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 linear differential operator to have a complete set of eigenfunctions.

4.1 Formal *vs.* concrete operators

We will call the object

$$L = p_0(x)\frac{d^n}{dx^n} + p_1(x)\frac{d^{n-1}}{dx^{n-1}} + \cdots + p_n(x), \tag{4.1}$$

which we also write as

$$p_0(x)\partial_x^n + p_1(x)\partial_x^{n-1} + \cdots + p_n(x), \tag{4.2}$$

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

$$(\partial_x + v)(\partial_x + w) = \partial_x^2 + w' + (w + v)\partial_x + vw, \tag{4.3}$$

or

$$(\partial_x + w)(\partial_x + v) = \partial_x^2 + v' + (w + v)\partial_x + vw, \tag{4.4}$$

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

$$L = -\partial_x^2 + q(x) \tag{4.5}$$

and

$$P = \partial_x^3 + a(x)\partial_x + \partial_x a(x). \tag{4.6}$$

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

$$\partial_x a = a\partial_x + a'. \tag{4.7}$$

We can now form the commutator $[P, L] \equiv PL - LP$. After a little effort, we find

$$[P, L] = (3q' + 4a')\partial_x^2 + (3q'' + 4a'')\partial_x + q''' + 2aq' + a'''. \tag{4.8}$$

If we choose $a = -\frac{3}{4}q$, the commutator becomes a pure multiplication operator, with no differential part:

$$[P, L] = \frac{1}{4}q''' - \frac{3}{2}qq'. \tag{4.9}$$

The equation

$$\frac{dL}{dt} = [P, L], \tag{4.10}$$

or, equivalently,

$$\dot{q} = \frac{1}{4}q''' - \frac{3}{2}qq', \tag{4.11}$$

has a formal solution

$$L(t) = e^{tP}L(0)e^{-tP}, \tag{4.12}$$

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. Because the theory of matrix operators makes much use of inner products and orthogonality, 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 $[a,b]$. Now a differential operator cannot act on *every* function in the Hilbert space because not all of them are differentiable. Even though we will 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 vector 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

$$L = p_0\partial_x^2 + p_1\partial_x + p_2 \tag{4.13}$$

on the interval $[a,b]$, we might impose

$$\begin{aligned} B_1[y] = \alpha_{11}y(a) + \alpha_{12}y'(a) + \beta_{11}y(b) + \beta_{12}y'(b) &= 0, \\ B_2[y] = \alpha_{21}y(a) + \alpha_{22}y'(a) + \beta_{21}y(b) + \beta_{22}y'(b) &= 0, \end{aligned} \tag{4.14}$$

but we will not, in defining the differential *operator*, impose *inhomogeneous* conditions, such as

$$\begin{aligned} B_1[y] = \alpha_{11}y(a) + \alpha_{12}y'(a) + \beta_{11}y(b) + \beta_{12}y'(b) &= A, \\ B_2[y] = \alpha_{21}y(a) + \alpha_{22}y'(a) + \beta_{21}y(b) + \beta_{22}y'(b) &= B, \end{aligned} \tag{4.15}$$

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 reasonable[1]: 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 an L^2 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

$$L = p_0(x)\frac{d^n}{dx^n} + p_1(x)\frac{d^{n-1}}{dx^{n-1}} + \cdots + p_n(x), \tag{4.16}$$

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

$$w\left(u^*Lv - v(L^\dagger u)^*\right) = \frac{d}{dx}Q[u,v], \tag{4.17}$$

[1]There is a deeper reason which we will explain in section 9.7.2.

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

$$\langle u, v \rangle_w = \int_a^b w u^* v \, dx, \tag{4.18}$$

and if the functions u and v have boundary conditions that make $Q[u, v]|_a^b = 0$, then

$$\langle u, Lv \rangle_w = \langle L^\dagger u, v \rangle_w, \tag{4.19}$$

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

$$L = -i\frac{d}{dx} \tag{4.20}$$

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^*:

$$\begin{aligned} u^*\left(-i\frac{d}{dx}v\right) &= \left(i\frac{d}{dx}u^*\right)v - i\frac{d}{dx}(u^*v) \\ &= \left(-i\frac{d}{dx}u\right)^* v - i\frac{d}{dx}(u^*v) \\ &\equiv v(L^\dagger u)^* + \frac{d}{dx}Q[u, v]. \end{aligned} \tag{4.21}$$

We have ended up with the Lagrange identity

$$u^*\left(-i\frac{d}{dx}v\right) - v\left(-i\frac{d}{dx}u\right)^* = \frac{d}{dx}(-iu^*v), \tag{4.22}$$

and found that

$$L^\dagger = -i\frac{d}{dx}, \quad Q[u,v] = -iu^*v. \tag{4.23}$$

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

$$L = p_0\frac{d^2}{dx^2} + p_1\frac{d}{dx} + p_2, \tag{4.24}$$

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

$$\begin{aligned} u^*\left[p_0v'' + p_1v' + p_2v\right] - v\left[(p_0u)'' - (p_1u)' + p_2u\right]^* \\ = \frac{d}{dx}\left[p_0(u^*v' - vu^{*\prime}) + (p_1 - p_0')u^*v\right]. \end{aligned} \tag{4.25}$$

From this we read off that

$$\begin{aligned} L^\dagger &= \frac{d^2}{dx^2}p_0 - \frac{d}{dx}p_1 + p_2 \\ &= p_0\frac{d^2}{dx^2} + (2p_0' - p_1)\frac{d}{dx} + (p_0'' - p_1' + p_2). \end{aligned} \tag{4.26}$$

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

$$\begin{aligned} p_0 &= p_0 \\ 2p_0' - p_1 &= p_1 \quad \Rightarrow \quad p_0' = p_1 \\ p_0'' - p_1' + p_2 &= p_2 \quad \Rightarrow \quad p_0'' = p_1'. \end{aligned} \tag{4.27}$$

We therefore require that $p_1 = p_0'$, and so

$$L = \frac{d}{dx}\left(p_0\frac{d}{dx}\right) + p_2, \tag{4.28}$$

which we recognize as a *Sturm-Liouville* operator.

Example: Reduction to Sturm-Liouville form. Another way to make the operator

$$L = p_0\frac{d^2}{dx^2} + p_1\frac{d}{dx} + p_2, \tag{4.29}$$

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

$$w = \frac{1}{p_0} \exp\left\{ \int_a^x \left(\frac{p_1}{p_0} \right) dx' \right\} \tag{4.30}$$

and observe that it is positive on (a, b), and that

$$Ly = \frac{1}{w}(wp_0y')' + p_2y. \tag{4.31}$$

Now

$$\langle u, Lv \rangle_w - \langle Lu, v \rangle_w = [wp_0(u^*v' - u^{*\prime}v)]_a^b, \tag{4.32}$$

where

$$\langle u, v \rangle_w = \int_a^b wu^*v \, dx. \tag{4.33}$$

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

$$Ly = \frac{1}{w}(wp_0y')' + p_2y, \tag{4.34}$$

the eigenvalue equation

$$Ly = \lambda y \tag{4.35}$$

can be written

$$(wp_0y')' + p_2wy = \lambda wy. \tag{4.36}$$

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

$$\langle P, Q \rangle = \frac{1}{\pi} \int d^2z \, e^{-z^*z} \, [P(z)]^* \, Q(z),$$

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 operator.[2]

Exercise 4.1: Consider the differential operator $\hat{L} = id/dx$. Find the formal adjoint of L with respect to the inner product $\langle u, v \rangle = \int wu^*v\,dx$, and find the corresponding surface term $Q[u, v]$.

[2]In deriving this result we have used the *Wirtinger calculus* where z and z^* are treated 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

$$T = -\partial_x^2, \quad \mathcal{D}(T) = \{y, Ty \in L^2[0,1] \,:\, y(0) = y(1) = 0\}. \tag{4.37}$$

With the inner product

$$\langle y_1, y_2\rangle = \int_0^1 y_1^* y_2\,dx \tag{4.38}$$

we have

$$\langle y_1, Ty_2\rangle - \langle Ty_1, y_2\rangle = [y_1'^* y_2 - y_1^* y_2']_0^1 = 0. \tag{4.39}$$

The integrated-out part is zero because both y_1 and y_2 satisfy the boundary conditions. We see that

$$\langle y_1, Ty_2\rangle = \langle Ty_1, y_2\rangle \tag{4.40}$$

and so T is *Hermitian* or *symmetric*.

The eigenfunctions and eigenvalues of T are

$$\left.\begin{array}{c} y_n(x) = \sin n\pi x \\ \lambda_n = n^2\pi^2 \end{array}\right\} \quad n = 1, 2, \ldots. \tag{4.41}$$

We see that:

i) the eigenvalues are *real*;
ii) the eigenfunctions for different λ_n are *orthogonal*,

$$2\int_0^1 \sin n\pi x \sin m\pi x\,dx = \delta_{nm}, \quad n = 1, 2, \ldots \tag{4.42}$$

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

$$y(x) = \sum_{n=1}^{\infty} a_n \sqrt{2}\sin n\pi x \tag{4.43}$$

where

$$a_n = \int_0^1 y(x)\sqrt{2}\sin n\pi x\, dx. \tag{4.44}$$

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

$$T = -i\partial_x, \quad \mathcal{D}(T) = \{y, Ty \in L^2[0,1] \,:\, y(0) = y(1) = 0\}. \tag{4.45}$$

Again

$$\begin{aligned} \langle y_1, Ty_2\rangle - \langle Ty_1, y_2\rangle &= \int_0^1 dx\, \{y_1^*(-i\partial_x y_2) - (-i\partial_x y_1)^* y_2\} \\ &= -i[y_1^* y_2]_0^1 = 0. \end{aligned} \tag{4.46}$$

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:

$$H = x^3 p + p x^3. \tag{4.47}$$

Now let

$$\psi_\lambda(x) = |x|^{-3/2} \exp\left\{-\frac{\lambda}{4x^2}\right\}, \tag{4.48}$$

where λ is real and positive. Show that

$$H\psi_\lambda = -i\lambda\psi_\lambda, \tag{4.49}$$

so ψ_λ is an eigenfunction with a purely imaginary eigenvalue. Examine the proof that Hermitian operators have real eigenvalues, and identify at which point it fails. (*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 $T : V \to V$ and an inner product $\langle\ ,\ \rangle$, 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 we set $T^\dagger u = w$.

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

$$T = -i\partial_x, \quad \mathcal{D}(T) = \{y, Ty \in L^2[0, 1]\ : y(1) = 0\}. \tag{4.50}$$

Now,

$$\begin{aligned}\int_0^1 dx\, u^*(-i\partial_x v) &= -i[u^*(1)v(1) - u^*(0)v(0)] + \int_0^1 dx(-i\partial_x u)^* v \\ &= -i[u^*(1)v(1) - u^*(0)v(0)] \quad + \quad \langle w, v\rangle, \end{aligned} \tag{4.51}$$

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 $T^\dagger$:

$$T^\dagger = -i\partial_x, \quad \mathcal{D}(T^\dagger) = \{y, Ty \in L^2[0,1] : y(0) = 0\}. \tag{4.52}$$

For our problematic operator

$$T = -i\partial_x, \quad \mathcal{D}(T) = \{y, Ty \in L^2[0,1] \ : y(0) = y(1) = 0\}, \tag{4.53}$$

we have

$$\begin{aligned} \int_0^1 dx\, u^*(-i\partial_x v) &= -i[u^* v]_0^1 + \int_0^1 dx(-i\partial_x u)^* v \\ &= \quad 0 \quad + \quad \langle w, v\rangle, \end{aligned} \tag{4.54}$$

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

$$T^\dagger = -i\partial_x, \quad \mathcal{D}(T^\dagger) = \{y, Ty \in L^2[0,1]\}. \tag{4.55}$$

Although any of these operators "$T = -i\partial_x$" is *formally* self-adjoint we have,

$$\mathcal{D}(T) \neq \mathcal{D}(T^\dagger), \tag{4.56}$$

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,

$$\int_0^1 dx\, u^*(-i\partial_x v) - \int_0^1 dx(-i\partial_x u)^* v = -i\Big(u^*(1)v(1) - u^*(0)v(0)\Big). \quad (4.57)$$

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 $n = \ldots, -2, -1, 0, 1, 2\ldots$ 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

$$\langle u, Lv\rangle - \langle Lu, v\rangle = [p(u^* v' - u'^* v)]_a^b. \tag{4.62}$$

Let us seek to impose boundary conditions separately at the two ends. Thus, at $x = a$ we want

$$(u^* v' - u'^* v)|_a = 0, \tag{4.63}$$

or

$$\frac{u'^*(a)}{u^*(a)} = \frac{v'(a)}{v(a)}, \tag{4.64}$$

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

$$\frac{v'(a)}{v(a)} = \frac{u'(a)}{u(a)} = \tan\theta_a \tag{4.65}$$

for some real angle θ_a, and similar boundary conditions with a θ_b at b. We can also write these boundary conditions as

$$\begin{aligned} \alpha_a y(a) + \beta_a y'(a) &= 0, \\ \alpha_b y(b) + \beta_b y'(b) &= 0. \end{aligned} \tag{4.66}$$

Deficiency indices and self-adjoint extensions

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 we define an initial domain $\mathcal{D}_0(L)$ for the operator L by imposing the strictest possible boundary conditions. This we do 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 extensions* $\mathcal{D}(L) \supset \mathcal{D}_0(L)$ of the initial tightly-restricted domain.

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

$$P_r = -i\partial_r, \quad \mathcal{D}_0(T) = \{y, P_r y \in L^2[0,\infty] \, : y(0) = 0\}. \tag{4.67}$$

We then have

$$P_r^\dagger = -i\partial_r, \quad \mathcal{D}(P_r^\dagger) = \{y, P_r^\dagger y \in L^2[0,\infty]\} \tag{4.68}$$

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

$$T = -\partial_x^2, \quad \mathcal{D}_0(T) = \{y, Ty \in L^2[0,\infty] \, : y(0) = y'(0) = 0\}. \tag{4.69}$$

We then have

$$T^\dagger = -\partial_x^2, \quad \mathcal{D}(T^\dagger) = \{y, T^\dagger y \in L^2[0,\infty]\}. \tag{4.70}$$

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

$$\begin{aligned} B_1[y] = \alpha_{11}y(a) + \alpha_{12}y'(a) + \beta_{11}y(b) + \beta_{12}y'(b) &= 0, \\ B_2[y] = \alpha_{21}y(a) + \alpha_{22}y'(a) + \beta_{21}y(b) + \beta_{22}y'(b) &= 0 \end{aligned}$$

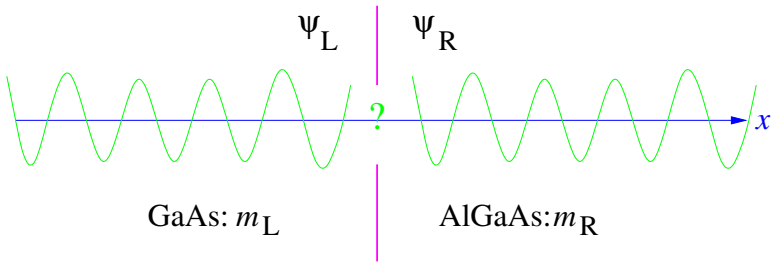

Figure 4.1: *Heterojunction and wavefunctions.*

Physics application: semiconductor heterojunction

We now demonstrate why we have spent so much time on identifying self-adjoint boundary conditions: the technique is important in practical physics problems.

A *heterojunction* is an atomically smooth interface between two related semiconductors, such as GaAs and $Al_xGa_{1-x}As$, which typically possess different band-masses. We wish to describe the conduction electrons 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 beween 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?

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

$$\begin{aligned} H &= -\frac{1}{2m_L}\frac{d^2}{dx^2} + V_L(x), \quad x < 0, \\ &= -\frac{1}{2m_R}\frac{d^2}{dx^2} + V_R(x), \quad x > 0. \end{aligned} \tag{4.71}$$

Integrating by parts, and keeping the terms at the interface gives us

$$\langle \psi_1, H\psi_2\rangle - \langle H\psi_1, \psi_2\rangle = \frac{1}{2m_L}\left\{\psi_{1L}^*\psi_{2L}' - \psi'^*_{1L}\psi_{2L}\right\} - \frac{1}{2m_R}\left\{\psi_{1R}^*\psi_{2R}' - \psi'^*_{1R}\psi_{2R}\right\}. \tag{4.72}$$

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:

$$\begin{pmatrix} \psi_{2L} \\ \psi_{2L}' \end{pmatrix} = \begin{pmatrix} a & b \\ c & d \end{pmatrix} \begin{pmatrix} \psi_{2R} \\ \psi_{2R}' \end{pmatrix}. \tag{4.73}$$

This relation involves four complex, and therefore eight real, parameters. Demanding that

$$\langle \psi_1, H\psi_2\rangle = \langle H\psi_1, \psi_2\rangle, \tag{4.74}$$

we find

$$\frac{1}{2m_L}\left\{\psi_{1L}^*(c\psi_{2R} + d\psi_{2R}') - \psi'^*_{1L}(a\psi_{2R} + b\psi_{2R}')\right\} = \frac{1}{2m_R}\left\{\psi_{1R}^*\psi_{2R}' - \psi'^*_{1R}\psi_{2R}\right\}, \tag{4.75}$$

and this must hold for arbitrary ψ_{2R}, ψ_{2R}', so, picking off the coefficients of these expressions and complex conjugating, we find

$$\begin{pmatrix} \psi_{1R} \\ \psi_{1R}' \end{pmatrix} = \begin{pmatrix} m_R \\ \overline{m_L} \end{pmatrix} \begin{pmatrix} d^* & -b^* \\ -c^* & a^* \end{pmatrix} \begin{pmatrix} \psi_{1L} \\ \psi_{1L}' \end{pmatrix}. \tag{4.76}$$

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

$$\begin{pmatrix} a & b \\ c & d \end{pmatrix}^{-1} = \begin{pmatrix} m_R \\ \overline{m_L} \end{pmatrix} \begin{pmatrix} d^* & -b^* \\ -c^* & a^* \end{pmatrix}. \tag{4.77}$$

Since

$$\begin{pmatrix} a & b \\ c & d \end{pmatrix}^{-1} = \frac{1}{ad-bc} \begin{pmatrix} d & -b \\ -c & a \end{pmatrix}, \tag{4.78}$$

we see that this requires

$$\begin{pmatrix} a & b \\ c & d \end{pmatrix} = e^{i\phi} \sqrt{\frac{m_L}{m_R}} \begin{pmatrix} A & B \\ C & D \end{pmatrix}, \tag{4.79}$$

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 calculation.[3] 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 $L^2[a,b]$ 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

[3] For example, see: T. Ando, S. Mori, *Surface Science* **113** (1982) 124.

the *point* spectrum when its associated eigenfunction is normalizable *i.e* is a *bona-fide* member of $L^2[a,b]$ 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 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

$$T\phi_n(x) = \lambda_n \phi_n(x), \tag{4.80}$$

where n is an integer. After multiplication by suitable constants, the ϕ_n are orthonormal,

$$\int \phi_n^*(x)\phi_m(x)\,dx = \delta_{nm}, \tag{4.81}$$

and complete. We can express the *completeness condition* as the statement that

$$\sum_n \phi_n(x)\phi_n^*(x') = \delta(x-x'). \tag{4.82}$$

If we take this representation of the delta function and multiply it by $f(x')$ and integrate over x', we find

$$f(x) = \sum_n \phi_n(x) \int \phi_n^*(x')f(x')\,dx'. \tag{4.83}$$

So,

$$f(x) = \sum_n a_n \phi_n(x) \tag{4.84}$$

with

$$a_n = \int \phi_n^*(x')f(x')\,dx'. \tag{4.85}$$

This means that if we can expand a delta function in terms of the $\phi_n(x)$, we can expand any (square integrable) function.

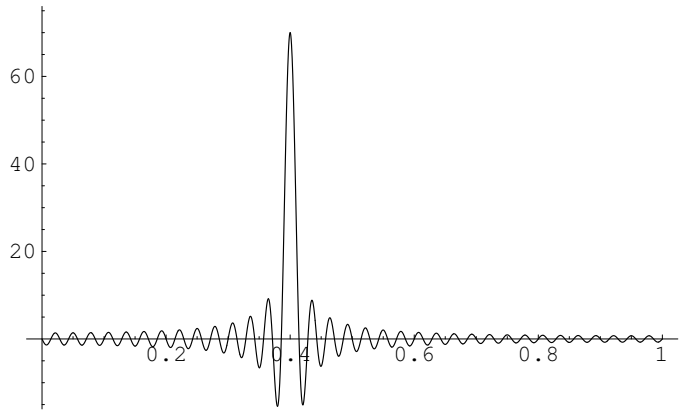

Figure 4.2: *The sum* $\sum_{n=1}^{70} 2\sin(n\pi x)\sin(n\pi x')$ *for* $x' = 0.4$. *Take note of the very disparate scales on the horizontal and vertical axes.*

Warning: 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 70 terms in the sum

$$\sum_{n=1}^{\infty} \sqrt{2}\sin(n\pi x)\sqrt{2}\sin(n\pi x') = \delta(x-x')$$

is shown in figure 4.2. The "wiggles" on both sides of the spike at $x = x'$ do not decrease in amplitude as the number of terms grows. They do, however, 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 $x = x'$.

Rayleigh-Ritz and completeness

For the Schrödinger eigenvalue problem

$$Ly = -y'' + q(x)y = \lambda y, \quad x \in [a,b], \tag{4.86}$$

the large eigenvalues are $\lambda_n \approx n^2\pi^2/(a-b)^2$. This is because the term qy eventually becomes negligeable compared to λy, and we can then solve the equation 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

$$Ly = -(py')' + qy = \lambda y, \quad x \in [a,b], \tag{4.87}$$

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

$$\lambda_0 = \inf_{y\in\mathcal{D}(L)} \frac{\langle y, Ly\rangle}{\langle y, y\rangle}. \tag{4.88}$$

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 Ritz.[4]

Suppose we have already found the first n normalized eigenfunctions $y_0, y_1, \ldots, y_{n-1}$. Let the space spanned by these functions be V_n. Then an obvious extension of the variational principle gives

$$\lambda_n = \inf_{y\in V_n^\perp} \frac{\langle y, Ly\rangle}{\langle y, y\rangle}. \tag{4.89}$$

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,

$$y = \sum_{m=0}^{\infty} a_m y_m, \tag{4.90}$$

[4] J. W. Strutt (later Lord Rayleigh), "In Finding the Correction for the Open End of an Organ-Pipe." *Phil. Trans.* **161** (1870) 77; W. Ritz, "Uber eine neue Methode zur Lösung gewisser Variationsprobleme der mathematischen Physik." *J. reine angew. Math.* **135** (1908).

where

$$a_m = \langle y_m, y \rangle, \tag{4.91}$$

then the sum does indeed converge to y.

Let

$$h_n = y - \sum_{m=0}^{n-1} a_m y_m \tag{4.92}$$

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

$$\langle h_n, Lh_n \rangle = \langle y, Ly \rangle - \sum_{m=0}^{n-1} \lambda_m |a_m|^2, \tag{4.93}$$

where we have made use of the orthonormality of the y_m. The subtracted sum is guaranteed positive, so

$$\langle h_n, Lh_n \rangle \leq \langle y, Ly \rangle. \tag{4.94}$$

Combining this inequality with Rayleigh-Ritz tells us that

$$\frac{\langle y, Ly \rangle}{\langle h_n, h_n \rangle} \geq \frac{\langle h_n, Lh_n \rangle}{\langle h_n, h_n \rangle} \geq \lambda_n. \tag{4.95}$$

In other words

$$\frac{\langle y, Ly \rangle}{\lambda_n} \geq \| y - \sum_{m=0}^{n-1} a_m y_m \|^2. \tag{4.96}$$

Since $\langle y, Ly \rangle$ is independent of n, and $\lambda_n \to \infty$, we have $\| y - \sum_0^{n-1} a_m y_m \|^2 \to 0$. 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

$$H = (-\partial_x + x)(\partial_x + x) + 1 = -\partial_x^2 + x^2. \tag{4.97}$$

This is in the form $Q^\dagger Q + 1$, where $Q = (\partial_x + x)$, and $Q^\dagger = (-\partial_x + x)$ is its formal adjoint. If we write these operators in the opposite order we have

$$QQ^\dagger = (\partial_x + x)(-\partial_x + x) = -\partial_x^2 + x^2 + 1 = H + 1. \tag{4.98}$$

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

$$Q^\dagger Q\psi = \lambda\psi \tag{4.99}$$

implies that

$$Q(Q^\dagger Q\psi) = \lambda Q\psi, \tag{4.100}$$

or

$$QQ^\dagger(Q\psi) = \lambda(Q\psi). \tag{4.101}$$

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

$$0 = \langle\psi, Q^\dagger Q\psi\rangle = \langle Q\psi, Q\psi\rangle, \tag{4.102}$$

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

$$\psi_0 = e^{-\frac{1}{2}x^2} \tag{4.103}$$

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

$$\psi = e^{+\frac{1}{2}x^2}, \tag{4.104}$$

which is not normalizable, and so not an element of $L^2[-\infty, \infty]$.

Since

$$H = Q^\dagger Q + 1 = QQ^\dagger - 1, \tag{4.105}$$

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

$$\psi_n = (Q^\dagger)^n \psi_0 \tag{4.106}$$

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

$$\psi_n(x) = H_n(x) e^{-\frac{1}{2}x^2}, \tag{4.107}$$

where

$$H_n(x) = (-1)^n e^{x^2} \frac{d^n}{dx^n} e^{-x^2} \tag{4.108}$$

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.

Problem 4.7: Schrödinger equations of the form

$$-\frac{d^2\psi}{dx^2} - l(l+1)\mathrm{sech}^2 x\, \psi = E\psi$$

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 $\psi = \exp\left\{-\int^x u(x')dx'\right\}$ 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)

$$H = -\frac{d}{dx}^2 - 2\,\mathrm{sech}^2 x.$$

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 $x \to \pm\infty$. 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

$$H = -\partial_x^2. \tag{4.109}$$

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 $L \to \infty$

The operator H has formal eigenfunctions

$$\varphi_k(x) = e^{ikx}, \tag{4.110}$$

corresponding to eigenvalues $\lambda = k^2$. Suppose we impose periodic boundary conditions at $x = \pm L/2$:

$$\varphi_k(-L/2) = \varphi_k(+L/2). \tag{4.111}$$

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

$$\chi_n(x) = \frac{1}{\sqrt{L}} e^{ik_n x}. \tag{4.112}$$

The completeness condition is

$$\sum_{n=-\infty}^{\infty} \frac{1}{L} e^{ik_n x} e^{-ik_n x'} = \delta(x - x'), \quad x, x' \in [-L/2, L/2]. \tag{4.113}$$

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

$$\sum_{n=-\infty}^{\infty} \Big\{ \dots \Big\} \to \int dn \Big\{ \dots \Big\} = \int dk \left(\frac{dn}{dk} \right) \Big\{ \dots \Big\}, \tag{4.114}$$

where

$$\frac{dn}{dk} = \frac{L}{2\pi} \tag{4.115}$$

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

$$\frac{dn}{dk} = \rho(k). \tag{4.116}$$

If we express the density of states in terms of the eigenvalue λ then, by an abuse of notation, we have

$$\rho(\lambda) \equiv \frac{dn}{d\lambda} = \frac{L}{2\pi\sqrt{\lambda}}. \tag{4.117}$$

[5]When 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, they 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 prefer to regard non-normalizable wavefunctions as being distributions in our rigged Hilbert space.

Note that

$$\frac{dn}{d\lambda} = 2\frac{dn}{dk}\frac{dk}{d\lambda}, \tag{4.118}$$

which looks a bit weird, but remember that *two* states, $\pm k_n$, correspond to the same λ and that the symbols

$$\frac{dn}{dk}, \quad \frac{dn}{d\lambda} \tag{4.119}$$

are ratios of measures, *i.e. Radon-Nikodym derivatives*, not ordinary derivatives.

In the $L \to \infty$ limit, the completeness condition becomes

$$\int_{-\infty}^{\infty} \frac{dk}{2\pi} e^{ik(x-x')} = \delta(x - x'), \tag{4.120}$$

and the length L has disappeared.

Suppose that we now apply boundary conditions $y = 0$ on $x = \pm L/2$. The normalized eigenfunctions are then

$$\chi_n = \sqrt{\frac{2}{L}} \sin k_n(x + L/2), \tag{4.121}$$

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

$$\rho(k) = \frac{dn}{dk} = \frac{L}{\pi}, \tag{4.122}$$

which is twice as large as in the periodic case, but the eigenvalue density of states is

$$\rho(\lambda) = \frac{L}{2\pi\sqrt{\lambda}}, \tag{4.123}$$

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 Peierls[6] 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

$$\left(-\frac{d^2}{dr^2} + V(r)\right)\psi = E\psi \tag{4.124}$$

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 $R \to \infty$ limit. Let us first deal with the simple case that $V(r) \equiv 0$; then the solutions are

$$\psi_k(r) \propto \sin kr, \tag{4.125}$$

with eigenvalue $E = k^2$, and with the allowed values of being given by $k_n R = n\pi$. Since

$$\int_0^R \sin^2(k_n r)\, dr = \frac{R}{2}, \tag{4.126}$$

[6]Peierls proved that the phonon contribution to the specific heat of a crystal could be correctly calculated by using periodic boundary conditions. Some sceptics had thought that such "unphysical" boundary conditions would give a result wrong by factors of two.

the normalized wavefunctions are

$$\psi_k = \sqrt{\frac{2}{R}} \sin kr, \tag{4.127}$$

and completeness reads

$$\sum_{n=1}^{\infty} \left(\frac{2}{R}\right) \sin(k_n r) \sin(k_n r') = \delta(r - r'). \tag{4.128}$$

As R becomes large, this sum goes over to an integral:

$$\begin{aligned} \sum_{n=1}^{\infty} \left(\frac{2}{R}\right) \sin(k_n r) \sin(k_n r') &\rightarrow \int_0^{\infty} dn \left(\frac{2}{R}\right) \sin(kr)\, \sin(kr'), \\ &= \int_0^{\infty} \frac{R dk}{\pi} \left(\frac{2}{R}\right) \sin(kr)\, \sin(kr') \end{aligned} \tag{4.129}$$

Thus,

$$\left(\frac{2}{\pi}\right) \int_0^{\infty} dk\, \sin(kr) \sin(kr') = \delta(r - r'). \tag{4.130}$$

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

$$\psi_k(r) = \sin\left(kr + \eta(k)\right), \tag{4.131}$$

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 $V(r) = \lambda\delta(r - a)$. See figure 4.3.

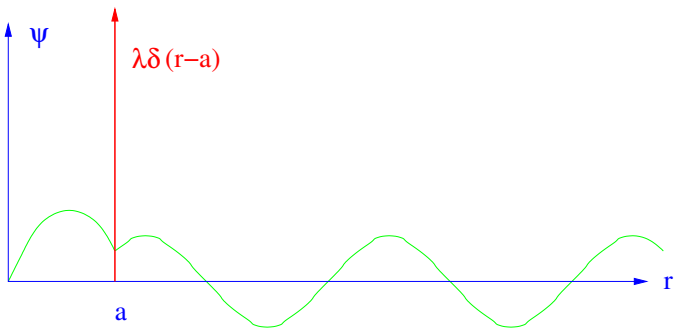

Figure 4.3: *Delta function shell potential.*

A solution with eigenvalue $E = k^2$ and satisfying the boundary condition at $r = 0$ is

$$\psi(r) = \begin{cases} A\sin(kr), & r < a, \\ \sin(kr + \eta), & r > a. \end{cases} \tag{4.132}$$

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,

$$\frac{\psi'(a + \epsilon)}{\psi(a)} - \frac{\psi'(a - \epsilon)}{\psi(a)} = \lambda, \tag{4.133}$$

or

$$\frac{k\cos(ka + \eta)}{\sin(ka + \eta)} - \frac{k\cos(ka)}{\sin(ka)} = \lambda. \tag{4.134}$$

Thus,

$$\cot(ka + \eta) - \cot(ka) = \frac{\lambda}{k}, \tag{4.135}$$

and

$$\eta(k) = -ka + \cot^{-1}\left(\frac{\lambda}{k} + \cot ka\right). \tag{4.136}$$

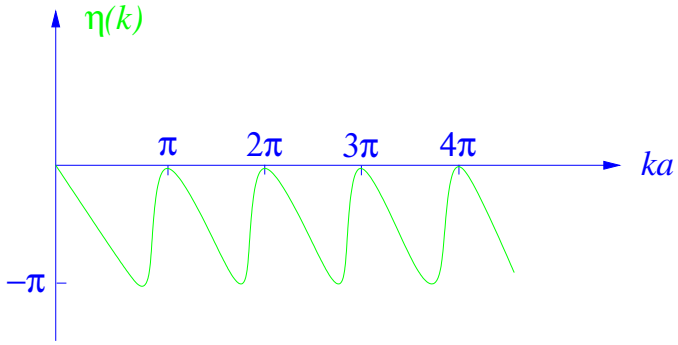

Figure 4.4: *The phase shift $\eta(k)$ of equation (4.136) plotted against ka.*

A sketch of $\eta(k)$ is shown in figure 4.4. The allowed values of k are required by the boundary condition

$$\sin(kR + \eta(k)) = 0 \tag{4.137}$$

to satisfy

$$kR + \eta(k) = n\pi. \tag{4.138}$$

This is a transcendental equation for k, and so finding the individual solutions k_n is not simple. We can, however, write

$$n = \frac{1}{\pi}\Big(kR + \eta(k)\Big) \tag{4.139}$$

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

$$\frac{dn}{dk} = \frac{1}{\pi}\left\{R + \frac{\partial\eta}{\partial k}\right\}. \tag{4.140}$$

The density of allowed k values is therefore

$$\rho(k) = \frac{1}{\pi}\left\{R + \frac{\partial\eta}{\partial k}\right\}. \tag{4.141}$$

For our delta-shell example, a plot of $\rho(k)$ appears in figure 4.5.

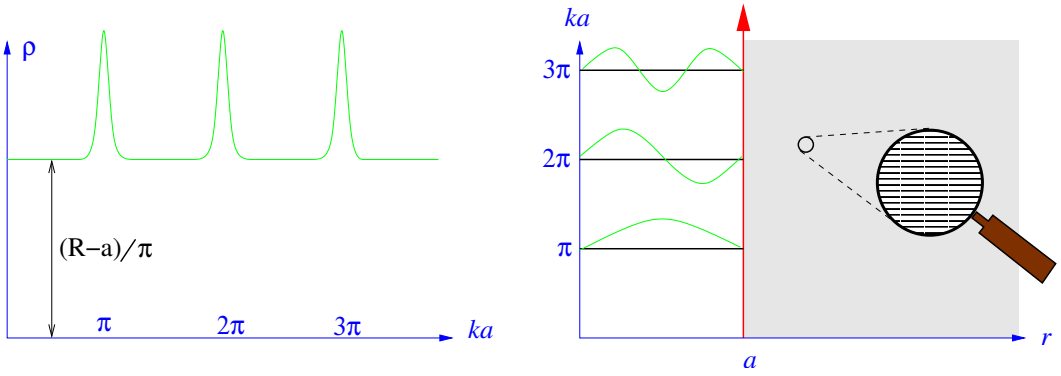

Figure 4.5: *The density of states for the delta-shell potential. The extended states are so close in energy that we need an optical aid to resolve individual levels. The almost-bound resonance levels have to squeeze in between them.*

This figure shows a sequence of 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

$$\int_0^R dr|\psi_k|^2 = N_k^{-2}, \tag{4.142}$$

so as to find the the normalized wavefunctions

$$\chi_k = N_k \psi_k. \tag{4.143}$$

Let $\psi_k(r)$ be a solution of

$$H\psi = \left(-\frac{d^2}{dr^2} + V(r)\right)\psi = k^2\psi \tag{4.144}$$

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

$$\begin{aligned}(k^2 - k'^2)\int_0^R dr\,\psi_k\,\psi_{k'} &= \int_0^R dr\,\{(H\psi_k)\psi_{k'} - \psi_k(H\psi_{k'})\} \\ &= [\psi_k\psi'_{k'} - \psi'_k\psi_{k'}]_0^R \\ &= \sin(kR+\eta)k'\cos(k'R+\eta) \\ &\quad -k\cos(kR+\eta)\sin(k'R+\eta).\end{aligned} \tag{4.145}$$

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

$$2k\int_0^R dr(\psi_k)^2 = -\frac{1}{2}\sin\Big(2(kR+\eta)\Big) + k\left\{R + \frac{\partial\eta}{\partial k}\right\}. \tag{4.146}$$

In other words,

$$\int_0^R dr(\psi_k)^2 = \frac{1}{2}\left\{R + \frac{\partial\eta}{\partial k}\right\} - \frac{1}{4k}\sin\Big(2(kR+\eta)\Big). \tag{4.147}$$

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

$$\int_0^R dr|\psi_k|^2 = \frac{1}{2}\left\{R + \frac{\partial\eta}{\partial k}\right\}. \tag{4.148}$$

Observe that the same expression occurs in both the density of states and the normalization integral. When we use these quantities to write down the contribution of the normalized states in the continuous spectrum to the completeness relation we find that

$$\int_0^\infty dk\left(\frac{dn}{dk}\right) N_k^2\psi_k(r)\psi_k(r') = \left(\frac{2}{\pi}\right)\int_0^\infty dk\,\psi_k(r)\psi_k(r'), \tag{4.149}$$

the density of states and normalization factor having cancelled and 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

$$\sum_{\text{bound states}} \psi_n(r)\psi_n(r') + \left(\frac{2}{\pi}\right)\int_0^\infty dk\,\psi_k(r)\,\psi_k(r') = \delta(r-r'). \tag{4.150}$$

Example: We will exhibit a completeness relation for a problem on the entire real line. We have already met the Pöschel-Teller equation,

$$H\psi = \left(-\frac{d^2}{dx^2} - l(l+1)\,\mathrm{sech}^2 x\right)\psi = E\psi \tag{4.151}$$

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

$$\psi_0(x) = \frac{1}{\sqrt{2}}\operatorname{sech} x. \tag{4.152}$$

The rest of the spectrum consists of a continuum of unbound states with eigenvalues $E(k) = k^2$ and eigenfunctions

$$\psi_k(x) = \frac{1}{\sqrt{1+k^2}} e^{ikx}(-ik + \tanh x). \tag{4.153}$$

Here, k is any real number. The normalization of $\psi_k(x)$ has been chosen so that, at large $|x|$, where $\tanh x \to \pm 1$, we have

$$\psi_k^*(x)\psi_k(x') \to e^{-ik(x-x')}. \tag{4.154}$$

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

$$\begin{aligned} I &= \delta(x-x') - \int_{-\infty}^{\infty} \frac{dk}{2\pi} \psi_k^*(x)\psi_k(x') \\ &= \int_{-\infty}^{\infty} \frac{dk}{2\pi} \left(e^{-ik(x-x)} - \psi_k^*(x)\psi_k(x') \right) \\ &= \int_{-\infty}^{\infty} \frac{dk}{2\pi} e^{-ik(x-x')} \frac{1 + ik(\tanh x - \tanh x') - \tanh x \tanh x'}{1+k^2}. \end{aligned} \tag{4.155}$$

We use the standard integral,

$$\int_{-\infty}^{\infty} \frac{dk}{2\pi} e^{-ik(x-x')} \frac{1}{1+k^2} = \frac{1}{2} e^{-|x-x'|}, \tag{4.156}$$

together with its x' derivative,

$$\int_{-\infty}^{\infty} \frac{dk}{2\pi} e^{-ik(x-x')} \frac{ik}{1+k^2} = \operatorname{sgn}(x-x') \frac{1}{2} e^{-|x-x'|}, \tag{4.157}$$

to find

$$I = \frac{1}{2}\Big\{ 1 + \operatorname{sgn}(x-x')(\tanh x - \tanh x') - \tanh x \tanh x' \Big\} e^{-|x-x'|}. \tag{4.158}$$

Assume, without loss of generality, that $x > x'$; then this reduces to

$$\begin{aligned} \frac{1}{2}(1+\tanh x)(1-\tanh x')e^{-(x-x')} &= \frac{1}{2}\operatorname{sech} x \operatorname{sech} x' \\ &= \psi_0(x)\psi_0(x'). \end{aligned} \tag{4.159}$$

Thus, the expected completeness condition

$$\psi_0(x)\psi_0(x') + \int_{-\infty}^{\infty} \frac{dk}{2\pi}\psi_k^*(x)\psi_k(x') = \delta(x-x'), \tag{4.160}$$

is confirmed.

4.4 Further 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 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.

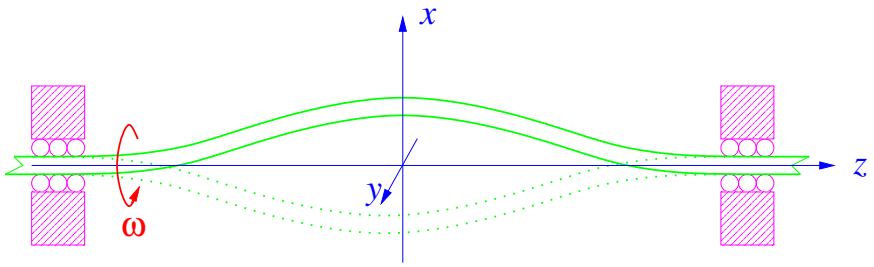

Figure 4.6: *The $n = 1$ even-parity mode of a whirling shaft.*

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 a frequency ω_{n+1}, at which the pattern is repeated. Our task is to understand why this happens.

The kinetic energy of the whirling shaft is

$$T = \frac{1}{2}\int_{-L}^{L} \rho\{\dot{x}^2 + \dot{y}^2\}dz,$$

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 negligeable 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 problem this.

Problem 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 $n = 1, 2, \ldots, N$;
- 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:

a) 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.

b) 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.

c) Consider the non-symmetric N-by-N matrix operator

$$D^2 u = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & \ldots & 0 \\ 1 & -2 & 1 & 0 & 0 & \ldots & 0 \\ 0 & 1 & -2 & 1 & 0 & \ldots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots \\ 0 & \ldots & 0 & 1 & -2 & 1 & 0 \\ 0 & \ldots & 0 & 0 & 1 & -2 & 1 \\ 0 & \ldots & 0 & 0 & 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} u_N \\ u_{N-1} \\ u_{N-2} \\ \vdots \\ u_3 \\ u_2 \\ u_1 \end{pmatrix}.$$

i) What vectors span the null space of D^2?

ii) To what continuum boundary conditions for d^2/dx^2 does this matrix correspond?

iii) 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: Let

$$\widehat{H} \;=\; \begin{pmatrix} -i\partial_x & m_1 - im_2 \\ m_1 + im_2 & i\partial_x \end{pmatrix}$$

$$= \quad -i\widehat{\sigma}_3\partial_x + m_1\widehat{\sigma}_1 + m_2\widehat{\sigma}_2$$

be a one-dimensional Dirac Hamiltonian. Here $m_1(x)$ and $m_2(x)$ are real functions and the $\widehat{\sigma}_i$ are the Pauli matrices. The matrix differential operator $\widehat{H}$ acts on the two-component "spinor"

$$\Psi(x) = \begin{pmatrix} \psi_1(x) \\ \psi_2(x) \end{pmatrix}.$$

a) Consider the eigenvalue problem $\widehat{H}\Psi = E\Psi$ on the interval $[a, b]$. Show that the boundary conditions

$$\frac{\psi_1(a)}{\psi_2(a)} = \exp\{i\theta_a\}, \quad \frac{\psi_1(b)}{\psi_2(b)} = \exp\{i\theta_b\}$$

where θ_a, θ_b are real angles, make $\widehat{H}$ into an operator that is self-adjoint with respect to the inner product

$$\langle \Psi_1, \Psi_2 \rangle = \int_a^b \Psi_1^\dagger(x)\Psi_2(x)\, dx.$$

b) Find the eigenfunctions Ψ_n and eigenvalues E_n in the case that $m_1 = m_2 = 0$ and the $\theta_{a,b}$ are arbitrary real angles.

Here are three further problems involving the completeness of operators with a continuous spectrum:

Problem 4.11: *Missing State.* In problem 4.7 you will have found that the Schrödinger equation

$$\left(-\frac{d^2}{dx^2} - 2\,\mathrm{sech}^2 x\right)\psi = E\,\psi$$

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 $\psi_0(x) = \frac{1}{\sqrt{2}} \operatorname{sech} x$.

Problem 4.12: *Continuum Completeness.* Consider the differential operator

$$\hat{L} = -\frac{d^2}{dx^2}, \qquad 0 \leq x < \infty$$

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

$$\int_{-\infty}^{\infty} \frac{dk}{2\pi} e^{ikx} \frac{1}{1+k^2t^2} = \frac{1}{2|t|} e^{-|x|/|t|}.$$

Take care! You should monitor how the bound state contribution switches on and off as θ is varied. Keeping track of the modulus signs $|\ldots|$ in the standard integral is essential for this.

Problem 4.13: *One-dimensional scattering redux.* Consider again the one-dimensional Schrödinger equation from chapter 3 problem 3.4:

$$-\frac{d^2\psi}{dx^2} + V(x)\psi = E\psi,$$

where $V(x)$ is zero except in a finite interval $[-a, a]$ near the origin.

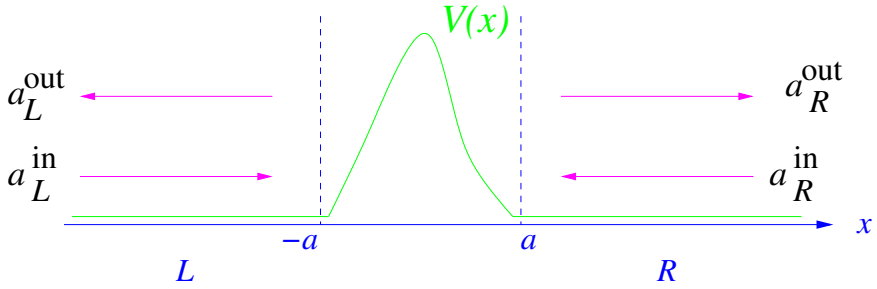

Figure 4.7: *Incoming and outgoing waves in problem 4.13. The asymptotic regions L and R are defined by $L = \{x < -a\}$ and $R = \{x > a\}$.*

For $k > 0$, consider solutions of the form

$$\psi(x) = \begin{cases} a_L^{\text{in}} e^{ikx} + a_L^{\text{out}} e^{-ikx}, & x \in L, \\ a_R^{\text{in}} e^{-ikx} + a_R^{\text{out}} e^{ikx}, & x \in R. \end{cases}$$

a) Show that, in the notation of problem 3.4, we have

$$\begin{bmatrix} a_L^{\text{out}} \\ a_R^{\text{out}} \end{bmatrix} = \begin{bmatrix} r_L(k) & t_R(-k) \\ t_L(k) & r_R(-k) \end{bmatrix} \begin{bmatrix} a_L^{\text{in}} \\ a_R^{\text{in}} \end{bmatrix},$$

and show that the S-matrix

$$S(k) \equiv \begin{bmatrix} r_L(k) & t_R(-k) \\ t_L(k) & r_R(-k) \end{bmatrix}$$

is unitary.

b) By observing that complex conjugation interchanges the "in" and "out" waves, show that it is natural to extend the definition of the transmission and reflection coefficients to all real k by setting $r_{L,R}(k) = r^*_{L,R}(-k)$, $t_{L,R}(k) = t^*_{L,R}(-k)$.

c) In problem 3.4 we introduced the particular solutions

$$\begin{aligned}\psi_k(x) &= \begin{cases} e^{ikx} + r_L(k)e^{-ikx}, & x \in L, \\ t_L(k)e^{ikx}, & x \in R, \end{cases} \quad k > 0, \\ &= \begin{cases} t_R(k)e^{ikx}, & x \in L, \\ e^{ikx} + r_R(k)e^{-ikx}, & x \in R. \end{cases} \quad k < 0.\end{aligned}$$

Show that, together with any bound states $\psi_n(x)$, these $\psi_k(x)$ satisfy the completeness relation

$$\sum_{\text{bound}} \psi^*_n(x)\psi_n(x') + \int_{-\infty}^{\infty} \frac{dk}{2\pi}\psi^*_k(x)\psi_k(x') = \delta(x - x')$$

provided that

$$\begin{aligned}-\sum_{\text{bound}} \psi^*_n(x)\psi_n(x') &= \int_{-\infty}^{\infty} \frac{dk}{2\pi} r_L(k)e^{-ik(x+x')}, \qquad x, x' \in L, \\ &= \int_{-\infty}^{\infty} \frac{dk}{2\pi} t_L(k)e^{-ik(x-x')}, \qquad x \in L,\ x' \in R, \\ &= \int_{-\infty}^{\infty} \frac{dk}{2\pi} t_R(k)e^{-ik(x-x')}, \qquad x \in R,\ x' \in L, \\ &= \int_{-\infty}^{\infty} \frac{dk}{2\pi} r_R(k)e^{-ik(x+x')}, \qquad x, x' \in R.\end{aligned}$$

d) Compute $r_{L,R}(k)$ and $t_{L,R}(k)$ for the potential $V(x) = -\lambda\delta(x)$,and verify that the conditions in part c) are satisfied.

If you are familiar with complex variable methods, look ahead to chapter 18 where problem 18.22 shows you how to use complex variable methods to evaluate the Fourier transforms in part c), and so confirm that the bound state $\psi_n(x)$ and the $\psi_k(x)$ together constitute a complete set of eigenfunctions.

Problem 4.14: *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 $\sin(kr + \eta(k))$. We fix the $2n\pi$ ambiguity in the definition of $\eta(k)$ by taking $\eta(\infty)$ to be zero, and requiring $\eta(k)$ to be a continuous function of 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

$$\frac{2}{\pi}\int_0^{k_f}\left(\int_0^R \left\{|\chi_k(x)|^2 - |\chi_k^0(x)|^2\right\}\, dr\right) dk = \frac{1}{\pi}\left[\eta(k_f) - \eta(0)\right] + \text{oscillations}.$$

  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 $R \to \infty$.
  (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 $k \to 0$.)

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

$$Q_{\rm tot} = \frac{1}{\pi}\eta(k_f).$$

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.