of this, it is traditional to define the *Neumann function*

$$N_\nu(x) = \frac{J_\nu(x) \cos \nu\pi - J_{-\nu}(x)}{\sin \nu\pi}, \quad (8.75)$$

as this remains an independent second solution even when ν becomes integral. At short distance, and for ν not an integer

$$\begin{aligned} J_\nu(x) &= \left(\frac{x}{2}\right)^\nu \frac{1}{\Gamma(\nu+1)} + \cdots, \\ N_\nu(x) &= \frac{1}{\pi} \left(\frac{x}{2}\right)^{-\nu} \Gamma(\nu) + \cdots. \end{aligned} \quad (8.76)$$

When ν tends to zero, we have

$$\begin{aligned} J_0(x) &= 1 - \frac{1}{4}x^2 + \cdots \\ N_0(x) &= \left(\frac{2}{\pi}\right) (\ln x/2 + \gamma) + \cdots, \end{aligned} \quad (8.77)$$

where $\gamma = .57721\dots$ denotes the Euler-Mascheroni constant. For fixed ν , and $x \gg \nu$ we have the asymptotic expansions

$$J_\nu(x) \sim \sqrt{\frac{2}{\pi x}} \cos\left(x - \frac{1}{2}\nu\pi - \frac{1}{4}\pi\right) \left(1 + O\left(\frac{1}{x}\right)\right), \quad (8.78)$$

$$N_\nu(x) \sim \sqrt{\frac{2}{\pi x}} \sin\left(x - \frac{1}{2}\nu\pi - \frac{1}{4}\pi\right) \left(1 + O\left(\frac{1}{x}\right)\right). \quad (8.79)$$

It is therefore natural to define the *Hankel functions*

$$H_\nu^{(1)}(x) = J_\nu(x) + iN_\nu(x) \sim \sqrt{\frac{2}{\pi x}} e^{i(x - \nu\pi/2 - \pi/4)}, \quad (8.80)$$

$$H_\nu^{(2)}(x) = J_\nu(x) - iN_\nu(x) \sim \sqrt{\frac{2}{\pi x}} e^{-i(x - \nu\pi/2 - \pi/4)}. \quad (8.81)$$

We will derive these asymptotic forms later.

Generating Function

The two-dimensional wave equation

$$\left(\nabla^2 - \frac{1}{c^2} \frac{\partial^2}{\partial t^2}\right) \Phi(r, \theta, t) = 0 \quad (8.82)$$

has solutions

$$\Phi = e^{i\omega t} e^{in\theta} J_n(kr), \quad (8.83)$$

where $k = |\omega|/c$. Equivalently, the two dimensional Helmholtz equation

$$(\nabla^2 + k^2)\Phi = 0, \quad (8.84)$$

has solutions $e^{in\theta} J_n(kr)$. It also has solutions with $J_n(kr)$ replaced by $N_n(kr)$, but these are not finite at the origin. Since the $e^{in\theta} J_n(kr)$ are the only solutions that are finite at the origin, any other finite solution should be expandable in terms of them. In particular, we should be able to expand a plane wave solution:

$$e^{iky} = e^{ikr \sin \theta} = \sum_n a_n e^{in\theta} J_n(kr). \quad (8.85)$$

As we will see in a moment, the a_n 's are all unity, so in fact

$$e^{ikr \sin \theta} = \sum_{n=-\infty}^{\infty} e^{in\theta} J_n(kr). \quad (8.86)$$

This *generating function* is the historical origin of the Bessel functions. They were introduced by the astronomer Wilhelm Bessel as a method of expressing the eccentric anomaly of a planetary position as a Fourier sine series in the mean anomaly — a modern version of Hipparchus' epicycles.

From the generating function we see that

$$J_n(x) = \frac{1}{2\pi} \int_0^{2\pi} e^{-in\theta + ix \sin \theta} d\theta. \quad (8.87)$$

Whenever you come across a formula like this, involving the Fourier integral of the exponential of a trigonometric function, you are probably dealing with a Bessel function.

The generating function can also be written as

$$e^{\frac{x}{2}(t-\frac{1}{t})} = \sum_{n=-\infty}^{\infty} t^n J_n(x). \quad (8.88)$$

Expanding the left-hand side and using the binomial theorem, we find

$$\begin{aligned} LHS &= \sum_{m=0}^{\infty} \left(\frac{x}{2}\right)^m \frac{1}{m!} \left[\sum_{r+s=m} \frac{(r+s)!}{r!s!} (-1)^s t^r t^{-s} \right], \\ &= \sum_{r=0}^{\infty} \sum_{s=0}^{\infty} (-1)^s \left(\frac{x}{2}\right)^{r+s} \frac{t^{r-s}}{r!s!}, \\ &= \sum_{n=-\infty}^{\infty} t^n \left\{ \sum_{s=0}^{\infty} \frac{(-1)^s}{s!(s+n)!} \left(\frac{x}{2}\right)^{2s+n} \right\}. \end{aligned} \quad (8.89)$$

We recognize that the sum in the braces is the series expansion defining $J_n(x)$. This therefore proves the generating function formula.

Bessel Identities

There are many identities and integrals involving Bessel functions. The standard reference is the monumental *Treatise on the Theory of Bessel Functions* by G. N. Watson. Here are just a few formulæ for your delectation:

i) Starting from the generating function

$$\exp \left\{ \frac{1}{2}x \left(t - \frac{1}{t} \right) \right\} = \sum_{n=-\infty}^{\infty} J_n(x) t^n, \quad (8.90)$$

we can, with a few lines of work, establish the recurrence relations

$$2J'_n(x) = J_{n-1}(x) - J_{n+1}(x), \quad (8.91)$$

$$\frac{2n}{x} J_n(x) = J_{n-1}(x) + J_{n+1}(x), \quad (8.92)$$

together with

$$J'_0(x) = -J_1(x), \quad (8.93)$$

$$J_n(x+y) = \sum_{r=-\infty}^{\infty} J_r(x) J_{n-r}(y). \quad (8.94)$$

ii) From the series expansion for $J_n(x)$ we find

$$\frac{d}{dx} \{x^n J_n(x)\} = x^n J_{n-1}(x). \quad (8.95)$$

iii) By similar methods, we find

$$\left(\frac{1}{x} \frac{d}{dx}\right)^m \{x^{-n} J_n(x)\} = (-1)^m x^{-n-m} J_{n+m}(x). \quad (8.96)$$

iv) Again from the series expansion, we find

$$\int_0^\infty J_0(ax) e^{-px} dx = \frac{1}{\sqrt{a^2 + p^2}}. \quad (8.97)$$

Semi-classical picture

The Schrödinger equation

$$-\frac{\hbar^2}{2m} \nabla^2 \psi = E \psi \quad (8.98)$$

can be separated in cylindrical polars, and has eigenfunctions

$$\psi_{k,l}(r, \theta) = J_l(kr) e^{il\theta}. \quad (8.99)$$

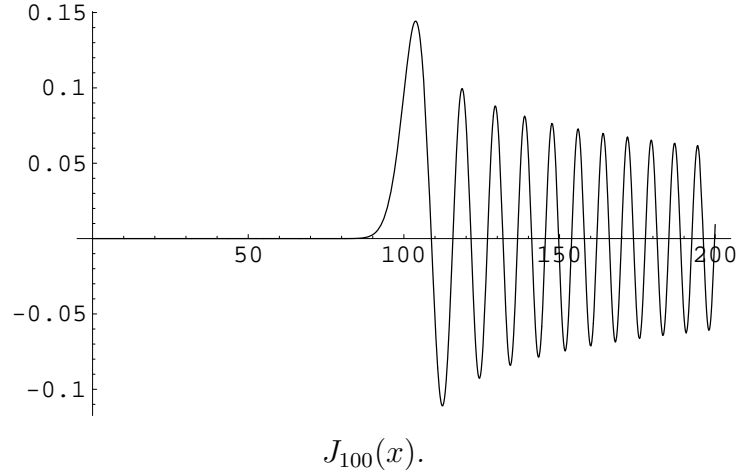
The eigenvalues are $E = \hbar^2 k^2 / 2m$. The quantity $L = \hbar l$ is the angular momentum of the Schrödinger particle about the origin. If we impose rigid-wall boundary conditions that $\psi_{k,l}(r, \theta)$ vanish on the circle $r = R$, then the allowed k form a discrete set $k_{l,n}$, where $J_l(k_{l,n}R) = 0$. To find the energy eigenvalues we therefore need to know the location of the zeros of $J_l(x)$. There is no closed form equation for these numbers, but they are tabulated. The zeros for $kR \gg l$ are also approximated by the zeros of the asymptotic expression

$$J_l(kR) \sim \sqrt{\frac{2}{\pi kR}} \cos(kR - \frac{1}{2}l\pi - \frac{1}{4}\pi), \quad (8.100)$$

which are located at

$$k_{l,n}R = \frac{1}{2}l\pi + \frac{1}{4}\pi + (2n+1)\frac{\pi}{2}. \quad (8.101)$$

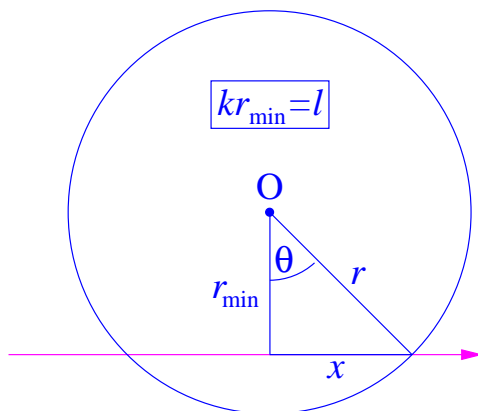
If we let $R \rightarrow \infty$, then the spectrum becomes continuous and we are describing unconfined scattering states. Since the particles are free, their classical motion is in a straight line at constant velocity. A classical particle making a closest approach at a distance r_{\min} , has angular momentum $L = pr_{\min}$. Since $p = \hbar k$ is the particle's linear momentum, we have $l = kr_{\min}$. Because the classical particle is never closer than r_{\min} , the quantum mechanical wavefunction representing such a particle will become evanescent (*i.e.* tend rapidly to zero) as soon as r is smaller than r_{\min} . We therefore expect that $J_l(kr) \approx 0$ if $kr < l$. This effect is dramatically illustrated by the following *Mathematica*TM plot.



Improved asymptotic expressions, which give a better estimate of the $J_l(kr)$ zeros, are the approximations

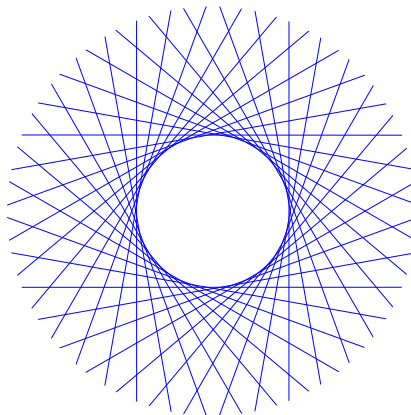
$$\begin{aligned} J_l(kr) &\approx \sqrt{\frac{2}{\pi kx}} \cos(kx - l\theta - \pi/4), \quad r \gg r_{\min}, \\ N_l(kr) &\approx \sqrt{\frac{2}{\pi kx}} \sin(kx - l\theta - \pi/4), \quad r \gg r_{\min}. \end{aligned} \quad (8.102)$$

Here $\theta = \cos^{-1}(r_{\min}/r)$ and $x = r \sin \theta$ are functions of r . They have a geometric interpretation in the right-angled triangle

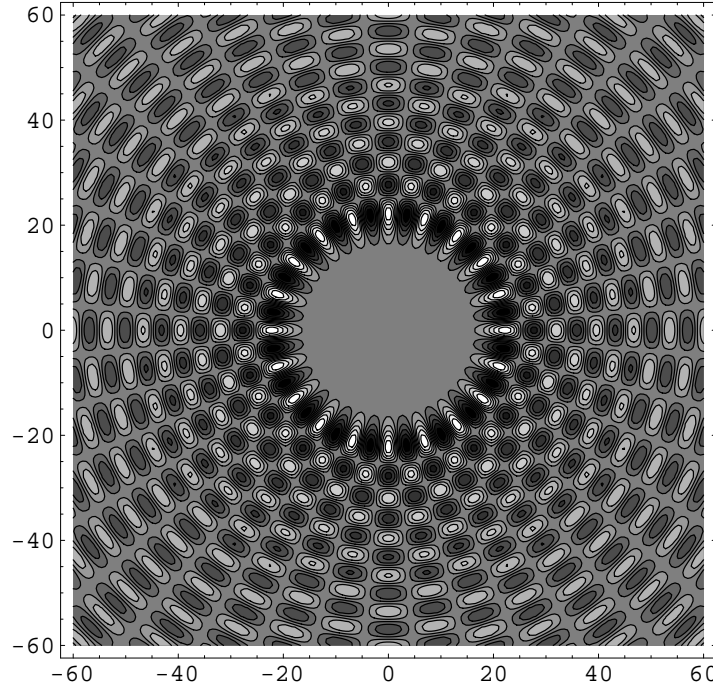


The parameter x has the physical interpretation of being the distance, measured from the point of closest approach to the origin, along the straight-line classical trajectory. The approximation is quite accurate once r exceeds r_{\min} by more than a few percent.

The asymptotic $r^{-1/2}$ fall-off of the Bessel function is also understandable in the semiclassical picture.



A collection of trajectories, each missing the origin by r_{\min} , leaves a “hole”.



The hole is visible in the real part of $\psi_{k,20}(r\theta) = e^{i20\theta} J_{20}(kr)$

By the uncertainty principle, a particle with definite angular momentum must have completely uncertain angular position. The wavefunction $J_l(kr)e^{il\theta}$ therefore represents a coherent superposition of beams of particles approaching from all directions, but all missing the origin by the same distance. The density of classical particle trajectories is infinite at $r = r_{\min}$, forming a caustic. By “conservation of lines”, the particle density falls off as $1/r$ as we move outwards. The particle density is proportional to $|\psi|^2$, so ψ itself decreases as $r^{-1/2}$. In contrast to the classical particle density, the quantum mechanical wavefunction amplitude remains finite at the caustic — the “geometric optics” infinity being tempered by diffraction effects.

Exercise 8.3: Recall that the WKB (Wentzel-Kramers-Brillouin) approximation to a solution of the Schrödinger equation

$$-\frac{d^2\psi}{dx^2} + V(x)\psi(x) = E\psi(x)$$

sets

$$\psi(x) \approx \frac{1}{\sqrt{\kappa(x)}} \exp \left\{ \pm i \int_a^x \kappa(\xi) d\xi \right\}$$

where $\kappa(x) = \sqrt{E - V(x)}$, and a is some conveniently chosen constant. This formula is valid in classically allowed regions, where κ is real, and away from “turning points” where κ goes to zero. In a classically forbidden region, where κ is imaginary, the solutions should decay exponentially. The *connection rule* that matches the standing wave in the classically allowed region onto the decaying solution is

$$\frac{1}{2\sqrt{|\kappa(x)|}} \exp \left\{ - \left| \int_a^x \kappa(\xi) d\xi \right| \right\} \rightarrow \frac{1}{\sqrt{\kappa(x)}} \cos \left\{ \left| \int_a^x \kappa(\xi) d\xi \right| - \frac{\pi}{4} \right\},$$

where a is the classical turning point. (The connection is safely made only in the direction of the arrow. This because a small error in the phase of the cosine will introduce a small admixture of the growing solution, which will eventually swamp the decaying solution.)

Show that setting $y(r) = r^{-1/2}\psi(r)$ in Bessel’s equation

$$-\frac{d^2y}{dr^2} - \frac{1}{r} \frac{dy}{dr} + \frac{l^2y}{r^2} = k^2y$$

reduces it to Schrödinger form

$$-\frac{d^2\psi}{dr^2} + \frac{(l^2 - 1/4)}{r^2}\psi = k^2\psi.$$

From this show that a WKB approximation to $y(r)$ is

$$\begin{aligned} y(r) &\approx \frac{1}{(r^2 - b^2)^{1/4}} \exp \left\{ \pm ik \int_b^r \frac{\sqrt{\rho^2 - b^2}}{\rho} d\rho \right\}, \quad r \gg b \\ &= \frac{1}{\sqrt{x(r)}} \exp \{ \pm i[kx(r) - l\theta(r)] \}, \end{aligned}$$

where $kb = \sqrt{l^2 - 1/4} \approx l$, and $x(r)$ and $\theta(r)$ were defined in connection with (8.102). Deduce that the expressions (8.102) are WKB approximations and are therefore accurate once we are away from the classical turning point at $r = b \equiv r_{\min}$

8.3.2 Orthogonality and Completeness

We can write the equation obeyed by $J_n(kr)$ in Sturm-Liouville form. We have

$$\frac{1}{r} \frac{d}{dr} \left(r \frac{dy}{dr} \right) + \left(k^2 - \frac{m^2}{r^2} \right) y = 0. \quad (8.103)$$

Comparison with the standard Sturm-Liouville equation shows that the weight function, $w(r)$, is r , and the eigenvalues are k^2 .

From Lagrange's identity we obtain

$$(k_1^2 - k_2^2) \int_0^R J_m(k_1 r) J_m(k_2 r) r dr = R [k_2 J_m(k_1 R) J'_m(k_2 R) - k_1 J_m(k_2 R) J'_m(k_1 R)]. \quad (8.104)$$

We have no contribution from the origin on the right-hand side because all J_m Bessel functions except J_0 vanish there, whilst $J'_0(0) = 0$. For each m we get a set of orthogonal functions, $J_m(k_n x)$, provided the $k_n R$ are chosen to be roots of $J_m(k_n R) = 0$ or $J'_m(k_n R) = 0$.

We can find the normalization constants by differentiating (8.104) with respect to k_1 and then setting $k_1 = k_2$ in the result. We find

$$\begin{aligned} \int_0^R [J_m(kr)]^2 r dr &= \frac{1}{2} R^2 \left[[J'_m(kR)]^2 + \left(1 - \frac{m^2}{k^2 R^2}\right) [J_m(kR)]^2 \right], \\ &= \frac{1}{2} R^2 [J_n(kR)]^2 - J_{n-1}(kR) J_{n+1}(kR). \end{aligned} \quad (8.105)$$

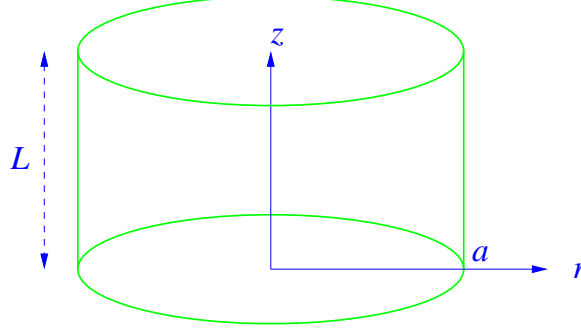
(The second equality follows on applying the recurrence relations for the $J_n(kr)$, and provides an expression that is perhaps easier to remember.) For Dirichlet boundary conditions we will require $k_n R$ to be zero of J_m , and so we have

$$\int_0^R [J_m(kr)]^2 r dr = \frac{1}{2} R^2 [J'_m(kR)]^2. \quad (8.106)$$

For Neumann boundary conditions we require $k_n R$ to be a zero of J'_m . In this case

$$\int_0^R [J_m(kr)]^2 r dr = \frac{1}{2} R^2 \left(1 - \frac{m^2}{k^2 R^2}\right) [J_m(kR)]^2. \quad (8.107)$$

Example: Harmonic function in cylinder.



We wish to solve $\nabla^2 V = 0$ within a cylinder of height L and radius a . The voltage is prescribed on the upper surface of the cylinder: $V(r, \theta, L) = U(r, \theta)$. We are told that $V = 0$ on all other parts of boundary.

The general solution of Laplace's equation in will be sum of terms such as

$$\left\{ \begin{array}{c} \sinh(kz) \\ \cosh(kz) \end{array} \right\} \times \left\{ \begin{array}{c} J_m(kr) \\ N_m(kr) \end{array} \right\} \times \left\{ \begin{array}{c} \sin(m\theta) \\ \cos(m\theta) \end{array} \right\}, \quad (8.108)$$

where the braces indicate a choice of upper or lower functions. We must take only the $\sinh(kz)$ terms because we know that $V = 0$ at $z = 0$, and only the $J_m(kr)$ terms because V is finite at $r = 0$. The k 's are also restricted by the boundary condition on the sides of the cylinder to be such that $J_m(ka) = 0$. We therefore expand the prescribed voltage as

$$U(r, \theta) = \sum_{m,n} \sinh(k_{nm}L) J_m(k_{nm}r) [A_{nm} \sin(m\theta) + B_{nm} \cos(m\theta)], \quad (8.109)$$

and use the orthonormality of the trigonometric and Bessel function to find the coefficients to be

$$A_{nm} = \frac{2 \operatorname{cosech}(k_{nm}L)}{\pi a^2 [J'_m(k_{nm}a)]^2} \int_0^{2\pi} d\theta \int_0^a U(r, \theta) J_m(k_{nm}r) \sin(m\theta) r dr, \quad (8.110)$$

$$B_{nm} = \frac{2 \operatorname{cosech}(k_{nm}L)}{\pi a^2 [J'_m(k_{nm}a)]^2} \int_0^{2\pi} d\theta \int_0^a U(r, \theta) J_m(k_{nm}r) \cos(m\theta) r dr, \quad m \neq 0, \quad (8.111)$$

and

$$B_{n0} = \frac{1}{2} \frac{2 \operatorname{cosech}(k_{n0}L)}{\pi a^2 [J'_0(k_{n0}a)]^2} \int_0^{2\pi} d\theta \int_0^a U(r, \theta) J_0(k_{n0}r) r dr. \quad (8.112)$$

Then we fit the boundary data expansion to the general solution, and so find

$$V(r, \theta, z) = \sum_{m,n} \sinh(k_{nm}z) J_m(k_{nm}r) [A_{nm} \sin(m\theta) + B_{nm} \cos(m\theta)]. \quad (8.113)$$

Hankel Transforms

When the radius, R , of the region in which we performing our eigenfunction expansion becomes infinite, the eigenvalue spectrum will become continuous, and the sum over the discrete k_n Bessel-function zeros must be replaced by an integral over k . By using the asymptotic approximation

$$J_n(kR) \sim \sqrt{\frac{2}{\pi kR}} \cos(kR - \frac{1}{2}n\pi - \frac{1}{4}\pi), \quad (8.114)$$

we may estimate the normalization integral as

$$\int_0^R [J_m(kr)]^2 r dr \sim \frac{R}{\pi k} + O(1). \quad (8.115)$$

We also find that the asymptotic density of Bessel zeros is

$$\frac{dn}{dk} = \frac{R}{\pi}. \quad (8.116)$$

Putting these two results together shows that the continuous-spectrum orthogonality and completeness relations are

$$\int_0^\infty J_n(kr) J_n(k'r) r dr = \frac{1}{k} \delta(k - k'), \quad (8.117)$$

$$\int_0^\infty J_n(kr) J_n(kr') k dk = \frac{1}{r} \delta(r - r'), \quad (8.118)$$

respectively. These two equations establish that the *Hankel transform* (also called the *Fourier-Bessel transform*) of a function $f(r)$, which is defined by

$$F(k) = \int_0^\infty J_n(kr) f(r) r dr, \quad (8.119)$$

has as its inverse

$$f(r) = \int_0^\infty J_n(kr) F(k) k dk. \quad (8.120)$$

Some Hankel transform pairs:

$$\begin{aligned}\int_0^\infty e^{-ar} J_0(kr) dr &= \frac{1}{\sqrt{k^2 + a^2}}, \\ \int_0^\infty \frac{J_0(kr)}{\sqrt{k^2 + a^2}} k dk &= \frac{e^{-ar}}{r}.\end{aligned}\tag{8.121}$$

$$\begin{aligned}\int_0^\infty \cos(ar) J_0(kr) dr &= \begin{cases} 1/\sqrt{k^2 - a^2}, & k > a, \\ 0, & k < a. \end{cases} \\ \int_a^\infty \frac{J_0(kr)}{\sqrt{k^2 - a^2}} k dk &= \frac{1}{r} \cos(ar).\end{aligned}\tag{8.122}$$

$$\begin{aligned}\int_0^\infty \sin(ar) J_0(kr) dr &= \begin{cases} 1/\sqrt{a^2 - k^2}, & k < a, \\ 0, & k > a. \end{cases} \\ \int_0^a \frac{J_0(kr)}{\sqrt{a^2 - k^2}} k dk &= \frac{1}{r} \sin(ar).\end{aligned}\tag{8.123}$$

8.3.3 Modified Bessel Functions

The Bessel function $J_n(kr)$ and the Neumann $N_n(kr)$ function oscillate at large distance, provided that k is real. When k is purely imaginary, it is convenient to combine them so as to have functions that grow or decay exponentially. These are the *modified Bessel functions*.

We define

$$I_\nu(x) = i^{-\nu} J_\nu(ix),\tag{8.124}$$

$$K_\nu(x) = \frac{\pi}{2 \sin \nu \pi} [I_{-\nu}(x) - I_\nu(x)].\tag{8.125}$$

The factor of $i^{-\nu}$ in the definition of $I_\nu(x)$ is inserted to make I_ν real. Our definition of $K_\nu(x)$ is that in Abramowitz and Stegun's *Handbook of Mathematical Functions*. It differs from that of Whittaker and Watson, who divide by $\tan \nu \pi$ instead of $\sin \nu \pi$.

At short distance

$$I_\nu(x) = \left(\frac{x}{2}\right)^\nu \frac{1}{\Gamma(\nu + 1)} + \dots,\tag{8.126}$$

$$K_\nu(x) = \frac{1}{2} \Gamma(\nu) \left(\frac{x}{2}\right)^{-\nu} + \dots.\tag{8.127}$$

When ν becomes an integer we must take limits, and in particular

$$I_0(x) = 1 + \frac{1}{4}x^2 + \cdots, \quad (8.128)$$

$$K_0(x) = -(\ln x/2 + \gamma) + \cdots. \quad (8.129)$$

The large x asymptotic behaviour is

$$I_\nu(x) \sim \frac{1}{\sqrt{2\pi x}} e^x, \quad x \rightarrow \infty, \quad (8.130)$$

$$K_\nu(x) \sim \frac{\pi}{\sqrt{2x}} e^{-x}, \quad x \rightarrow \infty. \quad (8.131)$$

From the expression for $J_n(x)$ as an integral, we have

$$I_n(x) = \frac{1}{2\pi} \int_0^{2\pi} e^{in\theta} e^{x \cos \theta} d\theta = \frac{1}{\pi} \int_0^\pi \cos(n\theta) e^{x \cos \theta} d\theta \quad (8.132)$$

for integer n . When n is not an integer we still have an expression for $I_\nu(x)$ as an integral, but now it is

$$I_\nu(x) = \frac{1}{\pi} \int_0^\pi \cos(\nu\theta) e^{x \cos \theta} d\theta - \frac{\sin \nu\pi}{\pi} \int_0^\infty e^{-x \cosh t - \nu t} dt. \quad (8.133)$$

Here we need $|\arg x| < \pi/2$ for the second integral to converge. The origin of the “extra” infinite integral must remain a mystery until we learn how to use complex integral methods for solving differential equations. From the definition of $K_\nu(x)$ in terms of I_ν we find

$$K_\nu(x) = \int_0^\infty e^{-x \cosh t} \cosh(\nu t) dt, \quad |\arg x| < \pi/2. \quad (8.134)$$

Physics Illustration: Light propagation in optical fibres. Consider the propagation of light of frequency ω_0 down a straight section of optical fibre. Typical fibres are made of two materials. An outer layer, or *cladding*, with refractive index n_2 , and an inner *core* with refractive index $n_1 > n_2$. The core of a fibre used for communication is usually less than $10\mu\text{m}$ in diameter.

We will treat the light field E as a scalar. This is not a particularly good approximation for real fibres, but the complications due to the vector character of the electromagnetic field are considerable. We suppose that E obeys

$$\frac{\partial^2 E}{\partial x^2} + \frac{\partial^2 E}{\partial y^2} + \frac{\partial^2 E}{\partial z^2} - \frac{n^2(x, y)}{c^2} \frac{\partial^2 E}{\partial t^2} = 0. \quad (8.135)$$

Here $n(x, y)$ is the refractive index of the fibre, which is assumed to lie along the z axis. We set

$$E(x, y, z, t) = \psi(x, y, z)e^{ik_0z - i\omega_0t} \quad (8.136)$$

where $k_0 = \omega_0/c$. The amplitude ψ is a (relatively) slowly varying envelope function. Plugging into the wave equation we find that

$$\frac{\partial^2 \psi}{\partial x^2} + \frac{\partial^2 \psi}{\partial y^2} + \frac{\partial^2 \psi}{\partial z^2} + 2ik_0 \frac{\partial \psi}{\partial z} + \left(\frac{n^2(x, y)}{c^2} \omega_0^2 - k_0^2 \right) \psi = 0. \quad (8.137)$$

Because ψ is slowly varying, we neglect the second derivative of ψ with respect to z , and this becomes

$$2ik_0 \frac{\partial \psi}{\partial z} = - \left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} \right) \psi + k_0^2 (1 - n^2(x, y)) \psi, \quad (8.138)$$

which is the two-dimensional time-dependent Schrödinger equation, but with t replaced by $z/2k_0$, where z is the distance down the fibre. The wave-modes that will be trapped and guided by the fibre will be those corresponding to bound states of the axisymmetric potential

$$V(x, y) = k_0^2(1 - n^2(r)). \quad (8.139)$$

If these bound states have (negative) “energy” E_n , then $\psi \propto e^{-iE_n z/2k_0}$, and so the actual wavenumber for frequency ω_0 is

$$k = k_0 - E_n/2k_0. \quad (8.140)$$

In order to have a unique propagation velocity for signals on the fibre, it is therefore necessary that the potential support one, and only one, bound state.

If

$$\begin{aligned} n(r) &= n_1, & r < a, \\ &= n_2, & r > a, \end{aligned} \quad (8.141)$$

then the bound state solutions will be of the form

$$\psi(r, \theta) = \begin{cases} e^{in\theta} e^{i\beta z} J_n(\kappa r), & r < a, \\ Ae^{in\theta} e^{i\beta z} K_n(\gamma r), & r > a, \end{cases} \quad (8.142)$$

where

$$\kappa^2 = (n_1^2 k_0^2 - \beta^2), \quad (8.143)$$

$$\gamma^2 = (\beta^2 - n_2^2 k_0^2). \quad (8.144)$$

To ensure that we have a solution decaying away from the core, we need β to be such that both κ and γ are real. We therefore require

$$n_1^2 > \frac{\beta^2}{k_0^2} > n_2^2. \quad (8.145)$$

At the interface both ψ and its radial derivative must be continuous, and so we will have a solution only if β is such that

$$\kappa \frac{J'_n(\kappa a)}{J_n(\kappa a)} = \gamma \frac{K'_n(\gamma a)}{K_n(\gamma a)}.$$

This Shrödinger approximation to the wave equation has other applications. It is called the *paraxial approximation*.

8.3.4 Spherical Bessel Functions

Consider the wave equation

$$\left(\nabla^2 - \frac{1}{c^2} \frac{\partial^2}{\partial t^2} \right) \varphi(r, \theta, \phi, t) = 0 \quad (8.146)$$

in spherical polar coordinates. To apply separation of variables, we set

$$\varphi = e^{i\omega t} Y_l^m(\theta, \phi) \chi(r), \quad (8.147)$$

and find that

$$\frac{d^2 \chi}{dr^2} + \frac{2}{r} \frac{d\chi}{dr} - \frac{l(l+1)}{r^2} \chi + \frac{\omega^2}{c^2} \chi = 0. \quad (8.148)$$

Substitute $\chi = r^{-1/2} R(r)$ and we have

$$\frac{d^2 R}{dr^2} + \frac{1}{r} \frac{dR}{dr} + \left(\frac{\omega^2}{c^2} - \frac{(l + \frac{1}{2})^2}{r^2} \right) R = 0. \quad (8.149)$$

This is Bessel's equation with $\nu^2 \rightarrow (l + \frac{1}{2})^2$. Therefore the general solution is

$$R = A J_{l+\frac{1}{2}}(kr) + B J_{-l-\frac{1}{2}}(kr), \quad (8.150)$$

where $k = |\omega|/c$. Now inspection of the series definition of the J_ν reveals that

$$J_{\frac{1}{2}}(x) = \sqrt{\frac{2}{\pi x}} \sin x, \quad (8.151)$$

$$J_{-\frac{1}{2}}(x) = \sqrt{\frac{2}{\pi x}} \cos x, \quad (8.152)$$

so these Bessel functions are actually elementary functions. This is true of all Bessel functions of half-integer order, $\nu = \pm 1/2, \pm 3/2, \dots$. We define the *spherical Bessel functions* by²

$$j_l(x) = \sqrt{\frac{\pi}{2x}} J_{l+\frac{1}{2}}(x), \quad (8.153)$$

$$n_l(x) = (-1)^{l+1} \sqrt{\frac{\pi}{2x}} J_{-(l+\frac{1}{2})}(x). \quad (8.154)$$

The first few are

$$\begin{aligned} j_0(x) &= \frac{1}{x} \sin x, \\ j_1(x) &= \frac{1}{x^2} \sin x - \frac{1}{x} \cos x, \\ j_2(x) &= \left(\frac{3}{x^3} - \frac{1}{x} \right) \sin x - \frac{3}{x^2} \cos x, \\ n_0(x) &= -\frac{1}{x} \cos x, \\ n_1(x) &= -\frac{1}{x^2} \cos x - \frac{1}{x} \sin x, \\ n_2(x) &= -\left(\frac{3}{x^3} - \frac{1}{x} \right) \cos x - \frac{3}{x^2} \sin x. \end{aligned}$$

Despite the appearance of negative powers of x , the $j_l(x)$ are all finite at $x = 0$. The $n_l(x)$ all diverge to $-\infty$ as $x \rightarrow 0$. In general

$$j_l(x) = f_l(x) \sin x + g_l(x) \cos(x), \quad (8.155)$$

$$n_l(x) = -f_l(x) \cos(x) + g_l(x) \sin x, \quad (8.156)$$

²We are using the definitions from Schiff's *Quantum Mechanics*.

where $f_l(x)$ and $g_l(x)$ are polynomials in $1/x$.

We also define the spherical Hankel functions by

$$h_l^{(1)}(x) = j_l(x) + in_l(x), \quad (8.157)$$

$$h_l^{(2)}(x) = j_l(x) - in_l(x). \quad (8.158)$$

These behave like

$$h_l^{(1)}(x) \sim \frac{1}{x} e^{i(x-[l+1]\pi/2)}, \quad (8.159)$$

$$h_l^{(2)}(x) \sim \frac{1}{x} e^{-i(x-[l+1]\pi/2)}, \quad (8.160)$$

at large x .

The solution to the wave equation regular at the origin is therefore a sum of terms such as

$$\varphi_{k,l,m}(r, \theta, \phi, t) = j_l(kr) Y_l^m(\theta, \phi) e^{-i\omega t}, \quad (8.161)$$

where $\omega = \pm ck$, with $k > 0$. For example, the plane wave e^{ikz} has expansion

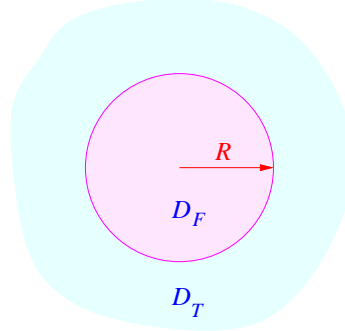
$$e^{ikz} = e^{ikr \cos \theta} = \sum_{l=0}^{\infty} (2l+1) i^l j_l(kr) P_l(\cos \theta), \quad (8.162)$$

or equivalently, using (8.66),

$$e^{i\mathbf{k} \cdot \mathbf{r}} = 4\pi \sum_{l=0}^{\infty} \sum_{m=-l}^l i^l j_l(kr) \left[Y_l^m(\hat{\mathbf{k}}) \right]^* Y_l^m(\hat{\mathbf{r}}) \quad (8.163)$$

where $\hat{\mathbf{k}}$, $\hat{\mathbf{r}}$, unit vectors in the direction of \mathbf{k} and \mathbf{r} respectively, are used as a shorthand notation to indicate the angles that should be inserted into the spherical harmonics. This angular-momentum-adapted expansion of a plane wave provides a useful tool in scattering theory.

Exercise 8.4: Peierl's Problem. Critical Mass. The core of a nuclear device consists of a sphere of fissile ^{235}U of radius R . It is surrounded by a thick shell of non-fissile material which acts as a neutron reflector, or *tamper*.



Fission core.

In the core, the fast neutron density $n(\mathbf{r}, t)$ obeys

$$\frac{\partial n}{\partial t} = \nu n + D_F \nabla^2 n. \quad (8.164)$$

Here the term with ν accounts for the production of additional neutrons due to induced fission. The term with D_F describes the diffusion of the fast neutrons. In the tamper the neutron flux obeys

$$\frac{\partial n}{\partial t} = D_T \nabla^2 n. \quad (8.165)$$

Both the neutron density n and flux $\mathbf{j} \equiv D_{F,T} \nabla n$, are continuous across the interface between the two materials. Find an equation determining the critical radius R_c above which the neutron density grows without bound. Show that the critical radius for an assembly with a tamper consisting of ^{238}U ($D_T = D_F$) is one-half of that for a core surrounded only by air ($D_T = \infty$), and so the use of a thick ^{238}U tamper reduces the critical mass by a factor of eight.

Factorization and Recurrence

The equation obeyed by the spherical Bessel function is

$$-\frac{d^2 \chi_l}{dx^2} - \frac{2}{x} \frac{d\chi_l}{dx} + \frac{l(l+1)}{x^2} \chi_l = k^2 \chi_l, \quad (8.166)$$

or, in Sturm-Liouville form,

$$-\frac{1}{x^2} \frac{d}{dx} \left(x^2 \frac{d\chi_l}{dx} \right) + \frac{l(l+1)}{x^2} \chi_l = k^2 \chi_l. \quad (8.167)$$

The corresponding differential operator is formally self-adjoint with respect to the inner product

$$\langle f, g \rangle = \int (f^* g) x^2 dx. \quad (8.168)$$

Now, the operator

$$D_l = -\frac{d^2}{dx^2} - \frac{2}{x} \frac{d}{dx} + \frac{l(l+1)}{x^2} \quad (8.169)$$

factorizes as

$$D_l = \left(-\frac{d}{dx} + \frac{l-1}{x} \right) \left(\frac{d}{dx} + \frac{l+1}{x} \right), \quad (8.170)$$

or as

$$D_l = \left(\frac{d}{dx} + \frac{l+2}{x} \right) \left(-\frac{d}{dx} + \frac{l}{x} \right). \quad (8.171)$$

Since, with respect to the $w = x^2$ inner product, we have

$$\left(\frac{d}{dx} \right)^\dagger = -\frac{1}{x^2} \frac{d}{dx} x^2 = -\frac{d}{dx} - \frac{2}{x}, \quad (8.172)$$

we can write

$$D_l = A_l^\dagger A_l = A_{l+1} A_{l+1}^\dagger, \quad (8.173)$$

where

$$A_l = \left(\frac{d}{dx} + \frac{l+1}{x} \right). \quad (8.174)$$

From this we can deduce

$$A_l j_l \propto j_{l-1}, \quad (8.175)$$

$$A_{l+1}^\dagger j_l \propto j_{l+1}. \quad (8.176)$$

The constants of proportionality are in each case unity. The same recurrence formulæ hold for the spherical Neumann functions n_l .

8.4 Singular Endpoints

In this section we will exploit our knowledge of the Laplace eigenfunctions in spherical and plane polar coordinates to illustrate Weyl's theory of self-adjoint boundary conditions at singular endpoints. We also connect Weyl's theory with concepts from scattering theory.

8.4.1 Weyl's Theorem

Consider the Sturm-Liouville eigenvalue problem

$$Ly \equiv -\frac{1}{w}[p(r)y']' + q(r)y = \lambda y \quad (8.177)$$

on the interval $[0, R]$. Here $p(r)$, $q(r)$ and $w(r)$ are all supposed real, so the equation is formally self-adjoint with respect to the inner product

$$\langle u, v \rangle_w = \int_0^R w u^* v dr. \quad (8.178)$$

If $r = 0$ is a singular point of (8.177), then we will be unable to impose boundary conditions of our accustomed form

$$ay(0) + by'(0) = 0 \quad (8.179)$$

because one or both of the linearly independent solutions $y_1(r)$ and $y_2(r)$ will diverge as $r \rightarrow 0$. The range of possibilities was enumerated by Weyl: *Theorem (Hermann Weyl, 1910): Suppose that $r = 0$ is a singular point and $r = R$ a regular point of the differential equation (8.177). Then*

I. Either:

- a) **Limit-circle case:** *There exists a λ_0 such that both of the linearly independent solutions to (8.177) have a w norm that is convergent in the vicinity of $r = 0$. In this case both solutions have convergent w norm for **all** values of λ .*

Or

- b) **limit-point case :** *No more than one solution has convergent w norm for any λ .*

II. In either case, whenever $\text{Im } \lambda \neq 0$, there is at least one finite-norm solution. When λ lies on the real axis there may or may not exist a finite norm solution.

We will not attempt to prove Weyl's theorem. The proof is not difficult and may be found in many standard texts³. It is just a little more technical than the level of this book. We will instead illustrate it with enough examples to make the result plausible, and its practical consequences clear.

³For example: Ivar Stackgold *Boundary Value Problems of Mathematical Physics*, Volume I (SIAM 2000).

When we come to construct the resolvent $R_\lambda(r, r')$ obeying

$$(L - \lambda I)R_\lambda(r, r') = \delta(r - r') \quad (8.180)$$

by writing it is a product of $y_<$ and $y_>$ we are obliged to choose a normalizable function for $y_<$, the solution obeying the boundary condition at $r = 0$. We must do this so that the range of R_λ will be in $L^2[0, R]$. In the limit-point case, and when $\text{Im } \lambda \neq 0$, there is only one choice for $y_<$. There is therefore a unique resolvent, a unique self-adjoint operator $L - \lambda I$ of which R_λ is the inverse, and hence L is a uniquely specified differential operator⁴.

In the limit-circle case there is more than one choice for $y_<$ and hence more than one way of making L into a self-adjoint operator. To what boundary conditions do these choices correspond?

Suppose that the two normalizable solutions for $\lambda = \lambda_0$ are $y_1(r)$ and $y_2(r)$. The essence of Weyl's theorem is that once we are sufficiently close to $r = 0$ the exact value of λ is unimportant and all solutions behave as a linear combination of these two. We can therefore impose as a boundary condition that the allowed solutions be proportional to a specified real linear combination

$$y(r) \propto ay_1(r) + by_2(r), \quad r \rightarrow 0. \quad (8.181)$$

This is a natural generalization of the regular case where we have a solution $y_1(r)$ with boundary conditions $y_1(0) = 1$, $y_1'(0) = 0$, so $y_1(r) \sim 1$, and a solution $y_2(r)$ with $y_2(0) = 0$, $y_2'(0) = 1$, so $y_2(r) \sim r$. The regular self-adjoint boundary condition

$$ay(0) + by'(0) = 0 \quad (8.182)$$

with real a, b then forces $y(r)$ to be

$$y(r) \propto by_1(r) - ay_2(r) \sim b(1 - ar), \quad r \rightarrow 0. \quad (8.183)$$

Example: Consider the radial part of the Laplace eigenvalue problem in two dimensions.

$$L\psi \equiv -\frac{1}{r} \frac{dr}{dr} \left(r \frac{d\psi}{dr} \right) + \frac{m^2}{r^2} \psi = k^2 \psi. \quad (8.184)$$

⁴When λ is on the real axis then there may be no normalizable solution, and R_λ cannot exist. This will occur only when λ is in the continuous spectrum of the operator L , and is not a problem as the same operator L is obtained for any λ .

The differential operator L is formally self-adjoint with respect to the inner product

$$\langle \psi, \chi \rangle = \int_0^R \psi^* \chi r dr. \quad (8.185)$$

When $k^2 = 0$, the $m^2 \neq 0$ equation has solutions $\psi = r^{\pm m}$, and, of the normalization integrals

$$\int_0^R |r^m|^2 r dr, \quad \int_0^R |r^{-m}|^2 r dr, \quad (8.186)$$

only the first, containing the positive power of r , is convergent. For $m \neq 0$ we are therefore in Weyl's *limit-point* case. For $m^2 = 0$, however, the $k^2 = 0$ solutions are $\psi_1(r) = 1$ and $\psi_2(r) = \ln r$. Both normalization integrals

$$\int_0^R 1^2 r dr, \quad \int_0^R |\ln r|^2 r dr \quad (8.187)$$

converge and we are in the *limit-circle* case at $r = 0$. When $k^2 > 0$ these solutions become

$$\begin{aligned} J_0(kr) &= 1 - \frac{1}{4}(kr)^2 + \dots \\ N_0(kr) &= \left(\frac{2}{\pi}\right) [\ln(kr/2) + \gamma] + \dots \end{aligned} \quad (8.188)$$

Both remain normalizable, in conformity with Weyl's theorem. The self-adjoint boundary conditions at $r \rightarrow 0$ are therefore that near $r = 0$ the allowed functions become proportional to

$$1 + \alpha \ln r \quad (8.189)$$

with α some specified real constant.

Example: Consider the radial equation that arises when we separate the Laplace eigenvalue problem in spherical polar coordinates.

$$-\frac{1}{r^2} \left(\frac{d}{dr} r^2 \frac{d\psi}{dr} \right) + \frac{l(l+1)}{r^2} \psi = k^2 \psi. \quad (8.190)$$

When $k = 0$ this has solutions $\psi = r^l, r^{-l-1}$. For non-zero l only the first of the normalization integrals

$$\int_0^R r^{2l} r^2 dr, \quad \int_0^R r^{-2l-2} r^2 dr, \quad (8.191)$$

is finite. Thus, for $l \neq 0$, we are again in the limit-point case, and the boundary condition at the origin is uniquely determined by the requirement that the solution be normalizable.

When $l = 0$, however, the two $k^2 = 0$ solutions are $\psi_1(r) = 1$ and $\psi_2(r) = 1/r$. Both integrals

$$\int_0^R r^2 dr, \quad \int_0^R r^{-2} r^2 dr \quad (8.192)$$

converge, so we are again in the limit-circle case. For positive k^2 , these solutions evolve into

$$\psi_{1,k}(r) = j_0(kr) = \frac{\sin kr}{kr}, \quad \psi_{2,k}(r) = -kn_0(kr) = \frac{\cos kr}{r} \quad (8.193)$$

Near $r = 0$, we have $\psi_{1,k} \sim 1$ and $\psi_{2,k} \sim 1/r$, exactly the same behaviour as the $k^2 = 0$ solutions.

We obtain a self-adjoint operator if we choose a constant a_s and demand that all functions in the domain be proportional to

$$\psi(r) \sim 1 - \frac{a_s}{r} \quad (8.194)$$

as we approach $r = 0$. If we write the solution with this boundary condition as

$$\begin{aligned} \psi_k(r) = \frac{\sin(kr + \delta)}{r} &= \cos \delta \left(\frac{\sin(kr)}{r} + \tan \delta \frac{\cos(kr)}{r} \right) \\ &\sim k \cos \delta \left(1 + \frac{\tan \delta}{kr} \right), \end{aligned} \quad (8.195)$$

we can read off the phase shift δ as

$$\tan \delta(k) = -ka_s. \quad (8.196)$$

These boundary conditions arise in quantum mechanics when we study the scattering of particles whose de Broglie wavelength is much larger than the range of the scattering potential. The incident wave is unable to resolve any of the internal structure of the potential and perceives its effect only as a singular boundary condition at the origin. In this context the constant a_s is called the *scattering length*. This physical model explains why only the $l = 0$

partial waves have a choice of boundary condition: classical particles with angular momentum $l \neq 0$ would miss the origin by a distance $r_{\min} = l/k$ and never see the potential.

The quantum picture also helps explain the physical origin of the distinction between the limit-point and limit-circle cases. A point potential can have a bound state that extends far beyond the short range of the potential. If the corresponding eigenfunction is normalizable, the bound particle has a significant amplitude to be found at non-zero r , and this amplitude must be included in the completeness relation and in the eigenfunction expansion of the Green function. When the state is not normalizable, however, the particle spends all its time very close to the potential, and its eigenfunction makes zero contribution to the Green function and completeness sum at any non-zero r . Any admixture of this non-normalizable state allowed by the boundary conditions can therefore be ignored, and, as far as the external world is concerned, all boundary conditions look alike. The next few exercises will illustrate this.

Exercise 8.5: The two-dimensional delta-function potential. Consider the quantum mechanical problem in \mathbb{R}^2

$$(-\nabla^2 + V(|\mathbf{r}|)) \psi = E\psi$$

with V an attractive circular square well.

$$V(r) = \begin{cases} -\lambda/\pi a^2, & r < a \\ 0, & r > a. \end{cases}$$

The factor of πa^2 has been inserted to make this a regulated version of $V(\mathbf{r}) = -\lambda \delta^2(\mathbf{r})$. Let $\mu = \sqrt{\lambda/\pi a^2}$.

i) By matching the functions

$$\psi(r) \propto \begin{cases} J_0(\mu r), & r < a \\ K_0(\kappa r), & r > a, \end{cases}$$

at $r = a$, show that in the limit $a \rightarrow 0$, we can scale $\lambda \rightarrow \infty$ in such a way that there remains a single bound state with binding energy

$$E_0 \equiv \kappa^2 = \frac{4}{a^2} e^{-2\gamma} e^{-4\pi/\lambda}.$$

- ii) Show that the associated wavefunction obeys

$$\psi(r) \rightarrow 1 + \alpha \ln r, \quad r \rightarrow 0$$

where

$$\alpha = \frac{1}{\gamma + \ln \kappa/2}.$$

Observe that this α can be any real number, and so the entire range of possible boundary conditions may be obtained by specifying the binding energy of an attractive potential.

- iii) Assume that we have fixed the boundary conditions by specifying κ , and consider the scattering of unbound particles off the short-range potential. It is natural to define the phase shift $\delta(k)$ so that

$$\begin{aligned} \psi_k(r) &= \cos \delta J_0(kr) - \sin \delta N_0(kr) \\ &\sim \sqrt{\frac{2}{\pi kr}} \cos(kr - \pi/4 + \delta), \quad r \rightarrow \infty. \end{aligned}$$

Show that

$$\cot \delta = \left(\frac{2}{\pi} \right) \ln k/\kappa.$$

Exercise 8.6: The three-dimensional delta-function potential. Repeat the calculation of the previous exercise for the case of a three-dimensional delta-function potential

$$V(r) = \begin{cases} -\lambda/(4\pi a^3/3), & r < a \\ 0, & r > a. \end{cases}$$

- i) Show that in the limit $a \rightarrow 0$, the delta-function strength λ can be scaled to infinity so that the scattering length

$$a_s = \left(\frac{\lambda}{4\pi a^2} - \frac{1}{a} \right)^{-1}$$

remains finite.

- ii) Show that when this a_s is positive, the attractive potential supports a single bound state with external wavefunction

$$\psi(r) \propto \frac{1}{r} e^{-\kappa r}$$

where $\kappa = a_s^{-1}$.

Exercise 8.7: The pseudo-potential. Consider a particle of mass μ confined in a large sphere of radius R . At the center of the sphere is a singular potential whose effects can be parameterized by its scattering length a_s and the resultant phase shift

$$\delta(k) \approx \tan \delta(k) = -a_s k.$$

In the absence of the potential, the normalized $l = 0$ wavefunctions would be

$$\psi_n(r) = \sqrt{\frac{1}{2\pi R}} \frac{\sin k_n r}{r}$$

where $k_n = n\pi/R$.

- i) Show that the presence of the singular potential perturbs the ψ_n eigenstate so that its energy E_n changes by an amount

$$\Delta E_n = \frac{\hbar^2}{2\mu} \frac{2a_s k_n^2}{R}.$$

- ii) Show this energy shift can be written as if it were the result of applying first-order perturbation theory

$$\Delta E_n \approx \langle n | V_{ps} | n \rangle \equiv \int d^3r |\psi_n|^2 V_{ps}(r)$$

to an artificial *pseudo-potential*

$$V_{ps}(r) = \frac{2\pi a_s \hbar^2}{\mu} \delta^3(r).$$

Although the energy shift is small when R is large, it is not a first-order perturbation effect and the pseudo-potential is a convenient fiction which serves to parameterize the effect of the true potential. Even the sign of the pseudo-potential may differ from that of the actual short distance potential. For our attractive “delta function”, for example, the pseudopotential changes from being attractive to being repulsive as the bound state is peeled off the bottom of the unbound continuum. The change of sign occurs not by a_s passing through zero, but by it passing through infinity. It is difficult to manipulate a single potential so as to see this dramatic effect, but when the particles have spin, and a spin-dependent interaction potential, it is possible to use a magnetic field to arrange for a bound state of one spin configuration to pass through the zero of energy of the other. The resulting *Feshbach resonance* has the same effect on the scattering length as the conceptually simpler *shape resonance* obtained by tuning the single potential.

The pseudo-potential formula is commonly used to describe the pairwise interaction of a dilute gas of particles of mass m , where it reads

$$V_{ps}(r) = \frac{4\pi a_s \hbar^2}{m} \delta^3(r). \quad (8.197)$$

The internal energy-density of the gas due to the two-body interaction then becomes

$$u(\rho) = \frac{1}{2} \frac{4\pi a_s \hbar^2}{m} \rho^2,$$

where ρ is the particle-number density.

The factor of two difference between the formula in the exercise and (8.197) arises because the μ in the exercise must be understood as the *reduced mass* $\mu = m^2/(m + m) = m/2$ of the pair of interacting particles.

Example: In n dimensions, the “ $l = 0$ ” part of the Laplace operator is

$$\frac{d^2}{dr^2} + \frac{(n-1)}{r} \frac{d}{dr}.$$

This formally self adjoint with respect to the natural inner product

$$\langle \psi, \chi \rangle_n = \int_0^\infty r^{n-1} \psi^* \chi dr. \quad (8.198)$$

The zero eigenvalue solutions are $\psi_1(r) = 1$ and $\psi_2(r) = r^{2-n}$. The second of these ceases to be normalizable once $n \geq 4$. In four space dimensions and above, therefore, we are always in the limit-point case. No point interaction — no matter how strong — can affect the physics. This non-interaction result extends, with slight modification, to the quantum field theory of relativistic particles. Here we find that contact interactions become *irrelevant* or *non-renormalizable* in more than four space-time dimensions.

8.5 Exercises and Problems

Here some further problems involving Legendre polynomials, associated Legendre functions and Bessel functions:

Exercise 8.8: A sphere of radius a is made by joining two conducting hemispheres along their equators. The hemispheres are electrically insulated from one another and maintained at two different potentials V_1 and V_2 .

- a) Starting from the general expression

$$V(r, \theta) = \sum_{l=0}^{\infty} \left(a_l r^l + \frac{b_l}{r^{l+1}} \right) P_l(\cos \theta)$$

find an integral expression for the coefficients a_l, b_l that are relevant to the electric field *outside* the sphere. Evaluate the integrals giving b_1, b_2 and b_3 .

- b) Use your results from part a) to compute the electric dipole moment of the sphere as function of the potential difference $V_1 - V_2$.
 c) Now the two hemispheres are electrically connected and the entire surface is at one potential. The sphere is immersed in a uniform electric field \mathbf{E} . What is its dipole moment now?

Exercise 8.9: Tides and Gravity . The Earth is not exactly spherical. Two major causes of the deviation from sphericity are the Earth's rotation and the tidal forces it feels from the Sun and the Moon. In this problem we will study the effects of rotation and tides on a self-gravitating sphere of fluid of uniform density ρ_0 .

- a) Consider the equilibrium of a nearly spherical body of fluid rotating homogeneously with angular velocity ω_0 . Show that the effect of rotation can be accounted for by introducing an “effective gravitational potential”

$$\varphi_{\text{eff}} = \varphi_{\text{grav}} + \frac{1}{3} \omega_0^2 R^2 (P_2(\cos \theta) - 1),$$

where R, θ are spherical coordinates defined with their origin in the centre of the body and \hat{z} along the axis of rotation.

- b) A small planet is in a circular orbit about a distant massive star. It rotates about an axis perpendicular to the plane of the orbit so that it always keeps the same face directed towards the star. Show that the planet experiences an effective external potential

$$\varphi_{\text{tidal}} = -\Omega^2 R^2 P_2(\cos \theta),$$

together with a potential, of the same sort as in part a), that arises from the once-per-orbit rotation. Here Ω is the orbital angular velocity, and R, θ are spherical coordinates defined with their origin at the centre of the planet and \hat{z} pointing at the star.

- c) The external potentials slightly deform the initially spherical planet and the surface is given by

$$R(\theta, \phi) = R_0 + \eta P_2(\cos \theta).$$

Show that, to first order in η , this deformation does not alter the volume of the body. Observe that positive η corresponds to a prolate spheroid and negative η to an oblate one.

- d) The gravitational field of the deformed spheroid can be found by approximating it as an undeformed homogeneous sphere of radius R_0 , together with a thin spherical shell of radius R_0 and surface mass density $\sigma = \rho_0 \eta P_2(\cos \theta)$. Use the general axisymmetric solution

$$\varphi(R, \theta, \phi) = \sum_{l=0}^{\infty} \left(A_l R^l + \frac{B_l}{R^{l+1}} \right) P_l(\cos \theta)$$

of Laplace's equation, together with Poisson's equation

$$\nabla^2 \varphi = 4\pi G \rho(\mathbf{r})$$

for the gravitational potential, to obtain expressions for φ_{shell} in the regions $R > R_0$ and $R \leq R_0$.

- e) The surface of the fluid will be an equipotential of the combined potentials of the homogeneous sphere, the thin shell, and the effective external potential of the tidal or centrifugal forces. Use this fact to find η (to lowest order in the angular velocities) for the two cases. Do not include the centrifugal potential from part b) when computing the tidal distortion. We never include the variation of the centrifugal potential across a planet when calculating tidal effects. This is because this variation is due to the once-per-year rotation, and contributes to the oblate equatorial bulge and not to the prolate tidal bulge⁵. (Answer: $\eta_{\text{rot}} = -\frac{5}{2} \frac{\omega_0^2 R_0}{4\pi G \rho_0}$, and $\eta_{\text{tide}} = \frac{15}{2} \frac{\Omega^2 R_0}{4\pi G \rho_0}$.)

Exercise 8.10: Dielectric Sphere. Consider a solid dielectric sphere of radius a and permittivity ϵ . The sphere is placed in a electric field which is takes the constant value $\mathbf{E} = E_0 \hat{\mathbf{z}}$ a long distance from the sphere. Recall that Maxwell's equations require that \mathbf{D}_{\perp} and \mathbf{E}_{\parallel} be continuous across the surface of the sphere.

- a) Use the expansions

$$\begin{aligned} \Phi_{in} &= \sum_l A_l r^l P_l(\cos \theta) \\ \Phi_{out} &= \sum_l (B_l r^l + C_l r^{-l-1}) P_l(\cos \theta) \end{aligned}$$

⁵Our earth rotates about its axis 365+1 times in a year, not 365 times. The "+1" is this effect.

and find all non-zero coefficients A_l , B_l , C_l .

- b) Show that the \mathbf{E} field inside the sphere is uniform and of magnitude $\frac{3\epsilon_0}{\epsilon+2\epsilon_0}E_0$.
 c) Show that the electric field is unchanged if the dielectric is replaced by the polarization-induced surface charge density

$$\sigma_{\text{induced}} = 3\epsilon_0 \left(\frac{\epsilon - \epsilon_0}{\epsilon + 2\epsilon_0} \right) E_0 \cos \theta.$$

(Some systems of units may require extra 4π 's in this last expression. In SI units $\mathbf{D} \equiv \epsilon\mathbf{E} = \epsilon_0\mathbf{E} + \mathbf{P}$, and the polarization induced charge density is $\rho_{\text{induced}} = -\nabla \cdot \mathbf{P}$)

Exercise 8.11: Hollow Sphere. The potential on a spherical surface of radius a is $\Phi(\theta, \phi)$. We want to express the potential inside the sphere as an integral over the surface in a manner analogous to the Poisson kernel in two dimensions.

- a) By using the generating function for Legendre polynomials, show that

$$\frac{1 - r^2}{(1 + r^2 - 2r \cos \theta)^{3/2}} = \sum_{l=0}^{\infty} (2l+1) r^l P_l(\cos \theta), \quad r < 1$$

- b) Starting from the expansion

$$\begin{aligned} \Phi_{\text{in}}(r, \theta, \phi) &= \sum_{l=0}^{\infty} \sum_{m=-l}^l A_{lm} r^l Y_l^m(\theta, \phi) \\ A_{lm} &= \frac{1}{a^l} \int_{S^2} [Y_l^m(\theta, \phi)]^* \Phi(\theta, \phi) d \cos \theta d\phi \end{aligned}$$

and using the addition formula for spherical harmonics, show that

$$\Phi_{\text{in}}(r, \theta, \phi) = \frac{a(a^2 - r^2)}{4\pi} \int_{S^2} \frac{\Phi(\theta', \phi')}{(r^2 + a^2 - 2ar \cos \gamma)^{3/2}} d \cos \theta' d\phi'$$

where $\cos \gamma = \cos \theta \cos \theta' + \sin \theta \sin \theta' \cos(\phi - \phi')$.

- c) By setting $r = 0$, deduce that a three dimensional harmonic function cannot have a local maximum or minimum.

Exercise 8.12: We have several times met with the Pöschel-Teller eigenvalue problem

$$\left(-\frac{d^2}{dx^2} + n(n+1) \operatorname{sech}^2 x \right) \psi = E\psi, \quad \star$$

in the particular case that $n = 1$. We now consider this problem for any positive integer n .

- a) Set $\xi = \tanh x$ in \star and show that it becomes

$$\left(\frac{d}{d\xi}(1 - \xi^2) \frac{d}{d\xi} + n(n+1) + \frac{E}{1 - \xi^2} \right) \psi = 0.$$

- b) Compare the equation in part a) with the associated Legendre equation and deduce that the bound-state eigenfunctions and eigenvalues of the original Pöschel-Teller equation are

$$\psi_m(x) = P_n^m(\tanh x), \quad E_m = -m^2, \quad m = 1, \dots, n,$$

where $P_n^m(\xi)$ is the associated Legendre function. Observe that this list of bound states does not include $\psi_0 = P_n^0(\tanh x) \equiv P_n(\tanh x)$. This is because ψ_0 is not normalizable, being the lowest of the unbound $E \geq 0$ continuous-spectrum states.

- c) Now seek continuous spectrum solutions to \star in the form

$$\psi_k(x) = e^{ikx} f(\tanh x),$$

and show if we take $E = k^2$, where k is any real number, then $f(\xi)$ obeys

$$(1 - \xi^2) \frac{d^2 f}{d\xi^2} + 2(ik - \xi) \frac{df}{d\xi} + n(n+1)f = 0. \quad \star\star$$

- d) Let us denote by $P_n^{(k)}(\xi)$ the solutions of $\star\star$ that reduce to the Legendre polynomial $P_n(\xi)$ when $k = 0$. Show that the first few $P_n^{(k)}(\xi)$ are

$$\begin{aligned} P_0^{(k)}(\xi) &= 1, \\ P_1^{(k)}(\xi) &= \xi - ik, \\ P_2^{(k)}(\xi) &= \frac{1}{2}(3\xi^2 - 1 - 3ik\xi - k^2). \end{aligned}$$

Explore the properties of the $P_n^{(k)}(\xi)$, and show that they include

- i) $P_n^{(k)}(-\xi) = (-1)^n P_n^{(-k)}(\xi)$.
- ii) $(n+1)P_{n+1}^{(k)}(\xi) = (2n+1)\xi P_n^{(k)}(\xi) - (n+k^2/n)P_{n-1}^{(k)}(\xi)$.
- iii) $P_n^{(k)}(1) = (1-ik)(2-ik)\dots(n-ik)/n!$.

(The $P_n^{(k)}(\xi)$ are the $\nu = -\mu = ik$ special case of the Jacobi polynomials $P_n^{(\nu, \mu)}(\xi)$)

Exercise 8.13: Bessel functions and impact parameters. In two dimensions we can expand a plane wave as

$$e^{iky} = \sum_{n=-\infty}^{\infty} J_n(kr) e^{in\theta}.$$

- a) What do you think the resultant wave will look like if we take only a finite segment of this sum? For example

$$\phi(x) = \sum_{l=10}^{17} J_l(kr) e^{in\theta}.$$

Think about:

- i) The quantum interpretation of $\hbar l$ as angular momentum = $\hbar k d$, where d is the *impact parameter*, the amount by which the incoming particle misses the origin.
 - ii) Diffraction: one cannot have a plane wave of finite width.
- b) After (writing down your best guess for the previous part, confirm your understanding by using Mathematica or other package to plot the real part of ϕ as defined above. The following Mathematica code may work.

```
Clear[bit,tot]
bit[l_,x_,y_] := Cos[l ArcTan[x,y]] BesselJ[l,Sqrt[x^2+y^2]]
tot[x_,y_] := Sum[bit[l,x,y],{l,10,17}]
ContourPlot[tot[x,y],{x,-40,40},{y,-40,40},PlotPoints ->200]
Display["wave",%,"EPS"]
```

Run it, or some similar code, as a batchfile. Try different ranges for the sum.

Exercise 8.14: Consider the the two-dimensional Fourier transform

$$\tilde{f}(\mathbf{k}) = \int e^{i\mathbf{k}\cdot\mathbf{x}} f(\mathbf{x}) d^2x$$

of a function that in polar co-ordinates is of the form $f(r, \theta) = \exp\{-il\theta\} f(r)$.

- a) Show that

$$\tilde{f}(\mathbf{k}) = 2\pi i^l e^{-il\theta_k} \int_0^\infty J_l(kr) f(r) r dr,$$

where k, θ_k are the polar co-ordinates of \mathbf{k} .

- b) Use the inversion formula for the two-dimensional Fourier transform to establish the inversion formula (8.120) for the Hankel transform

$$F(k) = \int_0^\infty J_l(kr) f(r) r dr.$$

Chapter 9

Integral Equations

A problem involving a differential equation can often be recast as one involving an integral equation. Sometimes this new formulation suggests a method of attack that would not have been apparent in the original language. It is also sometimes easier to extract general properties of the solution when the problem is expressed as an integral equation.

9.1 Illustrations

Here are some examples:

A boundary-value problem: Consider the differential equation for the unknown $u(x)$

$$-u'' + \lambda V(x)u = 0 \quad (9.1)$$

with the boundary conditions $u(0) = u(L) = 0$. To turn this into an integral equation we introduce the Green function

$$G(x, y) = \begin{cases} \frac{1}{L}x(y - L), & 0 \leq x \leq y \leq L, \\ \frac{1}{L}y(x - L), & 0 \leq y \leq x \leq L, \end{cases} \quad (9.2)$$

so that

$$-\frac{d^2}{dx^2}G(x, y) = \delta(x - y). \quad (9.3)$$

Then we can pretend that $\lambda V(x)u(x)$ in the differential equation is a known source term, and substitute it for “ $f(x)$ ” in the usual Green function solution.

We end up with

$$u(x) + \lambda \int_0^L G(x, y) V(y) u(y) dy = 0. \quad (9.4)$$

This *integral equation* for u has not solved the problem, but is equivalent to the original problem. Note, in particular, that the boundary conditions are implicit in this formulation: if we set $x = 0$ or L in the second term, it becomes zero because the Green function is zero at those points. The integral equation then says that $u(0)$ and $u(L)$ are both zero.

An initial value problem: Consider essentially the same differential equation as before, but now with initial data:

$$-u'' + V(x)u = 0, \quad u(0) = 0, \quad u'(0) = 1. \quad (9.5)$$

In this case, we claim that the inhomogeneous integral equation

$$u(x) - \int_0^x (x-t)V(t)u(t) dt = x, \quad (9.6)$$

is equivalent to the given problem. Let us check the claim. First, the initial conditions. Rewrite the integral equation as

$$u(x) = x + \int_0^x (x-t)V(t)u(t) dt, \quad (9.7)$$

so it is manifest that $u(0) = 0$. Now differentiate to get

$$u'(x) = 1 + \int_0^x V(t)u(t) dt. \quad (9.8)$$

This shows that $u'(0) = 1$, as required. Differentiating once more confirms that $u'' = V(x)u$.

These examples reveal that one advantage of the integral equation formulation is that the boundary or initial value conditions are automatically encoded in the integral equation itself, and do not have to be added as riders.

9.2 Classification of Integral Equations

The classification of linear integral equations is best described by a list:

- A) i) Limits on integrals fixed \Rightarrow Fredholm equation.
 ii) One integration limit is $x \Rightarrow$ Volterra equation.
- B) i) Unknown under integral only \Rightarrow Type I.
 ii) Unknown also outside integral \Rightarrow Type II.
- C) i) Homogeneous.
 ii) Inhomogeneous.

For example,

$$u(x) = \int_0^L G(x, y)u(y) dy \quad (9.9)$$

is a Type II homogeneous Fredholm equation, whilst

$$u(x) = x + \int_0^x (x - t)V(t)u(t) dt \quad (9.10)$$

is a Type II inhomogeneous Volterra equation.

The equation

$$f(x) = \int_a^b K(x, y)u(y) dy, \quad (9.11)$$

an inhomogeneous Type I Fredholm equation, is analogous to the matrix equation

$$\mathbf{K}\mathbf{x} = \mathbf{b}. \quad (9.12)$$

On the other hand, the equation

$$u(x) = \frac{1}{\lambda} \int_a^b K(x, y)u(y) dy, \quad (9.13)$$

a homogeneous Type II Fredholm equation, is analogous to the matrix eigenvalue problem

$$\mathbf{K}\mathbf{x} = \lambda\mathbf{x}. \quad (9.14)$$

Finally,

$$f(x) = \int_a^x K(x, y)u(y) dy, \quad (9.15)$$

an inhomogeneous Type I Volterra equation, is the analogue of a system of linear equations involving an upper triangular matrix.

The function $K(x, y)$ appearing in these in these expressions is called the *kernel*. The phrase “kernel of the integral operator” can therefore refer either to the function K or the nullspace of the operator. The context should make clear which meaning is intended.

9.3 Integral Transforms

When a Fredholm kernel is of the form $K(x - y)$, with x and y taking values on the entire real line, then it is translation invariant and we can solve the integral equation by using the Fourier transformation

$$\tilde{u}(k) = \mathcal{F}(u) = \int_{-\infty}^{\infty} u(x) e^{ikx} dx \quad (9.16)$$

$$u(x) = \mathcal{F}^{-1}(\tilde{u}) = \int_{-\infty}^{\infty} \tilde{u}(k) e^{-ikx} \frac{dk}{2\pi} \quad (9.17)$$

Integral equations involving translation-invariant Volterra kernels usually succumb to a Laplace transform

$$\tilde{u}(p) = \mathcal{L}(u) = \int_0^{\infty} u(x) e^{-px} dx \quad (9.18)$$

$$u(x) = \mathcal{L}^{-1}(\tilde{u}) = \frac{1}{2\pi i} \int_{\gamma-i\infty}^{\gamma+i\infty} \tilde{u}(p) e^{px} dp. \quad (9.19)$$

The Laplace inversion formula is the *Bromwich contour integral*, where γ is chosen so that all the singularities of $\tilde{u}(p)$ lie to the left of the contour. In practice one finds the inverse Laplace transform by using a table of Laplace transforms, such as the Bateman tables of integral transforms mentioned in the introduction to chapter 8.

For kernels of the form $K(x/y)$ the Mellin transform,

$$\tilde{u}(\sigma) = \mathcal{M}(u) = \int_0^{\infty} u(x) x^{\sigma-1} dx \quad (9.20)$$

$$u(x) = \mathcal{M}^{-1}(\tilde{u}) = \frac{1}{2\pi i} \int_{\gamma-i\infty}^{\gamma+i\infty} \tilde{u}(\sigma) x^{-\sigma} d\sigma, \quad (9.21)$$

is the tool of choice. Again the inversion formula requires a Bromwich contour integral, and so usually recourse to tables of Mellin transforms.

9.3.1 Fourier Methods

The class of problems that succumb to a Fourier transform can be thought of a continuous version of a matrix problem

The matrix form of the equation $\int_{-\infty}^{\infty} K(x-y)u(y) dy = f(x)$ where the entries in the matrix depend only on their distance from the main diagonal.

Example: Consider the type II Fredholm equation

$$u(x) - \lambda \int_{-\infty}^{\infty} e^{-|x-y|} u(y) dy = f(x), \quad (9.22)$$

where we will assume (for reasons that will become apparent) that $\lambda < 1/2$. Here the x -space kernel operator

$$K(x-y) = \delta(x-y) - \lambda e^{-|x-y|}. \quad (9.23)$$

has Fourier transform

$$\tilde{K}(k) = 1 - \frac{2\lambda}{k^2 + 1} = \frac{k^2 + (1 - 2\lambda)}{k^2 + 1} = \frac{k^2 + a^2}{k^2 + 1} \quad (9.24)$$

where $a^2 = 1 - 2\lambda$. From

$$\left(\frac{k^2 + a^2}{k^2 + 1} \right) \tilde{u}(k) = \tilde{f}(k) \quad (9.25)$$

we find

$$\begin{aligned} \tilde{u}(k) &= \left(\frac{k^2 + 1}{k^2 + a^2} \right) \tilde{f}(k) \\ &= \left(1 + \frac{1 - a^2}{k^2 + a^2} \right) \tilde{f}(k). \end{aligned} \quad (9.26)$$

Inverting the Fourier transform gives

$$\begin{aligned} u(x) &= f(x) + \frac{1 - a^2}{2a} \int_{-\infty}^{\infty} e^{-a|x-y|} f(y) dy \\ &= f(x) + \frac{\lambda}{\sqrt{1 - 2\lambda}} \int_{-\infty}^{\infty} e^{-\sqrt{1 - 2\lambda}|x-y|} f(y) dy. \end{aligned} \quad (9.27)$$

9.3.2 Laplace Transform Methods

The Volterra problem

$$\int_0^x K(x-y)u(y) dy = f(x), \quad 0 < x < \infty. \quad (9.28)$$

can also be solved by the application of an integral transform. In this case we observe that value of $K(x)$ is only needed for positive x , and this suggests that we take a *Laplace transform* over the positive real axis.

We only require the value of $K(x)$ for x positive, and u and f can be set to zero for $x < 0$.

Abel's equation

As an example of Laplace methods, consider Abel's equation

$$f(x) = \int_0^x \frac{1}{\sqrt{x-y}} u(y) dy, \quad (9.29)$$

where we are given $f(x)$ and wish to find $u(x)$. Here it is clear that we need $f(0) = 0$ for the equation to make sense. We have met this integral transformation before in the definition of the “half-derivative”. It is an example of the more general equation of the form

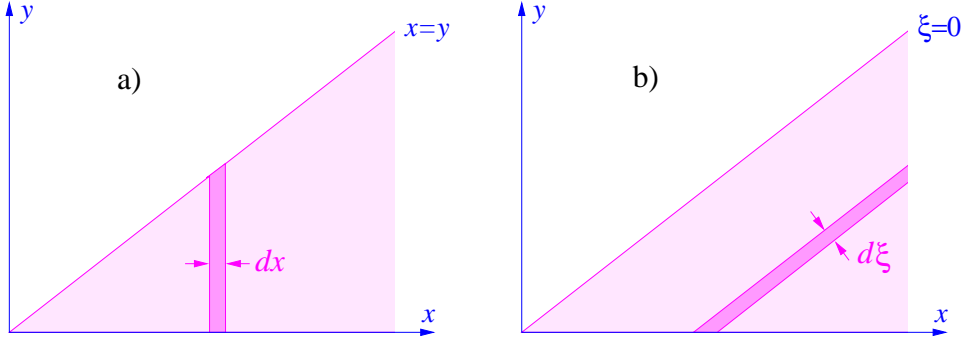
$$f(x) = \int_0^x K(x-y)u(y) dy. \quad (9.30)$$

Let us take the Laplace transform of both sides of (9.30):

$$\begin{aligned} \mathcal{L}f(p) &= \int_0^\infty e^{-px} \left(\int_0^x K(x-y)u(y) dy \right) dx \\ &= \int_0^\infty dx \int_0^x dy e^{-px} K(x-y)u(y). \end{aligned} \quad (9.31)$$

Now we make the change of variables

$$\begin{aligned} x &= \xi + \eta, \\ y &= \eta. \end{aligned} \quad (9.32)$$



Regions of integration for the convolution theorem: a) Integrating over y at fixed x , then over x ; b) Integrating over η at fixed ξ , then over ξ .

This has Jacobian

$$\frac{\partial(x, y)}{\partial(\xi, \eta)} = 1, \quad (9.33)$$

and the integral becomes

$$\begin{aligned} \mathcal{L}f(p) &= \int_0^\infty \int_0^\infty e^{-p(\xi+\eta)} K(\xi) u(\eta) d\xi d\eta \\ &= \int_0^\infty e^{-p\xi} K(\xi) d\xi \int_0^\infty e^{-p\eta} u(\eta) d\eta \\ &= \mathcal{L}K(p) \mathcal{L}u(p). \end{aligned} \quad (9.34)$$

Thus the Laplace transform of a Volterra convolution is the product of the Laplace transforms. We can now invert

$$u = \mathcal{L}^{-1}(\mathcal{L}f / \mathcal{L}K). \quad (9.35)$$

For Abel's equation, we have

$$K(x) = \frac{1}{\sqrt{x}}, \quad (9.36)$$

the Laplace transform of which is

$$\mathcal{L}K(p) = \int_0^\infty x^{\frac{1}{2}-1} e^{-px} dx = p^{-1/2} \Gamma\left(\frac{1}{2}\right) = p^{-1/2} \sqrt{\pi}. \quad (9.37)$$

Therefore, the Laplace transform of the solution $u(x)$ is

$$\mathcal{L}u(p) = \frac{1}{\sqrt{\pi}} p^{1/2} (\mathcal{L}f) = \frac{1}{\pi} (\sqrt{\pi} p^{-1/2} p \mathcal{L}f). \quad (9.38)$$

Now, Laplace transforms have the property that

$$p \mathcal{L}F = \mathcal{L}\left(\frac{d}{dx}F\right), \quad (9.39)$$

as may be seen by an integration by parts in the definition. Using this observation, and depending on whether we put the p next to f or outside the parenthesis, we conclude that the solution of Abel's equation can be written in two equivalent ways:

$$u(x) = \frac{1}{\pi} \frac{d}{dx} \int_0^x \frac{1}{\sqrt{x-y}} f(y) dy = \frac{1}{\pi} \int_0^x \frac{1}{\sqrt{x-y}} f'(y) dy. \quad (9.40)$$

Proving the equality of these two expressions was a problem we set ourselves in chapter 6.

Here is another way of establishing the equality: Assume for the moment that $K(0)$ is finite, and that, as we have already noted, $f(0) = 0$. Then,

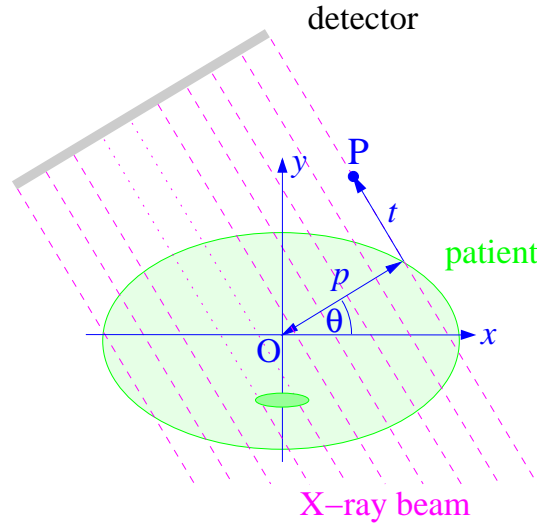
$$\frac{d}{dx} \int_0^x K(x-y) f(y) dy \quad (9.41)$$

is equal to

$$\begin{aligned} & K(0)f(x) + \int_0^x \partial_x K(x-y) f(y) dy, \\ &= K(0)f(x) - \int_0^x \partial_y K(x-y) f(y) dy \\ &= K(0)f(x) - \int_0^x \partial_y \left(K(x-y) f(y) \right) dy + \int_0^x K(x-y) f'(y) dy \\ &= K(0)f(x) - K(0)f(x) - K(x)f(0) + \int_0^x K(x-y) f'(y) dy \\ &= \int_0^x K(x-y) f'(y) dy. \end{aligned} \quad (9.42)$$

Since $K(0)$ cancelled out, we need not worry that it is divergent! More rigorously, we should regularize the improper integral by raising the lower limit on the integral to a small positive quantity, and then taking the limit to zero at the end of the calculation.

Radon Transforms



The geometry of the CAT scan Radon transformation, showing the location of the point P with co-ordinates $x = p \cos \theta - t \sin \theta$, $y = p \sin \theta + t \cos \theta$.

An Abel integral equation lies at the heart of the method for reconstructing the image in a computer aided tomography (CAT) scan. By rotating an X-ray source about a patient and recording the direction-dependent shadow, we measure the integral of his tissue density $f(x, y)$ along all lines in a slice (which we will take to be the x, y plane) through his body. The resulting information is the *Radon transform* F of the function f . If we parametrize the family of lines by p and θ , as shown in the figure, we have

$$\begin{aligned} F(p, \theta) &= \int_{-\infty}^{\infty} f(p \cos \theta - t \sin \theta, p \sin \theta + t \cos \theta) dt, \\ &= \int_{\mathbb{R}^2} \delta(x \cos \theta + y \sin \theta - p) f(x, y) dx dy. \end{aligned} \quad (9.43)$$

We will assume that f is zero outside some finite region (the patient), and so these integrals converge.

We wish to invert the transformation and recover f from the data $F(p, \theta)$. This problem was solved by Johann Radon in 1917. Radon made clever use of the Euclidean group to simplify the problem. He observed that we may take the point O at which we wish to find f to be the origin, and defined¹

$$F_O(p) = \frac{1}{2\pi} \int_0^{2\pi} \left\{ \int_{\mathbb{R}^2} \delta(x \cos \theta + y \sin \theta - p) f(x, y) dx dy \right\} d\theta. \quad (9.44)$$

Thus $F_O(p)$ is the angular average over all lines tangent to a circle of radius p about the desired inversion point. Radon then observed that if he additionally defines

$$\bar{f}(r) = \frac{1}{2\pi} \int_0^{2\pi} f(r \cos \phi, r \sin \phi) d\phi \quad (9.45)$$

then he can substitute $\bar{f}(r)$ for $f(x, y)$ in (9.44) without changing the value of the integral. Furthermore $\bar{f}(0) = f(0, 0)$. Hence, taking polar co-ordinates in the x, y plane, he has

$$F_O(p) = \frac{1}{2\pi} \int_0^{2\pi} \left\{ \int_{\mathbb{R}^2} \delta(r \cos \phi \cos \theta + r \sin \phi \sin \theta - p) \bar{f}(r) r d\phi dr \right\} d\theta. \quad (9.46)$$

We can now use

$$\delta(g(\phi)) = \sum_n \frac{1}{|g'(\phi_n)|} \delta(\phi - \phi_n), \quad (9.47)$$

where the sum is over the zeros ϕ_n of $g(\phi) = r \cos(\theta - \phi) - p$, to perform the ϕ integral. Any given point $x = r \cos \phi$, $y = r \sin \phi$ lies on two distinct lines if and only if $p < r$. Thus $g(\phi)$ has two zeros if $p < r$, but none if $r < p$. Consequently

$$F_O(p) = \frac{1}{2\pi} \int_0^{2\pi} \left\{ \int_p^\infty \frac{2}{\sqrt{r^2 - p^2}} \bar{f}(r) r dr \right\} d\theta. \quad (9.48)$$

Nothing in the inner integral depends on θ . The outer integral is therefore trivial, and so

$$F_O(p) = \int_p^\infty \frac{2}{\sqrt{r^2 - p^2}} \bar{f}(r) r dr. \quad (9.49)$$

¹We trust that the reader will forgive the anachronism of our expressing Radon's formulæ in terms of Dirac's delta function.

We can extract $F_O(p)$ from the data. We could therefore solve the Abel equation (9.49) and recover the complete function $\bar{f}(r)$. We are only interested in $\bar{f}(0)$, however, and it easier verify a claimed solution. Radon asserts that

$$f(0,0) = \bar{f}(0) = -\frac{1}{\pi} \int_0^\infty \frac{1}{p} \left(\frac{\partial}{\partial p} F_O(p) \right) dp. \quad (9.50)$$

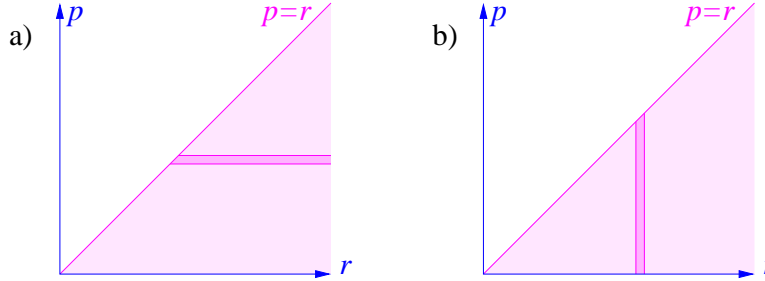
To prove that his claim is true we must first take the derivative of $F_O(p)$ and show that

$$\left(\frac{\partial}{\partial p} F_O(p) \right) = \int_p^\infty \frac{2p}{\sqrt{r^2 - p^2}} \left(\frac{\partial}{\partial r} \bar{f}(r) \right) dr. \quad (9.51)$$

The details of this computation are left as an exercise. It is little different from the differentiation of the integral transform at the end of the last section. We then substitute (9.51) into (9.50) and evaluate the resulting integral

$$I = -\frac{1}{\pi} \int_0^\infty \frac{1}{p} \left\{ \int_p^\infty \frac{2p}{\sqrt{r^2 - p^2}} \left(\frac{\partial}{\partial r} \bar{f}(r) \right) dr \right\} dp \quad (9.52)$$

by exchanging the order of the integrations, as shown in the figure.



a) In (9.52) we integrate first over r and then over p . The inner r integral is therefore from $r = p$ to $r = \infty$. b) In (9.53) we integrate first over p and then over r . The inner p integral therefore runs from $p = 0$ to $p = r$.

After the interchange we have

$$I = -\frac{2}{\pi} \int_0^\infty \left\{ \int_0^r \frac{1}{\sqrt{r^2 - p^2}} dp \right\} \left(\frac{\partial}{\partial r} \bar{f}(r) \right) dr. \quad (9.53)$$

Since

$$\int_0^r \frac{1}{\sqrt{r^2 - p^2}} dp = \frac{\pi}{2}, \quad (9.54)$$

the inner integral is independent of r . We thus obtain

$$I = - \int_0^\infty \left(\frac{\partial}{\partial r} \bar{f}(r) \right) dr = \bar{f}(0) = f(0, 0). \quad (9.55)$$

Radon's inversion formula is therefore correct.

Although Radon found a closed-form inversion formula, the numerical problem of reconstructing the image from the partial and noisy data obtained from a practical CAT scanner is quite delicate, and remains an active area of research.

9.4 Separable Kernels

Let

$$K(x, y) = \sum_{i=1}^N p_i(x) q_i(y), \quad (9.56)$$

where $\{p_i\}$ and $\{q_i\}$ are two linearly independent sets of functions. The range of K is therefore the span $\langle p_i \rangle$ of the set $\{p_i\}$. Such kernels are said to be *separable*. The theory of integral equations containing such kernels is especially transparent.

9.4.1 Eigenvalue problem

Consider the eigenvalue problem

$$\lambda u(x) = \int_D K(x, y) u(y) dy \quad (9.57)$$

for a separable kernel. Here, D is some range of integration, and $x \in D$. If $\lambda \neq 0$, we know that u has to be in the range of K , so we can write

$$u(x) = \sum_i \xi_i p_i(x). \quad (9.58)$$

Inserting this into the integral, we find that our problem reduces to the finite matrix eigenvalue equation

$$\lambda \xi_i = A_{ij} \xi_j, \quad (9.59)$$

where

$$A_{ij} = \int_D q_i(y) p_j(y) dy. \quad (9.60)$$

Matters are especially simple when $q_i = p_i^*$. In this case $A_{ij} = A_{ji}^*$ so the matrix A is Hermitian, and therefore has N linearly independent eigenvectors. Observe that none of the N associated eigenvalues can be zero. To see this, suppose that $v(x) = \sum_i \zeta_i p_i(x)$ is an eigenvector with zero eigenvalue. In other words, suppose that

$$0 = \sum_i p_i(x) \int_D p_i^*(y) p_j(y) \zeta_j dy. \quad (9.61)$$

Since the $p_i(x)$ are linearly independent, we must have

$$0 = \int_D p_i^*(y) p_j(y) \zeta_j dy = 0, \quad (9.62)$$

for each i separately. Multiplying by ζ_i^* and summing we find

$$0 = \int_D \left| \sum_j p_j(y) \zeta_j \right|^2 dy, \quad (9.63)$$

and $v(x)$ itself must have been zero. The remaining (infinite in number) eigenfunctions span $\langle q_i \rangle^\perp$ and have $\lambda = 0$.

9.4.2 Inhomogeneous problem

It is easiest to discuss inhomogeneous separable-kernel problems by example. Consider the equation

$$u(x) = f(x) + \mu \int_0^1 K(x, y) u(y) dy, \quad (9.64)$$

where $K(x, y) = xy$. Here, $f(x)$ and μ are given, and $u(x)$ is to be found. We know that $u(x)$ must be of the form

$$u(x) = f(x) + ax, \quad (9.65)$$

and the only task is to find the constant a . We plug u into the integral equation and, after cancelling a common factor of x , we find

$$a = \mu \int_0^1 y u(y) dy = \mu \int_0^1 y f(y) dy + a\mu \int_0^1 y^2 dy. \quad (9.66)$$

The last integral is equal to $\mu a/3$, so

$$a \left(1 - \frac{1}{3}\mu\right) = \mu \int_0^1 yf(y) dy, \quad (9.67)$$

and finally

$$u(x) = f(x) + x \frac{\mu}{(1 - \mu/3)} \int_0^1 yf(y) dy. \quad (9.68)$$

Notice that this solution is meaningless if $\mu = 3$. We can relate this to the eigenvalues of the kernel $K(x, y) = xy$. The eigenvalue problem for this kernel is

$$\lambda u(x) = \int_0^1 xyu(y) dy. \quad (9.69)$$

On substituting $u(x) = ax$, this reduces to $\lambda ax = ax/3$, and so $\lambda = 1/3$. All other eigenvalues are zero. Our inhomogeneous equation was of the form

$$(1 - \mu K)u = f \quad (9.70)$$

and the operator $(1 - \mu K)$ has an infinite set of eigenfunctions with eigenvalue 1, and a single eigenfunction, $u_0(x) = x$, with eigenvalue $(1 - \mu/3)$. The eigenvalue becomes zero, and hence the inverse ceases to exist, when $\mu = 3$.

A solution to the problem $(1 - \mu K)u = f$ may still exist even when $\mu = 3$. But now, applying the Fredholm alternative, we see that f must satisfy the condition that it be orthogonal to all solutions of $(1 - \mu K)^\dagger v = 0$. Since our kernel is Hermitian, this means that f must be orthogonal to the zero mode $u_0(x) = x$. For the case of $\mu = 3$, the equation is

$$u(x) = f(x) + 3 \int_0^1 xyu(y) dy, \quad (9.71)$$

and to have a solution f must obey $\int_0^1 yf(y) dy = 0$. We again set $u = f(x) + ax$, and find

$$a = 3 \int_0^1 yf(y) dy + a3 \int_0^1 y^2 dy, \quad (9.72)$$

but now this reduces to $a = a$. The general solution is therefore

$$u = f(x) + ax \quad (9.73)$$

with a arbitrary.

9.5 Singular Integral Equations

Equations involving principal-part integrals, such as the *airfoil equation*

$$\frac{P}{\pi} \int_{-1}^1 \varphi(x) \frac{1}{x-y} dx = f(y), \quad (9.74)$$

in which f is given and we are to find φ , are called *singular integral equations*. Their solution depends on what conditions are imposed on the unknown function $\varphi(x)$ at the endpoints of the integration region. We will consider only this simplest example here²

9.5.1 Solution via Tchebychef Polynomials

Recall the definition of the Tchebychef polynomials from chapter 2. We set

$$T_n(x) = \cos(n \cos^{-1} x), \quad (9.75)$$

$$U_{n-1}(x) = \frac{\sin(n \cos^{-1} x)}{\sin(\cos^{-1} x)} = \frac{1}{n} T'_n(x). \quad (9.76)$$

These are the Tchebychef Polynomials of the first and second kind, respectively. The orthogonality of the functions $\cos n\theta$ and $\sin n\theta$ over the interval $[0, \pi]$ translates into

$$\int_{-1}^1 \frac{1}{\sqrt{1-x^2}} T_n(x) T_m(x) dx = h_n \delta_{nm}, \quad n, m \geq 0, \quad (9.77)$$

where $h_0 = \pi$, $h_n = \pi/2$, $n > 0$, and

$$\int_{-1}^1 \sqrt{1-x^2} U_{n-1}(x) U_{m-1}(x) dx = \frac{\pi}{2} \delta_{nm}, \quad n, m > 0. \quad (9.78)$$

The sets $\{T_n(x)\}$ and $\{U_n(x)\}$ are complete in $L_w^2[0, 1]$ with the weight functions $w = (1-x^2)^{-1/2}$ and $w = (1-x^2)^{1/2}$, respectively.

Rather less obvious are the principal-part integral identities (valid for $-1 < y < 1$)

$$P \int_{-1}^1 \frac{1}{\sqrt{1-x^2}} \frac{1}{x-y} dx = 0, \quad (9.79)$$

$$P \int_{-1}^1 \frac{1}{\sqrt{1-x^2}} T_n(x) \frac{1}{x-y} dx = \pi U_{n-1}(y), \quad n > 0, \quad (9.80)$$

²The classic text is N. I. Muskhelishvili *Singular Integral Equations*.

and

$$P \int_{-1}^1 \sqrt{1-x^2} U_{n-1}(x) \frac{1}{x-y} dx = -\pi T_n(y). \quad (9.81)$$

These correspond, after we set $x = \cos \theta$ and $y = \cos \phi$, to the trigonometric integrals

$$P \int_0^\pi \frac{\cos n\theta}{\cos \theta - \cos \phi} d\theta = \pi \frac{\sin n\phi}{\sin \phi}, \quad (9.82)$$

and

$$P \int_0^\pi \frac{\sin \theta \sin n\theta}{\cos \theta - \cos \phi} d\theta = -\pi \cos n\phi, \quad (9.83)$$

respectively. We will motivate and derive these formulæ at the end of this section.

From these principal-part integrals we can solve the integral equation

$$\frac{P}{\pi} \int_{-1}^1 \varphi(x) \frac{1}{x-y} dx = f(y), \quad y \in [-1, 1], \quad (9.84)$$

for φ in terms of f , subject to the condition that φ be bounded at $x = \pm 1$. We will see that no solution exists unless f satisfies the condition

$$\int_{-1}^1 \frac{1}{\sqrt{1-x^2}} f(x) dx = 0, \quad (9.85)$$

but if f does satisfy this condition then there is a unique solution

$$\varphi(y) = -\frac{\sqrt{1-y^2}}{\pi} P \int_{-1}^1 \frac{1}{\sqrt{1-x^2}} f(x) \frac{1}{x-y} dx. \quad (9.86)$$

To understand why this is the solution, and why there is a condition on f , expand

$$f(x) = \sum_{n=1}^{\infty} b_n T_n(x). \quad (9.87)$$

Here, the condition on f translates into the absence of a term involving $T_0 \equiv 1$ in the expansion. Then,

$$\varphi(x) = \sqrt{1-x^2} \sum_{n=1}^{\infty} b_n U_{n-1}(x), \quad (9.88)$$

with b_n the coefficients that appear in the expansion of f , solves the problem. That this is so may be seen on substituting this expansion for φ into the integral equation and using second of the principal-part identities. Note that that this identity provides no way to generate a term with T_0 ; hence the constraint. Next we observe that the expansion for φ is generated term-by-term from the expansion for f by substituting this into the integral form of the solution and using the first principal-part identity.

Similarly, we can solve the for $\varphi(y)$ in

$$\frac{P}{\pi} \int_{-1}^1 \varphi(x) \frac{1}{x-y} dx = f(y), \quad y \in [-1, 1], \quad (9.89)$$

where now φ is permitted to be singular at $x = \pm 1$. In this case there is always a solution, but it is not unique. The solutions are

$$\varphi(y) = \frac{1}{\pi \sqrt{1-y^2}} P \int_{-1}^1 \sqrt{1-x^2} f(x) \frac{1}{x-y} dx + \frac{C}{\sqrt{1-y^2}}, \quad (9.90)$$

where C is an arbitrary constant. To see this, expand

$$f(x) = \sum_{n=1}^{\infty} a_n U_{n-1}(x), \quad (9.91)$$

and then

$$\varphi(x) = \frac{1}{\sqrt{1-x^2}} \left(\sum_{n=1}^{\infty} a_n T_n(x) + C T_0 \right), \quad (9.92)$$

satisfies the equation for any value of the constant C . Again the expansion for φ is generated from that of f by use of the second principal-part identity.

Explanation of the Principal-Part Identities

The principal-part identities can be extracted from the analytic properties of the resolvent operator $R_\lambda(n-n') \equiv (\hat{H} - \lambda I)_{n,n'}^{-1}$ for a tight-binding model of the conduction band in a one-dimensional crystal with nearest neighbour hopping. The eigenfunctions $u_E(n)$ for this problem obey

$$u_E(n+1) + u_E(n-1) = E u_E(n) \quad (9.93)$$

and are

$$u_E(n) = e^{in\theta}, \quad -\pi < \theta < \pi, \quad (9.94)$$

with energy eigenvalues $E = 2 \cos \theta$.

The resolvent $R_\lambda(n)$ obeys

$$R_\lambda(n+1) + R_\lambda(n-1) - \lambda R_\lambda(n) = \delta_{n0}, \quad n \in \mathbb{Z}, \quad (9.95)$$

and can be expanded in terms of the energy eigenfunctions as

$$R_\lambda(n-n') = \sum_E \frac{u_E(n)u_E^*(n')}{E-\lambda} = \int_{-\pi}^{\pi} \frac{e^{i(n-n')\theta}}{2 \cos \theta - \lambda} \frac{d\theta}{2\pi} \quad (9.96)$$

If we set $\lambda = 2 \cos \phi$, we observe that

$$\int_{-\pi}^{\pi} \frac{e^{in\theta}}{2 \cos \theta - 2 \cos \phi} \frac{d\theta}{2\pi} = \frac{1}{2i \sin \phi} e^{i|n|\phi}, \quad \text{Im } \phi > 0. \quad (9.97)$$

That this integral is correct can be confirmed by observing that it is evaluating the Fourier coefficient of the double geometric series

$$\sum_{n=-\infty}^{\infty} e^{-in\theta} e^{i|n|\phi} = \frac{2i \sin \phi}{2 \cos \theta - 2 \cos \phi}, \quad \text{Im } \phi > 0. \quad (9.98)$$

By writing $e^{in\theta} = \cos n\theta + i \sin n\theta$ and observing that the sine term integrates to zero, we find that

$$\int_0^{\pi} \frac{\cos n\theta}{\cos \theta - \cos \phi} d\theta = \frac{\pi}{i \sin \phi} (\cos n\phi + i \sin n\phi), \quad (9.99)$$

where $n > 0$, and again we have taken $\text{Im } \phi > 0$. Now let ϕ approach the real axis from above, and apply the Plemelj formula. We find

$$P \int_0^{\pi} \frac{\cos n\theta}{\cos \theta - \cos \phi} d\theta = \pi \frac{\sin n\phi}{\sin \phi}. \quad (9.100)$$

This is the first principal-part integral identity. The second identity,

$$P \int_0^{\pi} \frac{\sin \theta \sin n\theta}{\cos \theta - \cos \phi} d\theta = -\pi \cos n\phi, \quad (9.101)$$

is obtained from the first by using the addition theorems for the sine and cosine.

9.6 Wiener-Hopf equations

We have seen that Volterra equations of the form

$$\int_0^x K(x-y) u(y) dy = f(x), \quad 0 < x < \infty, \quad (9.102)$$

having translation invariant kernels, may be solved for u by using a Laplace transform. The apparently innocent modification

$$\int_0^\infty K(x-y) u(y) dy = f(x), \quad 0 < x < \infty \quad (9.103)$$

leads to an equation that is much harder to deal with. In these *Wiener-Hopf* equations, we are still only interested in the upper left quadrant of the continuous matrix,

The matrix form of (9.103).

and $K(x-y)$ still has entries depending only on their distance from the main diagonal. Now, however, we make use of the values of $K(x)$ for all of $-\infty < x < \infty$. This suggests the use of a Fourier transform. The problem is that, in order to Fourier transform, we must integrate over the entire real line on *both sides* of the equation and this requires us to know the values of $f(x)$ for negative values of x — but we have not been given this information (and do not really need it). We therefore make the replacement

$$f(x) \rightarrow f(x) + g(x), \quad (9.104)$$

where $f(x)$ is non-zero only for positive x , and $g(x)$ non-zero only for negative x . We then solve

$$\int_0^\infty K(x-y) u(y) dy = \begin{cases} f(x), & 0 < x < \infty, \\ g(x), & -\infty < x < 0, \end{cases} \quad (9.105)$$

so as to find u and g simultaneously. In other words, we extend the problem to one on the whole real line, but with the negative- x source term $g(x)$ chosen so that the solution $u(x)$ is non-zero only for positive x . We can represent this pictorially:

$$\begin{bmatrix} \text{grid} \\ K \end{bmatrix} \begin{bmatrix} u \\ 0 \end{bmatrix} = \begin{bmatrix} f \\ g \end{bmatrix}$$

The matrix form of (9.105) with both f and g

To find u and g we try to make an “LU” decomposition of the matrix K into the product $K = L^{-1}U$ of an upper triangular matrix $U(x - y)$ and a lower triangular matrix $L^{-1}(x - y)$. Written out in full, the product $L^{-1}U$ is

$$K(x - y) = \int_{-\infty}^{\infty} L^{-1}(x - t)U(t - y) dt. \quad (9.106)$$

Now the inverse of a lower triangular matrix is also lower triangular, and so $L(x - y)$ itself is lower triangular. This means that the function $U(x)$ is zero for negative x , whilst $L(x)$ is zero when x is positive.

$$\begin{bmatrix} \text{grid} \\ K \end{bmatrix} = \begin{bmatrix} 0 & 0 \\ L & 0 \end{bmatrix}^{-1} \begin{bmatrix} 0 & U \\ 0 & 0 \end{bmatrix}$$

The matrix decomposition $K = L^{-1}U$.

If we can find such a decomposition, then on multiplying both sides by L , equation (9.103) becomes

$$\int_0^x U(x - y)u(y) dy = h(x), \quad 0 < x < \infty, \quad (9.107)$$

where

$$h(x) \stackrel{\text{def}}{=} \int_x^{\infty} L(x - y)f(y) dy, \quad 0 < x < \infty. \quad (9.108)$$

These two equations come from the upper half of the full matrix equation represented in the figure:

$$\begin{bmatrix} \begin{array}{c|c} \text{shaded} & \text{shaded} \\ \hline 0 & U \\ \hline 0 & 0 \end{array} & \begin{array}{c} u \\ \hline 0 \end{array} \end{bmatrix} = \begin{bmatrix} \begin{array}{c|c} \text{shaded} & \text{shaded} \\ \hline 0 & 0 \\ \hline L & 0 \end{array} & \begin{array}{c} f \\ \hline g \end{array} \end{bmatrix} \equiv \begin{bmatrix} h \\ \hline 0 \end{bmatrix}$$

The equation (9.107) and the definition (9.108) correspond to the upper half of these two matrix equations.

The lower parts of the matrix equation have no influence on (9.107) and (9.108): The function $h(x)$ depends only on f , and while $g(x)$ should be chosen to give the column of zeros below h , we do not, in principle, need to know it. This is because we could solve the Volterra equation $Uu = h$ (9.107) *via* a Laplace transform. In practice (as we will see) it is easier to find $g(x)$, and then, knowing the (f, g) column vector, obtain $u(x)$ by solving (9.105). This we can do by Fourier transform.

The difficulty lies in finding the LU decomposition. For finite matrices this decomposition is a standard technique in numerical linear algebra. It equivalent to the method of *Gaussian elimination*, which, although we were probably never told its name, is the strategy taught in high school for solving simultaneous equations. For continuously infinite matrices, however, making such a decomposition demands techniques far beyond those learned in school. It is a particular case of the scalar *Riemann-Hilbert problem*, and its solution requires the use of complex variable methods.

On taking the Fourier transform of (9.106) we see that we are being asked to factorize

$$\tilde{K}(k) = [\tilde{L}(k)]^{-1} \tilde{U}(k) \quad (9.109)$$

where

$$\tilde{U}(k) = \int_0^\infty e^{ikx} U(x) dx \quad (9.110)$$

is analytic (*i.e.* has no poles or other singularities) in the region $\text{Im } k \geq 0$, and similarly

$$\tilde{L}(k) = \int_{-\infty}^0 e^{ikx} L(x) dx \quad (9.111)$$

has no poles for $\text{Im } k \leq 0$, these analyticity conditions being consequences of the vanishing conditions $U(x - y) = 0$, $x < y$ and $L(x - y) = 0$, $x > y$. There will be more than one way of factoring \tilde{K} into functions with these no-pole properties, but, because the inverse of an upper or lower triangular matrix is also upper or lower triangular, the matrices $U^{-1}(x - y)$ and $L^{-1}(x - y)$ have the same vanishing properties, and, because these inverse matrices correspond to the reciprocals of the Fourier transform, we must also demand that $\tilde{U}(k)$ and $\tilde{L}(k)$ have no *zeros* in the upper and lower half plane respectively. The combined no-poles, no-zeros conditions will usually determine the factors up to constants. If we are able to factorize $\tilde{K}(k)$ in this manner, we have effected the LU decomposition. When $\tilde{K}(k)$ is a rational function of k we can factorize by inspection. In the general case, more sophistication is required.

Example: Let us solve the equation

$$u(x) - \lambda \int_0^\infty e^{-|x-y|} u(y) dy = f(x), \quad (9.112)$$

where we will assume that $\lambda < 1/2$. Here the kernel function is

$$K(x, y) = \delta(x - y) - \lambda e^{-|x-y|}. \quad (9.113)$$

This has Fourier transform

$$\tilde{K}(k) = 1 - \frac{2\lambda}{k^2 + 1} = \frac{k^2 + (1 - 2\lambda)}{k^2 + 1} = \left(\frac{k + ia}{k + i} \right) \left(\frac{k - i}{k - ia} \right)^{-1}. \quad (9.114)$$

where $a^2 = 1 - 2\lambda$. We were able to factorize this by inspection with

$$\tilde{U}(k) = \frac{k + ia}{k + i}, \quad \tilde{L}(k) = \frac{k - i}{k - ia}. \quad (9.115)$$

having poles and zeros only in the lower (respectively upper) half-plane. We could now transform back into x space to find $U(x - y)$, $L(x - y)$ and solve the Volterra equation $Uu = h$. It is, however, less effort to work directly with the Fourier transformed equation in the form

$$\left(\frac{k + ia}{k + i} \right) \tilde{u}_+(k) = \left(\frac{k - i}{k - ia} \right) (\tilde{f}_+(k) + \tilde{g}_-(k)). \quad (9.116)$$

Here we have placed subscripts on $\tilde{f}(k)$, $\tilde{g}(k)$ and $\tilde{u}(k)$ to remind us that these Fourier transforms are analytic in the upper (+) or lower (-) half-plane. Since

the left-hand-side of this equation is analytic in the upper half-plane, so must be the right-hand-side. We therefore choose $\tilde{g}_-(k)$ to eliminate the potential pole at $k = ia$ that might arise from the first term on the right. This we can do by setting

$$\left(\frac{k-i}{k-ia}\right)g_-(k) = \frac{\alpha}{k-ia} \quad (9.117)$$

for some as yet undetermined constant α . (Observe that the resultant $g_-(k)$ is indeed analytic in the lower half-plane. This analyticity ensures that $g(x)$ is zero for positive x .) We can now solve for $\tilde{u}(k)$ as

$$\begin{aligned} \tilde{u}(k) &= \left(\frac{k+i}{k+ia}\right)\left(\frac{k-i}{k-ia}\right)\tilde{f}_+(k) + \left(\frac{k+i}{k+ia}\right)\frac{\alpha}{k-ia} \\ &= \frac{k^2+1}{k^2+a^2}\tilde{f}_+(k) + \alpha\frac{k+i}{k^2+a^2} \\ &= \tilde{f}_+(k) + \frac{1-a^2}{k^2+a^2}\tilde{f}_+(k) + \alpha\frac{k+i}{k^2+a^2} \end{aligned} \quad (9.118)$$

The inverse Fourier transform of

$$\frac{k+i}{k^2+a^2} \quad (9.119)$$

is

$$\frac{i}{2|a|}(1-|a|\operatorname{sgn}(x))e^{-|a||x|}, \quad (9.120)$$

and that of

$$\frac{1-a^2}{k^2+a^2} = \frac{2\lambda}{k^2+(1-2\lambda)} \quad (9.121)$$

is

$$\frac{\lambda}{\sqrt{1-2\lambda}}e^{-\sqrt{1-2\lambda}|x|}. \quad (9.122)$$

Consequently

$$\begin{aligned} u(x) &= f(x) + \frac{\lambda}{\sqrt{1-2\lambda}} \int_0^\infty e^{-\sqrt{1-2\lambda}|x-y|} f(y) dy \\ &\quad + \beta(1-\sqrt{1-2\lambda}\operatorname{sgn} x)e^{-\sqrt{1-2\lambda}|x|}. \end{aligned} \quad (9.123)$$

Here β is some multiple of α , and we have used the fact that $f(y)$ is zero for negative y to make the lower limit on the integral 0 instead of $-\infty$. We

determine the as yet unknown β from the requirement that $u(x) = 0$ for $x < 0$. We find that this will be the case if we take

$$\beta = -\frac{\lambda}{a(a+1)} \int_0^\infty e^{-ay} f(y) dy. \quad (9.124)$$

The solution is therefore, for $x > 0$,

$$\begin{aligned} u(x) = & f(x) + \frac{\lambda}{\sqrt{1-2\lambda}} \int_0^\infty e^{-\sqrt{1-2\lambda}|x-y|} f(y) dy \\ & + \frac{\lambda(\sqrt{1-2\lambda}-1)}{1-2\lambda+\sqrt{1-2\lambda}} e^{-\sqrt{1-2\lambda}x} \int_0^\infty e^{-\sqrt{1-2\lambda}y} f(y) dy. \end{aligned} \quad (9.125)$$

Not every invertible n -by- n matrix has a plain LU decomposition. For a related reason not every Wiener-Hopf equation can be solved so simply. Instead there is a topological *index theorem* that determines whether solutions can exist, and, if solutions do exist, whether they are unique. We shall therefore return to this problem once we have acquired a deeper understanding of the interaction between topology and complex analysis.

9.7 Some Functional Analysis

We have hitherto avoided, as far as it is possible, the full rigours of mathematics. For most of us, and for most of the time, we can solve our physics problems by using calculus rather than analysis. It is worth, nonetheless, being familiar with the proper mathematical language so that when something tricky comes up we know where to look for help. The modern setting for the mathematical study of integral and differential equations is the discipline of *functional analysis*, and the classic text for the mathematically inclined physicist is the four-volume set *Methods of Modern Mathematical Physics* by Michael Reed and Barry Simon. We cannot summarize these volumes in few paragraphs, but we can try to provide enough background that we explain a few issues that may have puzzled the alert reader.

Unlike most of the rest of this book, this section does require that the reader know what it means for a set to be compact.

9.7.1 Bounded and Compact Operators

- i) A linear operator $K : L^2 \rightarrow L^2$ is *bounded* if there is a positive number M such that

$$\|Kx\| \leq M\|x\|, \quad \forall x \in L^2. \quad (9.126)$$

If K is bounded then smallest such M is the *norm* of K , which we denote by $\|K\|$. Thus

$$\|Kx\| \leq \|K\| \|x\|. \quad (9.127)$$

For a finite-dimensional matrix, $\|K\|$ is the largest eigenvalue of K . A linear operator is a continuous function of its argument if, and only if, it is bounded. “Bounded” and “continuous” are therefore synonyms. Linear differential operators are *never* bounded, and this is the source of most of the complications in their theory.

- ii) If the operators A and B are bounded, then so is AB and

$$\|AB\| \leq \|A\| \|B\|. \quad (9.128)$$

- iii) A linear operator $K : L^2 \rightarrow L^2$ is *compact* (or *completely continuous*) if it maps bounded sets to relatively compact sets (sets whose closure is compact). Equivalently, K is compact if the image sequence Kx_n of every bounded sequence of functions, x_n , contains a convergent subsequence. Compact \Rightarrow continuous, but not *vice versa*. One can show that, given any positive number M , a compact self-adjoint operator has only a finite number of eigenvalues with λ outside the interval $[-M, M]$. The eigenvectors u_n with non-zero eigenvalues span the range of the operator. Any vector can therefore be written

$$u = u_0 + \sum_i a_i u_i, \quad (9.129)$$

where u_0 lies in the null space of K . The Green function of a linear differential operator defined on a finite interval is usually the integral kernel of a compact operator.

- iv) If K is compact then

$$H = I + K \quad (9.130)$$

is *Fredholm*. This means that H has a finite dimensional kernel and co-kernel, and that the Fredholm alternative applies.

v) An integral kernel is *Hilbert-Schmidt* if

$$\int |K(\xi, \eta)|^2 d\xi d\eta < \infty. \quad (9.131)$$

This means that K can be expanded in terms of a complete orthonormal set $\{\phi_m\}$ as

$$K(x, y) = \sum_{n,m=1}^{\infty} A_{nm} \phi_n(x) \phi_m^*(y) \quad (9.132)$$

in the sense that

$$\left\| \sum_{n,m=1}^{N,M} A_{nm} \phi_n \phi_m^* - K \right\| \rightarrow 0. \quad (9.133)$$

Now the finite sum

$$\sum_{n,m=1}^{N,M} A_{nm} \phi_n(x) \phi_m^*(y) \quad (9.134)$$

is automatically compact since it is bounded and has finite-dimensional range. (The unit ball in a Hilbert space is relatively compact \Leftrightarrow the space is finite dimensional). Thus, Hilbert-Schmidt implies that K is approximated in norm by compact operators. But a limit of compact operators is compact, so K itself is compact. Thus

Hilbert-Schmidt \Rightarrow compact.

It is easy to test a given kernel to see if it is Hilbert-Schmidt (simply use the definition) and therein lies the utility of the concept.

If we have a Hilbert-Schmidt Green function g , we can recast our differential equation as an integral equation with g as kernel, and this is why the Fredholm alternative works for a large class of linear differential equations.

Example: Consider the Legendre equation operator

$$Lu = -[(1-x^2)u']' \quad (9.135)$$

on the interval $[-1, 1]$ with boundary conditions that u be finite at the end-points. This operator has a normalized zero mode $u_0 = 1/\sqrt{2}$, so it does not have an inverse. There exists, however, a modified Green function $g(x, x')$ that satisfies

$$Lu = \delta(x - x') - \frac{1}{2}. \quad (9.136)$$

It is

$$g(x, x') = \ln 2 - \frac{1}{2} - \frac{1}{2} \ln(1 + x_>)(1 - x_<), \quad (9.137)$$

where $x_>$ is the greater of x and x' , and $x_<$ the lesser. We may verify that

$$\int_{-1}^1 \int_{-1}^1 |g(x, x')|^2 dx dx' < \infty, \quad (9.138)$$

so g is Hilbert-Schmidt and therefore the kernel of a compact operator. The eigenvalue problem

$$Lu_n = \lambda_n u_n \quad (9.139)$$

can be recast as the integral equation

$$\mu_n u_n = \int_{-1}^1 g(x, x') u_n(x') dx' \quad (9.140)$$

with $\mu_n = \lambda_n^{-1}$. The compactness of g guarantees that there is a complete set of eigenfunctions (these being the Legendre polynomials $P_n(x)$ for $n > 0$) having eigenvalues $\mu_n = 1/n(n+1)$. The operator g also has the eigenfunction P_0 with eigenvalue $\mu_0 = 0$. This example provides the justification for the claim that the “finite” boundary conditions we adopted for the Legendre equation in chapter 8 give us a self adjoint operator.

Note that $K(x, y)$ does not have to be bounded for K to be Hilbert-Schmidt.

Example: The kernel

$$K(x, y) = \frac{1}{(x - y)^\alpha}, \quad |x|, |y| < 1 \quad (9.141)$$

is Hilbert-Schmidt provided $\alpha < \frac{1}{2}$.

Example: The kernel

$$K(x, y) = \frac{1}{2m} e^{-m|x-y|}, \quad x, y \in \mathbb{R} \quad (9.142)$$

is not Hilbert-Schmidt because $|K(x - y)|$ is constant along the lines $x - y = \text{constant}$, which lie parallel to the diagonal. K has a continuous spectrum consisting of all real numbers less than $1/m^2$. It cannot be compact, therefore, but it is bounded, and $\|K\| = 1/m^2$.

9.7.2 Closed Operators

One motivation for our including a brief account of functional analysis is that the astute reader will have realized that some of the statements we have made in earlier chapters appear to be inconsistent. We have asserted in chapter 2 that no significance can be attached to the value of an L^2 function at any particular point — only integrated averages matter. In later chapters, though, we have happily imposed boundary conditions that require these very functions to take specified values at the endpoints of our interval. In this section we will resolve this paradox. The apparent contradiction is intimately connected with our imposing boundary conditions only on derivatives of lower order than that of the differential equation, but understanding why this is so requires some function-analytic language.

Differential operators L are never continuous; we cannot deduce from $u_n \rightarrow u$ that $Lu_n \rightarrow Lu$. Differential operators can be *closed*, however. A closed operator is one for which whenever a sequence u_n converges to a limit u and at the same time the image sequence Lu_n also converges to a limit f , then u is in the domain of L and $Lu = f$. The name is not meant to imply that the domain of definition is closed, but indicates instead that the *graph* of L — this being the set $\{u, Lu\}$ considered as a subset of $L^2[a, b] \times L^2[a, b]$ — contains its limit points and so is a closed set.

Any self-adjoint operator is automatically closed. To see why this is so, recall that in the defining the adjoint of an operator A , we say that y is in the domain of A^\dagger if there is a z such that $\langle y, Ax \rangle = \langle z, x \rangle$ for all x in the domain of A . We then set $A^\dagger y = z$. Now suppose that $y_n \rightarrow y$ and $A^\dagger y_n = z_n \rightarrow z$. The Cauchy-Schwartz-Bunyakovski inequality shows that the inner product is a continuous function of its arguments. Consequently, if x is in the domain of A , we can take the limit of $\langle y_n, Ax \rangle = \langle A^\dagger y_n, x \rangle = \langle z_n, x \rangle$ to deduce that $\langle y, Ax \rangle = \langle z, x \rangle$. But this means that y is in the domain of A^\dagger , and $z = A^\dagger y$. The adjoint of any operator is therefore a closed operator. A self-adjoint operator, being its own adjoint, is therefore necessarily closed.

A deep result states that a closed operator defined on a closed domain is bounded. Since they are always unbounded, the domain of a closed differential operator can never be a closed set.

An operator may not be closed but may be *closable*, in that we can make it closed by including additional functions in its domain. The essential requirement for closability is that we never have two sequences u_n and v_n which converge to the **same** limit, w , while Lu_n and Lv_n both converge, but

to **different** limits. Closability is equivalent to requiring that if $u_n \rightarrow 0$ and Lu_n converges, then Lu_n converges to zero.

Example: Let $L = d/dx$. Suppose that $u_n \rightarrow 0$ and $Lu_n \rightarrow f$. If φ is a smooth L^2 function that vanishes at 0, 1, then

$$\int_0^1 \varphi f \, dx = \lim_{n \rightarrow \infty} \int_0^1 \varphi \frac{du_n}{dx} \, dx = - \lim_{n \rightarrow \infty} \int_0^1 \varphi' u_n \, dx = 0. \quad (9.143)$$

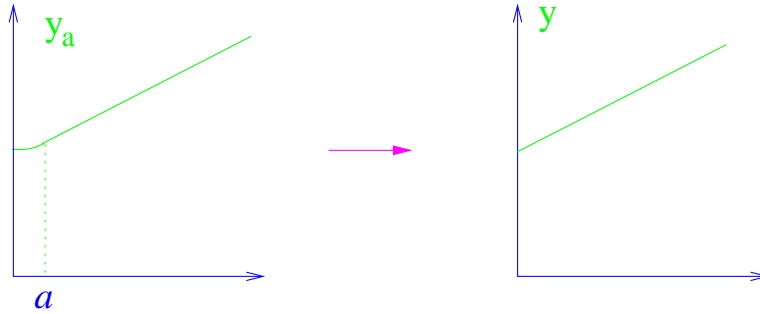
Here we have used the continuity of the inner product to justify the interchange the order of limit and integral. By the same arguments we used when dealing with the calculus of variations, we deduce that $f = 0$. Thus d/dx is closable.

If an operator is closable, we may as well add the extra functions to its domain and make it closed. Let us consider what closure means for the operator

$$L = \frac{d}{dx}, \quad \mathcal{D}(L) = \{y \in C^1[0, 1] : y'(0) = 0\}. \quad (9.144)$$

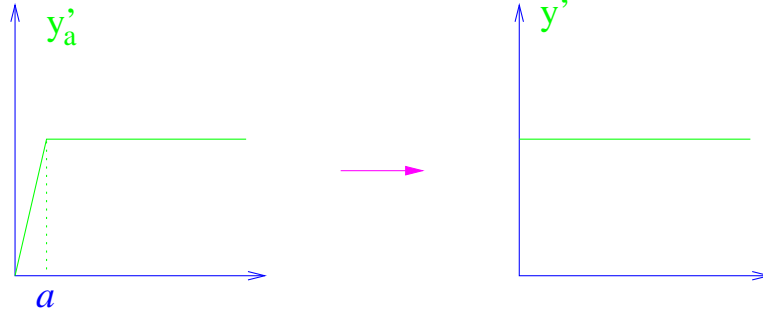
Here, in fixing the derivative at the endpoint, we are imposing a boundary condition of higher order than we ought.

Consider a sequence of differentiable functions y_a which have vanishing derivative at $x = 0$, but tend in L^2 to a function y whose derivative is non-zero at $x = 0$.



$$\lim_{a \rightarrow 0} y_a = y \text{ in } L^2[0, 1].$$

The derivative of these functions also converges in L^2 .



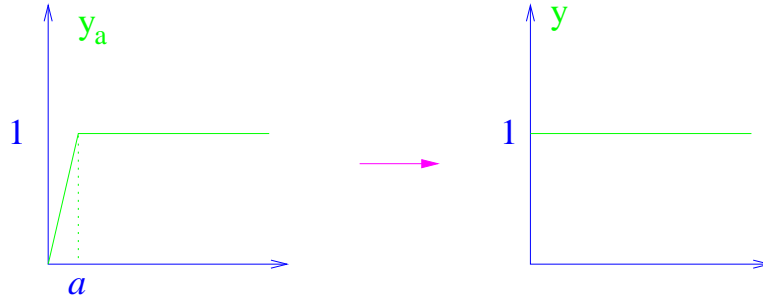
$$y'_a \rightarrow y' \text{ in } L^2[0, 1] .$$

If we want L to be closed, we should therefore extend the domain of definition of L to include functions with non-vanishing endpoint derivative. We can also use this method to add to the domain of L functions that are only *piecewise differentiable* — *i.e.* functions with a discontinuous derivative.

Now consider what happens if we try to extend the domain of

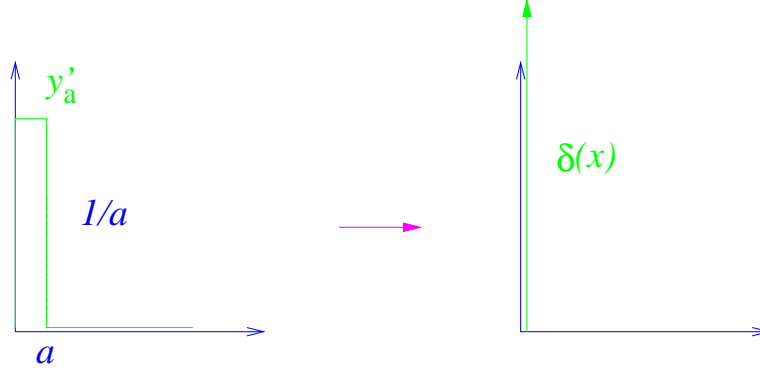
$$L = \frac{d}{dx}, \quad \mathcal{D}(L) = \{y, y' \in L^2 : y(0) = 0\}, \quad (9.145)$$

to include functions that do not vanish at the endpoint. Take a sequence of functions y_a that vanish at the origin, and converge in L^2 to a function that does not vanish at the origin:



$$\lim_{a \rightarrow 0} y_a = y \text{ in } L^2[0, 1].$$

Now the derivatives converge towards the derivative of the limit function — *together with a delta function near the origin*. The area under the functions $|y'_a(x)|^2$ grows without bound and the sequence Ly_a becomes infinitely far from the derivative of the limit function when distance is measured in the L^2 norm.



$y'_a \rightarrow \delta(x)$, but the delta function is not an element of $L^2[0, 1]$.

We therefore cannot use closure to extend the domain to include these functions. Another way of saying this is, that in order for the weak derivative of y to be in L^2 , and therefore for y to be in the domain of d/dx , the function y need not be classically differentiable, but its L^2 equivalence class must contain a *continuous* function — and continuous functions do have well-defined values. It is the values of this continuous representative that are constrained by the boundary conditions.

This story repeats for differential operators of any order: If we try to impose boundary conditions of too high an order, they are washed out in the process of closing the operator. Boundary conditions of lower order cannot be eliminated, however, and so make sense as statements involving functions in L^2 .

9.8 Series Solutions

9.8.1 Neumann Series

The geometric series

$$S = 1 - x + x^2 - x^3 + \cdots \quad (9.146)$$

converges to $1/(1+x)$ provided $|x| < 1$. Suppose we wish to solve

$$(I + \lambda K)\varphi = f \quad (9.147)$$

where K is an integral operator. It is then natural to write

$$\varphi = (I + \lambda K)^{-1}f = (1 - \lambda K + \lambda^2 K^2 - \lambda^3 K^3 + \cdots)f \quad (9.148)$$

where

$$K^2(x, y) = \int K(x, z)K(z, y) dz, \quad K^3(x, y) = \int K(x, z_1)K(z_1, z_2)K(z_2, y) dz_1 dz_2, \quad (9.149)$$

and so on. This *Neumann series* will converge, and yield a solution to the problem, provided that $\lambda\|K\| < 1$.

9.8.2 Fredholm Series

A familiar result from high-school algebra is *Cramer's rule* which gives the solution of a set of linear equations in terms of ratios of determinants. For example, the system of equations

$$\begin{aligned} a_{11}x_1 + a_{12}x_2 + a_{13}x_3 &= b_1, \\ a_{21}x_1 + a_{22}x_2 + a_{23}x_3 &= b_2, \\ a_{31}x_1 + a_{32}x_2 + a_{33}x_3 &= b_3, \end{aligned}$$

has solution

$$x_1 = \frac{1}{D} \begin{vmatrix} b_1 & a_{12} & a_{13} \\ b_2 & a_{22} & a_{23} \\ b_3 & a_{32} & a_{33} \end{vmatrix}, \quad x_2 = \frac{1}{D} \begin{vmatrix} a_{11} & b_1 & a_{13} \\ a_{21} & b_2 & a_{23} \\ a_{31} & b_3 & a_{33} \end{vmatrix}, \quad x_3 = \frac{1}{D} \begin{vmatrix} a_{11} & a_{12} & b_1 \\ a_{21} & a_{22} & b_2 \\ a_{31} & a_{32} & b_3 \end{vmatrix},$$

where

$$D = \begin{vmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{vmatrix}.$$

Although not as computationally efficient as standard Gaussian elimination, Cramer's rule is useful in that it is a closed-form solution. It is equivalent to the statement that the inverse of a matrix is given by the transposed matrix of the co-factors, divided by the determinant.

A similar formula for integral equations was given by Fredholm. The equations he considered were of the form

$$(I + \lambda K)\varphi = f. \quad (9.150)$$

We motivate Fredholm's formula by giving an expansion for the determinant of a finite matrix. Let

$$D(\lambda) = \det(\mathbf{I} + \lambda \mathbf{K}) \equiv \begin{vmatrix} 1 + \lambda K_{11} & \lambda K_{12} & \cdots & \lambda K_{1n} \\ \lambda K_{21} & 1 + \lambda K_{22} & \cdots & \lambda K_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ \lambda K_{n1} & \lambda K_{n2} & \cdots & 1 + \lambda K_{nn} \end{vmatrix}, \quad (9.151)$$

then

$$D(\lambda) = \sum_{m=0}^n \frac{\lambda^m}{m!} A_m, \quad (9.152)$$

where $A_0 = 1$, $A_1 = \text{tr } \mathbf{K} \equiv \sum_i K_{ii}$,

$$A_2 = \sum_{i_1, i_2=1}^n \begin{vmatrix} K_{i_1 i_1} & K_{i_1 i_2} \\ K_{i_2 i_1} & K_{i_2 i_2} \end{vmatrix}, \quad A_3 = \sum_{i_1, i_2, i_3=1}^n \begin{vmatrix} K_{i_1 i_1} & K_{i_1 i_2} & K_{i_1 i_3} \\ K_{i_2 i_1} & K_{i_2 i_2} & K_{i_2 i_3} \\ K_{i_3 i_1} & K_{i_3 i_2} & K_{i_3 i_3} \end{vmatrix}. \quad (9.153)$$

The pattern for the rest of the terms should be obvious, as should the proof.

As observed above, the inverse of a matrix is the reciprocal of the determinant of the matrix multiplied by the transposed matrix of the co-factors. So, if $D_{\mu\nu}$ is the co-factor of the term in $D(\lambda)$ associated with $K_{\nu\mu}$, then the solution of the equation

$$(\mathbf{I} + \lambda \mathbf{K})\mathbf{x} = \mathbf{b} \quad (9.154)$$

is

$$x_\mu = \frac{D_{\mu 1} b_1 + D_{\mu 2} b_2 + \cdots + D_{\mu n} b_n}{D(\lambda)}. \quad (9.155)$$

If $\mu \neq \nu$ we have

$$D_{\mu\nu} = \lambda K_{\mu\nu} + \lambda^2 \sum_i \begin{vmatrix} K_{\mu\nu} & K_{\mu i} \\ K_{i\nu} & K_{ii} \end{vmatrix} + \lambda^3 \frac{1}{2!} \sum_{i_1 i_2} \begin{vmatrix} K_{\mu\nu} & K_{\mu i_1} & K_{\mu i_2} \\ K_{i_1 \nu} & K_{i_1 i_1} & K_{i_1 i_2} \\ K_{i_2 \nu} & K_{i_2 i_1} & K_{i_2 i_2} \end{vmatrix} + \cdots. \quad (9.156)$$

When $\mu = \nu$ we have

$$D_{\mu\mu} = \delta_{\mu\mu} \tilde{D}(\lambda) \quad (9.157)$$

where $\tilde{D}(\lambda)$ is the expression analogous to $D(\lambda)$, but with the μ 'th row and column deleted.

These elementary results suggests the definition of the *Fredholm determinant* of the integral kernel $K(x, y)$ $a < x, y < b$, as

$$D(\lambda) = \text{Det } |I + \lambda K| \equiv \sum_{m=0}^{\infty} \frac{\lambda^m}{m!} A_m, \quad (9.158)$$

where $A_0 = 1$, $A_1 = \text{Tr } K \equiv \int_a^b K(x, x) dx$,

$$A_2 = \int_a^b \int_a^b \begin{vmatrix} K(x_1, x_1) & K(x_1, x_2) \\ K(x_2, x_1) & K(x_2, x_2) \end{vmatrix} dx_1 dx_2,$$

$$A_3 = \int_a^b \int_a^b \int_a^b \begin{vmatrix} K(x_1, x_1) & K(x_1, x_2) & K(x_1, x_3) \\ K(x_2, x_1) & K(x_2, x_2) & K(x_2, x_3) \\ K(x_3, x_1) & K(x_3, x_2) & K(x_3, x_3) \end{vmatrix} dx_1 dx_2 dx_3. \quad (9.159)$$

etc.. We also define

$$\begin{aligned} D(x, y, \lambda) = & \lambda K(x, y) + \lambda^2 \int_a^b \begin{vmatrix} K(x, y) & K(x, \xi) \\ K(\xi, y) & K(\xi, \xi) \end{vmatrix} d\xi \\ & + \lambda^3 \frac{1}{2!} \int_a^b \int_a^b \begin{vmatrix} K(x, y) & K(x, \xi_1) & K(x, \xi_2) \\ K(\xi_1, y) & K(\xi_1, \xi_1) & K(\xi_1, \xi_2) \\ K(\xi_2, y) & K(\xi_2, \xi_1) & K(\xi_2, \xi_2) \end{vmatrix} d\xi_1 d\xi_2 + \cdots, \end{aligned} \quad (9.160)$$

and then

$$\varphi(x) = f(x) + \frac{1}{D(\lambda)} \int_a^b D(x, y, \lambda) f(y) dy \quad (9.161)$$

is the solution of the equation

$$\varphi(x) + \lambda \int_a^b K(x, y) \varphi(y) dy = f(x). \quad (9.162)$$

If $|K(x, y)| < M$ in $[a, b] \times [a, b]$, the *Fredholm series* for $D(\lambda)$ and $D(x, y, \lambda)$ converge for all λ , and define entire functions. In this it is unlike the Neumann series, which has a finite radius of convergence.

The proof of these claims follows from the identity

$$D(x, y, \lambda) + \lambda D(\lambda) K(x, y) + \lambda \int_a^b D(x, \xi, \lambda) K(\xi, y) d\xi = 0, \quad (9.163)$$

or, more compactly with $G(x, y) = D(x, y, \lambda)/D(\lambda)$,

$$(I + G)(I + \lambda K) = I. \quad (9.164)$$

For details see Whitaker and Watson §11.2.

Example: The equation

$$\varphi(x) = x + \lambda \int_0^1 xy \varphi(y) dy \quad (9.165)$$

gives us

$$D(\lambda) = 1 - \frac{1}{3}\lambda, \quad D(x, y, \lambda) = \lambda xy \quad (9.166)$$

and so

$$\varphi(x) = \frac{3x}{3-\lambda}. \quad (9.167)$$

(We have seen this equation and solution before)

Exercise: Show that the equation

$$\varphi(x) = x + \lambda \int_0^1 (xy + y^2) \varphi(y) dy$$

gives

$$D(\lambda) = 1 - \frac{2}{3}\lambda - \frac{1}{72}\lambda^2$$

and

$$D(x, y, \lambda) = \lambda(xy + y^2) + \lambda^2\left(\frac{1}{2}xy^2 - \frac{1}{3}xy - \frac{1}{3}y^2 + \frac{1}{4}y\right).$$

Appendix A

Linear Algebra Review

In solving the differential equations of physics we have to work with infinite dimensional vector spaces. Navigating these vast regions is much easier if you have a sound grasp of the theory of finite dimensional spaces. Most physics students have studied this as undergraduates, but not always in a systematic way. In this appendix we gather together and review those parts of linear algebra that we will find useful in the main text.

A.1 Vector Space

A.1.1 Axioms

A *vector space* V over a field \mathbb{F} is a set equipped with two operations: a binary operation called *vector addition* which assigns to each pair of elements $\mathbf{x}, \mathbf{y} \in V$ a third element denoted by $\mathbf{x} + \mathbf{y}$, and *scalar multiplication* which assigns to an element $\mathbf{x} \in V$ and $\lambda \in \mathbb{F}$ a new element $\lambda\mathbf{x} \in V$. There is also a distinguished element $\mathbf{0} \in V$ such that the following axioms are obeyed¹:

- 1) Vector addition is commutative: $\mathbf{x} + \mathbf{y} = \mathbf{y} + \mathbf{x}$.
- 2) Vector addition is associative: $(\mathbf{x} + \mathbf{y}) + \mathbf{z} = \mathbf{x} + (\mathbf{y} + \mathbf{z})$.
- 3) Additive identity: $\mathbf{0} + \mathbf{x} = \mathbf{x}$.
- 4) Existence of additive inverse: for any $\mathbf{x} \in V$, there is an element $(-\mathbf{x}) \in V$, such that $\mathbf{x} + (-\mathbf{x}) = \mathbf{0}$.
- 5) Scalar distributive law i) $\lambda(\mathbf{x} + \mathbf{y}) = \lambda\mathbf{x} + \lambda\mathbf{y}$.
- 6) Scalar distributive law ii) $(\lambda + \mu)\mathbf{x} = \lambda\mathbf{x} + \mu\mathbf{x}$.

¹In this list $1, \lambda, \mu, \in \mathbb{F}$ and $\mathbf{x}, \mathbf{y}, \mathbf{0} \in V$.

7) Scalar multiplication is associative: $(\lambda\mu)\mathbf{x} = \lambda(\mu\mathbf{x})$.

8) Multiplicative identity: $1\mathbf{x} = \mathbf{x}$.

The elements of V are called *vectors*. We will only consider vector spaces over the field of the real numbers, $\mathbb{F} = \mathbb{R}$, or the complex numbers, $\mathbb{F} = \mathbb{C}$.

You have no doubt been working with vectors for years, and are saying to yourself “I know this stuff”. Perhaps so, but to see if you really understand these axioms try the following exercise. Its value lies not so much in the solution of its parts, which are easy, as in appreciating that these commonly used properties both can and need to be proved from the axioms. (Hint: work the problems in the order given; the later parts depend on the earlier.)

Exercise A.1: Use the axioms to show that:

- i) If $\mathbf{x} + \tilde{\mathbf{0}} = \mathbf{x}$, then $\tilde{\mathbf{0}} = \mathbf{0}$.
- ii) We have $0\mathbf{x} = \mathbf{0}$ for any $\mathbf{x} \in V$. Here 0 is the additive identity in \mathbb{R} .
- iii) If $\mathbf{x} + \mathbf{y} = \mathbf{0}$, then $\mathbf{y} = -\mathbf{x}$. Thus the additive inverse is unique.
- iv) Given \mathbf{x}, \mathbf{y} in V , there is a unique \mathbf{z} such that $\mathbf{x} + \mathbf{z} = \mathbf{y}$, to which $\mathbf{z} = \mathbf{x} - \mathbf{y}$.
- v) $\lambda\mathbf{0} = \mathbf{0}$ for any $\lambda \in \mathbb{F}$.
- vi) If $\lambda\mathbf{x} = \mathbf{0}$, then either $\mathbf{x} = \mathbf{0}$ or $\lambda = 0$.
- vii) $(-1)\mathbf{x} = -\mathbf{x}$.

A.1.2 Bases and components

Let V be a vector space over \mathbb{F} . For the moment, this space has no additional structure beyond that of the previous section — no inner product and so no notion of what it means for two vectors to be orthogonal. There is still much that can be done, though. Here are the most basic concepts and properties that you should understand:

- i) A set of vectors $\{\mathbf{e}_1, \mathbf{e}_2, \dots, \mathbf{e}_n\}$ is *linearly dependent* if there exist $\lambda^\mu \in \mathbb{F}$, not all zero, such that

$$\lambda^1\mathbf{e}_1 + \lambda^2\mathbf{e}_2 + \dots + \lambda^n\mathbf{e}_n = \mathbf{0}. \quad (\text{A.1})$$

- ii) If it is not linearly dependent, a set of vectors $\{\mathbf{e}_1, \mathbf{e}_2, \dots, \mathbf{e}_n\}$ is *linearly independent*. For a linearly independent set, a relation

$$\lambda^1\mathbf{e}_1 + \lambda^2\mathbf{e}_2 + \dots + \lambda^n\mathbf{e}_n = \mathbf{0} \quad (\text{A.2})$$

can hold only if all the λ^μ are zero.

- iii) A set of vectors $\{\mathbf{e}_1, \mathbf{e}_2, \dots, \mathbf{e}_n\}$ is said to *span* V if for any $\mathbf{x} \in V$ there are numbers x^μ such that \mathbf{x} can be written (not necessarily uniquely) as

$$\mathbf{x} = x^1 \mathbf{e}_1 + x^2 \mathbf{e}_2 + \dots + x^n \mathbf{e}_n. \quad (\text{A.3})$$

A vector space is *finite dimensional* if a finite spanning set exists.

- iv) A set of vectors $\{\mathbf{e}_1, \mathbf{e}_2, \dots, \mathbf{e}_n\}$ is a *basis* if it is a *maximal linearly independent set* (i.e. introducing any additional vector makes the set linearly dependent). An alternative definition declares a basis to be a *minimal spanning set* (i.e. deleting any of the \mathbf{e}_i destroys the spanning property). *Exercise:* Show that these two definitions are equivalent.
- v) If $\{\mathbf{e}_1, \mathbf{e}_2, \dots, \mathbf{e}_n\}$ is a basis then any $\mathbf{x} \in V$ can be written

$$\mathbf{x} = x^1 \mathbf{e}_1 + x^2 \mathbf{e}_2 + \dots + x^n \mathbf{e}_n, \quad (\text{A.4})$$

where the x^μ , the *components* of the vector with respect to this basis, are unique in that two vectors coincide if and only if they have the same components.

- vi) **Fundamental Theorem:** If the sets $\{\mathbf{e}_1, \mathbf{e}_2, \dots, \mathbf{e}_n\}$ and $\{\mathbf{f}_1, \mathbf{f}_2, \dots, \mathbf{f}_m\}$ are both bases for the space V then $m = n$. This invariant integer is the *dimension*, $\dim(V)$, of the space. For a proof (not difficult) see a mathematics text such as Birkhoff and McLane's *Survey of Modern Algebra*, or Halmos' *Finite Dimensional Vector Spaces*.

Suppose that $\{\mathbf{e}_1, \mathbf{e}_2, \dots, \mathbf{e}_n\}$ and $\{\mathbf{e}'_1, \mathbf{e}'_2, \dots, \mathbf{e}'_n\}$ are both bases, and that

$$\mathbf{e}_\nu = a^\mu_\nu \mathbf{e}'_\mu. \quad (\text{A.5})$$

Since $\{\mathbf{e}_1, \mathbf{e}_2, \dots, \mathbf{e}_n\}$ is a basis, the \mathbf{e}'_ν can also be uniquely expressed in terms of the \mathbf{e}_μ , and so the numbers a^μ_ν constitute an invertible matrix. (Note that we are, as usual, using the Einstein summation convention that repeated indices are to be summed over.) The components x'^μ of \mathbf{x} in the new basis are then found by comparing the coefficients of \mathbf{e}'_μ in

$$x'^\mu \mathbf{e}'_\mu = \mathbf{x} = x^\nu \mathbf{e}_\nu = x^\nu (a^\mu_\nu \mathbf{e}'_\mu) = (x^\nu a^\mu_\nu) \mathbf{e}'_\mu \quad (\text{A.6})$$

to be $x'^\mu = a^\mu_\nu x^\nu$, or equivalently, $x^\nu = (a^{-1})^\nu_\mu x'^\mu$. Note how the \mathbf{e}_μ and the x^μ transform in “opposite” directions. The components x^μ are therefore said to transform *contravariantly*.

A.2 Linear Maps

Let V and W be vector spaces having dimensions n and m respectively. A *linear map*, or *linear operator*, A is a function $A : V \rightarrow W$ with the property that

$$A(\lambda \mathbf{x} + \mu \mathbf{y}) = \lambda A(\mathbf{x}) + \mu A(\mathbf{y}). \quad (\text{A.7})$$

A.2.1 Matrices

A linear map is an object that exists independently of any basis. Given bases $\{\mathbf{e}_\mu\}$ for V and $\{\mathbf{f}_\nu\}$ for W , however, a map may be represented by an n -by- m *matrix*. We obtain this matrix

$$\mathbf{A} = \begin{pmatrix} a^1_1 & a^1_2 & \dots & a^1_n \\ a^2_1 & a^2_2 & \dots & a^2_n \\ \vdots & \vdots & \ddots & \vdots \\ a^m_1 & a^m_2 & \dots & a^m_n \end{pmatrix}, \quad (\text{A.8})$$

having entries a^ν_μ , by looking at the action of the map on the basis elements:

$$A(\mathbf{e}_\mu) = \mathbf{f}_\nu a^\nu_\mu. \quad (\text{A.9})$$

To make the right-hand-side of (A.9) look like a matrix product, where we sum over adjacent indices, the array a^ν_μ has been written to the *right* of the basis vector². The map $\mathbf{y} = A(\mathbf{x})$ is therefore

$$\mathbf{y} \equiv y^\nu \mathbf{f}_\nu = A(\mathbf{x}) = A(x^\mu \mathbf{e}_\mu) = x^\mu A(\mathbf{e}_\mu) = x^\mu (\mathbf{f}_\nu a^\nu_\mu) = (a^\nu_\mu x^\mu) \mathbf{f}_\nu, \quad (\text{A.10})$$

whence, comparing coefficients of \mathbf{f}_ν , we have

$$y^\nu = a^\nu_\mu x^\mu. \quad (\text{A.11})$$

The action of the linear map on *components* is therefore given by the usual matrix multiplication from the *left*: $\mathbf{y} = \mathbf{A}\mathbf{x}$, or more explicitly

$$\begin{pmatrix} y^1 \\ y^2 \\ \vdots \\ y^m \end{pmatrix} = \begin{pmatrix} a^1_1 & a^1_2 & \dots & a^1_n \\ a^2_1 & a^2_2 & \dots & a^2_n \\ \vdots & \vdots & \ddots & \vdots \\ a^m_1 & a^m_2 & \dots & a^m_n \end{pmatrix} \begin{pmatrix} x^1 \\ x^2 \\ \vdots \\ x^n \end{pmatrix}. \quad (\text{A.12})$$

²You have probably seen this “backward” action before in quantum mechanics. If we use Dirac notation $|n\rangle$ for an orthonormal basis, and insert a complete set of states, $|m\rangle\langle m|$, then $A|n\rangle = |m\rangle\langle m|A|n\rangle$. The matrix $\langle m|A|n\rangle$ representing the operator A operating on a vector from the *left* thus automatically appears to the *right* of the basis vectors used to expand the result.

The *identity map* $I : V \rightarrow V$ is represented by the n -by- n matrix

$$\mathbf{I}_n = \begin{pmatrix} 1 & 0 & 0 & \dots & 0 \\ 0 & 1 & 0 & \dots & 0 \\ 0 & 0 & 1 & \dots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & \dots & 1 \end{pmatrix}, \quad (\text{A.13})$$

which has the same entries in any basis.

Exercise A.2: Let U, V, W be vector spaces, and $A : V \rightarrow W, B : U \rightarrow V$ linear maps which are represented by the matrices \mathbf{A} with entries a^μ_ν and \mathbf{B} with entries b^μ_ν , respectively. Use the action of the maps on basis elements to show that the map $AB : U \rightarrow W$ is represented by the matrix product \mathbf{AB} whose entries are $a^\mu_\lambda b^\lambda_\nu$.

A.2.2 Range-nullspace theorem

Given a linear map $A : V \rightarrow W$, we can define two important subspaces:

- i) The *kernel* or *nullspace* is defined by

$$\text{Ker } A = \{\mathbf{x} \in V : A(\mathbf{x}) = \mathbf{0}\}. \quad (\text{A.14})$$

It is a subspace of V .

- ii) The *range* or *image* space is defined by

$$\text{Im } A = \{\mathbf{y} \in W : \mathbf{y} = A(\mathbf{x}), \mathbf{x} \in V\}. \quad (\text{A.15})$$

It is a subspace of the *target space* W .

The key result linking these spaces is the *range-nullspace theorem* which states that

$$\boxed{\dim(\text{Ker } A) + \dim(\text{Im } A) = \dim V}$$

It is proved by taking a basis, \mathbf{n}_μ , for $\text{Ker } A$ and extending it to a basis for the whole of V by appending $(\dim V - \dim(\text{Ker } A))$ extra vectors, \mathbf{e}_ν . It is easy to see that the vectors $A(\mathbf{e}_\nu)$ are linearly independent and span $\text{Im } A \subseteq W$. Note that this result is meaningless unless V is finite dimensional.

The number $\dim(\text{Im } A)$ is the number of linearly independent columns in the matrix, and is often called the (column) rank of the matrix.

A.2.3 The dual space

Associated with the vector space V is its *dual space*, V^* , which is the set of linear maps $f : V \rightarrow \mathbb{F}$. In other words the set of linear functions $f(\)$ that take in a vector and return a number. These functions are often also called *covectors*. (Mathematicians place the prefix *co-* in front of the name of a mathematical object to indicate a dual class of objects, consisting of the set of structure-preserving maps of the original objects into the field over which they are defined.)

Using linearity we have

$$f(\mathbf{x}) = f(x^\mu \mathbf{e}_\mu) = x^\mu f(\mathbf{e}_\mu) = x^\mu f_\mu. \quad (\text{A.16})$$

The set of numbers $f_\mu = f(\mathbf{e}_\mu)$ are the components of the covector $f \in V^*$. If we change basis $\mathbf{e}_\nu = a^\mu_\nu \mathbf{e}'_\mu$ then

$$f_\nu = f(\mathbf{e}_\nu) = f(a^\mu_\nu \mathbf{e}'_\mu) = a^\mu_\nu f(\mathbf{e}'_\mu) = a^\mu_\nu f'_\mu. \quad (\text{A.17})$$

Thus $f_\nu = a^\mu_\nu f'_\mu$ and the f_μ components transform in the same manner as the basis. They are therefore said to transform *covariantly*.

Given a basis \mathbf{e}_μ of V , we can define a *dual basis* for V^* as the set of covectors $\mathbf{e}^{*\mu} \in V^*$ such that

$$\mathbf{e}^{*\mu}(\mathbf{e}_\nu) = \delta^\mu_\nu. \quad (\text{A.18})$$

It should be clear that this is a basis for V^* , and that f can be expanded

$$f = f_\mu \mathbf{e}^{*\mu}. \quad (\text{A.19})$$

Although the spaces V and V^* have the same dimension, and are therefore isomorphic, there is no natural map between them. The assignment $\mathbf{e}_\mu \mapsto \mathbf{e}^{*\mu}$ is *unnatural* because it depends on the choice of basis.

One way of driving home the distinction between V and V^* is to consider the space V of fruit orders at a grocers. Assume that the grocer stocks only apples, oranges and pears. The elements of V are then vectors such as

$$\mathbf{x} = 3\text{kg } \mathbf{apples} + 4.5\text{kg } \mathbf{oranges} + 2\text{kg } \mathbf{pears}. \quad (\text{A.20})$$

Take V^* to be the space of possible price lists, an example element being

$$f = (\pounds 3.00/\text{kg}) \mathbf{apples}^* + (\pounds 2.00/\text{kg}) \mathbf{oranges}^* + (\pounds 1.50/\text{kg}) \mathbf{pears}^*. \quad (\text{A.21})$$

The evaluation of f on \mathbf{x}

$$f(\mathbf{x}) = 3 \times \pounds 3.00 + 4.5 \times \pounds 2.00 + 2 \times \pounds 1.50 = \pounds 21.00, \quad (\text{A.22})$$

then returns the total cost of the order. You should have no difficulty in distinguishing between a price list and box of fruit!

We may consider the original vector space V to be the dual space of V^* since, given vectors in $\mathbf{x} \in V$ and $f \in V^*$, we naturally define $\mathbf{x}(f)$ to be $f(\mathbf{x})$. Thus $(V^*)^* = V$. Instead of giving one space priority as being the set of linear functions on the other, we can treat V and V^* on an equal footing. We then speak of the *pairing* of $\mathbf{x} \in V$ with $f \in V^*$ to get a number in the field. It is then common to use the notation (f, \mathbf{x}) to mean either of $f(\mathbf{x})$ or $\mathbf{x}(f)$. **Warning:** despite the similarity of the notation, do not fall into the trap of thinking of the pairing (f, \mathbf{x}) as an inner product (see next section) of f with \mathbf{x} . The two objects being paired live in different spaces. In an inner product, the vectors being multiplied live in the same space.

A.3 Inner-Product Spaces

Some vector spaces V come equipped with an inner (or scalar) product. This additional structure allows us to relate V and V^* .

A.3.1 Inner products

We will use the symbol $\langle \mathbf{x}, \mathbf{y} \rangle$ to denote an *inner product*. An inner (or *scalar*) product is a conjugate-symmetric, sesquilinear, non-degenerate map $V \times V \rightarrow \mathbb{F}$. In this string of jargon, the phrase *conjugate symmetric* means that

$$\langle \mathbf{x}, \mathbf{y} \rangle = \langle \mathbf{y}, \mathbf{x} \rangle^*, \quad (\text{A.23})$$

where the “ $*$ ” denotes complex conjugation, and *sesquilinear*³ means

$$\langle \mathbf{x}, \lambda \mathbf{y} + \mu \mathbf{z} \rangle = \lambda \langle \mathbf{x}, \mathbf{y} \rangle + \mu \langle \mathbf{x}, \mathbf{z} \rangle, \quad (\text{A.24})$$

$$\langle \lambda \mathbf{x} + \mu \mathbf{y}, \mathbf{z} \rangle = \lambda^* \langle \mathbf{x}, \mathbf{z} \rangle + \mu^* \langle \mathbf{y}, \mathbf{z} \rangle. \quad (\text{A.25})$$

The product is therefore linear in the second slot, but *anti-linear* in the first. When our field is the real numbers \mathbb{R} then the complex conjugation is

³*Sesqui* is a Latin prefix meaning “one-and-a-half”.

redundant and the product will be symmetric

$$\langle \mathbf{x}, \mathbf{y} \rangle = \langle \mathbf{y}, \mathbf{x} \rangle, \quad (\text{A.26})$$

and bilinear

$$\langle \mathbf{x}, \lambda \mathbf{y} + \mu \mathbf{z} \rangle = \lambda \langle \mathbf{x}, \mathbf{y} \rangle + \mu \langle \mathbf{x}, \mathbf{z} \rangle, \quad (\text{A.27})$$

$$\langle \lambda \mathbf{x} + \mu \mathbf{y}, \mathbf{z} \rangle = \lambda \langle \mathbf{x}, \mathbf{z} \rangle + \mu \langle \mathbf{y}, \mathbf{z} \rangle. \quad (\text{A.28})$$

The term *non-degenerate* means that $\langle \mathbf{x}, \mathbf{y} \rangle = 0$ for all \mathbf{y} implies that $\mathbf{x} = \mathbf{0}$. Many inner products satisfy the stronger condition of being *positive definite*. This means that $\langle \mathbf{x}, \mathbf{x} \rangle > 0$, unless $\mathbf{x} = \mathbf{0}$, when $\langle \mathbf{x}, \mathbf{x} \rangle = 0$. Positive definiteness implies non-degeneracy, but not *vice-versa*.

Given a basis \mathbf{e}_μ , we can form the pairwise products

$$\langle \mathbf{e}_\mu, \mathbf{e}_\nu \rangle = g_{\mu\nu}. \quad (\text{A.29})$$

If the array of numbers $g_{\mu\nu}$ constituting the components of the *metric tensor* turns out to be $g_{\mu\nu} = \delta_{\mu\nu}$, then we say that the basis is *orthonormal* with respect to the inner product. We will not assume orthonormality without specifically saying so. The non-degeneracy of the inner product guarantees the existence of a matrix $g^{\mu\nu}$ which is the inverse of $g_{\mu\nu}$, *i.e.* $g_{\mu\nu} g^{\nu\lambda} = \delta_\mu^\lambda$.

If we take our field to be the real numbers \mathbb{R} then the additional structure provided by a non-degenerate inner product allows us to identify V with V^* . For any $f \in V^*$ we can find a vector $\mathbf{f} \in V$ such that

$$f(\mathbf{x}) = \langle \mathbf{f}, \mathbf{x} \rangle. \quad (\text{A.30})$$

In components, we solve the equation

$$f_\mu = g_{\mu\nu} f^\nu \quad (\text{A.31})$$

for f^ν . We find $f^\nu = g^{\nu\mu} f_\mu$. Usually, we simply identify f with \mathbf{f} , and hence V with V^* . We say that the *covariant components* f_μ are related to the *contravariant components* f^μ by *raising*

$$f^\mu = g^{\mu\nu} f_\nu, \quad (\text{A.32})$$

or *lowering*

$$f_\mu = g_{\mu\nu} f^\nu, \quad (\text{A.33})$$

the indices using the metric tensor. Obviously, this identification depends crucially on the inner product; a different inner product would, in general, identify an $f \in V^*$ with a completely different $\mathbf{f} \in V$.

A.3.2 Euclidean vectors

Consider \mathbb{R}^n equipped with its Euclidean metric and associated “dot” inner product. Given a vector \mathbf{x} and a basis \mathbf{e}_μ with $g_{\mu\nu} = \mathbf{e}_\mu \cdot \mathbf{e}_\nu$, we can define two sets of components for the same vector. Firstly the coefficients x^μ appearing in the basis expansion

$$\mathbf{x} = x^\mu \mathbf{e}_\mu,$$

and secondly the “components”

$$x_\mu = \mathbf{x} \cdot \mathbf{e}_\mu = g_{\mu\nu} x^\nu,$$

of \mathbf{x} along the basis vectors. The x_μ are obtained from the x^μ by the same “lowering” operation as before, and so x^μ and x_μ are naturally referred to as the contravariant and covariant components, respectively, of the vector \mathbf{x} . When the \mathbf{e}_μ constitute an orthonormal basis, then $g_{\mu\nu} = \delta_{\mu\nu}$ and the two sets of components are numerically coincident.

A.3.3 Bra and ket vectors

When our vector space is over the field of the complex numbers, the anti-linearity of the first slot of the inner product means we can no longer make a simple identification of V with V^* . Instead there is an *anti-linear* correspondence between the two spaces. The vector $\mathbf{x} \in V$ is mapped to $\langle \mathbf{x}, \rangle$ which, since it returns a number when a vector is inserted into its vacant slot, is an element of V^* . This mapping is anti-linear because

$$\lambda \mathbf{x} + \mu \mathbf{y} \mapsto \langle \lambda \mathbf{x} + \mu \mathbf{y}, \rangle = \lambda^* \langle \mathbf{x}, \rangle + \mu^* \langle \mathbf{y}, \rangle. \quad (\text{A.34})$$

This antilinear map is probably familiar to you from quantum mechanics, where V is the space of Dirac’s “ket” vectors $|\psi\rangle$ and V^* the space of “bra” vectors $\langle\psi|$. The symbol, here ψ , in each of these objects is a label distinguishing one state-vector from another. We often use the eigenvalues of some complete set of commuting operators. To each vector $|\psi\rangle$ we use the $(\dots)^\dagger$ map to assign it a dual vector

$$|\psi\rangle \mapsto |\psi\rangle^\dagger \equiv \langle\psi|$$

having the same labels. The dagger map is defined to be antilinear

$$(\lambda|\psi\rangle + \mu|\chi\rangle)^\dagger = \lambda^* \langle\psi| + \mu^* \langle\chi|, \quad (\text{A.35})$$

and Dirac denoted the number resulting from the pairing of the covector $\langle\psi|$ with the vector $|\chi\rangle$ by the “bra-c-ket” symbol $\langle\psi|\chi\rangle$:

$$\langle\psi|\chi\rangle \stackrel{\text{def}}{=} (\langle\psi|, |\chi\rangle). \quad (\text{A.36})$$

We can regard the dagger map as either determining the inner-product on V *via*

$$\langle|\psi\rangle, |\chi\rangle\rangle \stackrel{\text{def}}{=} (|\psi\rangle^\dagger, |\chi\rangle) = (\langle\psi|, |\chi\rangle) \equiv \langle\psi|\chi\rangle, \quad (\text{A.37})$$

or being determined by it as

$$|\psi\rangle^\dagger \stackrel{\text{def}}{=} \langle|\psi\rangle, \rangle \equiv \langle\psi|. \quad (\text{A.38})$$

When we represent our vectors by their components with respect to an orthonormal basis, the dagger map is the familiar operation of taking the conjugate transpose,

$$\begin{pmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{pmatrix} \mapsto \begin{pmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{pmatrix}^\dagger = (x_1^*, x_2^*, \dots, x_n^*) \quad (\text{A.39})$$

but this is not true in general. In a non-orthogonal basis the column vector with components x^μ is mapped to the row vector with components $(x^\dagger)_\mu = (x^\nu)^* g_{\nu\mu}$.

Much of Dirac notation tacitly assumes an orthonormal basis. For example, in the expansion

$$|\psi\rangle = \sum_n |n\rangle \langle n|\psi\rangle \quad (\text{A.40})$$

the expansion coefficients $\langle n|\psi\rangle$ should be the *contravariant* components of $|\psi\rangle$, but the $\langle n|\psi\rangle$ have been obtained from the inner product, and so are in fact its *covariant* components. The expansion (A.40) is therefore valid only when the $|n\rangle$ constitute an orthonormal basis. This will always be the case when the labels on the states show them to be the eigenvectors of a complete commuting set of observables, but sometimes, for example, we may use the integer “ n ” to refer to an orbital centered on a particular atom in a crystal, and then $\langle n|m\rangle \neq \delta_{mn}$. When using such a non-orthonormal basis it is safer not to use Dirac notation.

Conjugate operator

A linear map $A : V \rightarrow W$ automatically induces a map $A^* : W^* \rightarrow V^*$. Given $f \in W^*$ we can evaluate $f(A(\mathbf{x}))$ for any \mathbf{x} in V , and so $f(A(\cdot))$ is an element of V^* that we may denote by $A^*(f)$. Thus,

$$A^*(f)(\mathbf{x}) = f(A(\mathbf{x})). \quad (\text{A.41})$$

Functional analysts call A^* the *conjugate* of A . The word “conjugate” and the symbol A^* is rather unfortunate as it has the potential for generating confusion⁴ — not least because the $(\dots)^*$ map is *linear*. No complex conjugation is involved. Thus

$$(\lambda A + \mu B)^* = \lambda A^* + \mu B^*. \quad (\text{A.42})$$

Dirac deftly sidesteps this notational problem by writing $\langle \psi | A$ for the action of the conjugate of the operator $A : V \rightarrow V$ on the bra vector $\langle \psi | \in V^*$. After setting $f \rightarrow \langle \psi |$ and $\mathbf{x} \rightarrow |\chi\rangle$, equation (A.41) therefore reads

$$(\langle \psi | A) |\chi\rangle = \langle \psi | (A |\chi\rangle). \quad (\text{A.43})$$

This shows that it does not matter where we place the parentheses, so Dirac simply drops them and uses one symbol $\langle \psi | A |\chi\rangle$ to represent both sides of (A.43). Dirac notation thus avoids the non-complex-conjugating “*” by suppressing the distinction between an operator and its conjugate. If, therefore, for some reason we need to make the distinction, we cannot use Dirac notation.

Exercise A.3: If $A : V \rightarrow V$ and $B : V \rightarrow V$ show that $(AB)^* = B^* A^*$.

Exercise A.4: How does the reversal of the operator order in the previous exercise manifest itself in Dirac notation?

A.3.4 Adjoint operator

The “conjugate” operator of the previous section does not require an inner product for its definition, and is a map from V^* to V^* . When we do have an inner product, however, we can use it to define a different operator “conjugate” to A that, like A itself, is a map from V to V . This new conjugate is

⁴The terms *dual*, *transpose*, or *adjoint* are sometimes used in place of “conjugate.” Each of these words brings its own capacity for confusion.

called the *adjoint* or the *Hermitian conjugate* of A . To construct it, we first remind ourselves that for any linear map $f : V \rightarrow \mathbb{C}$, there is a vector $\mathbf{f} \in V$ such that $f(\mathbf{x}) = \langle \mathbf{f}, \mathbf{x} \rangle$. (To find it we simply solve $f_\nu = (f^\mu)^* g_{\mu\nu}$ for f^μ .) We next observe that $\mathbf{x} \mapsto \langle \mathbf{y}, A\mathbf{x} \rangle$ is such a linear map, and so there is a \mathbf{z} such that $\langle \mathbf{y}, A\mathbf{x} \rangle = \langle \mathbf{z}, \mathbf{x} \rangle$. It should be clear that \mathbf{z} depends linearly on \mathbf{y} , so we may define the adjoint linear map, A^\dagger , by setting $A^\dagger \mathbf{y} = \mathbf{z}$. This gives us the identity

$$\boxed{\langle \mathbf{y}, A\mathbf{x} \rangle = \langle A^\dagger \mathbf{y}, \mathbf{x} \rangle}$$

The correspondence $A \mapsto A^\dagger$ is anti-linear

$$(\lambda A + \mu B)^\dagger = \lambda^* A^\dagger + \mu^* B^\dagger. \quad (\text{A.44})$$

The adjoint of A depends on the inner product being used to define it. Different inner products give different A^\dagger 's.

In the particular case that our chosen basis \mathbf{e}_μ is orthonormal with respect to the inner product, *i.e.*

$$\langle \mathbf{e}_\mu, \mathbf{e}_\nu \rangle = \delta_{\mu\nu}, \quad (\text{A.45})$$

then the Hermitian conjugate A^\dagger of the operator A is represented by the Hermitian conjugate matrix \mathbf{A}^\dagger which is obtained from the matrix \mathbf{A} by interchanging rows and columns and complex conjugating the entries.

Exercise A.5: Show that $(AB)^\dagger = B^\dagger A^\dagger$.

Exercise A.6: When the basis is not orthonormal, show that

$$(A^\dagger)^\rho{}_\sigma = (g_{\sigma\mu} A^\mu{}_\nu g^{\nu\rho})^*. \quad (\text{A.46})$$

A.4 Sums and Differences of Vector Spaces

A.4.1 Direct sums

Suppose that U and V are vector spaces. We define their *direct sum* $U \oplus V$ to be the vector space of ordered pairs (\mathbf{u}, \mathbf{v}) with

$$\lambda(\mathbf{u}_1, \mathbf{v}_1) + \mu(\mathbf{u}_2, \mathbf{v}_2) = (\lambda\mathbf{u}_1 + \mu\mathbf{u}_2, \lambda\mathbf{v}_1 + \mu\mathbf{v}_2). \quad (\text{A.47})$$

The set of vectors $\{(\mathbf{u}, 0)\} \subset U \oplus V$ forms a copy of U , and $\{(0, \mathbf{v})\} \subset U \oplus V$ a copy of V . Thus U and V may be regarded as subspaces of $U \oplus V$.

If U and V are any pair of subspaces of W , we can form the space $U + V$ consisting of all elements of W that can be written as $\mathbf{u} + \mathbf{v}$ with $\mathbf{u} \in U$ and $\mathbf{v} \in V$. The decomposition $\mathbf{x} = \mathbf{u} + \mathbf{v}$ of an element $\mathbf{x} \in U + V$ into parts in U and V will be unique (in that $\mathbf{u}_1 + \mathbf{v}_1 = \mathbf{u}_2 + \mathbf{v}_2$ implies that $\mathbf{u}_1 = \mathbf{u}_2$ and $\mathbf{v}_1 = \mathbf{v}_2$) if and only if $U \cap V = \{\mathbf{0}\}$ where $\{\mathbf{0}\}$ is the subspace containing only the zero vector. In this case $U + V$ can be identified with $U \oplus V$.

If U is a subspace of W then we can seek a *complementary space* V such that $W = U \oplus V$, or, equivalently, $W = U + V$ with $U \cap V = \{\mathbf{0}\}$. Such complementary spaces are *not* unique. Consider \mathbb{R}^3 , for example, with U being the vectors in the x, y plane. If \mathbf{e} is any vector that does not lie in this plane then the one-dimensional space spanned by \mathbf{e} is a complementary space for U .

A.4.2 Quotient spaces

We have seen that if U is a subspace of W there are many complementary subspaces V such that $W = U \oplus V$. We may however define a *unique* space that we could write as $W - U$ and call it the difference of the two spaces. It is more common, however, to see this space written as W/U and referred to as the *quotient* of W *modulo* U . This quotient space is the vector space of *equivalence classes* of vectors, where we do not distinguish between two vectors in W if their difference lies in U . In other words

$$\mathbf{x} = \mathbf{y} \pmod{U} \iff \mathbf{x} - \mathbf{y} \in U. \quad (\text{A.48})$$

The collection of elements in W that are equivalent to $\mathbf{x} \pmod{U}$ composes a *coset*, written $\mathbf{x} + U$, a set whose elements are $\mathbf{x} + \mathbf{u}$ where \mathbf{u} is any vector in U . These cosets are the elements of W/U .

If we have a positive-definite inner product we can also define a unique *orthogonal complement* of $U \subset W$. We define U^\perp to be the set

$$U^\perp = \{\mathbf{x} \in W : \langle \mathbf{x}, \mathbf{y} \rangle = 0, \forall \mathbf{y} \in U\}. \quad (\text{A.49})$$

It is easy to see that this is a linear subspace and that $U \oplus U^\perp = W$. For finite dimensional spaces

$$\dim W/U = \dim U^\perp = \dim W - \dim U$$

and $(U^\perp)^\perp = U$. For infinite dimensional spaces we only have $(U^\perp)^\perp \supseteq U$. (Be careful, however. If the inner product is *not* positive definite, U and U^\perp may have non-zero vectors in common.)

Although they have the same dimensions, do not confuse W/U with U^\perp , and in particular do not use the phrase *orthogonal complement* without specifying an inner product.

A practical example of a quotient space occurs in digital imaging. A colour camera reduces the infinite-dimensional space \mathcal{L} of coloured light incident on each pixel to three numbers, R , G and B , these obtained by pairing the spectral intensity with the frequency response (an element of \mathcal{L}^*) of the red, green and blue detectors at that point. The space of distinguishable colours is therefore only three dimensional. Many different incident spectra will give the same output RGB signal, and are therefore equivalent as far as the camera is concerned. In the colour industry these equivalent colours are called *metamers*. Equivalent colours differ by spectral intensities that lie in the space \mathcal{B} of *metameric black*. There is no inner product here, so it is meaningless to think of the space of distinguishable colours as being \mathcal{B}^\perp . It is, however, precisely what we mean by \mathcal{L}/\mathcal{B} .

When we have a linear map $A : U \rightarrow V$, the quotient space $V/\text{Im } A$ is often called the *co-kernel* of A .

A.4.3 Projection-operator decompositions

An operator $P : V \rightarrow V$ that obeys $P^2 = P$ is called a *projection operator*. It projects a vector $\mathbf{x} \in V$ to $P\mathbf{x} \in \text{Im } P$ *along* $\text{Ker } P$ — in the sense of casting a shadow onto $\text{Im } P$ with the light coming from the direction $\text{Ker } P$. In other words all vectors lying in $\text{Ker } P$ are killed, whilst any vector already in $\text{Im } P$ is left alone by P . (If $\mathbf{x} \in \text{Im } P$ then $\mathbf{x} = P\mathbf{y}$ for some $\mathbf{y} \in V$, and $P\mathbf{x} = P^2\mathbf{y} = P\mathbf{y} = \mathbf{x}$.) The only vector common to both $\text{Ker } P$ and $\text{Im } P$ is $\mathbf{0}$, and so

$$V = \text{Ker } P \oplus \text{Im } P. \quad (\text{A.50})$$

Exercise A.7: Let P_1 be a projection operator. Show that $P_2 = I - P_1$ is also a projection operator and $P_1 P_2 = 0$. Show also that $\text{Im } P_2 = \text{Ker } P_1$ and $\text{Ker } P_2 = \text{Im } P_1$.

A.5 Inhomogeneous Linear Equations

Suppose we wish to solve the system of linear equations

$$a_{11}y_1 + a_{12}y_2 + \cdots + a_{1n}y_n = b_1$$

$$\begin{array}{rcl}
a_{21}y_1 + a_{22}y_2 + \cdots + a_{2n}y_n & = & b_2 \\
\vdots & & \vdots \\
a_{m1}y_1 + a_{m2}y_2 + \cdots + a_{mn}y_n & = & b_m
\end{array}$$

or, in matrix notation,

$$\mathbf{A}\mathbf{y} = \mathbf{b}, \quad (\text{A.51})$$

where \mathbf{A} is the n -by- m matrix with entries a_{ij} . Faced with such a problem, we should start by asking ourselves the questions:

- i) Does a solution exist?
- ii) If a solution does exist, is it unique?

These issues are best addressed by considering the matrix \mathbf{A} as a linear operator $A : V \rightarrow W$, where V is n dimensional and W is m dimensional. The natural language is then that of the range and nullspaces of A . There is no solution to the equation $\mathbf{A}\mathbf{y} = \mathbf{b}$ when $\text{Im } A$ is not the whole of W and \mathbf{b} does not lie in $\text{Im } A$. Similarly, the solution will not be unique if there are distinct vectors $\mathbf{x}_1, \mathbf{x}_2$ such that $A\mathbf{x}_1 = A\mathbf{x}_2$. This means that $A(\mathbf{x}_1 - \mathbf{x}_2) = \mathbf{0}$, or $(\mathbf{x}_1 - \mathbf{x}_2) \in \text{Ker } A$. These situations are linked, as we have seen, by the range null-space theorem:

$$\dim(\text{Ker } A) + \dim(\text{Im } A) = \dim V. \quad (\text{A.52})$$

Thus, if $m > n$ there are bound to be some vectors \mathbf{b} for which no solution exists. When $m < n$ the solution cannot be unique.

A.5.1 Rank and index

Suppose $V \equiv W$ (so $m = n$ and the matrix is square) and we chose an inner product, $\langle \mathbf{x}, \mathbf{y} \rangle$, on V . Then $\mathbf{x} \in \text{Ker } A$ implies that, for all \mathbf{y}

$$0 = \langle \mathbf{y}, A\mathbf{x} \rangle = \langle A^\dagger \mathbf{y}, \mathbf{x} \rangle, \quad (\text{A.53})$$

or that \mathbf{x} is perpendicular to the range of A^\dagger . Conversely, let \mathbf{x} be perpendicular to the range of A^\dagger ; then

$$\langle \mathbf{x}, A^\dagger \mathbf{y} \rangle = 0, \quad \forall \mathbf{y} \in V, \quad (\text{A.54})$$

which means that

$$\langle A\mathbf{x}, \mathbf{y} \rangle = 0, \quad \forall \mathbf{y} \in V, \quad (\text{A.55})$$

and, by the non-degeneracy of the inner product, this means that $A\mathbf{x} = \mathbf{0}$. The net result is that

$$\text{Ker } A = (\text{Im } A^\dagger)^\perp. \quad (\text{A.56})$$

Similarly

$$\text{Ker } A^\dagger = (\text{Im } A)^\perp. \quad (\text{A.57})$$

Now

$$\begin{aligned} \dim(\text{Ker } A) + \dim(\text{Im } A) &= \dim V, \\ \dim(\text{Ker } A^\dagger) + \dim(\text{Im } A^\dagger) &= \dim V, \end{aligned} \quad (\text{A.58})$$

but

$$\begin{aligned} \dim(\text{Ker } A) &= \dim(\text{Im } A^\dagger)^\perp \\ &= \dim V - \dim(\text{Im } A^\dagger) \\ &= \dim(\text{Ker } A^\dagger). \end{aligned}$$

Thus, for finite-dimensional square matrices, we have

$$\boxed{\dim(\text{Ker } A) = \dim(\text{Ker } A^\dagger)}$$

In particular, the row and column rank of a square matrix coincide.

Example: Consider the matrix

$$\mathbf{A} = \begin{pmatrix} 1 & 2 & 3 \\ 1 & 1 & 1 \\ 2 & 3 & 4 \end{pmatrix}$$

Clearly, the number of linearly independent rows is two, since the third row is the sum of the other two. The number of linearly independent columns is also two — although less obviously so — because

$$-\begin{pmatrix} 1 \\ 1 \\ 2 \end{pmatrix} + 2\begin{pmatrix} 2 \\ 1 \\ 3 \end{pmatrix} = \begin{pmatrix} 3 \\ 1 \\ 4 \end{pmatrix}.$$

Warning: The equality $\dim(\text{Ker } A) = \dim(\text{Ker } A^\dagger)$, need not hold in infinite dimensional spaces. Consider the space with basis $\mathbf{e}_1, \mathbf{e}_2, \mathbf{e}_3, \dots$ indexed by the positive integers. Define $A\mathbf{e}_1 = \mathbf{e}_2$, $A\mathbf{e}_2 = \mathbf{e}_3$, and so on. This operator has $\dim(\text{Ker } A) = 0$. The adjoint with respect to the natural inner

product has $A^\dagger \mathbf{e}_1 = \mathbf{0}$, $A^\dagger \mathbf{e}_2 = \mathbf{e}_1$, $A^\dagger \mathbf{e}_3 = \mathbf{e}_2$. Thus $\text{Ker } A^\dagger = \{\mathbf{e}_1\}$, and $\dim(\text{Ker } A^\dagger) = 1$. The difference $\dim(\text{Ker } A) - \dim(\text{Ker } A^\dagger)$ is called the *index* of the operator. The index of an operator is often related to topological properties of the space on which it acts, and in this way appears in physics as the origin of *anomalies* in quantum field theory.

A.5.2 Fredholm alternative

The results of the previous section can be summarized as saying that the *Fredholm Alternative* holds for finite square matrices. The Fredholm Alternative is the set of statements

I. Either

i) $A\mathbf{x} = \mathbf{b}$ has a *unique* solution,

or

ii) $A\mathbf{x} = \mathbf{0}$ has a solution.

II. If $A\mathbf{x} = \mathbf{0}$ has n linearly independent solutions, then so does $A^\dagger \mathbf{x} = \mathbf{0}$.

III. If alternative ii) holds, then $A\mathbf{x} = \mathbf{b}$ has *no* solution unless \mathbf{b} is orthogonal to all solutions of $A^\dagger \mathbf{x} = \mathbf{0}$.

It should be obvious that this is a recasting of the statements that

$$\dim(\text{Ker } A) = \dim(\text{Ker } A^\dagger),$$

and

$$(\text{Ker } A^\dagger)^\perp = \text{Im } A. \quad (\text{A.59})$$

Notice that finite-dimensionality is essential here. Neither of these statements is guaranteed to be true in infinite dimensional spaces.

A.6 Determinants

A.6.1 Skew-symmetric n -linear Forms

You will be familiar with the elementary definition of the determinant of an n -by- n matrix \mathbf{A} having entries a_{ij} :

$$\det \mathbf{A} \equiv \begin{vmatrix} a_{11} & a_{12} & \cdots & a_{1n} \\ a_{21} & a_{22} & \cdots & a_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ a_{n1} & a_{n2} & \cdots & a_{nn} \end{vmatrix} \stackrel{\text{def}}{=} \epsilon_{i_1 i_2 \dots i_n} a_{1i_1} a_{2i_2} \cdots a_{ni_n}. \quad (\text{A.60})$$

Here, $\epsilon_{i_1 i_2 \dots i_n}$ is the *Levi-Civita* symbol, which is skew-symmetric in all its indices and $\epsilon_{12 \dots n} = 1$. From this definition we see that the determinant changes sign if any pair of its rows are interchanged, and that it is linear in each row. In other words

$$\begin{vmatrix} \lambda a_{11} + \mu b_{11} & \lambda a_{12} + \mu b_{12} & \dots & \lambda a_{1n} + \mu b_{1n} \\ c_{21} & c_{22} & \dots & c_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ c_{n1} & c_{n2} & \dots & c_{nn} \end{vmatrix} = \lambda \begin{vmatrix} a_{11} & a_{12} & \dots & a_{1n} \\ c_{21} & c_{22} & \dots & c_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ c_{n1} & c_{n2} & \dots & c_{nn} \end{vmatrix} + \mu \begin{vmatrix} b_{11} & b_{12} & \dots & b_{1n} \\ c_{21} & c_{22} & \dots & c_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ c_{n1} & c_{n2} & \dots & c_{nn} \end{vmatrix}.$$

If we consider each row as being the components of a vector in an n -dimensional vector space V , we may regard the determinant as being a skew-symmetric n -linear form, *i.e.* a map

$$\omega : \overbrace{V \times V \times \dots V}^{n \text{ factors}} \rightarrow \mathbb{F} \quad (\text{A.61})$$

which is linear in each slot,

$$\omega(\lambda \mathbf{a} + \mu \mathbf{b}, \mathbf{c}_2, \dots, \mathbf{c}_n) = \lambda \omega(\mathbf{a}, \mathbf{c}_2, \dots, \mathbf{c}_n) + \mu \omega(\mathbf{b}, \mathbf{c}_2, \dots, \mathbf{c}_n), \quad (\text{A.62})$$

and changes sign when any two arguments are interchanged,

$$\omega(\dots, \mathbf{a}_i, \dots, \mathbf{a}_j, \dots) = -\omega(\dots, \mathbf{a}_j, \dots, \mathbf{a}_i, \dots). \quad (\text{A.63})$$

We will denote the space of skew-symmetric n -linear forms on V by the symbol $\bigwedge^n(V^*)$. Let ω be an arbitrary skew-symmetric n -linear form in $\bigwedge^n(V^*)$, and let $\{\mathbf{e}_1, \mathbf{e}_2, \dots, \mathbf{e}_n\}$ be a basis for V . If $\mathbf{a}_i = a_{ij} \mathbf{e}_j$ ($i = 1, \dots, n$) is a collection of n vectors⁵, we compute

$$\begin{aligned} \omega(\mathbf{a}_1, \mathbf{a}_2, \dots, \mathbf{a}_n) &= a_{1i_1} a_{2i_2} \dots a_{ni_n} \omega(\mathbf{e}_{i_1}, \mathbf{e}_{i_2}, \dots, \mathbf{e}_{i_n}) \\ &= a_{1i_1} a_{2i_2} \dots a_{ni_n} \epsilon_{i_1 i_2 \dots i_n} \omega(\mathbf{e}_1, \mathbf{e}_2, \dots, \mathbf{e}_n). \end{aligned} \quad (\text{A.64})$$

⁵The index j on a_{ij} should really be a superscript since a_{ij} is the j -th contravariant component of the vector \mathbf{a}_i . We are writing it as a subscript only for compatibility with other equations in this section.

In the first line we have exploited the linearity of ω in each slot, and in going from the first to the second line we have used skew-symmetry to rearrange the basis vectors in their canonical order. We deduce that all skew-symmetric n -forms are proportional to the determinant

$$\omega(\mathbf{a}_1, \mathbf{a}_2, \dots, \mathbf{a}_n) \propto \begin{vmatrix} a_{11} & a_{12} & \dots & a_{1n} \\ a_{21} & a_{22} & \dots & a_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ a_{n1} & a_{n2} & \dots & a_{nn} \end{vmatrix},$$

and that the proportionality factor is the number $\omega(\mathbf{e}_1, \mathbf{e}_2, \dots, \mathbf{e}_n)$. When the number of its slots is equal to the dimension of the vector space, there is therefore essentially only *one* skew-symmetric multilinear form and $\bigwedge^n(V^*)$ is a one-dimensional vector space.

Now we use the notion of skew-symmetric n -linear forms to give a powerful definition of the determinant of an *endomorphism*, i.e. a linear map $A : V \rightarrow V$. Let ω be a non-zero skew-symmetric n -linear form. The object

$$\omega_A(\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_n) = \omega(A\mathbf{x}_1, A\mathbf{x}_2, \dots, A\mathbf{x}_n). \quad (\text{A.65})$$

is also a skew-symmetric n -linear form. Since there is only one such object up to multiplicative constants, we must have

$$\omega(A\mathbf{x}_1, A\mathbf{x}_2, \dots, A\mathbf{x}_n) \propto \omega(\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_n). \quad (\text{A.66})$$

We define “ $\det A$ ” to be the constant of proportionality. Thus

$$\omega(A\mathbf{x}_1, A\mathbf{x}_2, \dots, A\mathbf{x}_n) = \det(A) \omega(\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_n). \quad (\text{A.67})$$

By writing this out in a basis where the linear map A is represented by the matrix \mathbf{A} , we easily see that

$$\det \mathbf{A} = \det A. \quad (\text{A.68})$$

The new definition is therefore compatible with the old one. The advantage of this more sophisticated definition is that it makes no appeal to a basis, and so shows that the determinant of an endomorphism is a basis-independent concept. A byproduct is an easy proof that $\det(AB) = \det(A)\det(B)$, a

result that is not so easy to establish with the elementary definition. We write

$$\begin{aligned}
 \det(AB)\omega(\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_n) &= \omega(AB\mathbf{x}_1, AB\mathbf{x}_2, \dots, AB\mathbf{x}_n) \\
 &= \omega(A(B\mathbf{x}_1), A(B\mathbf{x}_2), \dots, A(B\mathbf{x}_n)) \\
 &= \det(A)\omega(B\mathbf{x}_1, B\mathbf{x}_2, \dots, B\mathbf{x}_n) \\
 &= \det(A)\det(B)\omega(\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_n).
 \end{aligned} \tag{A.69}$$

Cancelling the common factor of $\omega(\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_n)$ completes the proof.

Exercise A.8: Let ω be a skew-symmetric n -linear form on an n -dimensional vector space. Assuming that ω does not vanish identically, show that a set of n vectors $\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_n$ is linearly independent, and hence forms a basis, if, and only if, $\omega(\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_n) \neq 0$.

Exercise A.9: Let

$$\mathbf{A} = \begin{pmatrix} \mathbf{a} & \mathbf{b} \\ \mathbf{c} & \mathbf{d} \end{pmatrix}$$

be a partitioned matrix where \mathbf{a} is m -by- m and \mathbf{d} n -by- n . By making a Gaussian decomposition

$$\mathbf{A} = \begin{pmatrix} \mathbf{I}_m & \mathbf{x} \\ \mathbf{0} & \mathbf{I}_n \end{pmatrix} \begin{pmatrix} \mathbf{\Lambda}_1 & \mathbf{0} \\ \mathbf{0} & \mathbf{\Lambda}_2 \end{pmatrix} \begin{pmatrix} \mathbf{I}_m & \mathbf{0} \\ \mathbf{y} & \mathbf{I}_n \end{pmatrix},$$

show that, for invertible \mathbf{d} , we have *Schur's determinant formula*⁶

$$\det \mathbf{A} = \det(\mathbf{d}) \det(\mathbf{a} - \mathbf{b}\mathbf{d}^{-1}\mathbf{c}).$$

A.6.2 The adjugate matrix

Given a square matrix

$$\mathbf{A} = \begin{pmatrix} a_{11} & a_{12} & \dots & a_{1n} \\ a_{21} & a_{22} & \dots & a_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ a_{n1} & a_{n2} & \dots & a_{nn} \end{pmatrix} \tag{A.70}$$

⁶I. Schur, J. für reine und angewandte Math. **147** (1917) 205-232.

and an element a_{ij} , we define the corresponding *minor* M_{ij} to be the determinant of the $(n-1)$ -by- $(n-1)$ matrix constructed by deleting from \mathbf{A} the row and column containing a_{ij} . The number

$$A_{ij} = (-1)^{i+j} M_{ij} \quad (\text{A.71})$$

is then called the *co-factor* of the element a_{ij} . (It is traditional to use uppercase letters to denote co-factors.) The basic result involving co-factors is that

$$\sum_j a_{ij} A_{i'j} = \delta_{ii'} \det \mathbf{A}. \quad (\text{A.72})$$

When $i = i'$, this is known as the *Laplace development* of the determinant about row i . We get zero when $i \neq i'$ because we are effectively developing a determinant with two equal rows. We now define the *adjugate matrix*⁷, $\text{Adj } \mathbf{A}$, to be the transposed matrix of the co-factors:

$$(\text{Adj } \mathbf{A})_{ij} = A_{ji}. \quad (\text{A.73})$$

In terms of this we have

$$\mathbf{A}(\text{Adj } \mathbf{A}) = (\det \mathbf{A})\mathbf{I}. \quad (\text{A.74})$$

In other words

$$\mathbf{A}^{-1} = \frac{1}{\det \mathbf{A}} \text{Adj } \mathbf{A}. \quad (\text{A.75})$$

Each entry in the adjugate matrix is a polynomial of degree $n-1$ in the entries of the original matrix. Thus, no division is required to form it, and the adjugate matrix exists even if the inverse matrix does not.

Cayley's theorem

You will know that the possible eigenvalues of the n -by- n matrix \mathbf{A} are given by the roots of its *characteristic equation*

$$0 = \det (\mathbf{A} - \lambda \mathbf{I}) = (-1)^n (\lambda^n - \text{tr}(\mathbf{A})\lambda^{n-1} + \cdots + (-1)^n \det(\mathbf{A})), \quad (\text{A.76})$$

and have probably met with *Cayley's theorem* that asserts that every matrix obeys its own characteristic equation.

$$\mathbf{A}^n - \text{tr}(\mathbf{A})\mathbf{A}^{n-1} + \cdots + (-1)^n \det(\mathbf{A})\mathbf{I} = \mathbf{0}. \quad (\text{A.77})$$

⁷Some authors rather confusingly call this the *adjoint matrix*.

The proof of Cayley's theorem involves the adjugate matrix. We write

$$\det(\mathbf{A} - \lambda \mathbf{I}) = (-1)^n (\lambda^n + \alpha_1 \lambda^{n-1} + \cdots + \alpha_n) \quad (\text{A.78})$$

and observe that

$$\det(\mathbf{A} - \lambda \mathbf{I}) \mathbf{I} = (\mathbf{A} - \lambda \mathbf{I}) \text{Adj}(\mathbf{A} - \lambda \mathbf{I}). \quad (\text{A.79})$$

Now $\text{Adj}(\mathbf{A} - \lambda \mathbf{I})$ is a matrix-valued polynomial in λ of degree $n - 1$, and it can be written

$$\text{Adj}(\mathbf{A} - \lambda \mathbf{I}) = \mathbf{C}_0 \lambda^{n-1} + \mathbf{C}_1 \lambda^{n-2} + \cdots + \mathbf{C}_{n-1}, \quad (\text{A.80})$$

for some matrix coefficients \mathbf{C}_i . On multiplying out the equation

$$(-1)^n (\lambda^n + \alpha_1 \lambda^{n-1} + \cdots + \alpha_n) \mathbf{I} = (\mathbf{A} - \lambda \mathbf{I})(\mathbf{C}_0 \lambda^{n-1} + \mathbf{C}_1 \lambda^{n-2} + \cdots + \mathbf{C}_{n-1}) \quad (\text{A.81})$$

and comparing like powers of λ , we find the relations

$$\begin{aligned} (-1)^n \mathbf{I} &= -\mathbf{C}_0, \\ (-1)^n \alpha_1 \mathbf{I} &= -\mathbf{C}_1 + \mathbf{A} \mathbf{C}_0, \\ (-1)^n \alpha_2 \mathbf{I} &= -\mathbf{C}_2 + \mathbf{A} \mathbf{C}_1, \\ &\vdots \\ (-1)^n \alpha_{n-1} \mathbf{I} &= -\mathbf{C}_{n-1} + \mathbf{A} \mathbf{C}_{n-2}, \\ (-1)^n \alpha_n \mathbf{I} &= \mathbf{A} \mathbf{C}_{n-1}. \end{aligned}$$

Multiply the first equation on the left by \mathbf{A}^n , the second by \mathbf{A}^{n-1} , and so on down the last equation which we multiply by $\mathbf{A}^0 \equiv \mathbf{I}$. Now add. We find that the sum telescopes to give Cayley's theorem,

$$\mathbf{A}^n + \alpha_1 \mathbf{A}^{n-1} + \cdots + \alpha_n \mathbf{I} = \mathbf{0},$$

as advertised.

A.6.3 Differentiating determinants

Suppose that the elements of \mathbf{A} depend on some parameter x . From the elementary definition

$$\det \mathbf{A} = \epsilon_{i_1 i_2 \dots i_n} a_{1 i_1} a_{2 i_2} \cdots a_{n i_n},$$

we find

$$\frac{d}{dx} \det \mathbf{A} = \epsilon_{i_1 i_2 \dots i_n} (a'_{1i_1} a_{2i_2} \dots a_{ni_n} + a_{1i_1} a'_{2i_2} \dots a_{ni_n} + \dots + a_{1i_1} a_{2i_2} \dots a'_{ni_n}). \quad (\text{A.82})$$

In other words,

$$\frac{d}{dx} \det \mathbf{A} = \begin{vmatrix} a'_{11} & a'_{12} & \dots & a'_{1n} \\ a_{21} & a_{22} & \dots & a_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ a_{n1} & a_{n2} & \dots & a_{nn} \end{vmatrix} + \begin{vmatrix} a_{11} & a_{12} & \dots & a_{1n} \\ a'_{21} & a'_{22} & \dots & a'_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ a_{n1} & a_{n2} & \dots & a_{nn} \end{vmatrix} + \dots + \begin{vmatrix} a_{11} & a_{12} & \dots & a_{1n} \\ a_{21} & a_{22} & \dots & a_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ a'_{n1} & a'_{n2} & \dots & a'_{nn} \end{vmatrix}.$$

The same result can also be written more compactly as

$$\frac{d}{dx} \det \mathbf{A} = \sum_{ij} \frac{da_{ij}}{dx} A_{ij}, \quad (\text{A.83})$$

where A_{ij} is cofactor of a_{ij} . Using the connection between the adjugate matrix and the inverse, this is equivalent to

$$\frac{1}{\det \mathbf{A}} \frac{d}{dx} \det \mathbf{A} = \text{tr} \left\{ \frac{d\mathbf{A}}{dx} \mathbf{A}^{-1} \right\}, \quad (\text{A.84})$$

or

$$\frac{d}{dx} \ln (\det \mathbf{A}) = \text{tr} \left\{ \frac{d\mathbf{A}}{dx} \mathbf{A}^{-1} \right\}. \quad (\text{A.85})$$

A special case of this formula is the result

$$\frac{\partial}{\partial a_{ij}} \ln (\det \mathbf{A}) = (\mathbf{A}^{-1})_{ji}. \quad (\text{A.86})$$

A.7 Diagonalization and Canonical Forms

An essential part of the linear algebra tool-kit is the set of techniques for the reduction of a matrix to its simplest, *canonical form*. This is often a diagonal matrix.

A.7.1 Diagonalizing linear maps

A common task is the diagonalization of a matrix \mathbf{A} representing a linear map A . Let us recall some standard material relating to this:

- i) If $A\mathbf{x} = \lambda\mathbf{x}$ for a non-zero vector \mathbf{x} , then \mathbf{x} is said to be an *eigenvector* of A with *eigenvalue* λ .
- ii) A linear operator A on a finite-dimensional vector space is said to be *self-adjoint*, or *Hermitian*, with respect to the inner product $\langle \cdot, \cdot \rangle$ if $A = A^\dagger$, or equivalently if $\langle \mathbf{x}, A\mathbf{y} \rangle = \langle A\mathbf{x}, \mathbf{y} \rangle$ for all \mathbf{x} and \mathbf{y} .
- iii) If A is Hermitian with respect to a positive definite inner product $\langle \cdot, \cdot \rangle$ then all the eigenvalues λ are real. To see that this is so, we write

$$\lambda \langle \mathbf{x}, \mathbf{x} \rangle = \langle \mathbf{x}, \lambda \mathbf{x} \rangle = \langle \mathbf{x}, A\mathbf{x} \rangle = \langle A\mathbf{x}, \mathbf{x} \rangle = \langle \lambda \mathbf{x}, \mathbf{x} \rangle = \lambda^* \langle \mathbf{x}, \mathbf{x} \rangle. \quad (\text{A.87})$$

Because the inner product is positive definite and \mathbf{x} is not zero, the factor $\langle \mathbf{x}, \mathbf{x} \rangle$ cannot be zero. We conclude that $\lambda = \lambda^*$.

- iii) If A is Hermitian and λ_i and λ_j are two distinct eigenvalues with eigenvectors \mathbf{x}_i and \mathbf{x}_j , respectively, then $\langle \mathbf{x}_i, \mathbf{x}_j \rangle = 0$. To prove this, we write

$$\lambda_j \langle \mathbf{x}_i, \mathbf{x}_j \rangle = \langle \mathbf{x}_i, A\mathbf{x}_j \rangle = \langle A\mathbf{x}_i, \mathbf{x}_j \rangle = \langle \lambda_i \mathbf{x}_i, \mathbf{x}_j \rangle = \lambda_i^* \langle \mathbf{x}_i, \mathbf{x}_j \rangle. \quad (\text{A.88})$$

But $\lambda_i^* = \lambda_i$, and so $(\lambda_i - \lambda_j) \langle \mathbf{x}_i, \mathbf{x}_j \rangle = 0$. Since, by assumption, $(\lambda_i - \lambda_j) \neq 0$ we must have $\langle \mathbf{x}_i, \mathbf{x}_j \rangle = 0$.

- iv) An operator A is said to be *diagonalizable* if we can find a basis for V that consists of eigenvectors of A . In this basis, A is represented by the matrix $\mathbf{A} = \text{diag}(\lambda_1, \lambda_2, \dots, \lambda_n)$, where the λ_i are the eigenvalues.

Not all linear operators can be diagonalized. The key element determining the diagonalizability of a matrix is the *minimal polynomial equation* obeyed by the matrix representing the operator. As mentioned in the previous section, the possible eigenvalues an n -by- n matrix \mathbf{A} are given by the roots of the *characteristic equation*

$$0 = \det(\mathbf{A} - \lambda \mathbf{I}) = (-1)^n (\lambda^n - \text{tr}(\mathbf{A})\lambda^{n-1} + \dots + (-1)^n \det(\mathbf{A})).$$

This is because a non-trivial solution to the equation

$$\mathbf{A}\mathbf{x} = \lambda\mathbf{x} \quad (\text{A.89})$$

requires the matrix $\mathbf{A} - \lambda \mathbf{I}$ to have a non-trivial nullspace, and so $\det(\mathbf{A} - \lambda \mathbf{I})$ must vanish. Cayley's Theorem, which we proved in the previous section, asserts that every matrix obeys its own characteristic equation:

$$\mathbf{A}^n - \text{tr}(\mathbf{A})\mathbf{A}^{n-1} + \dots + (-1)^n \det(\mathbf{A})\mathbf{I} = \mathbf{0}.$$

The matrix \mathbf{A} may, however, satisfy an equation of lower degree. For example, the characteristic equation of the matrix

$$\mathbf{A} = \begin{pmatrix} \lambda_1 & 0 \\ 0 & \lambda_1 \end{pmatrix} \quad (\text{A.90})$$

is $(\lambda - \lambda_1)^2$. Cayley therefore asserts that $(\mathbf{A} - \lambda_1 \mathbf{I})^2 = \mathbf{0}$. This is clearly true, but \mathbf{A} also satisfies the equation of first degree $(\mathbf{A} - \lambda_1 \mathbf{I}) = \mathbf{0}$.

The equation of lowest degree satisfied by \mathbf{A} is said to be the minimal polynomial equation. It is unique up to an overall numerical factor: if two distinct minimal equations of degree n were to exist, and if we normalize them so that the coefficients of \mathbf{A}^n coincide, then their difference, if non-zero, would be an equation of degree $\leq (n - 1)$ obeyed by \mathbf{A} — and a contradiction to the minimal equation having degree n .

If

$$P(\mathbf{A}) \equiv (\mathbf{A} - \lambda_1 \mathbf{I})^{\alpha_1} (\mathbf{A} - \lambda_2 \mathbf{I})^{\alpha_2} \cdots (\mathbf{A} - \lambda_n \mathbf{I})^{\alpha_n} = \mathbf{0} \quad (\text{A.91})$$

is the minimal equation then each root λ_i is an eigenvalue of \mathbf{A} . To prove this, we select one factor of $(\mathbf{A} - \lambda_i \mathbf{I})$ and write

$$P(\mathbf{A}) = (\mathbf{A} - \lambda_i \mathbf{I})Q(\mathbf{A}), \quad (\text{A.92})$$

where $Q(\mathbf{A})$ contains all the remaining factors in $P(\mathbf{A})$. We now observe that there must be some vector \mathbf{y} such that $\mathbf{x} = Q(\mathbf{A})\mathbf{y}$ is not zero. If there were no such \mathbf{y} then $Q(\mathbf{A}) = \mathbf{0}$ would be an equation of lower degree obeyed by \mathbf{A} in contradiction to the assumed minimality of $P(\mathbf{A})$. Since

$$\mathbf{0} = P(\mathbf{A})\mathbf{y} = (\mathbf{A} - \lambda_i \mathbf{I})\mathbf{x} \quad (\text{A.93})$$

we see that \mathbf{x} is an eigenvector of \mathbf{A} with eigenvalue λ_i .

Because all possible eigenvalues appear as roots of the characteristic equation, the minimal equation must have the same roots as the characteristic equation, but with equal or lower multiplicities α_i .

In the special case that \mathbf{A} is self-adjoint, or Hermitian, with respect to a positive definite inner product $\langle \ , \ \rangle$ the minimal equation has no repeated roots. Suppose that this were not so, and that \mathbf{A} has minimal equation $(\mathbf{A} - \lambda \mathbf{I})^2 R(\mathbf{A}) = \mathbf{0}$ where $R(\mathbf{A})$ is a polynomial in \mathbf{A} . Then, for all vectors \mathbf{x} we have

$$0 = \langle R\mathbf{x}, (\mathbf{A} - \lambda \mathbf{I})^2 R\mathbf{x} \rangle = \langle (\mathbf{A} - \lambda \mathbf{I})R\mathbf{x}, (\mathbf{A} - \lambda \mathbf{I})R\mathbf{x} \rangle. \quad (\text{A.94})$$

Now the vanishing of the rightmost expression shows that $(\mathbf{A} - \lambda \mathbf{I})R(\mathbf{A})\mathbf{x} = \mathbf{0}$ for all \mathbf{x} . In other words

$$(\mathbf{A} - \lambda \mathbf{I})R(\mathbf{A}) = \mathbf{0}. \quad (\text{A.95})$$

The equation with the repeated factor was not minimal therefore, and we have a contradiction.

If the equation of lowest degree satisfied by the matrix has no repeated roots, the matrix is diagonalizable; if there are repeated roots, it is not. The last statement should be obvious, because a diagonalized matrix satisfies an equation with no repeated roots, and this equation will hold in all bases, including the original one. The first statement, in combination with the observation that the minimal equation for a Hermitian matrix has no repeated roots, shows that a Hermitian (with respect to a positive definite inner product) matrix can be diagonalized.

To establish the first statement, suppose that \mathbf{A} obeys the equation

$$\mathbf{0} = P(\mathbf{A}) \equiv (\mathbf{A} - \lambda_1 \mathbf{I})(\mathbf{A} - \lambda_2 \mathbf{I}) \cdots (\mathbf{A} - \lambda_n \mathbf{I}), \quad (\text{A.96})$$

where the λ_i are all distinct. Then, setting $x \rightarrow \mathbf{A}$ in the identity⁸

$$\begin{aligned} 1 = & \frac{(x - \lambda_2)(x - \lambda_3) \cdots (x - \lambda_n)}{(\lambda_1 - \lambda_2)(\lambda_1 - \lambda_3) \cdots (\lambda_1 - \lambda_n)} + \frac{(x - \lambda_1)(x - \lambda_3) \cdots (x - \lambda_n)}{(\lambda_2 - \lambda_1)(\lambda_2 - \lambda_3) \cdots (\lambda_2 - \lambda_n)} + \cdots \\ & + \frac{(x - \lambda_1)(x - \lambda_2) \cdots (x - \lambda_{n-1})}{(\lambda_n - \lambda_1)(\lambda_n - \lambda_2) \cdots (\lambda_n - \lambda_{n-1})}, \end{aligned} \quad (\text{A.97})$$

where in each term one of the factors of the polynomial is omitted in both numerator and denominator, we may write

$$\mathbf{I} = \mathbf{P}_1 + \mathbf{P}_2 + \cdots + \mathbf{P}_n, \quad (\text{A.98})$$

where

$$\mathbf{P}_1 = \frac{(\mathbf{A} - \lambda_2 \mathbf{I})(\mathbf{A} - \lambda_3 \mathbf{I}) \cdots (\mathbf{A} - \lambda_n \mathbf{I})}{(\lambda_1 - \lambda_2)(\lambda_1 - \lambda_3) \cdots (\lambda_1 - \lambda_n)}, \quad (\text{A.99})$$

etc. Clearly $\mathbf{P}_i \mathbf{P}_j = \mathbf{0}$ if $i \neq j$, because the product contains the minimal equation as a factor. Multiplying (A.98) by \mathbf{P}_i therefore gives $\mathbf{P}_i^2 = \mathbf{P}_i$, showing that the \mathbf{P}_i are projection operators. Further $(\mathbf{A} - \lambda_i \mathbf{I})(\mathbf{P}_i) = \mathbf{0}$, so

$$(\mathbf{A} - \lambda_i \mathbf{I})(\mathbf{P}_i \mathbf{x}) = \mathbf{0} \quad (\text{A.100})$$

⁸The identity may be verified by observing that the difference of the left and right hand sides is a polynomial of degree $n-1$, which, by inspection, vanishes at the n points $x = \lambda_i$. But a polynomial which has more zeros than its degree, must be identically zero.

for any vector \mathbf{x} , and we see that $\mathbf{P}_i\mathbf{x}$, if not zero, is an eigenvector with eigenvalue λ_i . Thus \mathbf{P}_i projects onto the i -th eigenspace. Any vector can therefore be decomposed

$$\begin{aligned}\mathbf{x} &= \mathbf{P}_1\mathbf{x} + \mathbf{P}_2\mathbf{x} + \cdots + \mathbf{P}_n\mathbf{x} \\ &= \mathbf{x}_1 + \mathbf{x}_2 + \cdots + \mathbf{x}_n,\end{aligned}\tag{A.101}$$

where \mathbf{x}_i , if not zero, is an eigenvector with eigenvalue λ_i . Since any \mathbf{x} can be written as a sum of eigenvectors, the eigenvectors span the space.

Jordan decomposition

If the minimal polynomial has repeated roots, the matrix can still be reduced to the *Jordan canonical form*, which is diagonal except for some 1's immediately above the diagonal.

For example, suppose the characteristic equation for a 6-by-6 matrix \mathbf{A} is

$$0 = \det(\mathbf{A} - \lambda\mathbf{I}) = (\lambda_1 - \lambda)^3(\lambda_2 - \lambda)^3,\tag{A.102}$$

but the minimal equation is

$$0 = (\lambda_1 - \lambda)^3(\lambda_2 - \lambda)^2.\tag{A.103}$$

Then the Jordan form of \mathbf{A} might be

$$\mathbf{T}^{-1}\mathbf{A}\mathbf{T} = \begin{pmatrix} \lambda_1 & 1 & 0 & 0 & 0 & 0 \\ 0 & \lambda_1 & 1 & 0 & 0 & 0 \\ 0 & 0 & \lambda_1 & 0 & 0 & 0 \\ 0 & 0 & 0 & \lambda_2 & 1 & 0 \\ 0 & 0 & 0 & 0 & \lambda_2 & 0 \\ 0 & 0 & 0 & 0 & 0 & \lambda_2 \end{pmatrix}.\tag{A.104}$$

One may easily see that (A.103) is the minimal equation for this matrix. The minimal equation alone does not uniquely specify the pattern of λ_i 's and 1's in the Jordan form, though.

It is rather tedious, but quite straightforward, to show that any linear map can be reduced to a Jordan form. The proof is sketched in the following exercises:

Exercise A.10: Suppose that the linear operator T is represented by an $N \times N$ matrix, where $N > 1$. T obeys the equation

$$(T - \lambda I)^p = 0,$$

with $p = N$, but does not obey this equation for any $p < N$. Here λ is a number and I is the identity operator.

- i) Show that if T has an eigenvector, the corresponding eigenvalue must be λ . Deduce that T *cannot* be diagonalized.
- ii) Show that there exists a vector \mathbf{e}_1 such that $(T - \lambda I)^N \mathbf{e}_1 = 0$, but no lesser power of $(T - \lambda I)$ kills \mathbf{e}_1 .
- iii) Define $\mathbf{e}_2 = (T - \lambda I)\mathbf{e}_1$, $\mathbf{e}_3 = (T - \lambda I)^2 \mathbf{e}_1$, etc. up to \mathbf{e}_N . Show that the vectors $\mathbf{e}_1, \dots, \mathbf{e}_N$ are linearly independent.
- iv) Use $\mathbf{e}_1, \dots, \mathbf{e}_N$ as a basis for your vector space. Taking

$$\mathbf{e}_1 = \begin{pmatrix} 0 \\ \vdots \\ 0 \\ 1 \end{pmatrix}, \quad \mathbf{e}_2 = \begin{pmatrix} 0 \\ \vdots \\ 1 \\ 0 \end{pmatrix}, \quad \dots, \quad \mathbf{e}_N = \begin{pmatrix} 1 \\ 0 \\ \vdots \\ 0 \end{pmatrix},$$

write out the matrix representing T in the \mathbf{e}_i basis.

Exercise A.11:

Let $T : V \rightarrow V$ be a linear map and suppose that the minimal polynomial equation satisfied by T is

$$Q(T) = (T - \lambda_1 I)^{r_1} (T - \lambda_2 I)^{r_2} \dots (T - \lambda_n I)^{r_n} = 0.$$

Let V_{λ_i} denote the space of *generalized eigenvectors* for the eigenvalue λ_i . This is the set of \mathbf{x} such that $(T - \lambda_i I)^{r_i} \mathbf{x} = 0$. You will show that

$$V = \bigoplus_i V_{\lambda_i}.$$

- i) Consider the set of polynomials $Q_{\lambda_i, j}(t) = (t - \lambda_i)^{-(r_i - j + 1)} Q(t)$ where $j = 1, \dots, r_i$. Show that this set of $N \equiv \sum_i r_i$ polynomials forms a basis for the vector space $\mathcal{F}_{N-1}(t)$ of polynomials in t of degree no more than $N - 1$. (Since the number of $Q_{\lambda_i, j}$ is N , and this is equal to the dimension of $\mathcal{F}_{N-1}(t)$, the claim will be established if you can show that the polynomials are linearly independent. This is easy to do: suppose that

$$\sum_{\lambda_i, j} \alpha_{\lambda_i, j} Q_{\lambda_i, j}(t) = 0.$$

- Set $t = \lambda_i$ and deduce that $\alpha_{\lambda_i,1} = 0$. Knowing this, differentiate with respect to t and again set $t = \lambda_i$ and deduce that $\alpha_{\lambda_i,2} = 0$, and so on.)
- ii) Since the $Q_{\lambda_i,j}$ form a basis, and since $1 \in \mathcal{F}_{N-1}$, argue that we can find $\beta_{\lambda_i,j}$ such that

$$1 = \sum_{\lambda_i,j} \beta_{\lambda_i,j} Q_{\lambda_i,j}(t).$$

Now define

$$P_i = \sum_{j=1}^{r_i} \beta_{\lambda_i,j} Q_{\lambda_i,j}(T),$$

and so

$$I = \sum_{\lambda_i} P_i, \quad (\star)$$

- Use the minimal polynomial equation to deduce that $P_i P_j = 0$ if $i \neq j$. Multiplication of \star by P_i then shows that $P_i P_j = \delta_{ij} P_j$. Deduce from this that \star is a decomposition of the identity into a sum of mutually orthogonal projection operators P_i that project onto the spaces V_{λ_i} . Conclude that any \mathbf{x} can be expanded as $\mathbf{x} = \sum_i \mathbf{x}_i$ with $\mathbf{x}_i \equiv P_i \mathbf{x} \in V_{\lambda_i}$.
- iii) Show that the decomposition also implies that $V_{\lambda_i} \cap V_{\lambda_j} = \{\mathbf{0}\}$ if $i \neq j$. (Hint: a vector in V_{λ_i} is killed by all projectors with the possible exception of P_i and a vector in V_{λ_j} will be killed by all the projectors with the possible exception of P_j .)
- iv) Put these results together to deduce that V is a direct sum of the V_{λ_i} .
- v) Combine the result of part iv) with the ideas behind exercise A.10 to complete the proof of the Jordan decomposition theorem.

A.7.2 Diagonalizing quadratic forms

Do not confuse the notion of diagonalizing the matrix representing a *linear map* $A : V \rightarrow V$ with that of diagonalizing the matrix representing a *quadratic form*. A (real) quadratic form is a map $Q : V \rightarrow \mathbb{R}$, which is obtained from a symmetric bilinear form $B : V \times V \rightarrow \mathbb{R}$ by setting the two arguments, \mathbf{x} and \mathbf{y} , in $B(\mathbf{x}, \mathbf{y})$ equal:

$$Q(\mathbf{x}) = B(\mathbf{x}, \mathbf{x}). \quad (\text{A.105})$$

No information is lost by this specialization. We can recover the non-diagonal ($\mathbf{x} \neq \mathbf{y}$) values of B from the diagonal values, $Q(\mathbf{x})$, by using the *polarization trick*

$$B(\mathbf{x}, \mathbf{y}) = \frac{1}{2}[Q(\mathbf{x} + \mathbf{y}) - Q(\mathbf{x}) - Q(\mathbf{y})]. \quad (\text{A.106})$$

An example of a real quadratic form is the kinetic energy term

$$T(\dot{\mathbf{x}}) = \frac{1}{2} m_{ij} \dot{x}^i \dot{x}^j = \frac{1}{2} \dot{\mathbf{x}}^T \mathbf{M} \dot{\mathbf{x}} \quad (\text{A.107})$$

in a “small vibrations” Lagrangian. Here, \mathbf{M} , with entries m_{ij} , is the mass matrix.

Whilst one can diagonalize such forms by the tedious procedure of finding the eigenvalues and eigenvectors of the associated matrix, it is simpler to use Lagrange’s method, which is based on repeatedly completing squares.

Consider, for example, the quadratic form

$$Q = x^2 - y^2 - z^2 + 2xy - 4xz + 6yz = (x, y, z) \begin{pmatrix} 1 & 1 & -2 \\ 1 & -1 & 3 \\ -2 & 3 & -1 \end{pmatrix} \begin{pmatrix} x \\ y \\ z \end{pmatrix}. \quad (\text{A.108})$$

We complete the square involving x :

$$Q = (x + y - 2z)^2 - 2y^2 + 10yz - 5z^2, \quad (\text{A.109})$$

where the terms outside the squared group no longer involve x . We now complete the square in y :

$$Q = (x + y - 2z)^2 - (\sqrt{2}y - \frac{5}{\sqrt{2}}z)^2 + \frac{15}{2}z^2, \quad (\text{A.110})$$

so that the remaining term no longer contains y . Thus, on setting

$$\begin{aligned} \xi &= x + y - 2z, \\ \eta &= \sqrt{2}y - \frac{5}{\sqrt{2}}z, \\ \zeta &= \sqrt{\frac{15}{2}}z, \end{aligned}$$

we have

$$Q = \xi^2 - \eta^2 + \zeta^2 = (\xi, \eta, \zeta) \begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} \xi \\ \eta \\ \zeta \end{pmatrix}. \quad (\text{A.111})$$

If there are no x^2 , y^2 , or z^2 terms to get us started, then we can proceed by using $(x + y)^2$ and $(x - y)^2$. For example, consider

$$\begin{aligned}
 Q &= 2xy + 2yz + 2zy, \\
 &= \frac{1}{2}(x + y)^2 - \frac{1}{2}(x - y)^2 + 2xz + 2yz \\
 &= \frac{1}{2}(x + y)^2 + 2(x + y)z - \frac{1}{2}(x - y)^2 \\
 &= \frac{1}{2}(x + y + 2z)^2 - \frac{1}{2}(x - y)^2 - 4z^2 \\
 &= \xi^2 - \eta^2 - \zeta^2,
 \end{aligned}$$

where

$$\begin{aligned}
 \xi &= \frac{1}{\sqrt{2}}(x + y + 2z), \\
 \eta &= \frac{1}{\sqrt{2}}(x - y), \\
 \zeta &= \sqrt{2}z.
 \end{aligned}$$

A judicious combination of these two tactics will reduce the matrix representing any real quadratic form to a matrix with ± 1 's and 0's on the diagonal, and zeros elsewhere. As the egregiously asymmetric treatment of x , y , z in the last example indicates, this can be done in many ways, but *Cayley's Law of Inertia* asserts that the number of $+1$'s, -1 's and 0's will always be the same. Naturally, if we allow complex numbers in the redefinitions of the variables, we can always reduce the form to one with only $+1$'s and 0's.

The essential difference between diagonalizing linear maps and diagonalizing quadratic forms is that in the former case we seek matrices \mathbf{A} such that $\mathbf{A}^{-1}\mathbf{M}\mathbf{A}$ is diagonal, whereas in the latter case we seek matrices \mathbf{A} such that $\mathbf{A}^T\mathbf{M}\mathbf{A}$ is diagonal. Here, the superscript T denotes transposition.

Exercise A.12: Show that the matrix

$$\mathbf{Q} = \begin{pmatrix} a & b \\ b & c \end{pmatrix}$$

representing the quadratic form

$$Q(x, y) = ax^2 + 2bxy + cy^2$$

may be reduced to

$$\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \quad \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \quad \text{or} \quad \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix},$$

depending on whether the *discriminant*, $ac - b^2$, is respectively greater than zero, less than zero, or equal to zero.

Warning: You might be tempted to refer to the discriminant $ac - b^2$ as being the determinant of Q . It is indeed the determinant of the matrix \mathbf{Q} , but there is no such thing as the “determinant” of the quadratic form itself. You may compute the determinant of the matrix representing Q in some basis, but if you change basis and repeat the calculation you will get a different answer. For *real* quadratic forms, however, the *sign* of the determinant stays the same, and this is all that the discriminant cares about.

A.7.3 Block-diagonalizing symplectic forms

A skew-symmetric bilinear form $\omega : V \times V \rightarrow \mathbb{R}$ is often called a *symplectic form*. Such forms play an important role in Hamiltonian dynamics and in optics. Let $\{\mathbf{e}_i\}$ be a basis for V , and set

$$\omega(\mathbf{e}_i, \mathbf{e}_j) = \omega_{ij}. \quad (\text{A.112})$$

If $\mathbf{x} = x^i \mathbf{e}_i$ and $\mathbf{y} = y^j \mathbf{e}_j$, we therefore have

$$\omega(\mathbf{x}, \mathbf{y}) = \omega(\mathbf{e}_i, \mathbf{e}_j) x^i y^j = \omega_{ij} x^i y^j. \quad (\text{A.113})$$

The numbers ω_{ij} can be thought of as the entries in a real skew-symmetric matrix $\mathbf{\Omega}$, in terms of which $\omega(\mathbf{x}, \mathbf{y}) = \mathbf{x}^T \mathbf{\Omega} \mathbf{y}$. We cannot exactly “diagonalize” such a skew-symmetric matrix because a matrix with non-zero entries only on its principal diagonal is necessarily symmetric. We can do the next best thing, however, and reduce $\mathbf{\Omega}$ to *block diagonal* form with simple 2-by-2 skew matrices along the diagonal.

We begin by expanding ω as

$$\omega = \frac{1}{2} \omega_{ij} \mathbf{e}^{*i} \wedge \mathbf{e}^{*j} \quad (\text{A.114})$$

where the *wedge* (or *exterior*) product $\mathbf{e}^{*i} \wedge \mathbf{e}^{*j}$ of a pair of basis vectors in V^* denotes the particular skew-symmetric bilinear form

$$\mathbf{e}^{*i} \wedge \mathbf{e}^{*j}(\mathbf{e}_\alpha, \mathbf{e}_\beta) = \delta_\alpha^i \delta_\beta^j - \delta_\beta^i \delta_\alpha^j. \quad (\text{A.115})$$

Again, if $\mathbf{x} = x^i \mathbf{e}_i$ and $\mathbf{y} = y^j \mathbf{e}_j$, we have

$$\begin{aligned} \mathbf{e}^{*i} \wedge \mathbf{e}^{*j}(\mathbf{x}, \mathbf{y}) &= \mathbf{e}^{*i} \wedge \mathbf{e}^{*j}(x^\alpha \mathbf{e}_\alpha, y^\beta \mathbf{e}_\beta) \\ &= (\delta_\alpha^i \delta_\beta^j - \delta_\beta^i \delta_\alpha^j) x^\alpha y^\beta \\ &= x^i y^j - y^i x^j. \end{aligned} \quad (\text{A.116})$$

Consequently

$$\omega(\mathbf{x}, \mathbf{y}) = \frac{1}{2} \omega_{ij} (x^i y^j - y^i x^j) = \omega_{ij} x^i y^j, \quad (\text{A.117})$$

as before. We extend the definition of the wedge product to other elements of V^* by requiring “ \wedge ” to be associative and distributive, taking note that

$$\mathbf{e}^{*i} \wedge \mathbf{e}^{*j} = -\mathbf{e}^{*j} \wedge \mathbf{e}^{*i}, \quad (\text{A.118})$$

and so $0 = \mathbf{e}^{*1} \wedge \mathbf{e}^{*1} = \mathbf{e}^{*2} \wedge \mathbf{e}^{*2}$, etc.

We next show that there exists a basis $\{\mathbf{f}^{*i}\}$ of V^* such that

$$\omega = \mathbf{f}^{*1} \wedge \mathbf{f}^{*2} + \mathbf{f}^{*3} \wedge \mathbf{f}^{*4} + \cdots + \mathbf{f}^{*(p-1)} \wedge \mathbf{f}^{*p}. \quad (\text{A.119})$$

Here, the integer $p \leq n$ is the *rank* of ω . It is necessarily an even number.

The new basis is constructed by a skew-analogue of Lagrange’s method of completing the square. If

$$\omega = \frac{1}{2} \omega_{ij} \mathbf{e}^{*i} \wedge \mathbf{e}^{*j} \quad (\text{A.120})$$

is not identically zero, we can, after re-ordering the basis if necessary, assume that $\omega_{12} \neq 0$. Then

$$\omega = \left(\mathbf{e}^{*1} - \frac{1}{\omega_{12}} (\omega_{23} \mathbf{e}^{*3} + \cdots + \omega_{2n} \mathbf{e}^{*n}) \right) \wedge (\omega_{12} \mathbf{e}^{*2} + \omega_{13} \mathbf{e}^{*3} + \cdots + \omega_{1n} \mathbf{e}^{*n}) + \omega^{\{3\}} \quad (\text{A.121})$$

where $\omega^{\{3\}} \in \bigwedge^2(V^*)$ does not contain \mathbf{e}^{*1} or \mathbf{e}^{*2} . We set

$$\mathbf{f}^{*1} = \mathbf{e}^{*1} - \frac{1}{\omega_{12}} (\omega_{23} \mathbf{e}^{*3} + \cdots + \omega_{2n} \mathbf{e}^{*n}) \quad (\text{A.122})$$

and

$$\mathbf{f}^{*2} = \omega_{12} \mathbf{e}^{*2} + \omega_{13} \mathbf{e}^{*3} + \cdots + \omega_{1n} \mathbf{e}^{*n}. \quad (\text{A.123})$$

Thus,

$$\omega = \mathbf{f}^{*1} \wedge \mathbf{f}^{*2} + \omega^{\{3\}}. \quad (\text{A.124})$$

If the remainder $\omega^{\{3\}}$ is identically zero, we are done. Otherwise, we apply the same process to $\omega^{\{3\}}$ so as to construct $\mathbf{f}^{*3}, \mathbf{f}^{*4}$ and $\omega^{\{5\}}$; we continue in this manner until we find a remainder, $\omega^{\{p+1\}}$, that vanishes.

Let $\{\mathbf{f}_i\}$ be the basis for V dual to the basis $\{\mathbf{f}^{*i}\}$. Then $\omega(\mathbf{f}_1, \mathbf{f}_2) = -\omega(\mathbf{f}_2, \mathbf{f}_1) = \omega(\mathbf{f}_3, \mathbf{f}_4) = -\omega(\mathbf{f}_4, \mathbf{f}_3) = 1$, and so on, all other values being zero. This shows that if we define the coefficients a^i_j by expressing $\mathbf{f}^{*i} = a^i_j \mathbf{e}^{*j}$, and hence $\mathbf{e}_i = \mathbf{f}_j a^j_i$, then the matrix Ω has been expressed as

$$\Omega = \mathbf{A}^T \tilde{\Omega} \mathbf{A}, \quad (\text{A.125})$$

where \mathbf{A} is the matrix with entries a^i_j , and $\tilde{\Omega}$ is the matrix

$$\tilde{\Omega} = \begin{pmatrix} 0 & 1 & & & \\ -1 & 0 & & & \\ & & 0 & 1 & \\ & & -1 & 0 & \\ & & & & \ddots \end{pmatrix}, \quad (\text{A.126})$$

which contains $p/2$ diagonal blocks of

$$\begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}, \quad (\text{A.127})$$

and all other entries are zero.

Example: Consider the skew bilinear form

$$\omega(\mathbf{x}, \mathbf{y}) = \mathbf{x}^T \Omega \mathbf{y} = (x^1, x^2, x^3, x^4) \begin{pmatrix} 0 & 1 & 3 & 0 \\ -1 & 0 & 1 & 5 \\ -3 & -1 & 0 & 0 \\ 0 & -5 & 0 & 0 \end{pmatrix} \begin{pmatrix} y^1 \\ y^2 \\ y^3 \\ y^4 \end{pmatrix}. \quad (\text{A.128})$$

This corresponds to

$$\omega = \mathbf{e}^{*1} \wedge \mathbf{e}^{*2} + 3\mathbf{e}^{*1} \wedge \mathbf{e}^{*3} + \mathbf{e}^{*2} \wedge \mathbf{e}^{*3} + 5\mathbf{e}^{*2} \wedge \mathbf{e}^{*4}. \quad (\text{A.129})$$

Following our algorithm, we write ω as

$$\omega = (\mathbf{e}^{*1} - \mathbf{e}^{*3} - 5\mathbf{e}^{*4}) \wedge (\mathbf{e}^{*2} + 3\mathbf{e}^{*3}) - 15\mathbf{e}^{*3} \wedge \mathbf{e}^{*4}. \quad (\text{A.130})$$

If we now set

$$\begin{aligned} \mathbf{f}^{*1} &= \mathbf{e}^{*1} - \mathbf{e}^{*3} - 5\mathbf{e}^{*4}, \\ \mathbf{f}^{*2} &= \mathbf{e}^{*2} + 3\mathbf{e}^{*3}, \\ \mathbf{f}^{*3} &= -15\mathbf{e}^{*3}, \\ \mathbf{f}^{*4} &= \mathbf{e}^{*4}, \end{aligned} \tag{A.131}$$

we have

$$\omega = \mathbf{f}^{*1} \wedge \mathbf{f}^{*2} + \mathbf{f}^{*3} \wedge \mathbf{f}^{*4}. \tag{A.132}$$

We have correspondingly expressed the matrix $\mathbf{\Omega}$ as

$$\begin{pmatrix} 0 & 1 & 3 & 0 \\ -1 & 0 & 1 & 5 \\ -3 & -1 & 0 & 0 \\ 0 & -5 & 0 & 0 \end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ -1 & 3 & -15 & 0 \\ -5 & 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} 0 & 1 & & \\ -1 & 0 & & \\ & & 0 & 1 \\ & & -1 & 0 \end{pmatrix} \begin{pmatrix} 1 & 0 & -1 & -5 \\ 0 & 1 & 3 & 0 \\ 0 & 0 & -15 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}. \tag{A.133}$$

Exercise A.13: Let $\mathbf{\Omega}$ be a skew symmetric $2n$ -by- $2n$ matrix with entries $\omega_{ij} = -\omega_{ji}$. Define the *Pfaffian* of $\mathbf{\Omega}$ by

$$\text{Pf } \mathbf{\Omega} = \frac{1}{2^n n!} \sum \epsilon_{i_1 i_2 \dots i_{2n}} \omega_{i_1 i_2} \omega_{i_3 i_4} \dots \omega_{i_{2n-1} i_{2n}}.$$

Show that $\text{Pf}(\mathbf{M}^T \mathbf{\Omega} \mathbf{M}) = \det(\mathbf{M}) \text{Pf}(\mathbf{\Omega})$. By reducing $\mathbf{\Omega}$ to a suitable canonical form, show that $(\text{Pf } \mathbf{\Omega})^2 = \det \mathbf{\Omega}$.

Exercise A.14: Let $\omega(\mathbf{x}, \mathbf{y})$ be a non-degenerate skew symmetric bilinear form on \mathbb{R}^{2n} , and $\mathbf{x}_1, \dots, \mathbf{x}_{2n}$ a set of vectors. Prove *Weyl's identity*

$$\text{Pf}(\mathbf{\Omega}) \det |\mathbf{x}_1, \dots, \mathbf{x}_{2n}| = \frac{1}{2^n n!} \sum \epsilon_{i_1, \dots, i_{2n}} \omega(\mathbf{x}_{i_1}, \mathbf{x}_{i_2}) \dots \omega(\mathbf{x}_{i_{2n-1}}, \mathbf{x}_{i_{2n}}).$$

Here $\det |\mathbf{x}_1, \dots, \mathbf{x}_{2n}|$ is the determinant of the matrix whose rows are the \mathbf{x}_i and $\mathbf{\Omega}$ is the matrix corresponding to the form ω .

Now let $M : \mathbb{R}^{2n} \rightarrow \mathbb{R}^{2n}$ be a linear map. Show that

$$\begin{aligned} &\text{Pf}(\mathbf{\Omega}) (\det M) \det |\mathbf{x}_1, \dots, \mathbf{x}_{2n}| \\ &= \frac{1}{2^n n!} \sum \epsilon_{i_1, \dots, i_{2n}} \omega(M\mathbf{x}_{i_1}, M\mathbf{x}_{i_2}) \dots \omega(M\mathbf{x}_{i_{2n-1}}, M\mathbf{x}_{i_{2n}}), \end{aligned}$$

Deduce that if $\omega(M\mathbf{x}, M\mathbf{y}) = \omega(\mathbf{x}, \mathbf{y})$ for all vectors \mathbf{x}, \mathbf{y} , then $\det M = 1$. The set of such matrices M that preserve ω compose the *symplectic group* $\text{Sp}(2n, \mathbb{R})$

Appendix B

Fourier Series and Integrals.

Fourier series and Fourier integral representations are the most important examples of the expansion of a function in terms of a complete orthonormal set. The material in this appendix reviews features peculiar to these special cases, and is intended to complement the the general discussion of orthogonal series in chapter 2.

B.1 Fourier Series

A function defined on a finite interval may be expanded as a Fourier *series*.

B.1.1 Finite Fourier series

Suppose we have measured $f(x)$ in the interval $[0, L]$, but only at the discrete set of points $x = na$, where a is the sampling interval and $n = 0, 1, \dots, N-1$, with $Na = L$. We can then represent our data $f(na)$ by a *finite* Fourier series. This representation is based on the geometric sum

$$\sum_{m=0}^{N-1} e^{ik_m(n'-n)a} = \frac{e^{2\pi i(n-n')a} - 1}{e^{2\pi i(n'-n)a/N} - 1}, \quad (\text{B.1})$$

where $k_m \equiv 2\pi m/Na$. For integer n , and n' , the expression on the right hand side of (B.1) is zero unless $n' - n$ is an integer multiple of N , when it becomes indeterminate. In this case, however, each term on the left hand side is equal to unity, and so their sum is equal to N . If we restrict n and n'

to lie between 0 and $N - 1$, we have

$$\sum_{m=0}^{N-1} e^{ik_m(n'-n)a} = N\delta_{n'n}. \quad (\text{B.2})$$

Inserting (B.2) into the formula

$$f(na) = \sum_{n'=0}^{N-1} f(n'a) \delta_{n'n}, \quad (\text{B.3})$$

shows that

$$f(na) = \sum_{m=0}^{N-1} a_m e^{-ik_m na}, \quad \text{where} \quad a_m \equiv \frac{1}{N} \sum_{n=0}^{N-1} f(na) e^{ik_m na}. \quad (\text{B.4})$$

This is the finite Fourier representation.

When $f(na)$ is real, it is convenient to make the k_m sum symmetric about $k_m = 0$ by taking $N = 2M + 1$ and setting the summation limits to be $\pm M$. The finite geometric sum then becomes

$$\sum_{m=-M}^M e^{im\theta} = \frac{\sin(2M+1)\theta/2}{\sin \theta/2}. \quad (\text{B.5})$$

We set $\theta = 2\pi(n' - n)/N$ and use the same tactics as before to deduce that

$$f(na) = \sum_{m=-M}^M a_m e^{-ik_m na}, \quad (\text{B.6})$$

where again $k_m = 2\pi m/L$, with $L = Na$, and

$$a_m = \frac{1}{N} \sum_{n=0}^{2M} f(na) e^{ik_m na}. \quad (\text{B.7})$$

In this form it is manifest that f being real both implies and is implied by $a_{-m} = a_m^*$.

These finite Fourier expansions are algebraic identities. No limits have to be taken, and so no restrictions need be placed on $f(na)$ for them to be valid. They are all that is needed for processing experimental data.

Although the initial $f(na)$ was defined only for the finite range $0 \leq n \leq N - 1$, the Fourier sum (B.4) or (B.7) is defined for any n , and so extends f to a periodic function of n with period N .

B.1.2 Continuum limit

Now we wish to derive a Fourier representation for functions defined everywhere on the interval $[0, L]$, rather just at the sampling points. The natural way to proceed is to build on the results from the previous section by replacing the interval $[0, L]$ with a discrete lattice of $N = 2M + 1$ points at $x = na$, where a is a small lattice spacing which we ultimately take to zero. For any non-zero a the continuum function $f(x)$ is thus replaced by the finite set of numbers $f(na)$. If we stand back and blur our vision so that we can no longer perceive the individual lattice points, a plot of this discrete function will look little different from the original continuum $f(x)$. In other words, provided that f is slowly varying on the scale of the lattice spacing, $f(an)$ can be regarded as a smooth function of $x = an$.

The basic “integration rule” for such smooth functions is that

$$a \sum_n f(an) \rightarrow \int f(an) a \, dn \rightarrow \int f(x) \, dx, \quad (\text{B.8})$$

as a becomes small. A sum involving a Kronecker δ will become an integral containing a Dirac δ -function:

$$a \sum_n f(na) \frac{1}{a} \delta_{nm} = f(ma) \rightarrow \int f(x) \delta(x - y) \, dx = f(y). \quad (\text{B.9})$$

We can therefore think of the δ function as arising from

$$\frac{\delta_{nn'}}{a} \rightarrow \delta(x - x'). \quad (\text{B.10})$$

In particular, the divergent quantity $\delta(0)$ (in x space) is obtained by setting $n = n'$, and can therefore be understood to be the reciprocal of the lattice spacing, or, equivalently, the number of lattice points per unit volume.

Now we take the formal continuum limit of (B.7) by letting $a \rightarrow 0$ and $N \rightarrow \infty$ while keeping their product $Na = L$ fixed. The *finite* Fourier representation

$$f(na) = \sum_{m=-M}^M a_m e^{-\frac{2\pi i m}{Na} na} \quad (\text{B.11})$$

now becomes an *infinite* series

$$f(x) = \sum_{m=-\infty}^{\infty} a_m e^{-2\pi i m x / L}, \quad (\text{B.12})$$

whereas

$$a_m = \frac{a}{Na} \sum_{n=0}^{N-1} f(na) e^{\frac{2\pi im}{Na} na} \rightarrow \frac{1}{L} \int_0^L f(x) e^{2\pi imx/L} dx. \quad (\text{B.13})$$

The series (B.12) is the Fourier expansion for a function on a finite interval. The sum is equal to $f(x)$ in the interval $[0, L]$. Outside, it produces L -periodic translates of the original f .

This Fourier expansion (B.12, B.13) is same series that we would obtain by using the $L^2[0, L]$ orthonormality

$$\frac{1}{L} \int_0^L e^{2\pi imx/L} e^{-2\pi inx/L} dx = \delta_{nm}, \quad (\text{B.14})$$

and using the methods of chapter two. The arguments adduced there, however, guarantee convergence only in the L^2 sense. While our present “continuum limit” derivation is only heuristic, it does suggest that for reasonably-behaved functions f the Fourier series (B.12) converges *pointwise* to $f(x)$. It is relatively easy to show that any continuous function is sufficiently “well-behaved” for pointwise convergence. Furthermore, if the function f is smooth then the convergence is uniform. This is useful to know, but we often desire a Fourier representation for a function with discontinuities. A stronger result is that if f is *piecewise continuous* in $[0, L]$, *i.e.*, continuous with the exception of a finite number of discontinuities, then the Fourier series will converge pointwise (but not uniformly¹) to $f(x)$ at points where $f(x)$ is continuous, and to its average

$$F(x) = \frac{1}{2} \lim_{\epsilon \rightarrow 0} \{f(x + \epsilon) + f(x - \epsilon)\} \quad (\text{B.15})$$

at those points where $f(x)$ has jumps. In the section B.3.2 we shall explain why the series converges to this average, and examine the nature of this convergence.

Most functions of interest to engineers are piecewise continuous, and this result is then all that they require. In physics, however, we often have to work with a broader class of functions, and so other forms of convergence become relevant. In quantum mechanics, in particular, the probability interpretation of the wavefunction requires only convergence in the L^2 sense, and

¹If a sequence of continuous functions converges uniformly, then its limit function is continuous.

this demands no smoothness properties at all—the Fourier representation converging to f whenever the L^2 norm $\|f\|^2$ is finite.

Half-range Fourier series

The exponential series

$$f(x) = \sum_{m=-\infty}^{\infty} a_m e^{-2\pi i m x / L}. \quad (\text{B.16})$$

can be re-expressed as the trigonometric sum

$$f(x) = \frac{1}{2}A_0 + \sum_{m=1}^{\infty} \{A_m \cos(2\pi m x / L) + B_m \sin(2\pi m x / L)\}, \quad (\text{B.17})$$

where

$$\begin{aligned} A_m &= \begin{cases} 2a_0 & m = 0, \\ a_m + a_{-m}, & m > 0, \end{cases} \\ B_m &= i(a_{-m} - a_m). \end{aligned} \quad (\text{B.18})$$

This is called a *full-range* trigonometric Fourier series for functions defined on $[0, L]$. In chapter 2 we expanded functions in series containing only sines. We can expand any function $f(x)$ defined on a finite interval as such a *half-range* Fourier series. To do this, we regard the given domain of $f(x)$ as being the half interval $[0, L/2]$ (hence the name). We then extend $f(x)$ to a function on the whole of $[0, L]$ and expand as usual. If we extend $f(x)$ by setting $f(x + L/2) = -f(x)$ then the A_m are all zero and we have

$$f(x) = \sum_{m=1}^{\infty} B_m \sin(2\pi m x / L), \quad x \in [0, L/2], \quad (\text{B.19})$$

where,

$$B_m = \frac{4}{L} \int_0^{L/2} f(x) \sin(2\pi m x / L) dx. \quad (\text{B.20})$$

Alternatively, we may extend the range of definition by setting $f(x + L/2) = f(L/2 - x)$. In this case it is the B_m that become zero and we have

$$f(x) = \frac{1}{2}A_0 + \sum_{m=1}^{\infty} A_m \cos(2\pi m x / L), \quad x \in [0, L/2], \quad (\text{B.21})$$

with

$$A_m = \frac{4}{L} \int_0^{L/2} f(x) \cos(2\pi m x/L) dx. \quad (\text{B.22})$$

The difference between a full-range and a half-range series is therefore seen principally in the continuation of the function outside its initial interval of definition. A full range series repeats the function periodically. A half-range sine series changes the sign of the continued function each time we pass to an adjacent interval, whilst the half-range cosine series reflects the function as if each interval endpoint were a mirror.

B.2 Fourier Integral Transforms

When the function we wish represent is defined on the entirety of \mathbb{R} then we can use the Fourier *integral* representation.

B.2.1 Inversion formula

We can obtain this formally from the Fourier series for a function defined on $[-L/2, L/2]$, where

$$f(x) = \sum_{m=-\infty}^{\infty} a_m e^{-\frac{2\pi i m}{L} x}, \quad (\text{B.23})$$

$$a_m = \frac{1}{L} \int_{-L/2}^{L/2} f(x) e^{\frac{2\pi i m}{L} x} dx, \quad (\text{B.24})$$

by letting L become large. The discrete $k_m = 2\pi m/L$ then merge into the continuous variable k and

$$\sum_{m=-\infty}^{\infty} \rightarrow \int_{-\infty}^{\infty} dm = L \int_{-\infty}^{\infty} \frac{dk}{2\pi}. \quad (\text{B.25})$$

The product La_m remains finite, and becomes a function that we shall call $\tilde{f}(k)$. Thus

$$f(x) = \int_{-\infty}^{\infty} \tilde{f}(k) e^{-ikx} \frac{dk}{2\pi}, \quad (\text{B.26})$$

$$\tilde{f}(k) = \int_{-\infty}^{\infty} f(x) e^{ikx} dx. \quad (\text{B.27})$$

This is the Fourier integral transform and its inverse.

It is good practice when doing Fourier transforms in physics to treat x and k asymmetrically: always put the 2π 's with the dk 's. This is because, as (B.25) shows, $dk/2\pi$ has the physical meaning of the number of Fourier modes per unit (spatial) volume with wavenumber between k and $k + dk$.

The Fourier representation of the Dirac delta-function is

$$\delta(x - x') = \int_{-\infty}^{\infty} \frac{dk}{2\pi} e^{ik(x-x')}. \quad (\text{B.28})$$

Suppose we put $x = x'$. Then “ $\delta(0)$ ”, which we earlier saw can be interpreted as the inverse lattice spacing, and hence the density of lattice points, is equal to $\int_{-\infty}^{\infty} \frac{dk}{2\pi}$. This is the total number of Fourier modes per unit length.

Exchanging x and k in the integral representation of $\delta(x - x')$ gives us the Fourier representation for $\delta(k - k')$:

$$\int_{-\infty}^{\infty} e^{i(k-k')x} dx = 2\pi \delta(k - k'). \quad (\text{B.29})$$

Thus $2\pi\delta(0)$ (in k space), although mathematically divergent, has the physical meaning $\int dx$, the volume of the system. It is good practice to put a 2π with each $\delta(k)$ because this combination has a direct physical interpretation.

Take care to note that the symbol $\delta(0)$ has a very different physical interpretation depending on whether δ is a delta-function in x or in k space.

Parseval's identity

Note that with the Fourier transform pair defined as

$$\tilde{f}(k) = \int_{-\infty}^{\infty} e^{ikx} f(x) dx \quad (\text{B.30})$$

$$f(x) = \int_{-\infty}^{\infty} e^{-ikx} \tilde{f}(k) \frac{dk}{2\pi}, \quad (\text{B.31})$$

Parseval's theorem takes the form

$$\int_{-\infty}^{\infty} |f(x)|^2 dx = \int_{-\infty}^{\infty} |\tilde{f}(k)|^2 \frac{dk}{2\pi}. \quad (\text{B.32})$$

Parseval's theorem tells us that the Fourier transform is a unitary map from $L^2(\mathbb{R}) \rightarrow L^2(\mathbb{R})$.

B.2.2 The Riemann-Lebesgue lemma

There is a reciprocal relationship between the rates at which a function and its Fourier transform decay at infinity. The more rapidly the function decays, the more high frequency modes it must contain—and hence the slower the decay of its Fourier transform. Conversely, the smoother a function the fewer high frequency modes it contains and the faster the decay of its transform. Quantitative estimates of this version of Heisenberg's uncertainty principle are based on the *Riemann-Lebesgue lemma*.

Recall that a function f is in $L^1(\mathbb{R})$ if it is integrable (this condition excludes the delta function) and goes to zero at infinity sufficiently rapidly that

$$\|f\|_1 \equiv \int_{-\infty}^{\infty} |f| dx < \infty. \quad (\text{B.33})$$

If $f \in L^1(\mathbb{R})$ then its Fourier transform

$$\tilde{f}(k) = \int_{-\infty}^{\infty} f(x) e^{ikx} dx \quad (\text{B.34})$$

exists, is a continuous function of k , and

$$|\tilde{f}(k)| \leq \|f\|_1. \quad (\text{B.35})$$

The Riemann-Lebesgue lemma asserts that if $f \in L^1(\mathbb{R})$ then

$$\lim_{k \rightarrow \infty} \tilde{f}(k) = 0. \quad (\text{B.36})$$

We will not give the proof. For f integrable in the Riemann sense, it is not difficult, being almost a corollary of the definition of the Riemann integral. We must point out, however, that the “ $|\dots|$ ” modulus sign is essential in the L^1 condition. For example, the integral

$$I = \int_{-\infty}^{\infty} \sin(x^2) dx \quad (\text{B.37})$$

is convergent, but only because of extensive cancellations. The L^1 norm

$$\int_{-\infty}^{\infty} |\sin(x^2)| dx \quad (\text{B.38})$$

is *not* finite, and whereas the Fourier transform of $\sin(x^2)$, *i.e.*

$$\int_{-\infty}^{\infty} \sin(x^2) e^{ikx} dx = \sqrt{\pi} \cos\left(\frac{k^2 + \pi}{4}\right), \quad (\text{B.39})$$

is also convergent, it does not decay to zero as k grows large.

The Riemann-Lebesgue lemma tells us that the Fourier transform maps $L^1(\mathbb{R})$ into $C_\infty(\mathbb{R})$, the latter being the space of continuous functions vanishing at infinity. Be careful: this map is only *into* and not *onto*. The inverse Fourier transform of a function vanishing at infinity does not necessarily lie in $L^1(\mathbb{R})$.

We link the smoothness of $f(x)$ to the rapid decay of $\tilde{f}(k)$, by combining Riemann-Lebesgue with integration by parts. Suppose that both f and f' are in $L^1(\mathbb{R})$. Then

$$[\tilde{f}'](k) \equiv \int_{-\infty}^{\infty} f'(x) e^{ikx} dx = -ik \int_{-\infty}^{\infty} f(x) e^{ikx} dx = -ik \tilde{f}(k) \quad (\text{B.40})$$

tends to zero. (No boundary terms arise from the integration by parts because in order for a differentiable function f to be in L^1 , it must tend to zero at infinity.) Since $k\tilde{f}(k)$ tends to zero, $\tilde{f}(k)$ itself must go to zero faster than $1/k$. We can continue in this manner and see that each additional derivative of f that lies in $L^1(\mathbb{R})$ buys us an extra power of $1/k$ in the decay rate of \tilde{f} at infinity. If any derivative possesses a jump discontinuity, however, *its* derivative will contain a delta-function, and a delta-function is not in L^1 . Thus, if n is the largest integer for which $k^n \tilde{f}(k) \rightarrow 0$ we may expect $f^{(n)}(x)$ to be somewhere discontinuous. For example, the function $f(x) = e^{-|x|}$ has a first derivative that lies in L^1 , but is discontinuous. Its Fourier transform $\tilde{f}(k) = 2/(1+k^2)$ therefore decays as $1/k^2$, but no faster.

B.3 Convolution

Suppose that $f(x)$ and $g(x)$ are functions on the real line \mathbb{R} . We define their *convolution* $f * g$, when it exists, by

$$[f * g](x) \equiv \int_{-\infty}^{\infty} f(x - \xi) g(\xi) d\xi. \quad (\text{B.41})$$

A change of variable $\xi \rightarrow x - \xi$ shows that, despite the apparently asymmetric treatment of f and g in the definition, the $*$ product obeys $f * g = g * f$.

B.3.1 The convolution theorem

Now, let $\tilde{f}(k)$ denote the Fourier transforms of f , *i.e.*

$$\tilde{f}(k) = \int_{-\infty}^{\infty} e^{ikx} f(x) dx. \quad (\text{B.42})$$

We claim that

$$\widetilde{[f * g]} = \tilde{f} \tilde{g}. \quad (\text{B.43})$$

The following computation shows that this claim is correct:

$$\begin{aligned} \widetilde{[f * g]}(k) &= \int_{-\infty}^{\infty} e^{ikx} \left(\int_{-\infty}^{\infty} f(x - \xi) g(\xi) d\xi \right) dx \\ &= \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} e^{ikx} f(x - \xi) g(\xi) d\xi dx \\ &= \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} e^{ik(x-\xi)} e^{ik\xi} f(x - \xi) g(\xi) d\xi dx \\ &= \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} e^{ikx'} e^{ik\xi} f(x') g(\xi) d\xi dx' \\ &= \left(\int_{-\infty}^{\infty} e^{ikx'} f(x') dx' \right) \left(\int_{-\infty}^{\infty} e^{ik\xi} g(\xi) d\xi \right) \\ &= \tilde{f}(k) \tilde{g}(k). \end{aligned} \quad (\text{B.44})$$

Note that we have freely interchanged the order of integrations. This is not always permissible, but it is allowed if $f, g \in L^1(\mathbb{R})$, in which case $f * g$ is also in $L^1(\mathbb{R})$.

B.3.2 Apodization and Gibbs' phenomenon

The convolution theorem is useful for understanding what happens when we truncate a Fourier series at a finite number of terms, or cut off a Fourier integral at a finite frequency or wavenumber.

Consider, for example, the cut-off Fourier integral representation

$$f_{\Lambda}(x) \equiv \frac{1}{2\pi} \int_{-\Lambda}^{\Lambda} \tilde{f}(k) e^{-ikx} dk, \quad (\text{B.45})$$

where $\tilde{f}(k) = \int_{-\infty}^{\infty} f(x) e^{ikx} dx$ is the Fourier transform of f . We can write this as

$$f_{\Lambda}(x) = \frac{1}{2\pi} \int_{-\infty}^{\infty} \theta_{\Lambda}(k) \tilde{f}(k) e^{-ikx} dk \quad (\text{B.46})$$

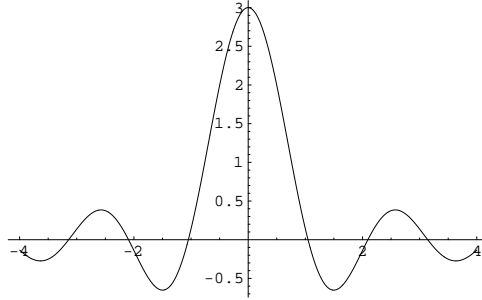
where $\theta_{\Lambda}(k)$ is unity if $|k| < \Lambda$ and zero otherwise. Written this way, the Fourier transform of f_{Λ} becomes the product of the Fourier transform of the original f with θ_{Λ} . The function f_{Λ} itself is therefore the convolution

$$f_{\Lambda}(x) = \int_{-\infty}^{\infty} \delta_{\Lambda}^{\text{F}}(x - \xi) f(\xi) d\xi \quad (\text{B.47})$$

of f with

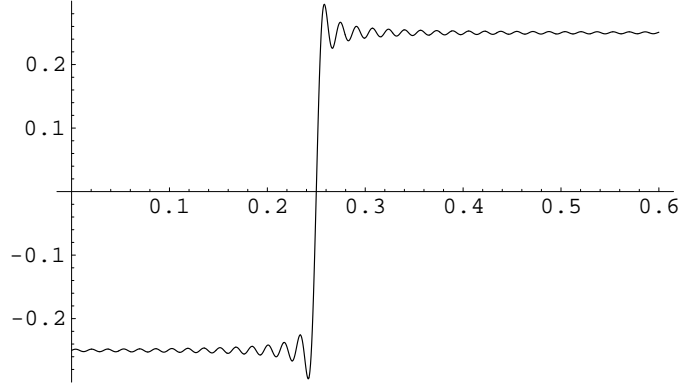
$$\delta_{\Lambda}^{\text{F}}(x) \equiv \frac{1}{\pi} \frac{\sin(\Lambda x)}{x} = \frac{1}{2\pi} \int_{-\infty}^{\infty} \theta_{\Lambda}(k) e^{-ikx} dk, \quad (\text{B.48})$$

which is the inverse Fourier transform of $\theta_{\Lambda}(x)$. We see that $f_{\Lambda}(x)$ is a kind of local average of the values of $f(x)$ smeared by the approximate delta-function $\delta_{\Lambda}^{\text{F}}(x)$. (The superscript F stands for “Fourier”).



A plot of $\pi\delta_{\Lambda}^{\text{F}}(x)$ for $\Lambda = 3$.

When $f(x)$ can be treated as a constant on the scale ($\approx 2\pi/\Lambda$) of the oscillation in $\delta_{\Lambda}^{\text{F}}(x)$, all that matters is that $\int_{-\infty}^{\infty} \delta_{\Lambda}^{\text{F}}(x) dx = 1$, and so $f_{\Lambda}(x) \approx f(x)$. This is the case if $f(x)$ is smooth and Λ is sufficiently large. However, if $f(x)$ possesses a discontinuity at x_0 , say, then we can never treat it as a constant and the rapid oscillations in $\delta_{\Lambda}^{\text{F}}(x)$ cause a “ringing” in $f_{\Lambda}(x)$ whose amplitude does not decrease (although the *width* of the region surrounding x_0 in which the effect is noticeable will decrease) as Λ grows. This ringing is known as *Gibbs’ phenomenon*.



The Gibbs phenomenon: A Fourier reconstruction of a piecewise constant function that jumps discontinuously from $y = -0.25$ to $+0.25$ at $x = 0.25$.

The amplitude of the ringing is largest immediately on either side of the point of discontinuity, where it is about 9% of the jump in f . This magnitude is determined by the area under the central spike in $\delta_\Lambda^F(x)$, which is

$$\frac{1}{\pi} \int_{-\pi/\Lambda}^{\pi/\Lambda} \frac{\sin(\Lambda x)}{x} dx = 1.18 \dots, \quad (\text{B.49})$$

independent of Λ . For x *exactly* at the point of discontinuity, $f_\Lambda(x)$ receives equal contributions from both sides of the jump and hence converges to the average

$$\lim_{\Lambda \rightarrow \infty} f_\Lambda(x) = \frac{1}{2} \{f(x_+) + f(x_-)\}, \quad (\text{B.50})$$

where $f(x_\pm)$ are the limits of f taken from the right and left, respectively. When $x = x_0 - \pi/\Lambda$, however, the central spike lies entirely to the left of the point of discontinuity and

$$\begin{aligned} f_\Lambda(x) &\approx \frac{1}{2} \{(1 + 1.18)f(x_-) + (1 - 1.18)f(x_+)\} \\ &\approx f(x_-) + 0.09\{f(x_-) - f(x_+)\}. \end{aligned} \quad (\text{B.51})$$

Consequently, $f_\Lambda(x)$ overshoots its target $f(x_-)$ by approximately 9% of the discontinuity. Similarly when $x = x_0 + \pi/\Lambda$

$$f_\Lambda(x) \approx f(x_+) + 0.09\{f(x_+) - f(x_-)\}. \quad (\text{B.52})$$

The ringing is a consequence of the abrupt truncation of the Fourier sum. If, instead of a sharp cutoff, we gradually de-emphasize the higher frequencies by the replacement

$$\tilde{f}(k) \rightarrow \tilde{f}(k) e^{-\alpha k^2/2} \quad (\text{B.53})$$

then

$$\begin{aligned} f_\alpha(x) &= \frac{1}{2\pi} \int_{-\infty}^{\infty} \tilde{f}(k) e^{-\alpha k^2/2} e^{-ikx} dk \\ &= \int_{-\infty}^{\infty} \delta_\alpha^G(x - \xi) f(\xi) d\xi \end{aligned} \quad (\text{B.54})$$

where

$$\delta_\alpha^G(x) = \frac{1}{\sqrt{2\pi\alpha}} e^{-x^2/2\alpha}, \quad (\text{B.55})$$

is a non-oscillating Gaussian approximation to a delta function. The effect of this convolution is to smooth out, or *mollify*, the original f , resulting in a C^∞ function. As α becomes small, the limit of $f_\alpha(x)$ will again be the local average of $f(x)$, so at a discontinuity f_α will converge to the mean $\frac{1}{2}\{f(x_+) + f(x_-)\}$.

When reconstructing a signal from a finite range of its Fourier components—for example from the output of an aperture-synthesis radio-telescope—it is good practice to smoothly suppress the higher frequencies in such a manner. This process is called *apodizing* (*i.e.* cutting off the feet of) the data. If we fail to apodize then any interesting sharp feature in the signal will be surrounded by “diffraction ring” artifacts.

Exercise B.1: Suppose that we exponentially suppress the higher frequencies by multiplying the Fourier amplitude $\tilde{f}(k)$ by $e^{-\epsilon|k|}$. Show that the original signal is smoothed by convolution with a *Lorentzian* approximation to a delta function

$$\delta_\epsilon^L(x - \xi) = \frac{1}{\pi} \frac{\epsilon}{\epsilon^2 + (x - \xi)^2}.$$

Observe that

$$\lim_{\epsilon \rightarrow 0} \delta_\epsilon^L(x) = \delta(x).$$

Exercise B.2: Consider the apodized Fourier series

$$f_r(\theta) = \sum_{n=-\infty}^{\infty} a_n r^{|n|} e^{in\theta},$$

where the parameter r lies in the range $0 < r < 1$, and the coefficients are

$$a_n \equiv \frac{1}{2\pi} \int_0^{2\pi} e^{-in\theta} f(\theta) d\theta.$$

Assuming that it is legitimate to interchange the order of the sum and integral, show that

$$\begin{aligned} f_r(\theta) &= \int_0^{2\pi} \delta_r^P(\theta - \theta') f(\theta') d\theta' \\ &\equiv \frac{1}{2\pi} \int_0^{2\pi} \left(\frac{1 - r^2}{1 - 2r \cos(\theta - \theta') + r^2} \right) f(\theta') d\theta'. \end{aligned}$$

Here the superscript P stands for Poisson because $\delta_r^P(\theta)$ is the *Poisson kernel* that solves the Dirichlet problem in the unit disc. Show that $\delta_r^P(\theta)$ tends to a delta function as $r \rightarrow 1$ from below.

Exercise B.3: The periodic Hilbert transform. Show that in the limit $r \rightarrow 1$ the sum

$$\sum_{n=-\infty}^{\infty} \operatorname{sgn}(n) e^{in\theta} r^{|n|} = \frac{re^{i\theta}}{1 - re^{i\theta}} - \frac{re^{-i\theta}}{1 - re^{-i\theta}}, \quad 0 < r < 1$$

becomes the principal-part distribution

$$P\left(i \cot\left(\frac{\theta}{2}\right)\right).$$

Let $f(\theta)$ be a smooth function on the unit circle, and define its *Hilbert transform* $\mathcal{H}f$ to be

$$(\mathcal{H}f)(\theta) = \frac{1}{2\pi} P \int_0^{2\pi} f(\theta') \cot\left(\frac{\theta - \theta'}{2}\right) d\theta'$$

Show the original function can be recovered from $(\mathcal{H}f)(\theta)$, together with knowledge of the angular average $\bar{f} = \int_0^{2\pi} f(\theta) d\theta / 2\pi$, as

$$\begin{aligned} f(\theta) &= -\frac{1}{2\pi} P \int_0^{2\pi} (\mathcal{H}f)(\theta') \cot\left(\frac{\theta - \theta'}{2}\right) d\theta' + \frac{1}{2\pi} \int_0^{2\pi} f(\theta') d\theta' \\ &= -(\mathcal{H}^2 f)(\theta) + \bar{f}. \end{aligned}$$

Exercise B.4: Find a closed-form expression for the sum

$$\sum_{n=-\infty}^{\infty} |n| e^{in\theta} r^{2|n|}, \quad 0 < r < 1.$$

Now let $f(\theta)$ be a smooth function defined on the unit circle and

$$a_n = \frac{1}{2\pi} \int_0^{2\pi} f(\theta) e^{-in\theta} d\theta$$

its n -th Fourier coefficient. By taking a limit $r \rightarrow 1$, show that

$$\pi \sum_{n=-\infty}^{\infty} |n| a_n a_{-n} = \frac{\pi}{4} \int_0^{2\pi} \int_0^{2\pi} [f(\theta) - f(\theta')]^2 \operatorname{cosec}^2 \left(\frac{\theta - \theta'}{2} \right) \frac{d\theta}{2\pi} \frac{d\theta'}{2\pi},$$

both the sum and integral being convergent. Show that these last two expressions are equal to

$$\frac{1}{2} \iint_{r < 1} |\nabla \varphi|^2 r dr d\theta$$

where $\varphi(r, \theta)$ is the function harmonic in the unit disc, whose boundary value is $f(\theta)$.

Exercise B.5: Let $\tilde{f}(k)$ be the Fourier transform of the smooth real function $f(x)$. Take a suitable limit in the previous problem to show that that

$$S[f] \equiv \frac{1}{4\pi} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \left\{ \frac{f(x) - f(x')}{x - x'} \right\}^2 dx dx' = \frac{1}{2} \int_{-\infty}^{\infty} |k| |\tilde{f}(k)|^2 \frac{dk}{2\pi}.$$

Exercise B.6: By taking a suitable limit in exercise B.3 show that, when acting on smooth functions f such that $\int_{-\infty}^{\infty} |f| dx$ is finite, we have $\mathcal{H}(\mathcal{H}f) = -f$, where

$$(\mathcal{H}f)(x) = \frac{P}{\pi} \int_{-\infty}^{\infty} \frac{f(x')}{x - x'} dx'$$

defines the Hilbert transform of a function on the real line. (Because \mathcal{H} gives zero when acting on a constant, some condition, such as $\int_{-\infty}^{\infty} |f| dx$ being finite, is necessary if \mathcal{H} is to be invertible.)

B.4 The Poisson Summation Formula

Suppose that $f(x)$ is a smooth function that tends rapidly to zero at infinity. Then the series

$$F(x) = \sum_{n=-\infty}^{\infty} f(x + nL) \quad (\text{B.56})$$

converges to a smooth function of period L . It therefore has a Fourier expansion

$$F(x) = \sum_{m=-\infty}^{\infty} a_m e^{-2\pi i m x / L} \quad (\text{B.57})$$

and we can compute the Fourier coefficients by integrating term-by-term

$$\begin{aligned} a_m &= \frac{1}{L} \int_0^L F(x) e^{2\pi i m x / L} dx \\ &= \frac{1}{L} \sum_{n=-\infty}^{\infty} \int_0^L f(x + nL) e^{2\pi i m x / L} dx \\ &= \frac{1}{L} \int_{-\infty}^{\infty} f(x) e^{2\pi i m x / L} dx \\ &= \frac{1}{L} \tilde{f}(2\pi m / L). \end{aligned} \quad (\text{B.58})$$

Thus

$$\sum_{n=-\infty}^{\infty} f(x + nL) = \frac{1}{L} \sum_{m=-\infty}^{\infty} \tilde{f}(2\pi m / L) e^{-2\pi i m x / L}. \quad (\text{B.59})$$

If we set $x = 0$, this becomes

$$\sum_{n=-\infty}^{\infty} f(nL) = \frac{1}{L} \sum_{m=-\infty}^{\infty} \tilde{f}(2\pi m / L). \quad (\text{B.60})$$

The equality of this pair of doubly infinite sums is called the *Poisson summation formula*.

Example: As the Fourier transform of a Gaussian is another Gaussian, the Poisson formula with $L = 1$ applied to $f(x) = \exp(-\kappa x^2)$ gives

$$\sum_{m=-\infty}^{\infty} e^{-\kappa m^2} = \sqrt{\frac{\pi}{\kappa}} \sum_{m=-\infty}^{\infty} e^{-m^2 \pi^2 / \kappa}, \quad (\text{B.61})$$

and (rather more usefully) applied to $\exp(-\frac{1}{2}tx^2 + ix\theta)$ gives

$$\sum_{n=-\infty}^{\infty} e^{-\frac{1}{2}tn^2 + in\theta} = \sqrt{\frac{2\pi}{t}} \sum_{n=-\infty}^{\infty} e^{-\frac{1}{2t}(\theta + 2\pi n)^2}. \quad (\text{B.62})$$

The last identity is known as *Jacobi's imaginary transformation*. It reflects the equivalence of the eigenmode expansion and the method-of-images solution of the diffusion equation

$$\frac{1}{2} \frac{\partial^2 \varphi}{\partial x^2} = \frac{\partial \varphi}{\partial t} \quad (\text{B.63})$$

on the unit circle. Notice that when t is small the sum on the right-hand side converges very slowly, whereas the sum on the left converges very rapidly. The opposite is true for large t . The conversion of a slowly converging series into a rapidly converging one is a standard application of the Poisson summation formula. It is the prototype of many *duality maps* that exchange a physical model with a large coupling constant for one with weak coupling.

If we take the limit $t \rightarrow 0$ in (B.62), the right hand side approaches a sum of delta functions, and so gives us the useful identity

$$\frac{1}{2\pi} \sum_{n=-\infty}^{\infty} e^{inx} = \sum_{n=-\infty}^{\infty} \delta(x + 2\pi n). \quad (\text{B.64})$$

The right-hand side of (B.64) is sometimes called the “Dirac comb.”

Exercise B.7: By applying the Poisson summation formula to the Fourier transform pair

$$f(x) = e^{-\epsilon|x|} e^{-ix\theta}, \quad \text{and} \quad \tilde{f}(k) = \frac{2\epsilon}{\epsilon^2 + (k - \theta)^2},$$

where $\epsilon > 0$, deduce that

$$\frac{\sinh \epsilon}{\cosh \epsilon - \cos(\theta - \theta')} = \sum_{n=-\infty}^{\infty} \frac{2\epsilon}{\epsilon^2 + (\theta - \theta' + 2\pi n)^2}. \quad (\text{B.65})$$

Hence show that the Poisson kernel is equivalent to an infinite periodic sum of Lorentzians

$$\frac{1}{2\pi} \left(\frac{1 - r^2}{1 - 2r \cos(\theta - \theta') + r^2} \right) = -\frac{1}{\pi} \sum_{n=-\infty}^{\infty} \frac{\ln r}{(\ln r)^2 + (\theta - \theta' + 2\pi n)^2}.$$

Appendix C

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