Mathematical Methods for Physics
PHYS 30672

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Contents

Chapter 1

Introduction and Prerequisites

This document is based on a summary of the main mathematical results of the course initially prepared by Graham Shaw. We hope they have turned into a reasonably complete (and accurate) guide to the material presented in the course.

I would suggest you come back to this from time to time, as this is always very much a work in progress. Please let me know if you find any typos or slips, so I can fix them.

This is not intended to be an absolutely complete set of notes, so do not be surprised if some derivations and examples of applying the results are not given, or are very much abbreviated. Of course, this does not imply you do not need to be able to derive or apply these results. Nor need you necessarily memorise very complicated equations, just because they are included here. Common sense must be applied; use of good textbooks next to these notes is advisable.

There are many different ways to remember mathematics and much of physics. One that is generally useful is to understand a number of the key principles underlying the work, so that you can derive most results quickly. Combined with practice from both the example sheets and additional material as can be found in the textbooks, should prepare you quite well for this course.

1.1 Prerequisites

PHYS 20171, Mathematics of Waves and Fields, is a prerequisite for this course. Most students will also have taken PHYS 30201, Mathematical Fundamentals of Quantum Mechanics. There is some overlap between those courses and the introductory material in these notes.

In addition, the Section on Green's Functions requires basic knowledge of contour integration and the residue theorem. The latter material has been covered in PHYS 20672, but it is not essential for understanding the lectures nor will it be tested in the exam.

Some students who have not attended PHYS 20672 may still want to get the gist of the Green's-function application of contour integration. They should read Appendix A (about 10 pages) and the first two or three pages of section 3.3 of Mathews and Walker, Mathematical Methods of Physics. (The later pages of section 3.3 involve integrating around cuts and branch points, which will not be required here.) There is also a Mathematica notebook (`Contour.nb`) available on the course web site, as well as a pdf file (`Contour.pdf`), and much of the material is also summarised in Appendix A.

1.2 Notation for scalar products

There are currently *two* editions of the notes, to cater to different tastes:

- In `Notes.pdf` and in the lectures I use $(\mathbf{a}, \mathbf{b})$ for the scalar product of vectors $\mathbf{a}$ and $\mathbf{b}$. There is a small chance that $\lambda\,(\mathbf{a}, \mathbf{b})$ (meaning the product of λ with $(\mathbf{a}, \mathbf{b})$) could be mistaken for a function λ with two arguments $\mathbf{a}$ and $\mathbf{b}$, but the correct reading can always be determined from the context.

- In `NotesBK.pdf` the scalar product is represented by $\langle \mathbf{a}|\mathbf{b}\rangle$, which is the notation most often found in textbooks of quantum mechanics and the one that students sometimes ask for. Please let me know if the automatic translation from $(\mathbf{a}, \mathbf{b})$ to $\langle \mathbf{a}|\mathbf{b}\rangle$ has missed any cases: I haven't checked every line.
- Followers of fashion should note that $\langle \mathbf{a}, \mathbf{b}\rangle$ is yet another notation for the scalar product; it is often found in the recent mathematical literature. *Any* appropriate notation is acceptable in answers to exam questions.
- The scalar product is denoted by $(\mathbf{a}, \mathbf{b})$ in the edition of the notes that you are currently reading.

Chapter 2

Linear vector spaces

2.1 Definition of a linear vector space

A linear vector space V over a scalar set S (we shall typically consider sets $S = \mathbb{R}$ or $\mathbb{C}$) is a set of objects (called vectors) $\mathbf{a}$, $\mathbf{b}$, $\mathbf{c}$, ... with two operations:

1. *Addition* of any two vectors, $\mathbf{c} = \mathbf{a} + \mathbf{b}$;
2. *Multiplication* by a scalar $\lambda \in S$, $\mathbf{b} = \lambda\mathbf{a}$.

These must satisfy the following conditions

1. V is closed under addition, $\forall \mathbf{a}, \mathbf{b} \in V : \mathbf{a} + \mathbf{b} \in V$.
2. Addition is commutative:
$$\forall \mathbf{a}, \mathbf{b} \in V : \mathbf{a} + \mathbf{b} = \mathbf{b} + \mathbf{a}$$
and associative
$$\forall \mathbf{a}, \mathbf{b}, \mathbf{c} \in V : (\mathbf{a} + \mathbf{b}) + \mathbf{c} = \mathbf{a} + (\mathbf{b} + \mathbf{c}).$$
3. There exists a *null vector* $\mathbf{0} \in V$, $\forall \mathbf{a} \in V : \mathbf{a} + \mathbf{0} = \mathbf{a}$.
4. Every element $\mathbf{a} \in V$ has an inverse $-\mathbf{a} \in V$ such that $\mathbf{a} + (-\mathbf{a}) = \mathbf{0}$.
5. The set V is closed under multiplication by a scalar, $\forall \mathbf{a} \in V, \lambda \in S : \lambda\mathbf{a} \in V$.
6. The multiplication is distributive for addition of both vectors and scalars,
$$\begin{aligned} \forall \mathbf{a}, \mathbf{b} \in V, \lambda \in S : &\quad \lambda(\mathbf{a} + \mathbf{b}) = \lambda\mathbf{a} + \lambda\mathbf{b}, \\ \forall \mathbf{a} \in V, \lambda, \mu \in S : &\quad (\lambda + \mu)\mathbf{a} = \lambda\mathbf{a} + \mu\mathbf{a}, \end{aligned}$$
and associative,
$$\forall \mathbf{a} \in V, \lambda, \mu \in S : \lambda(\mu\mathbf{a}) = (\lambda\mu)\mathbf{a}.$$
7. There is a unit element 1 in S, such that $1\mathbf{a} = \mathbf{a}$.

Note that we have not defined subtraction; it is a derived operation, and is defined through the addition of an inverse element.

Example 2.1:

The space $\mathbb{R}^3$ of vectors $\mathbf{r} = \begin{pmatrix} x \\ y \\ z \end{pmatrix} = x\mathbf{i} + y\mathbf{j} + z\mathbf{k}$ is a vector space over the set $S = \mathbb{R}$.

Example 2.2:

The space of two-dimensional complex spinors

$$\begin{pmatrix} \alpha \\ \beta \end{pmatrix} = \alpha \begin{pmatrix} 1 \\ 0 \end{pmatrix} + \beta \begin{pmatrix} 0 \\ 1 \end{pmatrix},$$

$\alpha, \beta \in \mathbb{C}$, is a vector space.

Note: If we look at the space of up and down spins, we must require that the length of the vectors (the probability), $|\alpha|^2 + |\beta|^2$, is 1. This is not a vector space, since

$$\left| \begin{pmatrix} \alpha_1 \\ \beta_1 \end{pmatrix} + \begin{pmatrix} \alpha_2 \\ \beta_2 \end{pmatrix} \right|^2 = |\alpha_1 + \alpha_2|^2 + |\beta_1 + \beta_2|^2 = |\alpha_1|^2 + |\beta_1|^2 + |\alpha_2|^2 + |\beta_2|^2 + 2\Re(\alpha_1^* \alpha_2 + \beta_1^* \beta_2),$$

which is not necessarily equal to 1.

Example 2.3:

The space of all square integrable (i.e., all functions f with $\int dx\, |f(x)|^2 < \infty$) complex functions f of a real variable, $f : \mathbb{R} \mapsto \mathbb{C}$ is a vector space, for $S = \mathbb{C}$.

The space defined above is of crucial importance in Quantum Mechanics. These wave functions are normalisable (i.e., we can define one with total probability 1).

The space of all functions f, $f : \mathbb{R} \mapsto \mathbb{C}$ with $\int dx\, |f(x)|^2 < \infty$ is denoted as $\mathcal{L}^2(\mathbb{R})$.

2.1.1 Problems

1. Show that the zero vector $\mathbf{0}$ is unique, and that for each $\mathbf{a}$ there is only one inverse $-\mathbf{a}$.

2.2 Linear independence and basis vectors

A set of vectors $\mathbf{a}, \mathbf{b}, \ldots, \mathbf{u}$ is said to be linearly independent provided the equation

$$\lambda\mathbf{a} + \mu\mathbf{b} + \ldots + \sigma\mathbf{u} = \mathbf{0}$$

has no solution except $\lambda = \mu = \ldots = \sigma = 0$.

This can be used to show that when you pick one of the vectors $\mathbf{a}, \mathbf{b}, \ldots, \mathbf{u}$, it can not be expressed as a sum over the rest. In cases where there is a largest number of independent vectors:

The dimension n of a space is the *largest* possible number of linearly independent vectors which can be found in the space.

Any set of n linearly independent vectors $\mathbf{e}_1, \mathbf{e}_2, \ldots, \mathbf{e}_n$ in an n-dimensional space is said to form a *complete set of basis vectors*, since one can show that any vector $\mathbf{x}$ in the space can be expanded in the form

$$\mathbf{x} = x_1\mathbf{e}_1 + x_2\mathbf{e}_2 + ... + x_n\mathbf{e}_n, \tag{2.1}$$

where the numbers x_i are called the *components* of $\mathbf{x}$ in the basis $\mathbf{e}_1, \mathbf{e}_2, \ldots, \mathbf{e}_n$.

Example 2.4:

Show that the vectors $(1,1,0)$, $(1,0,1)$ and $(0,1,1)$ are linearly independent. Find the component of a general vector (x,y,z) in this basis.

Solution:

We get the three coupled equations

$$\begin{aligned} x &= x_1 + x_2, \\ y &= x_1 + x_3, \\ z &= x_2 + x_3. \end{aligned}$$

These have a unique solution if the determinant is not zero,

$$\det \begin{pmatrix} 1 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 1 \end{pmatrix} \neq 0.$$

This is true, since the determinant equals -2. The components are found by solving the equations (Gaussian elimination is quite easy in this case):

$$x_1 = \frac{1}{2}(x+y-z), \quad x_2 = \frac{1}{2}(x+z-y), \quad x_3 = \frac{1}{2}(y+z-x).$$

Theorem 2.1. *The decomposition (2.1) is unique.*

Proof. Suppose that there is a second decomposition, $\mathbf{x} = y_1\mathbf{e}_1 + y_2\mathbf{e}_2 + ... + y_n\mathbf{e}_n$. Subtract the left- and right-hand sides of the two decompositions, collecting terms:

$$\mathbf{0} = (x_1 - y_1)\mathbf{e}_1 + (x_2 - y_1)\mathbf{e}_2 + ... + (x_n - y_n)\mathbf{e}_n.$$

Linear independence of the vectors $\{\mathbf{e}_i\}$ implies that $x_i = y_i$, which contradicts our assumption of a second decomposition, and thus it is unique. □

Let us look at an example in an *infinite dimensional space*:

Example 2.5:

The *Fourier decomposition* of a function defined only on the interval $[-\pi, \pi]$ is given by

$$f(x) = a_0 + \sum_{n=1}^{\infty} \left(a_n \cos nx + b_n \sin nx\right).$$

This means that for the Fourier series the basis functions are:

$$1, \{\sin nx, \cos nx\}, \quad n = 1, \ldots, \infty \quad .$$

It is not at all easy to show that this basis is complete! This is a general complication in infinite dimensional spaces.

2.2.1 The scalar product

For any two vectors $\mathbf{a}, \mathbf{b}$ we can define a scalar product[1] $(\mathbf{a}, \mathbf{b})$ [a generalizable notation for $\mathbf{a} \cdot \mathbf{b}$], which satisfies:

$$(\mathbf{a}, \mathbf{b}) = (\mathbf{b}, \mathbf{a})^*, \tag{2.2}$$

$$(\mathbf{a}, \lambda\mathbf{b} + \mu\mathbf{c}) = \lambda(\mathbf{a}, \mathbf{b}) + \mu(\mathbf{a}, \mathbf{c}) \quad , \tag{2.3}$$

together with

$$(\mathbf{a}, \mathbf{a}) \geq 0, \tag{2.4}$$

where the equality holds for $\mathbf{a} = \mathbf{0}$ only.
Note: The inner product is sometimes described as a mapping from $V \otimes V \mapsto S$, which is another way of saying that it is a scalar function of a pair of vectors in V.

We can use the inner product to define the norm (a more correct description of the length) of the vector $\mathbf{a}$,

$$\|\mathbf{a}\| = (\mathbf{a}, \mathbf{a})^{1/2}.$$

One can define a length without an inner product. A good example is the so-called "1-norm" of a vector, $||\mathbf{x}||_1 = \sum_n |x_n|$, which is used quite commonly in numerical analysis of linear algebra.

One of the important uses of an inner product is to test whether two vectors are at straight angles:

The vectors $\mathbf{a}$ and $\mathbf{b}$ are said to be *orthogonal* if $(\mathbf{a}, \mathbf{b}) = 0$.

Triangle and Cauchy–Schwartz inequality

The triangle inequality is the 'obvious' statement that the length of the sum of two vectors is less than the sum of the lengths,

$$\|\mathbf{a} + \mathbf{b}\| \leq \|\mathbf{a}\| + \|\mathbf{b}\|.$$

From the triangle inequality we could prove the Cauchy–Schwartz inequality, but we take a different approach here:

Theorem 2.2. *For any two vectors* $\mathbf{a}$, $\mathbf{b}$, *we have*

$$|(\mathbf{a}, \mathbf{b})| \leq \|\mathbf{a}\| \, \|\mathbf{b}\|. \tag{2.5}$$

Proof. The proof is simple. We suppose that $\mathbf{b} \neq \mathbf{0}$, because if $\mathbf{b} = \mathbf{0}$, Eq. (2.5) holds as a trivial equality, $0 = 0$. Consider the non-negative function $f(x)$ defined by

$$f(x) = (\mathbf{a} + x\mathbf{b}, \mathbf{a} + x\mathbf{b}) \geq 0\,,$$

where x is a complex variable. By using the properties of the scalar product, this can expanded to give

$$f(x) = (\mathbf{a}, \mathbf{a}) + x^*(\mathbf{b}, \mathbf{a}) + x(\mathbf{a}, \mathbf{b}) + |x|^2(\mathbf{b}, \mathbf{b}) \geq 0\,. \tag{2.6}$$

For the special value $x = -(\mathbf{b}, \mathbf{a})/\|\mathbf{b}\|^2$, (2.6) becomes

$$\|\mathbf{a}\|^2 - |(\mathbf{a}, \mathbf{b})|^2/\|\mathbf{b}\|^2 \geq 0\,,$$

which is easily rearranged to give the Cauchy–Schwartz inequality, Eq. (2.5). □

[1] We shall also use the term inner product for this operation.

You might want to show for yourself that the 'special' value of x that we needed in the proof is actually the value for which $f(x)$ takes its smallest possible value. Note, if you try this, that f is *not* an analytic function of x (why not?), so a little care will be needed to find the minimum: you could, for example, minimize with respect to the real and imaginary parts of x separately.

Orthogonalisation and orthonormalisation

There are several ways to turn an arbitrary set of vectors into an orthogonal set—one where every pair of vectors is orthogonal—, or even better an orthonormal set: an orthogonal set where each vector has length one. We discuss only two of these methods.

The traditional approach is the Gram-Schmidt procedure. This procedure is defined recursively. In the mth step of the algorithm one defines the vector $\mathbf{e}'_m$ that is orthonormal to the $m-1$ orthonormal vectors defined in previous steps. Thus

$$\begin{aligned} 1: &\mathbf{e}''_m = \mathbf{e}_m - \sum_{i=1}^{m-1} (\mathbf{e}'_i, \mathbf{e}_m)\mathbf{e}'_i; \\ 2: &\mathbf{e}'_m = \mathbf{e}''_m / \|\mathbf{e}''_m\|. \end{aligned}$$

The first line above removes all components parallel to the $m-1$ previous normalised and orthogonal vectors (check!), the second step normalises the result, so that $\mathbf{e}'_m$ is normalised.

A more modern approach (using numerical linear algebra) is based on the construction of the "overlap matrix" N (also called norm matrix, which is why we use the symbol), with entries $N_{ij} = (\mathbf{e}_i, \mathbf{e}_j)$. This matrix is Hermitian (or symmetric if the basis is real), and we can now define a matrix $N^{-1/2}$, such that $N^{-1/2}NN^{-1/2} = I$. This can then be used to define the orthonormal basis

$$\mathbf{e}'_k = (N^{-1/2})_{lk}\, \mathbf{e}_l.$$

For a *real symmetric matrix* M (and similarly for an Hermitian one, but we shall concentrate on the first case here) we can define matrix powers in a simple and unique way by requiring that the powers are also symmetric matrices.
The easiest way to get the result is first to diagonalise the matrix M, i.e., to find its eigenvalues λ_i and eigenvectors $e^{(i)}_j$. We can then write $M = O\,\mathrm{diag}(\lambda)O^T$, with O the matrix with the normalised eigenvectors as columns, $O_{ij} = e^{(j)}_i$. The eigenvectors are orthonormal, and thus $O^TO = I$. The matrix diag(..) has the eigenvalues λ on the diagonal, and is zero elsewhere. (Convince yourself that $O^TO = I$ and $O^TMO = \mathrm{diag}(\lambda)$.)
We then define arbitrary powers of M by

$$M^a = O\,\mathrm{diag}(\lambda^a)O^T. \tag{2.7}$$

Orthonormal basis functions: For discrete[2] vector spaces one can always choose an orthonormal set of basis functions satisfying

$$(\mathbf{e}_i, \mathbf{e}_j) = \delta_{ij}. \tag{2.8}$$

Here we have introduced the *Kronecker delta* δ_{ij}, defined for integer i, j. This object is zero unless $i = j$, when it is 1.

[2]Discrete here means that we can label the basis vectors by a finite or infinite set of integers. It contrasts to continuous bases, as discussed in the next section.

For such an orthonormal basis the completeness relation can be written as

$$\sum_i (\mathbf{e}_i)_a \, (\mathbf{e}_i)_b^* = \delta_{ab}, \tag{2.9}$$

where $(\mathbf{e}_i)_a$ denotes the ath component of ith basis vector $\mathbf{e}_i$.

2.2.2 Problems

2. Use the definition of independence to show that Eq. (2.1) holds for any set of independent functions.

3. Show that M^a, defined by Eq. (2.7), is a symmetric matrix.

4. *Harder:* Show that the eigenvalues of the overlap matrix N are positive, and deduce that $N^{-1/2}$ is Hermitian; the matrix is defined up to a choice of sign for the square root.

2.3 Function spaces

2.3.1 Continuous basis functions: Fourier Transforms

For a vector space of complex valued functions $f\colon \mathbb{R} \mapsto \mathbb{C}$ one can choose basis functions[3]

$$\mathbf{e}_k = \phi_k(x) = \frac{1}{\sqrt{2\pi}} e^{ikx}, \qquad -\infty < k < \infty,$$

and expand in these functions,

$$f(x) = \int_{-\infty}^{\infty} dk \, \phi_k(x) \tilde{f}(k). \tag{2.10}$$

The expansion coefficient is nothing but the Fourier transform,

$$\tilde{f}(k) = \int_{-\infty}^{\infty} dx \, \phi_k^*(x) f(x). \tag{2.11}$$

In much of physics, one traditionally does not normalise the ϕ_k, but uses $\phi_k(x) = e^{ikx}$. In that case an explicit factor 2π enters in the Fourier transforms, but not in the inverse one,

$$f(x) = \int_{-\infty}^{\infty} \frac{dk}{2\pi} \, e^{ikx} \tilde{f}(k),$$
$$\tilde{f}(k) = \int_{-\infty}^{\infty} dx \, e^{-ikx} f(x).$$

In order to figure out the orthogonality relations, we substitute (2.11) into (2.10), which gives the relation

$$f(x) = \int_{-\infty}^{\infty} dk \, \phi_k(x) \int_{-\infty}^{\infty} dx' \, \phi_k^*(x') f(x'), \tag{2.12}$$

which must hold for any $f(x)$. We now swap the order of integration, and find

$$f(x) = \int_{-\infty}^{\infty} dx' \left[\int_{-\infty}^{\infty} dk \, \phi_k(x) \phi_k^*(x') \right] f(x'). \tag{2.13}$$

[3] If we work in a real function space we should use the real and imaginary parts as a basis for real functions, but it is often easier to deal even with real functions as if they are complex. Think about the Fourier transform of a real function, see below.

We call the object between square brackets the "Dirac delta function" $\delta(x-x')$, where $\delta(y)$ can be defined using the explicit definition of the functions ϕ_k, as

$$\delta(y) = \frac{1}{2\pi}\int_{-\infty}^{\infty} dz\, e^{iyz}. \tag{2.14}$$

(See the appendix to this chapter, 2.4, for additional properties.)

From the definition (2.14) of the delta function, we can show that the basis states satisfy the orthonormality relation

$$(\phi_k, \phi_{k'}) = \int_{-\infty}^{\infty} dx\, \phi_k^*(x)\phi_{k'}(x) = \delta(k-k')$$

and the completeness relation

$$\int_{-\infty}^{\infty} dk\, \phi_k^*(x)\phi_k(x') = \delta(x-x').$$

2.3.2 General orthogonality and completeness in function spaces

We start with a space of functions, where the scalar product is assumed to be defined by[4]

$$(\phi, \psi) = \int dx\, \phi^*(x)\psi(x),$$

where the space from which ϕ and ψ are chosen is such that the integral is finite for any pair. In general:

Any vector space of functions with a scalar product, where all functions have finite norm, is called a *Hilbert space*.

Suppose in this space we have a discrete (i.e., labelled by integers), but let us assume infinite, set of basis functions ϕ_n, chosen to be orthonormal (similar to Eq. (2.8))

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

using orthogonalisation if necessary. Then an arbitrary $\psi(x)$ can be decomposed as

$$\psi(x) = \sum_n c_n \phi_n(x). \tag{2.15}$$

The coefficients c_n can be determined from the orthogonality relation, multiplying (2.15) from the left with ϕ_m^*, integrating with respect to x, exchanging the order of the summation and the integration on the right-hand side, we find that

$$(\phi_m, \psi) = \sum_n c_n(\phi_m, \phi_n) = \sum_n c_n \delta_{mn},$$

from which we conclude that

$$c_m = (\phi_m, \psi). \tag{2.16}$$

Substituting Eq. (2.16) into Eq. (2.15) we find

$$\begin{aligned}\psi(x) &= \sum_n \int dx'\, \phi_n(x')^*\psi(x')\phi_n(x) \\ &= \int dx' \left[\sum_n \phi_n(x')^*\phi_n(x)\right]\psi(x) \quad ,\end{aligned}$$

[4] More general definitions are possible, but apart from some minor changes to the algebra, the final results hold for all scalar products

where we have interchanged the summation and integration (which mathematicians will tell you may be incorrect!). From this we conclude that

$$\sum_n \phi_n(x')^* \phi_n(x) = \delta(x - x'),$$

which is the form of the completeness relation for a basis labelled by a discrete variable. If the basis is labelled by a continuous label, as for the Fourier transformation, we get the completeness relations discussed for that case, Eqs. (2.12,2.13). This leads to

$$(\phi_k, \phi_k) = \delta(0).$$

In this case we do not speak of a Hilbert space, since the basis is not normalisable, the norm of the basis states is necessarily infinite. We might instead speak of a "pre-Hilbert" space, a vector space of functions endowed with a scalar product, but without the assumption of a finite norm.

2.3.3 Example from Quantum Mechanics

Much of what we have stated in this section can be illustrated for quantum mechanical problems. Like all linear wave problems, QM relies heavily on the *principle of superposition*:

For any physical system, if $\psi_1(x,t)$ and $\psi_2(x,t)$ are possible wave functions, then so is

$$\psi(x,t) = \lambda\psi_1(x,t) + \mu\psi_2(x,t),$$

where λ and μ are arbitrary complex numbers.[a]

[a] This superposition principle is not a QM property, but one that is common to all (wave) solutions to linear wave equations.

This implies that the space of all ψ is a *linear vector space* (over x, since t is a *parameter* that describes the time evolution).

A very important statement can now be found in the fact that:

Theorem 2.3. *The eigenfunctions $\psi_n(x)$ of any physical operator form a complete set. (Can be proven for specific cases only.)*

This implies that

$$\psi(x,t) = \sum_n c_n(t)\psi_n(x).$$

A very clear example are the eigenstates of the harmonic oscillator Hamiltonian,

$$\hat{H} = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + \frac{1}{2}m\omega^2 x^2.$$

The solutions of the Schrödinger equation

$$\hat{H}\psi(x,t) = i\hbar\partial_t\psi(x,t)$$

are $\psi_n(x) = \exp(-x^2/(2b^2))H_n(x/b)$, with H_n a Hermite polynomial. In this case the time-dependence is determined by the eigenenergies, and we conclude that

$$\psi(x,t) = \sum_n a_n e^{-i(n+1/2)\omega t}\psi_n(x).$$

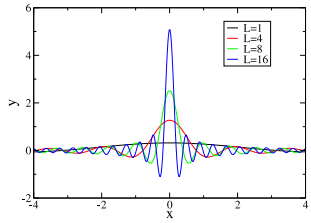

Figure 2.1: A sketch of $\frac{1}{2\pi}\frac{2}{x}\sin(Lx)$ for a few values of L. This function converges to a Dirac delta function

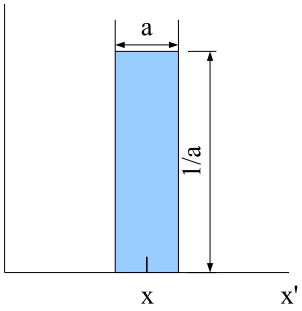

Figure 2.2: A sketch of a piecewise constant function, that in the limit $a \to 0$ gives the Dirac delta function

2.4 The Dirac delta function

The Dirac delta function $\delta(x)$ is defined by the "reproducing" property, i.e.,

$$\int dx'\, \delta(x-x')f(x') = f(x)$$

for *any* function $f(x)$.[5] This is equivalent to the following explicit definition (further forms are discussed in the Mathematica examples), see also Fig. 2.1.

$$\delta(x) = \frac{1}{2\pi}\int_{-\infty}^{\infty} dz\, e^{izx} \equiv \frac{1}{2\pi}\lim_{L\to\infty}\int_{-L}^{L} dz\, e^{izx} = \frac{1}{2\pi}\lim_{L\to\infty}\frac{2}{x}\sin(Lx) \quad .$$

It is often useful to think of the δ function as the limit of a simple function, and one example is an infinitely narrow spike, as in Fig. 2.2 for $a \to 0$.

Important properties

Since integration with the δ function "samples" $f(x')$ at the single point $x' = x$, we must conclude that

$$\delta(x-x') = 0 \text{ for } x \neq x'.$$

The area under the δ function is 1, as can be seen from taking $f(x') = 1$. Combining the last two results leads to an interesting expression for the area under the curve,

$$\int_{x-\epsilon}^{x+\epsilon} dx'\, \delta(x-x') = 1 \text{ for any } \epsilon > 0.$$

[5] The δ function is strictly speaking not a function, it is only defined *inside* an integral! A "function" of this kind is usually called a *distribution*, but we won't labour the distinction in this course.

A very useful relation is obtained when we scale the variables in the delta function, writing $y = ax$. Now, for $a < 0$, $x \to \pm\infty$ corresponds to $y \to \mp\infty$, so that

$$\int_{-\infty}^{\infty} dx'\, \delta(a(x-x'))f(x') = \text{sign}(a)\frac{1}{a}\int_{-\infty}^{\infty} dy'\, \delta(y-y')f(y'/a)\,,$$

where $\text{sign}(a)$ is the so-called signum function, $\text{sign}(a) = +1$ for $a > 0$ and -1 for $a < 0$: the sign-change that appears for $a < 0$ comes from reversing the limits of integration and the factor of $1/a$ arises from the change of variables. From this we find

$$\int_{-\infty}^{\infty} dx'\, \delta(a(x-x'))f(x') = \frac{f(y/a)}{|a|} = \frac{f(x)}{|a|}.$$

We can interpret the result as the contribution from the slope of the argument of the delta function, which appears inversely in front of the function at the point where the argument of the δ function is zero. Since the δ function is even, the answer only depends on the absolute value of a. Also note that we only need to integrate from below to above the singularity; it is not necessary to integrate over the whole infinite interval.

This result can now be generalised to a δ-function with a function $g(x)$ as argument: we need to sum over all zeroes of g inside the integration interval, and the quantity a above becomes the slope dg/dx at each of the zeroes,

$$\int_a^b dx\, f(x)\,\delta\left(g(x)\right) = \sum_i \left\{\frac{f(x)}{|dg/dx|}\right\}_{x=x_i}$$

where the sum extends over all points x_i such that $g(x_i) = 0$ and $a < x_i < b$.

Example 2.6:

Calculate the integral

$$\int_{-\infty}^{\infty} dx\, f(x)\delta(x^2 - c^2t^2).$$

Solution:

Let us first calculate the zeroes of $x^2 - c^2t^2$, $x = \pm ct$. The derivative of $x^2 - c^2t^2$ at these points is $\pm 2ct$, and thus

$$\int_{-\infty}^{\infty} dx\, f(x)\delta(x^2 - c^2t^2) = \frac{1}{2c|t|}\left(f(ct) + f(-ct)\right).$$

Integrals such as these occur in electromagnetic wave propagation.

Chapter 3

Operators, Eigenvectors and Eigenvalues

3.1 Linear operators

A linear operator L acts on vectors $\mathbf{a}, \mathbf{b} \ldots$ in a linear vector space V to give new vectors $L\mathbf{a}$, $L\mathbf{b}, \ldots$ such that[1]

$$L(\lambda\mathbf{a} + \mu\mathbf{b}) = \lambda L\mathbf{a} + \mu L\mathbf{b}$$

Example 3.1:

1. Matrix multiplication of a column vector by a fixed matrix is a linear operation, e.g.

$$L\mathbf{x} = \begin{pmatrix} 1 & 2 & 3 \\ 4 & 8 & -1 \end{pmatrix} \mathbf{x}.$$

2. Differentiation is a linear operation, e.g.,

$$Lf(x) = \frac{d}{dx} f(x).$$

3. Integration is linear as well,

$$(L_1 f)(x) = \int_0^x f(x')dx',$$
$$(L_2 f)(x) = \int_0^1 G(x, x')f(x')dx',$$

are both linear (see example sheet).

3.1.1 Domain, Codomain and Range

If the operators L maps the vector $\mathbf{f}$ on the vector $\mathbf{g}$, $L\mathbf{f} = \mathbf{g}$, the vector space of $\mathbf{f}$'s (the domain) can be different from the vector space of $\mathbf{g}$'s (the codomain or target). L is an operator which maps the domain onto the codomain, and even though it is defined for every element of the domain, the image of the domain (called the "range of L" or the "image of L") is in general only a subset of the codomain, see Fig. 3.1, even though in many physical applications the range and codomain do in fact coincide.

[1] This changes in the most general case where multiplication is not commutative!

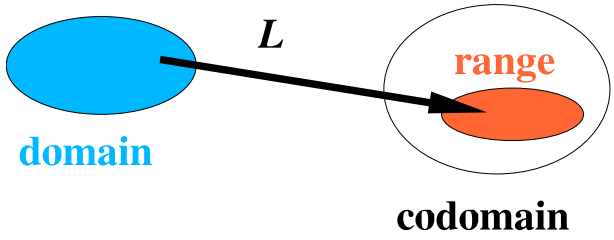

Figure 3.1: The definition of domain, codomain and range

Example 3.2:

1. The operator L: $\mathbb{C}^n \to \mathbb{C}$ defined by $L\mathbf{a} = (\mathbf{b}, \mathbf{a})$ with $\mathbf{b}$ a fixed vector, is a linear operator.
2. The matrix $\begin{pmatrix} 3 & 2 & 1 \\ 6 & 4 & 2 \end{pmatrix}$ maps from the space $\mathbb{R}^3$ of 3-vectors to the codomain $\mathbb{R}^2$ of 2-vectors. The range is the 1D subset of vectors $\lambda \begin{pmatrix} 1 \\ 2 \end{pmatrix}$, $\lambda \in \mathbb{R}$.
3. The (3D) gradient operator ∇ maps from the space of scalar fields ($f(\mathbf{x})$ is a real function of 3 variables) to the space of vector fields ($\nabla f(x)$ is a real 3-component vector function of 3 variables).

3.1.2 Matrix representations of linear operators

Let L be a linear operator, and $\mathbf{y} = l\mathbf{x}$. Let $\mathbf{e}_1$, $\mathbf{e}_2$, ...and $\mathbf{u}_1$, $\mathbf{u}_2$, ...be chosen sets of basis vectors in the domain and codomain, respectively, so that

$$\mathbf{x} = \sum_i \mathbf{e}_i x_i, \qquad \mathbf{y} = \sum_i \mathbf{u}_i y_i.$$

Then the components are related by the matrix relation

$$y_j = \sum_i L_{ji} x_i,$$

where the matrix L_{ji} is defined by

$$L\mathbf{e}_i = \sum_j \mathbf{u}_j L_{ji} = \sum_j \left(L^T\right)_{ij} \mathbf{u}_j. \tag{3.1}$$

Notice that the transformation relating the components x and y is the *transpose* of the matrix that connects the basis. This difference is related to what is sometimes called the active or passive view of transformations: in the active view, the components change, and the basis remains the same. In the passive view, the components remain the same but the basis changes. Both views represent the *same* transformation!

If the two basis sets $\{\mathbf{e}_i\}$ and $\{\mathbf{u}_j\}$ are *both orthonormal*, we can find the matrix elements of L as an inner product,

$$L_{ji} = (\mathbf{u}_j, L\mathbf{e}_i). \tag{3.2}$$

Example 3.3:

Find a matrix representation of the differential operator $\frac{d}{dx}$ in the space of functions on the interval $(-\pi, \pi)$.

Solution:

Since domain and codomain coincide, the bases in both spaces are identical; the easiest and most natural choice is the discrete Fourier basis $1, \{\cos nx, \sin nx\}_{n=1}^{\infty}$. With this choice, using $(\cos nx)' = -n \sin nx$ and $(\sin nx)' = n \cos nx$, we find

$$\frac{d}{dx}\begin{pmatrix} 1 \\ \cos x \\ \sin x \\ \cos 2x \\ \sin 2x \\ \vdots \end{pmatrix} = \begin{pmatrix} 0 \\ -\sin x \\ \cos x \\ -2\sin 2x \\ 2\cos 2x \\ \vdots \end{pmatrix} = M^T \begin{pmatrix} 1 \\ \cos x \\ \sin x \\ \cos 2x \\ \sin 2x \\ \vdots \end{pmatrix}.$$

We can immediately see that the matrix representation "M" takes the form

$$M^T = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & \dots \\ 0 & 0 & -1 & 0 & 0 & \\ 0 & 1 & 0 & 0 & 0 & \\ 0 & 0 & 0 & 0 & -2 & \\ 0 & 0 & 0 & 2 & 0 & \\ \vdots & & & & & \ddots \end{pmatrix}.$$

Matrix representation of the time-independent Schrödinger equation

Another common example is the matrix representation of the Schrödinger equation. Suppose we are given an *orthonormal* basis $\{\phi_i\}_{i=1}^{\infty}$ for the Hilbert space in which the operator $\hat{H}$ acts. By decomposing an eigenstate ψ of the Schrödinger equation,

$$\hat{H}\psi(x) = E\psi(x)$$

in the basis $\phi_j(x)$ as $\psi = \sum_j c_j \phi_j$, we get the matrix form

$$\sum_j H_{ij} c_j = E c_i\,, \tag{3.3}$$

with

$$H_{ij} = (\phi_i, \hat{H}\phi_j) = \int dx\, \phi_i(x)^* H \phi_j(x)\,.$$

This is clearly a form of Eq. (3.2).

The result in Eq. (3.3) is obviously an infinite-dimensional matrix problem, and no easier to solve than the original problem. Suppose, however, that we truncate both the sum over j and the set of coefficients c to contain only N terms. This can then be used to find an approximation to the eigenvalues and eigenvectors. See the Mathematica notebook `heisenberg.nb` for an example how to apply this to real problems.

3.1.3 Adjoint operator and Hermitian operators

You should be familiar with the Hermitian conjugate (also called adjoint) of a matrix, the generalisation of transpose: The Hermitian conjugate of a matrix is the complex conjugate of its transpose,

$$(M^\dagger)_{ij} = (M_{ji})^*, \quad \text{or} \quad M^\dagger = (M^T)^*.$$

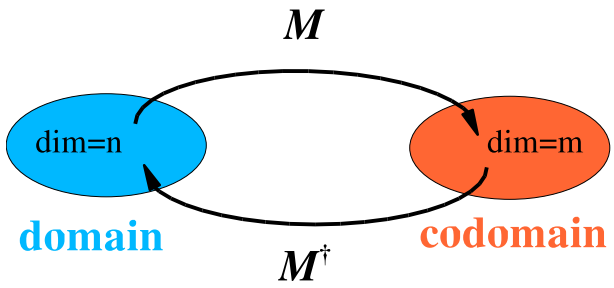

Figure 3.2: The definition of a matrix and its Hermitian conjugate

Thus

$$\begin{pmatrix} 0 & i \\ i & 0 \end{pmatrix}^\dagger = \begin{pmatrix} 0 & -i \\ -i & 0 \end{pmatrix}, \qquad \begin{pmatrix} 0 & i \\ -i & 0 \end{pmatrix}^\dagger = \begin{pmatrix} 0 & i \\ -i & 0 \end{pmatrix}.$$

We can also define the Hermitian conjugate of a column vector, if

$$\mathbf{v} = \begin{pmatrix} v_1 \\ \vdots \\ v_n \end{pmatrix}, \quad \mathbf{v}^\dagger = (v_1^*, \ldots, v_n^*).$$

This allows us to write the inner product as a matrix product,

$$(\mathbf{w}, \mathbf{v}) = \mathbf{w}^\dagger \mathbf{v}.$$

The most useful definition of Hermitian conjugate, which will be generalised below, is through the inner product:

> The Hermitian conjugate $M^\dagger$ of a matrix M has the property that for any two vectors $\mathbf{a}$ and $\mathbf{b}$ in the codomain and domain of M, respectively,
>
> $$(\mathbf{a}, M\mathbf{b}) = (M^\dagger \mathbf{a}, \mathbf{b}).$$

Thus, with a little algebra,

$$(\mathbf{a}, M\mathbf{b}) = \sum_{ij} a_i^* M_{ij} b_j = \sum_{ij} a_i^* (M_{ji}^\dagger)^* b_j = \sum_{ij} (M_{ji}^\dagger a_i)^* b_j = (M^\dagger \mathbf{a}, \mathbf{b}), \tag{3.4}$$

see Fig. 3.2. From the examples above, and the definition, we conclude that if M is an $m \times n$ matrix, $M^\dagger$ is an $n \times m$ matrix.

We now use our result (3.4) above for an operator, and define

$$\forall a \in \text{codomain}, b \in \text{domain}: \quad (a, Lb) = (L^\dagger a, b) = (b, L^\dagger a)^*$$

where the last two terms are identical, as follows from the basic properties of the scalar product, Eq. (2.2). A linear operator L maps the domain onto the codomain; its adjoint $L^\dagger$ maps the codomain back on to the domain.

As can be gleaned from Fig. 3.3, we can also use a basis in both the domain and codomain to use the matrix representation of linear operators (3.1,3.2), and find that the matrix representation of an operator satisfies the same relations as that for a finite matrix,

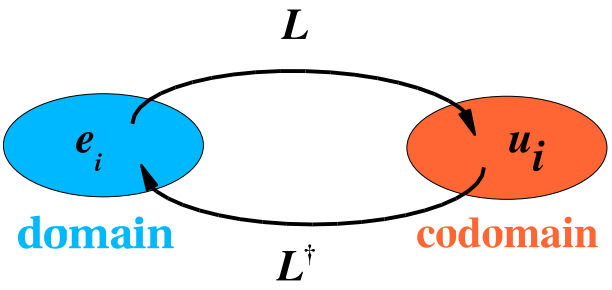

Figure 3.3: The definition of an operator and its Hermitian conjugate

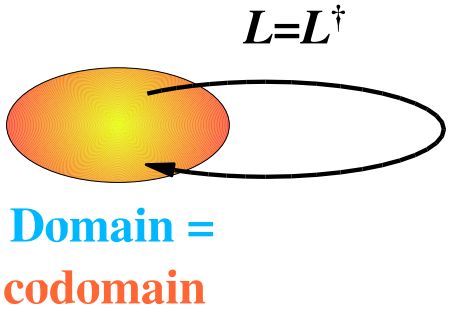

Figure 3.4: A schematic representation of a self-adjoint operator.

$$(L^\dagger)_{ik} = (L_{ki})^*.$$

A final important definition is that of

A self-adjoint or Hermitian operator L equals its adjoint,

$$L^\dagger = L.$$

Thus we also require that domain and codomain coincide, see Fig. 3.4.

3.2 Eigenvalue equations

We have all seen simple matrix eigenvalue problems; this is now generalised to linear operators, and we shall first of all consider eigenvalue equations of the form

$$L\mathbf{a} = \lambda\mathbf{a}.$$

Theorem 3.1. *For an Hermitian operator L,*

1. *the eigenvalues are real and*
2. *eigenvectors corresponding to different eigenvalues are orthogonal.*

Proof. Let's consider the first property first. Calculate

$$(\mathbf{a}, L\mathbf{a}) = \lambda(\mathbf{a}, \mathbf{a}),$$
$$(L^\dagger\mathbf{a}, \mathbf{a}) = \lambda^*(\mathbf{a}, \mathbf{a}),$$

but Hermiticity says the left-hand sides are equal. Subtract both sides of the equations and find

$$0 = (\lambda - \lambda^*)(\mathbf{a}, \mathbf{a}).$$

Positivity of $(\mathbf{a}, \mathbf{a})$, ($(\mathbf{a}, \mathbf{a}) \geq 0$ and is only 0 if $\mathbf{a} = \mathbf{0}$) allows us to conclude that $\lambda = \lambda^*$.

For the second property we consider two cases. First assume there is a second solution to the eigenvalue problem of the form $L\mathbf{b} = \mu\mathbf{b}$, with $\lambda \neq \mu$, $\lambda, \mu \in \mathbb{R}$. Then, using Hermiticity we can show that we have two expressions (obtained by having L act on $\mathbf{a}$ or $L^\dagger = L$ on $\mathbf{b}$) for

$$(\mathbf{b}, L\mathbf{a}) = \lambda(\mathbf{b}, \mathbf{a}) = \mu(\mathbf{b}, \mathbf{a}).$$

Taking the difference between the two right-hand sides, we find $(\lambda - \mu)(\mathbf{a}, \mathbf{b}) = 0$, and since $\mu \neq \lambda$, $(\mathbf{a}, \mathbf{b}) = 0$.

This does not apply to the case when we have two different eigenvalues for the same eigenvector (degeneracy). There is no rule precluding $(\mathbf{a}, \mathbf{b})$ to be zero, just no requirement for it to be so. In that case we can construct from the subspace of degenerate eigenvalues a set of vectors that are orthogonal, using the procedures set out in the previous chapter, since any linear combination of the degenerate eigenvectors still correspond to the same eigenvalue. □

Example 3.4:

Find the eigenvalues and eigenvectors of the matrix ("diagonalise the matrix")

$$M = \begin{pmatrix} 4 & 1 & 1 \\ 1 & 4 & 1 \\ 1 & 1 & 4 \end{pmatrix}$$

Solution:

The eigenvalues can be found from

$$M\mathbf{e} = \lambda\mathbf{e}.$$

This equation only has interesting (non-zero) solutions if the determinant of coefficients is zero,

$$\begin{aligned} 0 &= \det(M - \lambda I) \\ &= (4-\lambda)((4-\lambda)^2 - 1) - 1((4-\lambda) - 1) + 1(1 - (4-\lambda)) \\ &= (4-\lambda)((4-\lambda)^2 - 3) + 2 \\ &= -\lambda^3 + 12\lambda^2 - 45\lambda + 54\,. \end{aligned}$$

A little guesswork shows that this can be factorized as

$$-(\lambda - 3)^2(\lambda - 6) = 0.$$

The unique eigenvalue 6 has an eigenvector satisfying

$$\begin{pmatrix} -2 & 1 & 1 \\ 1 & -2 & 1 \\ 1 & 1 & -2 \end{pmatrix} \mathbf{e} = 0,$$

which has as normalised solution $\mathbf{e}_3 = \begin{pmatrix} 1 \\ 1 \\ 1 \end{pmatrix} / \sqrt{3}$. The degenerate eigenspace for $\lambda = 3$ has eigenvectors satisfying

$$\begin{pmatrix} 1 & 1 & 1 \\ 1 & 1 & 1 \\ 1 & 1 & 1 \end{pmatrix} \mathbf{e} = 0,$$

which describes a plane through the origin, orthogonal to $(1,1,1)$. We can find non-orthogonal eigenvectors, e.g. $(1,1,-2)$ and $(1,0,-1)$, but we can use the Gram–Schmidt procedure to find orthonormal eigenvectors of the form $\mathbf{e}_1 = (1,1,-2)/\sqrt{6}$ and $\mathbf{e}_2 = (1,-1,0)/\sqrt{2}$. The general eigenvector for eigenvalue 3 is then $a\mathbf{e}_1 + b\mathbf{e}_2$.

This example shows the reality of the eigenvalues, the orthogonality of the eigenvectors, etc.

Weight functions. For function spaces, one often meets the generalised eigenvalue equation

$$Ly(x) = \lambda\rho(x)y(x),$$

where L is a differential operator, $\rho(x)$ is a real and positive "weight function".

Theorem 3.2. *For an operator L, Hermitian with respect to the ordinary inner product $(u,v) = \int u(x)^* v(x)\,dx$, the eigenvalues are real and eigenvectors $u(x)$, $v(x)$ corresponding to different eigenvalues are "orthogonal with a weight function $\rho(x)$", i.e.*

$$(u,v)_\rho = \int dx\,\rho(x)u^*(x)v(x) = 0. \tag{3.5}$$

3.2.1 Problems

1. Show that the definition (3.5) satisfies the conditions (2.2–2.4).

3.3 Sturm–Liouville equations

There is a physically very important class of operators with a weight function. These occur in the so-called Sturm–Liouville equations, which are eigenvalue equations of the form

$$Ly(x) = \lambda\rho(x)y(x),$$

where $\rho(x) > 0$ is a given real positive weight function and the operator L is of the special *Sturm–Liouville* type,

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

where $p(x)$, $q(x)$ are given real functions and $p(x)$ is positive. The dot denotes the place the argument of the operator must be inserted. Explicitly, using (3.3) and (3.3), we see that they are homogeneous second order equations of the form

$$-\frac{d}{dx}\left(p(x)\frac{d}{dx}y(x)\right) + q(x)y(x) - \lambda\rho(x)y(x) = 0,$$

or equivalently, expanding out the derivatives,

$$p(x)\frac{d^2y}{dx^2} + \frac{dp}{dx}\frac{dy}{dx} - q(x)y(x) + \lambda\rho(x)y(x) = 0. \tag{3.6}$$

Many equations can be put in S-L form by multiplying by a suitably chosen function $\alpha(x)$, which is determined by requiring a differential equation of the form Eq. (3.6), see the next section.

Table 3.1: A few well-known examples of Sturm–Liouville problems that occur in mathematical physics

Name	$p(x)$	$q(x)$	$\rho(x)$	$[a,b]$
QM particle in a box	1	0	1	$[0,L]$, L finite
Legendre's equation	$(1-x^2)$	0	1	$[-1,1]$
Laguerre's equation	xe^{-x}	0	e^{-x}	$[0,\infty)$
Hermite's equation	e^{-x^2}	0	e^{-x^2}	$(-\infty,\infty)$
Chebyshev's equations	$(1-x^2)^{1\pm\frac{1}{2}}$	0	$(1-x^2)^{\pm 1/2}$	$[-1,1]$
Bessel's equation	x	ν^2/x	x	$[0,R]$, R finite
...and many others.				

3.3.1 How to bring an equation to Sturm–Liouville form

Given a general second order differential equation, that we suspect might be written as Sturm–Liouville equation, how do we find out whether this is true?

We start from a "canonical form". It is straightforward to rewrite any second order differential equation so that the coefficient of the second derivative is 1,

$$y''(x) + \alpha(x)y'(x) + \beta(x)y(x) + \lambda\tau(x)y(x) = 0,$$

so let us assume an equation of that form.

We shall show below that $\tau > 0$ for a Sturm–Liouville equation. Suppose first that we are given the function $p(x)$ in the Sturm–Liouville operator. We can then multiply both sides of the equation with p, and find

$$p(x)y''(x) + p(x)\alpha(x)y'(x) + p(x)\beta(x)y(x) + \lambda p(x)\tau(x)y(x) = 0.$$

If we compare this with equation (3.6) above we see that

$$p'(x) = \alpha(x)p(x), \qquad q(x) = -\beta(x)p(x), \qquad \rho(x) = \tau(x)p(x). \tag{3.7}$$

If we do *not* know p, we can solve (3.7) for $p(x)$,

$$\frac{d\ln(p(x))}{dx} = \alpha(x),$$
$$p(x) = \exp\left(\int^x \alpha(x')dx'\right).$$

We have thus found the function p to bring it to Sturm–Liouville form. The function $\rho = \tau p$ must be positive, and thus since p is positive, τ must be positive.

There are many well-known examples in physics, see Table 3.1. Almost all cases we meet in physics are Hermitian Sturm–Liouville operators. Some of these will be investigated further below, but first we need a useful property of Sturm–Liouville operators

3.3.2 A useful result

In general, one can show that for any two real functions $u(x)$, $v(x)$ defined for $x \in [a,b]$, and a Sturm–Liouville operator L also defined on $[a,b]$,

$$\begin{aligned} vLu - (Lv)u &= -v(x)\frac{d}{dx}\left(p(x)\frac{d}{dx}u(x)\right) + v(x)q(x)u(x) \\ &\quad + \left[\frac{d}{dx}\left(p(x)\frac{d}{dx}v(x)\right)\right]u(x) - v(x)q(x)u(x) \\ &= -v(pu')' + u(pv')' \\ &= \left[-vpu' + upv'\right]'. \end{aligned} \tag{3.8}$$

After integration we thus conclude that

$$\begin{aligned} \int_a^b dx\,[vLu - (Lv)u] &= (v, Lu) - (u, Lv) \\ &= \left[p(uv' - vu')\right]_a^b. \end{aligned} \tag{3.9}$$

3.3.3 Hermitian Sturm–Liouville operators

From the useful identity (3.9) we can draw some interesting conclusions about Hermitian Sturm–Liouville operators. By definition, an operator L is Hermitian if

$$\int_a^b dx\,[vLu - (Lv)u] = 0$$

for any two vectors u, v in the space. Hence, from this and (3.9), a S-L operator is Hermitian if and only if the boundary conditions at a and b are such that

$$\left[p(uv' - vu')\right]_a^b = p(b)W(b) - p(a)W(a) = 0, \tag{3.10}$$

where the Wronskian W is defined as

$$W(x) = \begin{vmatrix} u(x) & v(x) \\ u'(x) & v'(x) \end{vmatrix} = u(x)v'(x) - u'(x)v(x).$$

In mathematical physics the domain is often delimited by endpoints a and b where $p(a) = p(b) = 0$. At these endpoints, we typically add a boundary condition that for all solutions $y(x)$, the functions $y(x)$ and $p(x)y'(x)$ remain finite, and we require $Ay = Bpy'$, where A and B are not *both* zero (and are not necessarily the same at each endpoint). You can confirm that such a boundary condition leads to the satisfaction of (3.10), and hence makes L self-adjoint. In fact, the boundary condition is *stronger* than is required for self-adjointness alone, since $p(x)W(x) = 0$ at each endpoint, $x = a$ and b; we can say in this case that the boundary conditions have been *separated*.

Note that separated boundary conditions forbid "second solutions"—see next section.

3.3.4 Second solutions, singularities

Since a Sturm–Liouville equation is by definition second order, there are two independent solutions. If we have already obtained one (finite) solution $u(x)$ for a given λ, we would like to know the second solution, which we call $v(x)$. Thus

$$Lu(x) - \lambda\rho u(x) = 0, \tag{3.11}$$

$$Lv(x) - \lambda\rho v(x) = 0. \tag{3.12}$$

We now multiply (3.11) by $v(x)$ and (3.12) by $u(x)$, and subtract:

$$uLv - vLu = 0$$

or, using the result above

$$\frac{d}{dx}\left[puv' - pvu'\right] = 0.$$

Hence

$$puv' - pvu' = c\,,$$

i.e.,

$$uv' - vu' = \frac{c}{p(x)}\,.$$

Since u is known, this is a first-order differential equation for v. The technique applicable is the integrating factor or substitution of $v = uw$,

$$\begin{aligned} uu'w + uuw' - uu'w = c/p \implies \\ w' = \frac{c}{pu^2} \implies \\ w(x) = c\int^x \frac{1}{p(x')u(x')^2}dx' \quad . \end{aligned}$$

We can of course add a constant to w, but that would just add a contribution proportional to u in the solution, which we already know is allowed. We can also take $c = 1$, since the multiplication by c is a trivial reflection of linearity.

These solutions do not exist (i.e., diverge) for points such that $p(x) = 0$, which are called singular points. This may sound like a superficial remark, but in many cases the interval $[a, b]$, on which the Sturm–Liouville operator is defined, is delimited by such special singular points where $p(a) = p(b) = 0$.

Consider a second order differential equation

$$y''(x) + P(x)y'(x) + Q(x)y(x) = 0.$$

If at a point $x = x_0$ $P(x)$ or $Q(x)$ diverges, but $(x - x_0)P(x)$ and $(x - x_0)^2Q(x)$ are finite, x_0 is called a regular singular point. If $P(x)$ diverges faster than $1/(x - x_0)$ and/or $Q(x)$ diverges faster than $1/(x - x_0)^2$ we speak of an irregular singular point.

3.3.5 Eigenvectors and eigenvalues

For S-L operators with separated boundary conditions, we state without proof that:

1. The eigenvalues are real and non-degenerate, i.e., there exists only one finite solution $u_n(x)$ for each eigenvalue λ_n.

   Since the S-L equation is real and its solution $u_n(x)$ for any eigenvalue is unique, this implies $u_n(x) = u_n^*(x)$, up to a factor of unit modulus. Hence one can (and we will) always choose real eigenfunctions.

2. There exists a lowest eigenvalue λ_0 (this relies on the positivity of $p(x)$), and the sequence

   $$\lambda_0 < \lambda_1 < \ldots < \lambda_n < \ldots\,.$$

   is unbounded, $\lambda_n \to \infty$ as $n \to \infty$.

3. The number of nodes in the nth eigenvector, if the corresponding eigenvalues are ordered as above, is exactly equal to n. (The "nodes" referred to here are zeroes of the function at points *other than* the endpoints!)

4. Eigenfunctions u_m, u_n with $m \neq n$ are orthogonal with weight function $\rho(x)$,

$$(u_m, u_n)_\rho = \int_a^b dx\, \rho(x) u_m^*(x) u_n(x) = 0\,.$$

5. The eigenfunctions

$$u_1(x), u_2(x), \ldots, u_n(x), \ldots$$

form a complete basis set for functions on the interval $[a, b]$, satisfying the boundary conditions. (Proof will be given in the Variational Calculus section, but not necessarily discussed in class.)

3.4 Series solutions and orthogonal polynomials

You should all be familiar with one example from the Legendre polynomials discussed in the second year math course PHYS 20171. Orthogonal polynomials also arise naturally in the problem of the one-dimensional quantum-mechanical harmonic oscillator.

3.4.1 The quantum-mechanical oscillator and Hermite polynomials

The quantum-mechanical harmonic oscillator has the time independent Schrödinger equation

$$-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\psi(x) + \tfrac{1}{2}m\omega^2 x^2 \psi(x) = E\psi(x).$$

Solutions to such equations are usually required to be normalisable,

$$\int_{-\infty}^{\infty} |\psi^2(x)| dx < \infty,$$

i.e., $\psi \in \mathcal{L}^2(\mathbb{R})$.

Mathematical functions other than simple polynomials always act on pure numbers (since otherwise the result of the function would contain a mixture of quantities of different dimensions, as we can see by Taylor expanding). This holds here as well, and we must be able to define "dimensionless variables". We combine all the parameters of the problem to define two scales, a harmonic oscillator length

$$b = \left(\frac{\hbar}{m\omega}\right)^{1/2}$$

and a scale for energy $E_\omega = \hbar\omega$. We can then define a dimensionless coordinate and energy

$$z = x/b, \quad \lambda = E/E_\omega.$$

In these variables the Schrödinger equation reads

$$\frac{d^2}{dz^2}\psi(z) + (2\lambda - z^2)\psi(z) = 0. \tag{3.13}$$

Functions in $\mathcal{L}^2(\mathbb{R})$ must decay sufficiently fast at infinity: not all solutions to (3.13) have that property! Look at large z, where $\lambda \ll z^2$, and we find that a function of the form $\psi(z) = \exp(\pm z^2/2)$ satisfies exactly the equation

$$\frac{d^2}{dz^2}\psi(z) - z^2\psi(z) = 0.$$

for large z. Since we have neglected a constant to obtain this result, we can conclude that any behaviour of the form $z^a \exp(\pm z^2/2)$ is allowed, since the pre-factor gives subleading terms—please check. Since the wave function must vanish at infinity, we find the only acceptable option is a wave function of the form

$$\psi(z) = f(z)\exp(-z^2/2),$$

where $f(z)$ does not grow faster than a power as $z \to \infty$.

The easiest thing to do is substitute this into (3.13) and find an equation for f,

$$f''(z) - 2zf'(z) + (2\lambda - 1)f(z) = 0. \tag{3.14}$$

The last equation is *not* of Sturm–Liouville form, but if we multiply it by $p(z) = e^{-z^2}$ we obtain

$$[\exp(-z^2)f'(z)]' + (2\lambda - 1)\exp(-z^2)f(z) = 0. \tag{3.15}$$

This *is* a Sturm–Liouville equation, with eigenvalue $2\lambda - 1$ and weight function $e^{-z^2/2}$. The points $z = \pm\infty$ are singular, since p vanishes there. Thus $[a, b]$ is actually $(-\infty, \infty)$, as we would expect. (Of course, the original Schrödinger equation and (3.13) were *also* of Sturm–Liouville form, but with constant weight function; 3.14) is just a little easier to solve.)

So how do we tackle Hermite's equation (3.14)? The technique should be familiar: we try a Taylor series around $z = 0$,

$$f(z) = \sum_{n=0}^{\infty} c_n z^n,$$

substitute it into Hermite's equation and equate to zero the coefficient of each power of z,

$$(l+2)(l+1)c_{l+2} - (2l - (2\lambda - 1))c_l = 0.$$

This recurrence relation can be used to bootstrap our way up from c_0 or c_1. It terminates only if $(2\lambda - 1)$ is an even integer—and termination is required for power-law behaviour at infinity. We are thus only interested in even or odd polynomials, and we only have non-zero c's for the odd part (if $\lambda - 1/2$ is odd) or even part (when $\lambda - 1/2$ is even).

If we write $\lambda = n + 1/2$, with integer $n \geq 0$, the solutions are $H_n(z)$, where $H_0(z) = 1$, $H_1(z) = 2z$, $H_2(z) = 4z^2 - 2$, ...[2] These are orthogonal with respect to the weighted inner product

$$\int_{-\infty}^{\infty} \exp(-z^2)H_n(z)H_m(z)\,dz = k_n\delta_{nm},$$

but we shall not pause to determine k_n, which we we would need to normalize the solutions. This shows that the eigenfunctions of the harmonic oscillator are all of the form

$$\psi_n(x) = \frac{1}{\sqrt{bk_n}}\exp[-x^2/(2b^2)]H_n(x/b)$$

with eigenvalue $(n + \frac{1}{2})\hbar\omega$.

3.4.2 Legendre polynomials

A differential equation that you have seen a few times before, is Legendre's equation,

$$\Big[(1 - x^2)y'(x)\Big]' + \lambda y(x) = 0. \tag{3.16}$$

[2] The unlikely-looking factors of 2 arise from the conventional definition of the Hermite polynomials, which uses a generating function

$$\exp[-t^2 + 2tz] = \sum_{n=0}^{\infty} H_n(z)\frac{t^n}{n!}.$$

Clearly $x = \pm 1$ are singular points of this equation, which coincides with the fact that in most physically relevant situations $x = \cos\theta$, which only ranges from -1 to 1. As usual, we substitute a power series around the regular point $x = 0$, $y(x) = \sum_n c_n x^n$. From the recurrence relation for the coefficients,

$$c_{m+2} = \frac{m(m+1) - \lambda}{(m+1)(m+2)} c_m,$$

we see that the solutions are terminating (i.e., polynomials) if $\lambda = n(n+1)$ for $n \in \mathbb{N}$. These polynomials are denoted by $P_n(x)$. Solutions for other values of λ diverge at $x = 1$ or $x = -1$.

Since Eq. (3.16) is of Sturm–Liouville form, the polynomials are orthogonal,

$$\int_{-1}^{1} P_n(x) P_m(x)\, dx = 0 \text{ if } n \neq m.$$

As for all linear equations, the P_n's are defined up to a constant. This is fixed by requiring $P_n(1) = 1$.

Generating function

A common technique in mathematical physics is to combine all the solutions in a single object, called a "generating function", in this case

$$f(x,t) = \sum_n t^n P_n(x).$$

We shall now prove that

$$(1 - 2tx + t^2)^{-1/2} = \sum_n t^n P_n(x), \qquad (t \in [-1,1]), \tag{3.17}$$

and show that we can use this to prove a multitude of interesting relations on the way. The calculation is rather lengthy, so keep in mind where we do wish to end up: The coefficients of t^n in Eq. (3.17) satisfy Eq. (3.16).

1. First we differentiate (3.17) w.r.t. to x and t,

$$t(1 - 2tx + t^2)^{-3/2} = \sum_n t^n P_n'(x), \tag{3.18}$$

$$(x - t)(1 - 2tx + t^2)^{-3/2} = \sum_n n t^{n-1} P_n(x). \tag{3.19}$$

2. We then replace $(1 - 2tx + t^2)^{-1/2}$ on the l.h.s. of (3.18) by a $\sum_n t^n P_n(x)$, multiplying both sides with $(1 - 2tx + t^2)$,

$$\sum t^{n+1} P_n(x) = \sum_n P_n'(x)(t^n - 2xt^{n+1} + t^{n+2}).$$

   Equating coefficients of the same power in t, we find

$$P_n(x) = P_{n+1}'(x) - 2xP_n'(x) + P_{n-1}'(x). \tag{3.20}$$

3. Since $(x - t)$ times the l.h.s. of (3.18) equals t times the l.h.s. of (3.19), we can also equate the right-hand sides,

$$(x - t)\sum_n t^n P_n'(x) = t\sum_n n t^{n-1} P_n(x),$$

   from which we conclude that

$$xP_n'(x) - P_{n-1}'(x) = nP_n(x). \tag{3.21}$$

4. Combine (3.20) with (3.21) to find

$$(n+1)P_n(x) = P_{n+1}'(x) - xP_n'(x). \tag{3.22}$$

5. Let n go to $n-1$ in (3.22), and subtract (3.21) times x to find

$$(1-x^2)P_n'(x) = n\left(P_{n-1}(x) - xP_n(x)\right).$$

6. Differentiate this last relation,

$$\begin{aligned}\left[(1-x^2)P_n'(x)\right]' &= nP_{n-1}'(x) - nP_n(x) - nxP_n'(x)\\ &= -n(n+1)P_n(x),\end{aligned}$$

where we have applied (3.21) one more time.

This obviously completes the proof.

We can now easily convince ourselves that the normalisation of the P_n's derived from the generating function is correct,

$$f(1,t) = 1/(1-t) = \sum_n t^n = \sum_n t^n P_n(1),$$

i.e., $P_n(1) = 1$ as required.

This also shows why t should be less than 1; the expansion of $1/(1-t)$ has radius of convergence equal to 1.

Expansion of $|\mathbf{r}_1 - \mathbf{r}_2|^{-1}$.

One of the simplest physical applications is the expansion of $|\mathbf{r}_1 - \mathbf{r}_2|^{-1}$ in orthogonal functions of the angle between the two vectors.

Let us first assume $r_2 > r_1$,

$$\begin{aligned}|\mathbf{r}_1 - \mathbf{r}_2|^{-1} &= \frac{1}{\sqrt{r_1^2 + r_2^2 - 2r_1r_2\cos\theta}}\\ &= \frac{1}{r_2\sqrt{(r_1/r_2)^2 + 1 - 2r_1/r_2\cos\theta}}\\ &= \frac{1}{r_2}\sum_n \left(\frac{r_1}{r_2}\right)^n P_n(\cos\theta),\end{aligned} \tag{3.23}$$

where we have used the generating function with $t = r_1/r_2$.

Since the expression is symmetric between r_1 and r_2, we find the general result

$$\frac{1}{|\mathbf{r}_1 - \mathbf{r}_2|} = \sum_n \frac{r_<^n}{r_>^{n+1}} P_n(\cos\theta),$$

where $r_{<,>}$ is the smaller (larger) or r_1 and r_2.

Normalisation

When developing a general "Legendre series", $f(x) = \sum_n c_n P_n(x)$, we need to know the normalisation of $P_n(x)$. This can be obtained from the generating function, using orthogonality,

$$\int_{-1}^{1}\left(\sum_n t^n P_n(x)\right)^2 dx = \sum_n t^{2n}\int_{-1}^{1} P_n(x)^2\,dx.$$

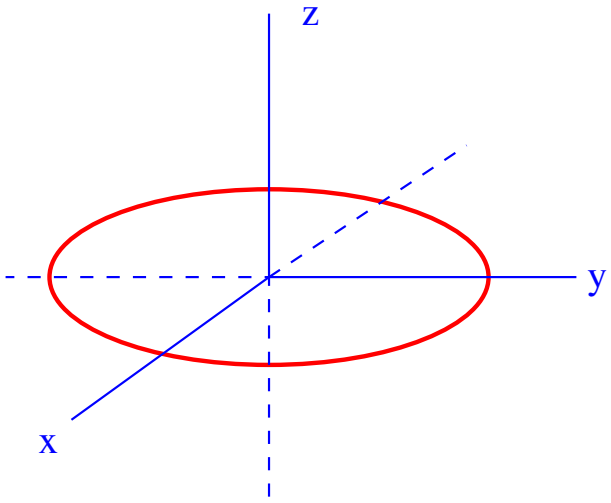

Figure 3.5: A homogeneously charged ring in the xy plane.

Substituting the generating function, we find

$$\begin{aligned}\int_{-1}^{1}(1-2xt+t^2)^{-1}\,dx &= \frac{1}{t}\ln\left(\frac{1+t}{1-t}\right)\\ &= \frac{1}{t}\sum_{m=1}^{\infty}\frac{1}{m}t^m-\frac{1}{m}(-t)^m\\ &= \sum_{m=2n+1}\frac{2}{2n+1}t^{2n}.\end{aligned} \tag{3.24}$$

Thus

$$\int_{-1}^{1}P_n(x)^2\,dx=\frac{2}{2n+1}.$$

Electrostatic potential due to a ring of charge

As a final example we discuss the case of a homogeneously charged ring of radius a in the xy plane, see fig. 3.5.

The equation to solve is $\Delta V = 0$, apart from on the ring itself. The problem can easily be tackled by separation of variables in polar coordinates, and we see from symmetry that the potential can only depend on r and θ. The angular equation gives Legendre polynomials, and the radial equation is trivial to solve (it has a power of r as solution), resulting in the expansion

$$V=\sum_{n=0}^{\infty}c_n\frac{a^n}{r^{n+1}}P_n(\cos\theta). \tag{3.25}$$

where we have imposed the boundary condition $V(\infty)=0$. Actually, we can be slightly more specific and use the fact that from far away the ring looks like a point charge, $V\to q/(4\pi\epsilon_0 r)$ for $r\to\infty$.

Now how do we determine the coefficients c_n in (3.25)? The simplest technique is based on a calculation of the potential on the positive z axis. You should have derived the result before (it is a standard example in basic electrostatics)

$$V(z)=\frac{q}{4\pi\epsilon_0\sqrt{z^2+a^2}}\quad .$$

This can easily be expanded in powers of a/z, and if we use $\sqrt{z^2} = z$ we get

$$V(z) = \frac{q}{4\pi\epsilon_0 z} \sum_{m=0}^{\infty} (-1)^m \frac{(2m-1)!!}{2^m m!} \left(\frac{a}{z}\right)^{2m}.$$

Since on the positive z axis $r = z$ and $P_n(\cos\theta) = P_n(1) = 1$, we conclude that

$$V(r,\theta) = \frac{q}{4\pi\epsilon_0 z} \sum_{m=0}^{\infty} (-1)^m \frac{(2m-1)!!}{2^m m!} \left(\frac{a}{r}\right)^{2m} P_{2m}(\cos\theta).$$

3.4.3 Bessel functions and the circular drum

Bessel's equation of order ν takes the form

$$x^2 y''(x) + x\,y'(x) + (x^2 - \nu^2) y(x) = 0.$$

This equation has a regular singular point at $x = 0$, and the point $x = \infty$ is regular. It is thus not of Sturm–Liouville form, without additional boundary conditions (see below).

The solutions can be found in many places: we substitute a generalised power series around $x = 0$,

$$y(x) = x^\gamma \sum_{n=0}^{\infty} c_n x^n.$$

From the index equation (lowest power in x) we find $\gamma = \pm\nu$; this leads to two independent solutions if ν is not a half-integer. The recurrence relations are

$$c_n = \frac{-1}{n(n \pm 2\nu)} c_{n-2}.$$

The main result are the Bessel functions (regular solutions) for $\nu \geq 0$,

$$J_\nu(x) = \sum_{k=0}^{\infty} \frac{(-1)^k}{k!\Gamma(\nu + k + 1)} \left(\frac{x}{2}\right)^{\nu+2k}.$$

The simplest use of these regular solutions is for example in the caculation of the modes in a circular drum. With $u(r,\phi) = R(r)e^{im\phi}$ we find that

$$r^2 R''(r) + rR'(r) + \lambda r^2 R(r) - m^2 R(r) = 0, \tag{3.26}$$

with the explicit boundary condition $y(a) = 0$ and the implicit boundary condition $y(0)$ is finite. With these conditions we have an Sturm–Liouville problem!

We can move λ into the variable by using the transformation

$$x = \sqrt{\lambda} r, \quad R(r) = y(x),$$

which turns the equation into Bessel's equation of order m. Thus

$$y = cJ_m(x), \quad R(r) = cJ_m(\sqrt{\lambda} r),$$

with the boundary condition

$$J_m(\sqrt{\lambda} a) = 0.$$

If we are given the zeroes x_n of $J_m(x)$, we find that

$$\lambda_n = \left(\frac{x_n}{a}\right)^2.$$

We tabulate the zeroes of $J_m(x)$ in Tab. 3.2.

Table 3.2: The eigenvalues as a function of m and n, divided by the lowest one.

	$m = 0$	$m = 1$	$m = 2$	$m = 3$
$n = 1$	1.	2.5387339670887545	4.5605686201597395	7.038761346947694
$n = 2$	5.2689404316052215	8.510612772447574	12.25103245391653	16.47492803352439
$n = 3$	12.949091948711432	17.89661521491159	23.347115194125884	29.291025900157134
$n = 4$	24.042160379641803	30.696015647982048	37.85459961832423	45.51139388242945
$n = 5$	38.5483546692039	46.90868597534144	55.77464019991307	65.14149844841049
$n = 6$	56.46772471517244	66.53458968257806	77.10759560464034	88.18317085819912
$n = 7$	77.80028714289776	89.5737132318928	101.85360724822897	114.63717276642296
$n = 8$	102.54604874469128	116.02605067898523	130.01274014487907	144.50386866809274
$n = 9$	130.70501270873422	145.89159908441692	161.58502760864766	177.78345128038563
$n = 10$	162.2771806904681	179.1703568603581	196.57048815295988	214.47603043403043

Chapter 4

Green's functions

4.1 General properties

The Green's function technique is used to solve differential equations of the form

$$(L_x u)(x) = f(x) \qquad \text{plus boundary conditions} \tag{4.1}$$

where L_x is a linear operator (not always Hermitian) with specified boundary conditions and $f(x)$ is a given "source term". We shall normally suppress the subscript x on L.

The solution of (4.1) can always be written as

$$u(x) = \int dx'\, G(x,x') f(x'), \tag{4.2}$$

where the Green's function $G(x,x')$ is defined by

$$LG(x,x') = \delta(x-x') \qquad \text{plus boundary conditions,} \tag{4.3}$$

where L acts on x, but not on x'. We also have the same boundary conditions as before! The proof is straightforward:

$$L\int dx'\, G(x,x')f(x') = \int dx'\, LG(x,x')f(x') = \int dx'\, \delta(x-x')f(x') = f(x). \tag{4.4}$$

Note by solving this equation, one obtains the solution of (4.1) for all possible $f(x)$, and thus it is very useful technique to solve inhomogeneous equations where the right-hand side takes on many different forms.

4.1.1 First example: Electrostatics

In your physics courses you have already been exposed to a Green's function, without it ever being made explicit. The problem of interest is the determination of the electrostatic potential $\Phi(\mathbf{x})$ for a *static* charge distribution $\rho(\mathbf{x})$. From $\nabla\cdot\mathbf{E} = \rho/\epsilon_0$ and $\mathbf{E} = -\nabla\Phi$ we can easily show that

$$\nabla^2\Phi(\mathbf{x}) = -\rho(\mathbf{x})/\epsilon_0, \tag{4.5}$$

with the boundary condition that $\Phi(\mathbf{x}) \to 0$ as $|\mathbf{x}| \to \infty$.

For a point charge q at position $\mathbf{x}'$, Eq. (4.5) becomes

$$\nabla^2\Phi(\mathbf{x}) = -(q/\epsilon_0)\delta(\mathbf{x}-\mathbf{x}').$$

[Note that $\mathbf{x}$ is a 3-vector, and that the notation $\delta(\mathbf{x})$ stands for the three-dimensional delta function, $\delta(x)\delta(y)\delta(z)$. Occasionally we like to make the dimensionality explicit by writing $\delta^{(3)}(\mathbf{x})$; however, we should normally be able to remember the dimensionality of the space we are working in!] We all know the solution, which is the Coulomb potential,

$$\Phi(\mathbf{x}) = \frac{q}{4\pi\epsilon_0}\frac{1}{|\mathbf{x}-\mathbf{x}'|}.$$

In other words, the Green's function G which solves

$$\nabla^2 G(\mathbf{x},\mathbf{x}') = \delta(\mathbf{x}-\mathbf{x}')$$

is

$$G(\mathbf{x},\mathbf{x}') = -\frac{1}{4\pi}\frac{1}{|\mathbf{x}-\mathbf{x}'|}. \tag{4.6}$$

This leads to the well known superposition principle for a general charge distribution,

$$\Phi(\mathbf{x}) = \frac{1}{4\pi\epsilon_0}\int d^3x' \frac{\rho(\mathbf{x}')}{|\mathbf{x}-\mathbf{x}'|}.$$

This is usually derived using the statement that each "small charge" $\delta Q(\mathbf{x}') = d^3x'\rho(\mathbf{x}')$ contributes $\frac{1}{4\pi\epsilon_0}\frac{\delta Q(\mathbf{x}')}{|\mathbf{x}-\mathbf{x}'|}$ to the potential Φ, and we simply superimpose all these contributions.

4.1.2 The eigenstate method

For linear *Hermitian* operators where we know the eigenvalues and eigenfunctions, one can easily show that the Green's functions can be written in the form

$$G(x,x') = \sum_n \frac{1}{\lambda_n} u_n(x) u_n(x')^*. \tag{4.7}$$

This relies on the fact that $u_n(x)$ is a complete and orthonormal set of eigenfunctions of L, obtained by solving

$$Lu_n(x) = \lambda_n u_n(x), \tag{4.8}$$

where we have made the assumption that there are no zero eigenvalues. For this special case of the Green's function of an Hermitian operator, (4.7) implies

$$G(x,x') = [G(x',x)]^*, \tag{4.9}$$

which is the *reciprocity relation* for the Green's function of an Hermitian operator.

If there are zero eigenvalues—and many important physical problems have "zero modes"—we have to work harder. Let us look at the case of a single zero eigenvalue, $\lambda_0 = 0$. The easiest way to analyse this problem is to decompose $u(x)$ and $f(x)$ in the eigenfunctions,

$$\begin{aligned} u(x) &= \sum_n c_n u_n(x), \\ f(x) &= \sum_n d_n u_n(x). \end{aligned} \tag{4.10}$$

We know that $d_n = (u_n, f)$, etc.

Now substitute (4.10) into (4.8) and find

$$\sum_n u_n(x) c_n \lambda_n = \sum_n u_n(x) d_n.$$

Linear independence of the set u_n gives

$$c_n\lambda_n = d_n = (u_n, f),$$

and of most interest

$$0 = c_0\lambda_0 = d_0. \tag{4.11}$$

Clearly this equation only has a solution if $d_0 = 0$. In other words we must require that $(u_0, f) = 0$, and thus the driving term f is orthogonal to the zero mode. In that case, c_0 is not determined at all, and we have the family of solutions

$$\begin{aligned} u(x) = \sum_n c_n u_n(x) &= c_0 u_0(x) + \sum_{n=1}^{\infty} \frac{d_n}{\lambda_n} u_n(x) \\ &= c_0 u_0(x) + \sum_{n=1}^{\infty} \frac{1}{\lambda_n} \int u_n(x) u_n(x')^* f(x') dx' \\ &= c_0 u_0(x) + \int \tilde{G}(x, x') f(x') dx' \quad . \end{aligned} \tag{4.12}$$

Here

$$\tilde{G}(x, x') = \sum_{n \neq 0} \frac{u_n(x) u_n(x')^*}{\lambda_n}$$

is a modified Green's function which excludes the zero mode. We could, if we wished, include an arbitrary multiple of u_0 in $\tilde{G}$ without changing (4.12), but there is no pressing reason to do so here.

The driven vibrating string

Consider a string with fixed endpoints (such as a violin string) driven by an oscillating position-dependent external force density,

$$F = F(x) \sin \omega t \quad .$$

If we now consider a small section of the string, see Fig. 4.1, and assume small displacements from equilibrium, we can use the fact that the tension in the string and its density are constant, and we can use the *tranvserse* component of Newton's equation for teh resulting transverse waves,

$$\underbrace{\rho dx}_{\text{mass}}\, \ddot{u} = \underbrace{T\frac{du}{dx}(x + dx)}_{\text{force at end}} - \underbrace{T\frac{du}{dx}(x)}_{\text{force at beginning}} - \underbrace{F dx}_{\text{external force}}$$

Using a Taylor series expansion of u and taking the limit $dx \downarrow 0$, we find

$$\rho \frac{\partial^2 u}{\partial t^2} = T \frac{\partial^2 u}{\partial x^2} - F(x) \sin \omega t.$$

We know how such a problem works; there is a transient period, after which a steady state oscillations is reached at the driving frequency, $u(x, t) = v(x) \sin \omega t$, i.e.,

$$\frac{\partial^2 u}{\partial t^2} = -\omega^2 u.$$

Using this relation, we obtain a complicated equation for the steady state amplitude $v(x)$,

$$\frac{d^2 v}{dx^2} + \frac{\rho\omega^2}{T} v = \frac{F(x)}{T}.$$

This can be simplified by writing $k^2 = \rho\omega^2/T$ and $f(x) = F(x)/T$,

$$v'' + k^2 v = f(x), \tag{4.13}$$

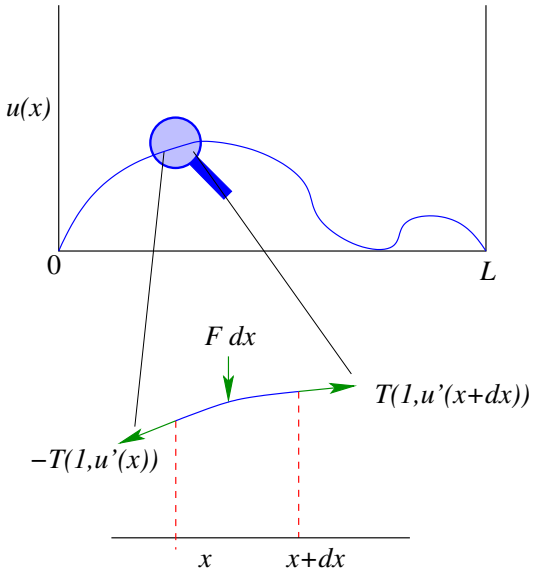

Figure 4.1: The balance of forces in a driven string

with boundary conditions $v = 0$ at $x = 0$ and $x = L$.

Now follow the eigenstate method for Green's functions. First we must solve

$$v_n'' + k^2 v_n = \lambda_n v_n.$$

If we write this as $v_n'' = (\lambda_n - k^2)v_n$, we recognise a problem of the simple form $y'' = \text{const.} \times y$, which is solved by functions that are either oscillatory or exponential. The boundary conditions only allow for solutions of the form $v_n = \sqrt{2/L}\sin k_n x$ with $k_n = n\pi/L$. From this we conclude that $\lambda_n = k^2 - k_n^2$, and thus

$$G(x, x') = \sum_{n=1}^{\infty} \frac{2}{L} \frac{\sin k_n x \sin k_n x'}{k^2 - k_n^2}.$$

The solution becomes

$$v(x) = \int_0^L G(x, x') f(x') dx' = \sum_n d_n \sqrt{\frac{2}{L}} \frac{\sin k_n x}{k^2 - k_n^2},$$

where

$$d_n = \int_0^L f(x)\sqrt{2/L}\sin k_n x \, dx.$$

Clearly, we have not discussed the case where takes on the values $k = k_m$, for any integer $m \geq 1$. From the discussion before we see that as k approaches such a point the problem becomes more and more sensitive to components in f of the mth mode. This is the situation of *resonance*, such as the wolf-tone of string instrument.

4.1.3 The continuity method

The continuity method can be used to find the Green's function of an ordinary differential equation of *any* order; we illustrate it here for the special case of a second-order equation.

For any second-order ODE, the equation for the Green's function can be put in the form

$$\left[\alpha(x)\frac{\partial^2}{\partial x^2} + \beta(x)\frac{\partial}{\partial x} + \gamma(x)\right] G(x, x') = \delta(x - x')\,. \tag{4.14}$$

Some would regard the *partial* derivatives here as being overly pedantic; we have used them to emphasize that G is a function of both x and x' and the differential operator acts only on the x-dependence of $G(x,x')$. To solve (4.14) one

(a) solves (4.14) for fixed x' in the regions $x < x'$ and $x > x'$, where it reduces to

$$LG(x,x') = 0 \qquad \text{plus boundary conditions .}$$

(b) fixes the remaining unknown functions of x' by using the continuity of $G(x,x')$ at $x = x'$; the discontinuity of the derivative is the inverse of the coefficient of the second derivative in the ODE,

$$\left[\frac{\partial}{\partial x}G(x,x')\right]_{x'-\epsilon}^{x'+\epsilon} = \frac{1}{\alpha(x')}\,, \quad \epsilon \to 0.$$

You should verify this for yourself, by integrating (4.14) between $x' - \epsilon$ and $x' + \epsilon$; you will need to use integration "by parts" *and* the continuity of $G(x,x')$ at $x = x'$ to show that the terms involving β and γ give contributions of order ϵ, and so are negligible as $\epsilon \to 0$.

It should not be hard to see how this general approach can be applied to ODEs of higher and lower order. For example, if the equation is of first order, $G(x,x')$ will be discontinuous at $x = x'$. Similarly, for a third-order equation, $G(x,x')$ and $\partial_x G(x,x')$ will be continuous at $x = x'$, but $\partial_x^2 G(x,x')$ will be discontinuous. In every case, the magnitude of any discontinuity is obtained by integrating the differential equation satisfied by $G(x,x')$.

Let us illustrate the method for the example of the driven vibrating string discussed above,

$$\left(\frac{d^2}{dx^2} + k^2\right) u(x) = f(x),$$

and the corresponding equation for the Green's function,

$$\left(\frac{\partial^2}{\partial x^2} + k^2\right) G(x,x') = \delta(x - x'), \tag{4.15}$$

with boundary conditions $G(x,x') = 0$ for $x = 0, L$. This can also be given a physical interpretation as the effect (i.e., the displacement) at x due to a point force acting at x'.

We first solve the problem

$$\frac{\partial^2}{\partial x^2}G(x,x') + k^2 G(x,x') = 0.$$

in the two regions $x < x'$, $x > x'$, which differ in boundary conditions,

For $x < x'$

$$G(x,x') = A(x')\sin(kx)$$

since $G(0,x') = 0$ falls within this domain.

For $x > x'$

$$G(x,x') = N(x')\sin(k(L-x))$$

since $G(L,x') = 0$ falls within this domain.

We now require that $G(x,x')$ is continuous in x at $x = x'$ (a point force doesn't break the string), and that $\partial_x G(x,x')$ is discontinuous at $x = x'$ (since a point force "kinks" the string).

To find this discontinuity, we integrate (4.15) from $x = x' - \epsilon$ to $x = x' + \epsilon$, where ϵ is a small quantity:

$$\int_{x'-\epsilon}^{x'+\epsilon} \left(\frac{\partial^2}{\partial x^2} + k^2\right) G(x,x')\,dx = \int_{x'-\epsilon}^{x'+\epsilon} \delta(x - x')\,dx,$$

which, up to terms of first order in ϵ, gives

$$-\left[\frac{\partial}{\partial x}G(x,x')\right]_{x'-\epsilon}^{x'+\epsilon} + k^2 G(x',x')2\epsilon = 1.$$

In the limit $\epsilon \to 0$ we find that

$$-\left(\frac{\partial G}{\partial x}\right)_{x=x'+\epsilon} + \left(\frac{\partial G}{\partial x}\right)_{x=x'-\epsilon} = 1.$$

From the form of G derived above, we conclude that

$$\begin{aligned} A(x')\sin kx' &= B(x')\sin k(L-x') \\ -B(x')k\cos k(L-x') - A(x')k\cos kx' &= 1 \end{aligned} \tag{4.16}$$

with as solution (as can be checked using the formula $\sin A\cos B + \cos A\sin B = \sin(A+B)$)

$$A(x') = -\frac{\sin k(L-x')}{k\sin kL} \quad \text{and} \quad B(x') = -\frac{\sin kx'}{k\sin kL}.$$

After putting these results together we find

$$G(x,x') = \begin{cases} -\dfrac{\sin kx\sin k(L-x')}{k\sin kL}, & x < x' \\ -\dfrac{\sin kx'\sin k(L-x)}{k\sin kL}, & x > x'. \end{cases}$$

Note the symmetry under interchange of x and x', which we could have predicted from the reciprocity relation (4.9) for the Green's function of an Hermitian operator; in this case there is no complex conjugation—can you explain why? Use of the reciprocity relation (where appropriate) can often simplify the task of finding a Green's function by the continuity method.

As a challenge problem, you may wish to check that this form is the same as the one derived by the eigenfunction method in the previous section (see also the mathematica based coursework).

4.2 Quantum mechanical scattering

We consider scattering from a finite range potential, which can be expressed in the more precise mathematical relation $rV(r) \to 0$ as $r \to \infty$. We use the "time-independent approach"; see Mandl, Quantum Mechanics, Chapter 11.

The idea is that a beam of particles, that is not very dense so that they don't significantly interact which each other, impinges on a target described by the the potential $V(r)$. If we observe the particles far away, we are really interested in their energy which must be *positive* for scattering states. Thus we write

$$\psi(\mathbf{r},t) = \phi(\mathbf{r})e^{-iEt/\hbar} \quad ,$$

where ϕ satisfies the time-independent Schrödinger equation

$$-\frac{\hbar^2}{2m}\nabla^2\phi(\mathbf{r}) + V(\mathbf{r})\phi(\mathbf{r}) = E\phi(\mathbf{r}).$$

For positive energy we introduce a wave number k, $E = \hbar^2k^2/(2m)$, and find

$$(\nabla^2 + k^2)\phi(\mathbf{r}) = \frac{2m}{\hbar^2}V(\mathbf{r})\phi(\mathbf{r}) = \rho(\mathbf{r}).$$

Here we replaced the right-hand side temporarily by an independent function, for reasons that will become apparent below.

As usual we still need to determine the boundary conditions. We have two processes that describe those: there is an incoming beam that outside the range of interaction becomes a plane wave, $\phi(\mathbf{r}) \to e^{ikz}$, and we do have the scattered particles, which are a result of the interaction with the potential. These are most naturally described in terms of outgoing spherical waves.

Spherical waves are eigenfunctions of the radial part of the Laplace operator,

$$-\frac{1}{r^2}\frac{d}{dr}r^2\frac{d}{dr}f(r) = k^2 f(r)\,,$$

and have the form $e^{\pm ikr}/r$. Using the radial component of the momentum operator, $p_r = -i\hbar\, d/dr$, we find that the plus sign in the exponent corresponds to outward travelling waves; the minus sign is thus for an incoming wave.

Outgoing spherical waves are of the form

$$f(\theta,\phi)\frac{e^{ikr}}{r}, \quad r \text{ large} \quad ,$$

so we have the "asymptotic" boundary condition

$$\phi(\mathbf{r}) \to e^{ikz} + f(\theta,\phi)\frac{e^{ikr}}{r} \qquad \text{for } r \to \infty \quad .$$

Also, the scattering amplitude $f(\theta,\phi)$ goes to zero as V goes to zero.

If we ignore the fact that ρ depends on ϕ (for the time being!) and write $\phi(\mathbf{r}) = e^{ikz} + \chi(\mathbf{r})$, we find we have to solve the equation

$$(\nabla^2 + k^2)\chi(\mathbf{r}) = \rho(\mathbf{r}),$$

subject to the boundary condition

$$\chi(\mathbf{r}) \to f(\theta,\phi)\frac{e^{ikr}}{r} \qquad \text{for } r \to \infty.$$

We can solve this by the Green's function method,

$$(\nabla^2 + k^2)G(\mathbf{r},\mathbf{r}') = \delta(\mathbf{r}-\mathbf{r}') \quad ,$$

where, by using translational invariance, we can write $G(\mathbf{r},\mathbf{r}') \equiv G(|\mathbf{r}-\mathbf{r}'|)$, so that

$$(\nabla^2 + k^2)G(\mathbf{r}) = \delta(\mathbf{r}) \quad .$$

Actually, since we know that

$$\nabla^2\left(\frac{1}{r}\right) = -4\pi\delta(\mathbf{r})\,,$$

we realize that G must approach this form for $r \to 0$. Together with the fact that

$$(\nabla^2 + k^2)\frac{e^{\pm ikr}}{r} = 0$$

for $r \neq 0$, we conclude that there are two independent solutions for G,

$$G_\pm(\mathbf{r},\mathbf{r}') = -\frac{1}{4\pi}\frac{e^{\pm ik|\mathbf{r}-\mathbf{r}'|}}{|\mathbf{r}-\mathbf{r}'|}.$$

Since, as we have argued above, the wave function can be written as the superposition of an incoming plane wave and an outgoing scattered wave, it is most natural to use the solution G_+.

By using the divergence theorem, it is not hard to show that

$$\begin{aligned}\int_{r\le R}(\nabla^2+k^2)\frac{e^{ikr}}{r}\,dV &= \oint_{r=R}\nabla\left(\frac{e^{ikr}}{r}\right)\cdot d\mathbf{S}+k^2\int_{r\le R}\frac{e^{ikr}}{r}\,dV\\ &= 4\pi R^2\left[\frac{d}{dr}\frac{e^{ikr}}{r}\right]_{r=R}+4\pi k^2\int_0^R e^{ikr}r\,dr\\ &= 4\pi e^{ikR}(ikR-1)+4\pi\left(-1-e^{ikR}(ikR-1)\right)\\ &= -4\pi.\end{aligned}$$

This also shows we really do have a delta function.

We thus find, substituting the solution for χ and its relation to ϕ,

$$\phi(\mathbf{r}) = e^{ikz}+\int d^3r' G_+(\mathbf{r},\mathbf{r}')\rho(\mathbf{r}').$$

If we also remember how ρ is related to ϕ, we get the integral equation for scattering,

$$\phi(\mathbf{r}) = e^{ikz}+\frac{2m}{\hbar^2}\int d^3r' G_+(\mathbf{r},\mathbf{r}')V(\mathbf{r}')\phi(\mathbf{r}') \quad . \tag{4.17}$$

This equation is called the *Lippmann–Schwinger* equation (in the coordinate representation).

One might reasonably ask what happens if we choose the *incoming* spherical wave solution for the Green's function. In that case we can *still* write down a solution of the form

$$\phi(\mathbf{r}) = \phi_0(\mathbf{r})+\frac{2m}{\hbar^2}\int d^3r' G_-(\mathbf{r},\mathbf{r}')V(\mathbf{r}')\phi(\mathbf{r}') \quad , \tag{4.18}$$

where ϕ_0 is a solution of the homogeneous equation

$$\nabla^2\phi_0+k^2\phi_0 = 0\,;$$

i.e., ϕ_0 is what we called a *zero mode* in Section 4.1.2. The only difficulty with (4.18) is to get the right large-distance behaviour of $\phi(\mathbf{r})$: the function ϕ_0 has to include the incident plane wave, the outgoing scattered wave, and must also *cancel out* the the incoming waves introduced by G_-. You can easily verify that

$$\phi_0(\mathbf{r}) = e^{ikz}+\frac{2m}{\hbar^2}\int d^3r'[G_+(\mathbf{r},\mathbf{r}')-G_-(\mathbf{r},\mathbf{r}')]V(\mathbf{r}')\phi(\mathbf{r}')$$

does all three jobs, and that $[G_+(\mathbf{r},\mathbf{r}')-G_-(\mathbf{r},\mathbf{r}')]$ is a solution of the homogeneous equation: the two delta functions cancel when (∇^2+k^2) is applied. So, by taking this route we are quickly led back to the Lippmann–Schwinger equation in its usual form (4.17).

The Born approximation

One way to tackle the scattering problem for a weak potential is to solve the problem by iteration, i.e., each time a ϕ appears we replace it by the right-hand side of (4.17). This results in the equation

$$\begin{aligned}\phi(\mathbf{r}) = e^{ikz}&+\frac{2m}{\hbar^2}\int d^3r' G_+(\mathbf{r},\mathbf{r}')V(\mathbf{r}')e^{ikz'}\\ &+\left(\frac{2m}{\hbar^2}\right)^2\int d^3r'd^3r'' G_+(\mathbf{r},\mathbf{r}')V(\mathbf{r}')G_+(\mathbf{r}',\mathbf{r}'')V(\mathbf{r}'')e^{ikz''}\\ &+\ldots\end{aligned}$$

For weak potentials we can truncate at first order:

$$\phi(\mathbf{r}) = e^{ikz} - \frac{m}{2\pi\hbar^2}\int d^3r' \frac{e^{ik|\mathbf{r}-\mathbf{r}'|}}{|\mathbf{r}-\mathbf{r}'|} V(\mathbf{r}')e^{ikz'} \quad .$$

To extract $f(\theta,\phi)$ we only need to know the behaviour for large r. Write $\mathbf{k} = k\hat{\mathbf{z}}$, so that $kz = \mathbf{k}\cdot\mathbf{r}$. Also define $\mathbf{k}' \equiv k(\mathbf{r}/r)$. For $r \gg r'$,

$$|\mathbf{r}-\mathbf{r}'| \approx r\left[1 - \mathbf{r}\cdot\mathbf{r}'/r^2 + \ldots\right]$$

so

$$\phi(\mathbf{r}) \to e^{ikz} + f(\theta,\phi)\frac{e^{ikr}}{r} \quad ,$$

with

$$f(\theta,\phi) = -\frac{m}{2\pi\hbar^2}\int d^3r' V(r')e^{i(\mathbf{k}-\mathbf{k}')\cdot\mathbf{r}} \quad .$$

This is called the *Born approximation*.

This is a good approximation in electron scattering from atoms, for example.

4.3 Time-dependent wave equation

In electromagnetism, you have met the equations for the scalar potential Φ and vector potential $\mathbf{A}$,

$$\Box\Phi = \frac{\rho(\mathbf{r},t)}{\epsilon_0}, \qquad \Box\mathbf{A} = \mu_0\mathbf{j}(\mathbf{r},t)\,, \qquad \text{where} \quad \Box = \frac{1}{c^2}\frac{\partial^2}{\partial t^2} - \nabla^2\,;$$

these equations are satisfied if the potentials are chosen so as to satisfy the Lorentz gauge condition,

$$\nabla\cdot\mathbf{A} + \frac{1}{c^2}\frac{\partial\Phi}{\partial t} = 0\,.$$

Since we would like to know what happens for arbitrary sources, we are immediately led to the study of the Green's function for the d'Alembertian or wave operator $\Box$,

$$\Box G(\mathbf{r},t;\mathbf{r}',t) = \delta(\mathbf{r}-\mathbf{r}')\delta(t-t').$$

The boundary conditions are

1. that the potentials should go to zero far from sources, $G(\mathbf{r},t;\mathbf{r}',t) \to 0$ as $r \to \infty$.
2. that the effect of a source always occurs after its cause (causality) $G(\mathbf{r},t;\mathbf{r}',t) = 0$ if $t < t'$.

For Galilean invariant problems, where we are free to change our origin in space and time, it is simple to show that the Green's function only depends on $\mathbf{r}-\mathbf{r}'$ and $t-t'$,

$$G(\mathbf{r},t;\mathbf{r}',t) \equiv G(\mathbf{r}-\mathbf{r}',t-t') \quad .$$

To obtain the functional form of G it is enough to solve for $\mathbf{r}' = 0$, $t' = 0$, i.e.

$$\left(\frac{1}{c^2}\frac{\partial^2}{\partial t^2} - \nabla^2\right) G(\mathbf{r},t) = \delta(\mathbf{r})\delta(t). \tag{4.19}$$

4.3.1 Solution for the Green's function by Fourier transforms

This standard method for time dependent wave equations is in several steps: First define the Fourier transform of G

> It is easier to use the asymmetric definition of the Fourier and inverse Fourier transform, so that is what we shall use here.

$$\begin{aligned}
\tilde{G}(\mathbf{k},\omega) &= \int d^3r \int dt\, G(\mathbf{r},t) \exp[-i(\mathbf{k}\cdot\mathbf{r}-\omega t)] \quad , \\
G(\mathbf{r},t) &= \int \frac{d^3k}{(2\pi)^3} \int \frac{d\omega}{2\pi}\, \tilde{G}(\mathbf{k},\omega) \exp[i(\mathbf{k}\cdot\mathbf{r}-\omega t)] \quad , \\
\delta(\mathbf{r})\delta(t) &= \int \frac{d^3k}{(2\pi)^3} \int \frac{d\omega}{2\pi} \exp[i(\mathbf{k}\cdot\mathbf{r}-\omega t)] \quad ,
\end{aligned} \tag{4.20}$$

and solve for the Fourier transform $\tilde{G}(\mathbf{k},\omega)$ by substituting the second of these relations into Eq. (4.19): This equation becomes

$$\begin{aligned}
\left(\frac{1}{c^2}\frac{\partial^2}{\partial t^2} - \nabla^2\right) G(\mathbf{r},t) &= \int \frac{d^3k}{(2\pi)^3} \int \frac{d\omega}{2\pi}\, \tilde{G}(\mathbf{k},\omega) \left(-\frac{\omega^2}{c^2}+k^2\right) \exp[i(\mathbf{k}\cdot\mathbf{r}-\omega t)] \\
&= \int \frac{d^3k}{(2\pi)^3} \int \frac{d\omega}{2\pi} \exp[i(\mathbf{k}\cdot\mathbf{r}-\omega t)] \quad .
\end{aligned}$$

If we now equate the integrands, we find that

$$\begin{aligned}
\tilde{G}(\mathbf{k},\omega)\left(-\frac{\omega^2}{c^2}+k^2\right) &= 1 \quad , \\
\tilde{G}(\mathbf{k},\omega) &= \frac{-c^2}{\omega^2 - c^2k^2} \quad .
\end{aligned}$$

We now substitute $\tilde{G}(\mathbf{k},\omega)$ back into (4.20)

$$G(\mathbf{r},t) = -c^2 \int \frac{d^3k}{(2\pi)^3} \int \frac{d\omega}{2\pi} \frac{\exp[i(\mathbf{k}\cdot\mathbf{r}-\omega t)]}{\omega^2 - c^2k^2} \quad . \tag{4.21}$$

Integration over solid angle

The d^3k part of the integral (4.21) is of the generic form

$$I = \int d^3k\, e^{i\mathbf{k}\cdot\mathbf{r}} f(k^2)$$

Integrals of this type can be dealt with in a standard way: We are free to choose the k_3 axis to our benefit, since we integrate over all k, and this preferred direction makes no difference to the value of the integral. Thus, we choose the k_3-axis parallel to $\mathbf{r}$, and find

$$\begin{aligned}
I &= \int k^2 dk\, \sin\theta\, d\theta\, d\phi\, e^{ikr\cos\theta} f(k^2) \\
&= 2\pi \int_0^\infty k^2 dk \left[\frac{-e^{ikr\cos\theta}}{ikr}\right]_0^\pi f(k^2) \\
&= 2\pi \int_0^\infty \frac{k\,dk}{ir} \left[e^{ikr} - e^{-ikr}\right] f(k^2) \\
&= 2\pi \int_{-\infty}^\infty \frac{k\,dk}{ir} e^{ikr} f(k^2) \quad .
\end{aligned}$$

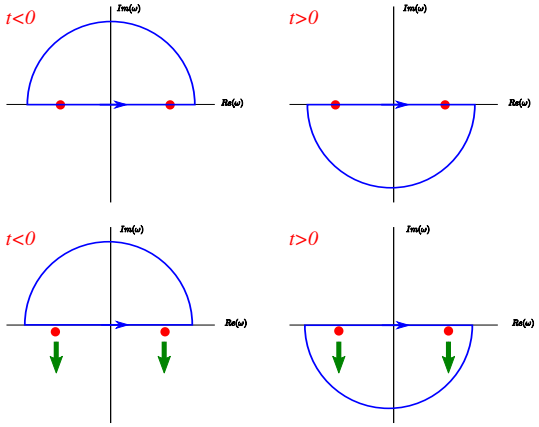

Figure 4.2: The contours used in the ω integral (4.23).

Note the trick used to transform the penultimate line into the last one: we change the second term in square brackets into an integral over $(-\infty, 0]$.

We can now apply this simplification to (4.21) to find

$$G(\mathbf{r},t) = -\frac{c^2}{(2\pi)^2 ir}\int_{-\infty}^{\infty} k\,dk \int_{-\infty}^{\infty}\frac{d\omega}{2\pi}\,\frac{\exp[i(kr-\omega t)]}{\omega^2-c^2k^2}. \tag{4.22}$$

We now tackle the ω integral,

$$\int_{-\infty}^{\infty}\frac{d\omega}{2\pi}\,\frac{e^{-i\omega t}}{\omega^2-c^2k^2}. \tag{4.23}$$

The problem with this integrand is that we have poles at $\omega = \pm ck$ on the real axis, and we have to integrate around these in some way. Here the boundary conditions enter. We shall use contour integration by closing off the integration contour by a semicircle in the complex ω plane. The position of the semicircle will be different for positive and negative t: Look at

$$\omega = Re^{i\phi},$$

where R is the radius of the semicircle (which we shall take to infinity), and ϕ is the variable that describes the movement along the semicircle. We find that

$$\exp[-i\omega t] = \exp[-iRt\cos\phi]\exp[Rt\sin\phi].$$

Since we want to add a semicircle without changing the integral, we must require that

$$\exp[Rt\sin\phi] \to 0 \text{ as } R\to\infty,$$

so that no contribution is made to the integral. This occurs if $t\sin\phi < 0$. Thus, if $t < 0$, we close the contour in the upper half plane, and if $t > 0$ in the lower one; see Fig. 4.2.

Now we have turned our ω integral into a contour integral, we need to decide how to deal with the poles, which lie on the real acis. Our time boundary condition (causality) states that $G = 0$ if $t < 0$, and thus we want to move the poles to just below the contour, as in the second part of Fig. 4.2, or by shifting the integration up by an infinitesimal amount above the real axis (these two ways of doing the integral are equivalent). The integral for $t > 0$ can then be done by residues, since we have two poles inside a closed contour. Note that the orientation of the contour is clockwise, and we just have a minus sign in the residue theorem,

$$\int_{-\infty}^{\infty}\frac{d\omega}{2\pi}\,\frac{e^{-i\omega t}}{\omega^2-c^2k^2} = \oint\frac{dz}{2\pi}\,\frac{e^{-izt}}{(z-ck)(z+ck)} = -2\pi i(R_+ + R_-) \quad .$$

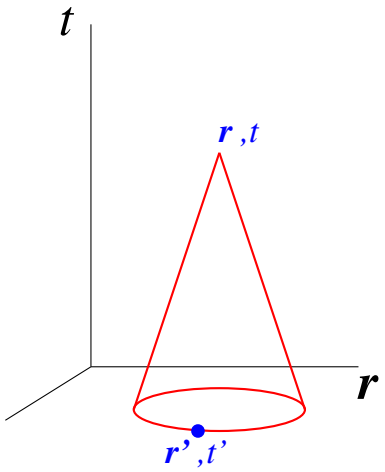

Figure 4.3: The backward light cone starting from $\mathbf{r}, t$

Here $R_\pm$ is the residue of the poles (the "strength" of the pole),

$$R_+ = \frac{1}{2\pi}\frac{e^{-ickt}}{2ck}, \qquad R_- = \frac{1}{2\pi}\frac{e^{+ickt}}{(-2ck)},$$

and we thus find that

$$\int_{-\infty}^{\infty}\frac{d\omega}{2\pi}\frac{e^{-i\omega t}}{\omega^2 - c^2k^2} = -\frac{i}{2ck}\left(e^{-ickt} - e^{ickt}\right).$$

If we substitute this into (4.22) we find that

$$\begin{aligned} G(\mathbf{r},t) &= \frac{c}{(2\pi)^2 2r}\int_{-\infty}^{\infty} dk\left(e^{ik(r-ct)} - e^{ik(r+ct)}\right) \\ &= \frac{c}{4\pi r}\left(\delta(r-ct) - \delta(r+ct)\right) \\ &= \frac{c}{4\pi r}\delta(r-ct). \end{aligned}$$

We were able to discard the second delta function above because its argument $r + ct > 0$ if $t > 0$, making the delta function zero.

If we now reinstate t' and $\mathbf{r}'$ using Galilean invariance, we find that

$$G(\mathbf{r},t;\mathbf{r}',t) = \frac{c}{4\pi|\mathbf{r}-\mathbf{r}'|}\delta\left(|\mathbf{r}-\mathbf{r}'| - c(t-t')\right). \tag{4.24}$$

For reasons that will become clear below, this is called the retarded Green's function. It vanishes everywhere except on the backward light cone, $|\mathbf{r}-\mathbf{r}'| = c(t-t')$; see Fig. 4.3.

Two special cases can be obtained simply:

1. For a static charge distribution (and no current), we find

$$\begin{aligned} \Phi(\mathbf{x}) &= \int d^3\mathbf{r}'dt'\frac{c}{4\pi|\mathbf{r}-\mathbf{r}'|}\delta\left(|\mathbf{r}-\mathbf{r}'| - c(t-t')\right)\frac{\rho(\mathbf{r}')}{\epsilon_0} \\ &= \int d^3\mathbf{r}'\frac{\rho(\mathbf{r}')}{4\pi\epsilon_0|\mathbf{r}-\mathbf{r}'|}, \end{aligned}$$

where we have used

$$\int dt'\,\delta\left(|\mathbf{r}-\mathbf{r}'| - c(t-t')\right) = \frac{1}{c}.$$

2. If $\rho(\mathbf{r}', t')$ describes a single moving charged particle, which is at a position $\mathbf{s}(t')$ at time t', we use $\rho = q\delta(\mathbf{r}' - \mathbf{s}(t'))$ and we find the potential,

$$\begin{aligned}\Phi(\mathbf{x}, t) &= \int d^3\mathbf{r}' dt' \frac{c}{4\pi|\mathbf{r} - \mathbf{r}'|}\delta\left(|\mathbf{r} - \mathbf{r}'| - c(t - t')\right) q\delta(\mathbf{r}' - \mathbf{s}(t'))/\epsilon_0 \\ &= \int dt' \frac{qc}{4\pi\epsilon_0|\mathbf{r} - \mathbf{s}(t')|}\delta\left(|\mathbf{r} - \mathbf{s}(t')| - c(t - t')\right).\end{aligned}$$

The path followed by the charge intersects the light-cone (with apex $\mathbf{r}, t$) at $\mathbf{s}(t'), t'$, so that the delta function in effect selects an *event*: the emission of the radiation that is observed at point $\mathbf{r}$ at time t. In the second problems sheet, you are asked to show that the above expression reduces to the usual formula for the Liénard–Wiechert potential.

4.3.2 Wave equations in $(2+1)$ dimensions

Green's functions for wave equations in (2+1) dimensions (two spatial, one time) can be solved directly by the Fourier transform method; or, if you know the result in (3+1) dimensions, they can also be obtained by "integrating out" the extra dimensions:

$$G^{(2)}(x - x', y - y', t - t') = \int dz'\, G(\mathbf{r} - \mathbf{r}', t - t') \tag{4.25}$$

for $t > t'$.

This can be checked quite simply. From

$$\Box G(\mathbf{r} - \mathbf{r}', t - t') = \delta(\mathbf{r} - \mathbf{r}')\delta(t - t')$$

we find that

$$\int dz'\, \Box G(\mathbf{r} - \mathbf{r}', t - t') = \int dz'\, \delta(\mathbf{r} - \mathbf{r}')\delta(t - t').$$

If we now swap differentiation and integration, we get

$$\Box \int dz'\, G(\mathbf{r} - \mathbf{r}', t - t') = \delta(x - x')\delta(y - y')\delta(t - t').$$

Since $\int dz'\, G(\mathbf{r} - \mathbf{r}', t - t') = G^{(2)}(x - x', y - y', t - t')$ is independent of z, we find that $\partial_z^2 G^{(2)} = 0$, and thus $G^{(2)}$ is indeed the Green's function for the two-dimensional wave equation.

From equation (4.24) we find

$$\int dz' \frac{c}{4\pi|\mathbf{r} - \mathbf{r}'|}\delta\big(|\mathbf{r} - \mathbf{r}'| - c(t - t')\big)$$

Integrate using the delta function, which is nonzero at $z'_\pm = z \pm \sqrt{c^2(t - t')^2 - (x - x')^2 - (y - y')^2}$, and thus

$$\delta\big(|\mathbf{r} - \mathbf{r}'| - c(t - t')\big) = \frac{|z - z'|}{\sqrt{c^2(t - t')^2 - (x - x')^2 - (y - y')^2}} \sum_{\alpha=\pm} \delta(z' - z'_\pm) \quad .$$

Both poles give the same contribution, and the retarded Green's function is thus

$$G^{(2)}(\mathbf{x} - \mathbf{x}', t - t') = \frac{c}{2\pi} \frac{1}{(c^2(t - t')^2 - |\mathbf{x} - \mathbf{x}'|^2)^{1/2}} \tag{4.26}$$

for $t > t'$, where $\mathbf{x}$ is a 2-dimensional space vector $\mathbf{x} = (x, y)$. In contrast to the 3+1 case, this is non-vanishing in the whole of the backward light-cone, not just on it!

Chapter 5

Integral Equations

5.1 Classification of linear integral equations

An integral equation is any equation in which an unknown function (to be determined) appears under an integral sign. We shall consider only equations of the general form

$$\theta f(x) = g(x) + \lambda \int_a^b K(x,y) f(y)\, dy\,. \tag{5.1}$$

The function g is usually given; λ is a constant, which can play the part of an eigenvalue (if $g = 0$), or may (sometimes) be a "small" parameter. It is usual to make a distinction between the following cases:

1. if $g = 0$ the equation is said to be *homogeneous*;
2. if $K(x,y) = 0$ for $y > x$ we have a *Volterra equation*
$$\theta f(x) = g(x) + \lambda \int_a^x K(x,y) f(y)\, dy\,;$$
3. if $\theta = 0$ we have a *Fredholm equation of the first kind*, whereas if $\theta = 1$ we have a Fredholm equation of the *second* kind.

The terminology can be difficult to get used to, but you won't be tested on it. The important thing is to *recognise* the different cases and apply appropriate methods to solve them.

5.1.1 Examples equivalent to differential equations

1. As we saw in the last chapter, the differential equation
$$Lg = f(x)\,,$$
where L is a Sturm–Liouville operator and $g(x)$ satisfies suitable SL boundary conditions at $x = a$ and b, has the Green's-function solution
$$g(x) = \int_a^b G(x,y) f(y)\, dy\,.$$
The last equation could be regarded as an integral equation to be solved for f; it is a Fredholm equation of the first kind.

2. Similarly, the eigenvalue equation
$$Lu = \lambda u$$
can be rewritten as a *homogeneous* Fredholm equation of the second kind,
$$u(x) = \lambda \int_a^b G(x,y)u(y)\,dy\,;$$
note, in particular, that no boundary conditions need to be imposed on the solution $u(x)$, because these are already contained in the Green's function.

3. The survival equation
$$\frac{dP}{dt} = -\alpha(t)P(t)\,, \quad \alpha \geq 0, \quad P(0) = 1,$$
can be integrated with respect to t to give a Volterra equation,
$$P(t) = 1 - \int_0^t \alpha(t')P(t')\,dt'\,,$$
where the constant 1 on the right-hand side arises from the initial condition $P(0) = 1$.

4. The "solution" to the quantum mechanical scattering problem, derived in the last chapter,
$$\psi(\mathbf{r}) = e^{i\mathbf{k}\cdot\mathbf{r}} + \frac{2m}{\hbar^2}\int G_+(\mathbf{r},\mathbf{r}')V(\mathbf{r}')\psi(\mathbf{r}')\,d^3\mathbf{r}'\,,$$
is a Fredholm equation of the second kind for ψ, equivalent to Schrödinger's equation plus boundary conditions.

The last three examples all illustrate an important reason for sometimes preferring an integral equation to an equivalent differential equation, where one exists: unlike the differential equation, in many cases *the integral equation already has the boundary conditions built in to it*—they don't have to be imposed on the solution by hand.

5.1.2 Examples that are *not* equivalent to differential equations

In the preceding examples, the integral equation was derived from an equivalent differential equation plus boundary conditions, and we might suppose that we could manage without the integral equation. For many physical problems, however, it is actually more natural to formulate the problem as an integral equation from the outset, and the resulting equation may not be equivalent to any differential equation of finite order:

1. Suppose, for example, that we are given a photograph of a spherically-symmetrical globular cluster of stars and want to deduce the 3D distribution of stars in the cluster from the 2D distribution in the photo. The 2D distribution $\sigma(R)$ (where $R = \sqrt{x^2+y^2}$) is essentially the projection of the 3D density $\rho(r)$ on to the (x,y) plane,
$$\sigma(R) = \int_{-\infty}^{\infty} \rho\big(\sqrt{R^2+z^2}\big)\,dz\,,$$
which is an integral equation for the unknown $\rho(r)$. It can be made to resemble (5.1) by making the change of variable $t = \sqrt{R^2+z^2}$, which gives
$$\sigma(R) = 2\int_R^{\infty} \frac{t\,\rho(t)}{\sqrt{t^2-R^2}}\,dt\,,$$
which we class as a Volterra equation, because the independent variable R appears as one of the limits of integration.

2. Many problems in statistical physics are most naturally formulated as integral equations. As an example, consider the steady flow of a gas at very low density along a tube of circular cross section. At sufficiently low density, the mean free path of molecules in the gas is much greater than the diameter of the tube, so that the rate of flow is limited only by collisions between the molecules and the walls.

   If the tube has length L and is aligned with the x-axis, we can suppose that the molecules arrive from $x < 0$ at a rate $s(x)$ per unit length of tube. When a molecule collides with the wall of the tube, it sticks for a short time and then leaves in a random direction; the molecule may subsequently make further collisions with the wall, or it may emerge from either end of the tube.

   If we consider the rate $\nu(x)\Delta x$ at which molecules leave length Δx of the wall of the tube, this must (in the steady state) equal the rate of arrival from outside, $s(x)\Delta x$, plus the rate of arrival from other portions of the tube surface:

$$\nu(x)\Delta x = s(x)\Delta x + \int_0^L \{p(|x-x'|)\Delta x\}\,\nu(x')\,dx', \tag{5.2}$$

   where $p(|x-x'|)\Delta x$ is the probability that a molecule arrives at the portion of tube $[x, x+\Delta x]$, given that it left the surface from point x'. As shown in the Mathematica notebook `MolecularFlow.nb`, the function $p(x)$ (and hence the arrival rate $s(x)$) can be calculated from the geometry of the tube; the precise expressions are not of great interest here, but if we divide each side of (5.2) by Δx we obtain

$$\nu(x) = s(x) + \int_0^L p(|x-x'|)\nu(x')\,dx',$$

   which is a Fredholm equation of the second kind, to be solved for $\nu(x)$.

5.2 Solution of integral equations

Just as with a differential equation, the possibility of solving an integral equation *analytically* depends crucially on its form. Before we consider some particular kinds of integral equation that happen to have simple methods of solution, it is worth pointing out that numerical methods are often more feasible than analytical solution. Various numerical methods exist, but an obvious one is to approximate the integral by a sum and solve the resulting linear equations. For example, for the Fredholm equation of the second kind,

$$f(x) = g(x) + \int_a^b K(x,y)f(y)\,dy\,,$$

we could divide the range of integration into $N-1$ sub-intervals of width $h = (b-a)/(N-1)$, on the assumption that, for $N \gg 1$, K, f and g will vary very little across each sub-interval. If we define

$$\begin{aligned} x_i &= a + ih, \quad i = 0, 1, \ldots, N-1 \\ f_i &= f(x_i) \\ g_i &= g(x_i) \\ K_{ij} &= h\,K(x_i, x_j)\,, \end{aligned}$$

our approximation to the integral equation will be

$$f_i = g_i + K_{ij}\,g_j \qquad \text{(summation convention)} \tag{5.3}$$

or, in matrix form,

$$(I-K)\mathbf{f} = \mathbf{g}\,,$$

where I is the $N \times N$ unit matrix. Large sets of linear equations can be set up and solved using Mathematica or MATLAB, or with the help of C/Fortran subroutine libraries. An example is given in the Mathematica notebook `MolecularFlow.nb`.

5.2.1 Equations soluble by simple methods

When they can be found, exact solutions of integral equations can be useful in ways that numerical solutions are not; for example, if we need to know precisely how the solution behaves as some parameter becomes very large or small. The *methods* used may also be helpful in suggesting a numerical approach to solving an integral equation. With this in mind, we consider a few kinds of integral equation where there are known, general methods of solution—though this list is not exhaustive.

A. Degenerate (or separable) kernel

A kernel is said to be *degenerate* or *separable* if it can be written in the form

$$K(x,y) = \sum_{i=1}^{N} \phi_i(x)\,\psi_i(y)\,. \tag{5.4}$$

The corresponding integral equation can always be reduced to a set of linear algebraic equations. We look at a specific case first, to get an idea of the method.

- Consider the equation

$$f(x) = x + \int_0^1 (1+xy) f(y)\,dy\,, \tag{5.5}$$

which has a degenerate kernel

$$K(x,y) \equiv 1 + xy = 1 \times 1 + x \times y\,.$$

On the right-hand side of (5.5) there are two distinct integrals,

$$A = \int_0^1 f(y)\,dy \quad \text{and} \quad B = \int_0^1 y\,f(y)\,dy\,,$$

so that (by using (5.5)),

$$f(x) = x + A + Bx\,.$$

If we now use this form for $f(x)$ in the equations defining A and B, we obtain

$$A = \int_0^1 (y + A + By)\,dy = \tfrac{1}{2} + A + \tfrac{1}{2}B$$
$$B = \int_0^1 y(y + A + By)\,dy = \tfrac{1}{3} + \tfrac{1}{2}A + \tfrac{1}{3}B\,,$$

whose solution is $A = -2$, $B = -1$. The integral equation (5.5) therefore has the unique solution $f(x) = -2$.

We can follow the same method for the general case. We have

$$\begin{aligned} f(x) &= g(x) + \int_a^b K(x,y) f(y)\,dy \\ &= g(x) + \sum_{j=1}^{N} \phi_j(x)\,(\psi_j, f) \end{aligned} \tag{5.6}$$

Writing f_i for the integral (ψ_i, f), we can project both sides of (5.6) onto $\psi_i(x)$ to obtain

$$\begin{aligned} f_i &= (\psi_i, g) + \sum_{j=1}^{N} (\psi_i, \phi_j)\, f_j \\ &\equiv g_i + K_{ij}\, f_j\,, \end{aligned} \tag{5.7}$$

where $g_i = (\psi_i, g)$ and $K_{ij} = (\psi_i, \phi_j)$. This set of linear equations for the quantities f_i has the same form as (5.3) and can be solved by the same methods—numerical, if N is large—and the final solution for $f(x)$ is given by the right-hand side of (5.6).

Later in this chapter we shall see that an *Hermitian* kernel can always be expanded in the form (5.4), though N may be infinite. If $K(x, y)$ can be approximated by truncating the expansion at some finite value of N, a numerical solution of (5.7) may be useful as an approximation to the exact $f(x)$.

We can often take short-cuts when solving equations with degenerate kernels. Consider the eigenvalue problem

$$f(x) = \lambda \int_0^{2\pi} \cos(x - y)\, f(y)\, dy\,.$$

The kernel $\cos(x - y) = \cos x \cos y + \sin x \sin y$ is separable, and it is clear by inspection that the right-hand side of the equation will give us

$$f(x) = A \cos x + B \sin x\,.$$

By using this form for f on both sides of the integral equation we obtain

$$\begin{aligned} A \cos x + B \sin x &= \lambda \int_0^{2\pi} [\cos x \cos y + \sin x \sin y][A \cos y + B \sin y]\, dy \\ &= \lambda\pi[A \cos x + B \sin x]\,, \end{aligned}$$

in which, for consistency, we must have $\lambda = 1/\pi$. Corresponding to this eigenvalue, there are *two* independent eigenfunctions, which we can take to be $\sin x$ and $\cos x$, or any two linear combinations of these functions.

B. Displacement (or convolution) kernel, limits of integration $-\infty$, ∞

Integral equations with a kernel of the form $K(x - y)$ are said to have a *displacement kernel* or *convolution kernel*. If the limits of integration are $-\infty$ and ∞, a solution can be found by taking the Fourier transform. As usual in this course, we define the Fourier transforms by

$$\tilde{f}(q) = \int_{-\infty}^{\infty} f(x)\, e^{-iqx}\, dx\,, \quad \text{etc.}$$

Taking the Fourier transform of each side of

$$f(x) = g(x) + \lambda \int_{-\infty}^{\infty} K(x - y) f(y)\, dy \tag{5.8}$$

gives us

$$\tilde{f}(q) = \tilde{g}(q) + \lambda \tilde{K}(q) \tilde{f}(q)\,, \tag{5.9}$$

where the convolution theorem has been used and it is assumed that the required transforms all exist. Rearranging this equation then yields

$$\tilde{f}(q) = \frac{\tilde{g}(q)}{1 - \lambda \tilde{K}(q)}\,;$$

of course, $\tilde{f}(q)$ must still be inverted to obtain the solution $f(x)$.

C. Displacement kernel, limits of integration 0, x

If the kernel is of displacement form and the limits of integration are 0 and x, as in a Volterra equation, the integral has the form of the convolution that appears in Laplace transform theory, where the Laplace

transform $\hat{f}(s)$ is defined by

$$\hat{f}(s) = \int_0^\infty f(x)\, e^{-sx}\, dx\,.$$

Taking the Laplace transform of each side of

$$f(x) = g(x) + \lambda \int_0^x K(x-y) f(y)\, dy$$

gives us

$$\hat{f}(s) = \hat{g}(s) + \lambda \hat{K}(s) \hat{f}(s)$$

whose solution is

$$\hat{f}(s) = \frac{\hat{g}(s)}{1 - \lambda \hat{K}(s)}\,.$$

Again, we need to be able to invert the integral transform, either by consulting a table of Laplace transforms, which will cover most cases, or—if desperate[1]—by using the Bromwich integral

$$f(x) = \frac{1}{2\pi i} \int_{\gamma - i\infty}^{\gamma + i\infty} \hat{f}(z)\, e^{zx}\, dz\,,$$

where the path of integration in the complex plane passes to the *right* of all singularities of $\hat{f}(z)$.

D. Reduction to a differential equation

It is often worth trying to reduce an integral equation to a more familiar differential equation. As we noted earlier, this may not always be possible, but one can look for clues: e.g., the kernel may become simpler when differentiated (a polynomial is the obvious case), or it may be converted into itself if differentiated enough times (trig functions and exponentials). There is no completely *general* strategy for spotting these cases, so we'll simply give two examples of Volterra equations that can be converted to differential equations.

1. Consider

$$f(x) = x - \int_0^x (x-y) f(y)\, dy\,, \tag{5.10}$$

an equation which could be solved by Laplace transform. However, if we differentiate twice with respect to x, we find

$$f'(x) = 1 - (x-x)f(x) - \int_0^x f(y)\, dy = 1 - \int_0^x f(y)\, dy \tag{5.11}$$

and

$$f''(x) = -f(x)\,,$$

which has the general solution $f(x) = A\cos x + B\sin x$. We can fix the constants A and B from the initial conditions $f(0) = 0$ (from (5.10)) and $f'(0) = 1$ (from (5.11)), which give $A = 0$ and $B = 1$; the solution is therefore

$$f(x) = \sin x\,.$$

Note especially that the initial conditions (and hence the constants) are derived from the original integral equation: we don't need to look elsewhere for boundary conditions.

[1] I don't mean to disparage the Bromwich integral: it can be very helpful for obtaining analytic approximations to $f(x)$, e.g., for $x \to \infty$; it is even possible to evaluate the contour integral numerically. But if there's a reasonable chance of an *exact* solution to your problem, it is likely that someone else will have encountered it before, and recorded the result in a table. Mathematica, of course, is a useful (but not foolproof) alternative to tables.

2. Often we have to use a little more ingenuity. For example, when we differentiate

$$f(x) = x + \int_0^x xy\, f(y)\, dy\,, \tag{5.12}$$

we obtain

$$\begin{aligned} f'(x) &= 1 + x^2 f(x) + \int_0^x y\, f(y)\, dy \\ &= x^2 f(x) + \frac{f(x)}{x}\,, \end{aligned} \tag{5.13}$$

where we have recycled (5.12) to express the integral in terms of $f(x)$. The last equation is separable, and has the solution

$$f(x) = A x\, e^{x^3/3}\,,$$

where A is a constant of integration. The constant can be determined either by substituting f back into (5.12), or from (5.13), which gives $f'(0) = 1$. But the solution we derived has $f'(0) = A$, so for consistency we must have $A = 1$. Again, the constant of integration is determined from the integral equation.

Four of the problems in Examples 3 will give you some practice in converting integral equations to differential equations.

5.3 Neumann series solution

Sometimes the parameter λ in an integral equation can be regarded as small, so we might hope to obtain a solution as a series of terms in increasing powers of λ. The Born approximation in scattering theory is an example of this.

Starting from

$$f(x) = g(x) + \lambda \int K(x,y)\, f(y)\, dy\,, \tag{5.14}$$

we make the replacement

$$f(x) \to g(x) + \lambda \int K(x,y)\, f(y)\, dy$$

where f appears on the right-hand side of (5.14):

$$\begin{aligned} f(x) &= g(x) + \lambda \int K(x,y_1)\, f(y_1)\, dy_1 \\ &= g(x) + \lambda \int K(x,y_1)\, g(y_1)\, dy_1 \\ &\qquad + \lambda^2 \int\int K(x,y_1)\, K(y_1,y_2)\, f(y_2)\, dy_2\, dy_1 \\ &= g(x) + \lambda \int K(x,y_1)\, g(y_1)\, dy_1 \\ &\qquad + \lambda^2 \int\int K(x,y_1)\, K(y_1,y_2)\, g(y_2)\, dy_2\, dy_1 \\ &\qquad + \lambda^3 \int\int\int K(x,y_1)\, K(y_1,y_2)\, K(y_2,y_3)\, g(y_3)\, dy_3\, dy_2\, dy_1 \\ &\qquad + \ldots \end{aligned}$$

5.3.1 Convergence of Neumann series

Does the Neumann series converge? If are g and K are *bounded*—$|g| \leq g_{\max}$ and $|K| \leq K_{\max}$—and the ranges of integration are finite, we can obtain an upper bound on each term by replacing the functions g and K by their maximum values:

$$\begin{aligned}|f(x)| \leq g_{\max} &+ |\lambda| K_{\max} g_{\max} \int dy_1 \\ &+ |\lambda|^2 K_{\max}^2 g_{\max} \int\int dy_2\, dy_1 \\ &+ |\lambda|^3 K_{\max}^3 g_{\max} \int\int\int dy_3\, dy_2\, dy_1 \\ &+ \ldots\end{aligned}$$

So far we have left the limits of integration undefined, but these are important: as we shall see, there is an interesting difference in the behaviour of the Neumann series for the solution of a Volterra equation when compared with the series for a more general Fredholm equation.

Volterra equations

For convenience, suppose that the lower limit of integration is zero. Then, from the condition $K(y_n, y_{n+1}) = 0$ for $y_n < y_{n+1}$, we can assume $x \geq y_1 \geq y_2 \geq \ldots \geq 0$, so that the n-fold integrations are

$$\begin{aligned}\int_0^x \cdots \int_0^{y_{n-2}} \int_0^{y_{n-1}} dy_n\, dy_{n-1}\, dy_{n-2} \ldots dy_1 &= \int_0^x \cdots \int_0^{y_{n-2}} \frac{y_{n-1}}{1}\, dy_{n-1}\, dy_{n-2} \ldots dy_1 \\ &= \int_0^x \cdots \int_0^{y_{n-3}} \frac{y_{n-2}^2}{2\times 1}\, dy_{n-2} \ldots dy_1 \\ &= \ldots \\ &= \frac{x^n}{n!}\,.\end{aligned}$$

From this, our bound on $f(x)$ is

$$|f(x)| \leq g_{\max} \sum_{n=0}^{\infty} \frac{\{|\lambda| g_{\max} K_{\max} x\}^n}{n!} = g_{\max} \exp\{|\lambda| K_{\max} x\}\,,$$

which is finite for all finite λ and x. Accordingly, the Neumann series *always* converges for a Volterra equation with bounded g and K.

General Fredholm equation of the second kind

The picture is less rosy in the more general case, where the n-fold integration is

$$\int_a^b \cdots \int_a^b dy_n \ldots dy_1 = (b-a)^n\,.$$

In this case our bound becomes

$$|f(x)| \leq g_{\max}\{1 + |\lambda| K_{\max}(b-a) + |\lambda|^2 K_{\max}^2 (b-a)^2 + \ldots\},$$

a geometric series which converges for $|\lambda| < 1/[K_{\max}(b-a)]$. If the latter condition is violated, the Neumann series may or may not diverge as the number of terms increases. Further investigation is then required, and the result will depend on the specific form of the kernel, $K(x,y)$—we can be sure of that, because a Volterra equation (with bounded kernel) is just a *special kind* of Fredholm equation, for which the Neumann series *always* converges.

As we shall see when we consider the Hilbert–Schmidt theory of integral equations, for certain problems (those with Hermitian kernels) we can be precise about the radius of convergence of the Neumann series expansion.

5.3.2 Resolvent kernels

The higher-order terms of the Neumann series expansions can be a little awkward to manipulate: the function $g(x)$ is buried deep inside a nest of integrals. It can therefore be helpful to re-write the solution of (5.14) in the form

$$f(x) = g(x) - \lambda \int R(x,y;\lambda)\, g(y)\, dy\,, \tag{5.15}$$

which (provided a solution exists) defines the *resolvent kernel*, $R(x,y;\lambda)$ of the integral equation (5.14).

> You might wonder why the resolvent has been defined so that an awkward-looking minus-sign appears in (5.15). One reason is that we can then write
>
> $$g(x) = f(x) + \lambda \int R(x,y;\lambda)\, g(y)\, dy\,, \tag{5.16}$$
>
> which is an integral equation of the same form as (5.14), but with the roles of f and g exchanged, and with K replaced by R; in fact, $K(x,y)$ is the resolvent kernel of (5.16).

We can use Neumann's method to develop a series expansion for the resolvent kernel. To be definite, suppose that we want to solve the Volterra equation

$$f(x) = g(x) + \lambda \int_0^x K(x,y)\, f(y)\, dy\,. \tag{5.17}$$

After the first iteration, we have

$$f(x) = g(x) + \lambda \int_0^x K(x,y)\, g(y)\, dy + \lambda \int_0^x K(x,y) \left(\lambda \int_0^y K(y,z)\, f(z)\, dz \right) dy\,.$$

Since our aim is always to have f (and later g) appear in the outermost integral, we now reverse the order of the y and z integrations. After noting that the region of integration in the (y,z) plane is the triangle $z < y < x$ (draw a diagram to illustrate this), we find

$$\begin{aligned} f(x) &= g(x) + \lambda \int_0^x K(x,y)\, g(y)\, dy + \lambda \int_0^x \left(\lambda \int_z^x K(x,y)\, K(y,z)\, dy \right) f(z)\, dz \\ &= g(x) + \lambda \int_0^x K(x,y)\, g(y)\, dy + \lambda^2 \int_0^x K_2(x,z)\, f(z)\, dz\,, \end{aligned} \tag{5.18}$$

where the "iterated kernel" K_2 is defined by

$$K_2(x,z) = \int_z^x K(x,y)\, K(y,z)\, dy\,.$$

It is plausible that the procedure leading to (5.18) might be extended to give a series of the form

$$f(x) = g(x) + \sum_{m=1}^{N-1} \lambda^m \int_0^x K_m(x,y)\, g(y)\, dy + \lambda^N \int_0^x K_N(x,y)\, f(y)\, dy\,, \tag{5.19}$$

and we can construct a proof by induction to show this.

Proof

First suppose that (5.19) holds for a particular value of N. Make the substitution (5.17) on the right-hand side of (5.19) to obtain

$$\begin{aligned} f(x) = g(x) &+ \sum_{m=1}^{N-1} \lambda^m \int_0^x K_m(x,y)\, g(y)\, dy \\ &+ \lambda^N \int_0^x K_N(x,y)\, g(y)\, dy \\ &+ \lambda^N \int_0^x K_N(x,y) \left(\lambda \int_0^y K(y,z)\, f(z)\, dz \right) dy \\ = g(x) &+ \sum_{m=1}^{N} \lambda^m \int_0^x K_m(x,y)\, g(y)\, dy \\ &+ \lambda^{N+1} \int_0^x \left(\int_z^x K_N(x,y)\, K(y,z)\, dy \right) f(z)\, dz\,, \end{aligned} \tag{5.20}$$

where the last line has been obtained by reversing the order of integration, in exactly the same way that (5.18) was obtained. As required, the result (5.20) is of the same form as (5.19), with $N \to N+1$, provided we define

$$K_{N+1}(x,z) = \int_z^x K_N(x,y)\, K(y,z)\, dy\,.$$

All we need to complete the proof is to point out that (5.19) does indeed hold for some value of N: (5.18) is already of this form, with $N = 2$, if we make the identification $K_1 \equiv K$. Hence, by the induction, (5.19) holds also for $N = 3$, $N = 4$, and for all subsequent values of N.

Series expansion of the resolvent kernel

Finally, we take the limit $N \to \infty$ in (5.19) and reverse the order of summation and integration to obtain

$$f(x) = g(x) + \int_0^x \left(\sum_{m=1}^{\infty} \lambda^m K_m(x,y) \right) g(y)\, dy\,;$$

comparison with (5.15) then gives

$$R(x,y;\lambda) = -\sum_{m=1}^{\infty} \lambda^{m-1} K_m(x,y)$$

as the series expansion for the resolvent kernel.

> The argument above is easily modified to provide a series expansion for the resolvent kernel of a more general Fredholm equation of the second kind. You should check *for yourself* that the only change is to the limits of integration, which become a and b in all cases.

Example 5.1:

Find the solution of

$$f(x) = g(x) + \lambda \int_0^1 xy f(y)\, dy\,,$$

for any $g(x)$.

Solution:

It would probably be easiest to use the separable kernel method in this case, but the equation can also be solved by constructing the Neumann series for the resolvent. We have $K(x,y) = xy$, so

$$K_2(x,y) = \int_0^1 (xz)(zy)\,dz = \frac{xy}{3}\,,$$
$$K_3(x,y) = \int_0^1 K_2(x,z)\,K(z,y)\,dz = \frac{xy}{3^2}\,,$$

and, in general, $K_n(x,y) = xy/3^{n-1}$. Using this expression in the expansion for the resolvent gives

$$R(x,y;\lambda) = -\sum_{n=1}^{\infty} \frac{\lambda^{n-1}}{3^{n-1}}\,xy = \frac{-xy}{1-\lambda/3}\,.$$

Note that the power-series expansion of the resolvent converges only for $|\lambda| < 3$, but the resummed series is an expression which is analytic for any $\lambda \neq 3$. From this, the general solution for $\lambda \neq 3$ is

$$f(x) = g(x) + \frac{\lambda x}{1-\lambda/3}\int_0^1 y\,g(y)\,dy\,.$$

5.4 Hilbert–Schmidt theory

The Hilbert–Schmidt theory offers a general approach to integral equations in which the kernel is *Hermitian*,

$$K(x,y) = K(y,x)^*\,.$$

The theory is based on the eigenfunctions $\{u_i\}$ and eigenvalues $\{\lambda_i\}$ of the kernel,

$$u_i(x) = \lambda_i \int_a^b K(x,y)\,u_i(y)\,dy\,.$$

A central result of the Hilbert–Schmidt theory is that (under certain conditions) these eigenfunctions can be proved to *exist*—for example, if the kernel is bounded and the range of integration is finite. We shall not be concerned with this relatively technical (but important) issue.[2] Instead, we shall assume that the eigenfunctions exist and use them to construct the solution of the Fredholm equation of the second kind.

- Prove for yourself that the eigenvalues of an Hermitian kernel are real, and show that the eigenfunctions satisfy the orthogonality condition

$$(u_i,u_j) = \int_a^b u_i^*(x)\,u_j(x)\,dx = 0 \quad \text{for} \quad \lambda_i \neq \lambda_j\,.$$

Eigenfunctions corresponding to the *same* eigenvalue can be orthogonalized by using the Gram–Schmidt procedure. We shall always assume that this has been done, and that the eigenfunctions are normalized so that $(u_i,u_j) = \delta_{ij}$.

A further result of the Hilbert–Schmidt theory is that these eigenfunctions span the space of "source-representable" functions: any square-integrable function $f(x)$ that can be represented in the form

$$f(x) = \int_a^b K(x,y)\,g(y)\,dy$$

[2] F. G. Tricomi's book *Integral Equations* is a useful introduction to the subject.

can also be represented by a convergent eigenfunction expansion

$$f(x) = \sum_i (u_i, f)\, u_i(x)\,.$$

The term *source-representable* comes from electrostatics: the potential can be expressed as

$$\phi(\mathbf{r}) = \frac{1}{4\pi\epsilon_0} \int \frac{\rho(\mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|}\, d^3\mathbf{r}'$$

i.e., in terms of its *source*, ρ, where the Coulomb potential takes the role of the kernel.

The restriction to source-representable functions is an essential one, as we can see by considering the trivial kernel $K(x,y) = v(x)\, v^*(y)$, whose only eigenfunction $u_1(x)$ is proportional to $v(x)$. Clearly, the only source-representable functions in this case are simple multiples of $v(x)$.

5.4.1 Eigenfunction expansion of the kernel

We can seek an eigenfunction expansion of the kernel,

$$K(x,y) = \sum_i k_i^*(y)\, u_i(x) = \sum_i k_i(x)\, u_i^*(y)\,,$$

where we have used the fact that K is Hermitian to obtain the second expression. If we multiply both sides by $\lambda_n\, u_n(y)$ and integrate, we obtain

$$\lambda_n \int_a^b K(x,y)\, u_n(y)\, dy = \lambda_n \sum_i k_i(x)\, (u_i, u_n) = \lambda_n\, k_n(x)\,,$$

where we have used the orthogonality condition $(u_i, u_n) = \delta_{in}$. But, by using the definition of an eigenfunction, the left-hand side of the last equation can be written more simply as $u_n(x)$, so we have

$$k_n(x) = \frac{u_n(x)}{\lambda_n} \quad \text{and} \quad K(x,y) = \sum_n \frac{u_n(x)\, u_n^*(y)}{\lambda_n}\,.$$

Unsurprisingly (why?) the last expression has the same form as the eigenfunction expansion of the Green's function of an Hermitian differential operator.[3]

5.4.2 Hilbert–Schmidt solution of integral equations

We re-write the Fredholm equation of the second kind in the form

$$f(x) - g(x) = \lambda \int_a^b K(x,y)\, f(y)\, dy \tag{5.21}$$

to emphasize the fact that, if a solution exists, $f - g$ is source-representable, and so can be written in terms of the eigenfunctions as

$$f(x) - g(x) = \sum_n c_n\, u_n(x)\,.$$

[3] *Technical note:* If the number of eigenfunctions is *infinite*, the expansion of $K(x,y)$ may not converge, so the equals-sign is too optimistic. Nevertheless, if we multiply both sides by a square-integrable function $g(y)$ and integrate, the result *is* an equality—and this is the only way that the eigenfunction expansion of K is used in practice.

Using this expansion on both sides of (5.21) then gives

$$\begin{aligned}\sum_n c_n\, u_n(x) &= \lambda \int_a^b K(x,y)\, f(y)\, dy \\ &= \lambda \int_a^b K(x,y)\, [f(y) - g(y)]\, dy + \lambda \int_a^b K(x,y)\, g(y)\, dy \\ &= \lambda \sum_n \frac{c_n}{\lambda_n}\, u_n(x) + \lambda \sum_n \frac{(u_n, g)}{\lambda_n}\, u_n(x)\,,\end{aligned}$$

where the eigenfunction expandion of $K(x,y)$ has been used to obtain the last line. By equating coefficients of $u_n(x)$ on each side, we obtain

$$c_n = \frac{\lambda}{\lambda_n}\, c_n + \frac{\lambda}{\lambda_n}\, (u_n, g)$$

or

$$c_n = \frac{\lambda}{\lambda_n - \lambda}\, (u_n, g)\,.$$

This last expression for c_n can then be used to obtain the solution of the integral equation, since

$$\begin{aligned}f(x) - g(x) &= \sum_n c_n\, u_n(x) \\ &= \sum_n \frac{\lambda}{\lambda_n - \lambda}\, u_n(x) \int_a^b u_n^*(y)\, g(y)\, dy \\ &\equiv -\lambda \int_a^b R(x,y)\, g(y)\, dy\,,\end{aligned}$$

where

$$R(x,y) = \sum_n \frac{u_n(x)\, u_n^*(y)}{\lambda - \lambda_n} \tag{5.22}$$

is the resolvent kernel of the Fredholm equation. Our solution for $f(x)$ is finally

$$f(x) = g(x) - \lambda \int_a^b R(x,y)\, g(y)\, dy\,. \tag{5.23}$$

Equations (5.23) and (5.22) show that the solution $f(x)$ diverges as λ approaches an eigenvalue λ_n, provided (u_n, g) is non-zero for that particular n. From this we can deduce that the Neumann series solution of the Fredholm equation converges only for $|\lambda| < |\lambda_1|$, the smallest of the eigenvalues.

Example 5.2:

Obtain the eigenfunction expansion of the resolvent of

$$f(x) = g(x) + \lambda \int_0^1 xy f(y)\, dy\,.$$

Solution:

First we note that the kernel $K(x,y) = xy$ has only *one* eigenfunction, $u_1(x) = C\,x$. If $u_1(x)$ is normalized to unity, we must have

$$\int_0^1 |u_1(x)|^2\, dx = |C|^2 \int_0^1 x^2\, dx = 1\,,$$

which gives $|C| = \sqrt{3}$.

From the definition of an eigenfunction, we also have

$$Cx = \lambda_1 \int_0^1 (xy)\, Cy\, dy = \lambda_1\, Cx/3\,;$$

hence $\lambda_1 = 3$. Putting the results for u_1 and λ_1 together, we get

$$R(x,y;\lambda) = \frac{u_1(x)u_1^*(y)}{\lambda - \lambda_1} = \frac{3xy}{\lambda - 3}\,,$$

equivalent to the result found earlier by summing the Neumann series, which converged only for $|\lambda| < 3$, the eigenvalue of $K(x,y)$.

Chapter 6

Variational calculus

6.1 Functionals and stationary points

As will be illustrated below, we can generalize the concept of a function to that of a functional, a mapping of a function onto a number. An example could be

$$I[y] = \int_a^b y(x)\,dx,$$

where we have also introduced a "square-brackets notation" to distinguish this from a function. In short, a functional $I[y]$ has a definite numerical value for each function $x \to y(x)$.

Example 6.1:

An example of a functional is

$$I[y] = \int_0^\pi y(x)\,dx.$$

Some illustrative values of the functional are

$y(x)$	$I[y]$
$\sin x$	2
$\cos x$	0
x	$\pi^2/2$
x^2	$\pi^3/3$
$\vdots$	$\vdots$

6.2 Stationary points

For a function we speak of a stationary point when the function doesn't change under a small change, i.e., if we take $x \to x + \delta x$, and thus $f \to f + \delta f$, the change in f, $\delta f = 0$, to first order in δx. This leads to the obvious relation $\frac{df}{dx} = 0$.

As for functions, we are extremely interested in stationary points of functionals:

A functional has a stationary point for any function y such that a small change $y(x) \to y(x) + \epsilon(x)$ leads to *no* change in $I[y]$ to first order in $\epsilon(x)$.

A key difference with the stationary points of functions is that smallness of $\epsilon(x)$ only implies that as a function it is everywhere (mathematician would say "uniformly") close to zero, but can still vary arbitrarily.

An important class of functionals is given by

$$I[y] = \int_a^b dx\, F(y(x), y'(x), x) \quad , \tag{6.1}$$

where a, b are fixed, and y is specified at the boundaries, i.e., the values of $y(a)$ and $y(b)$ are specified as boundary conditions. Thus under a (small) change $y(x) \to y(x) + \epsilon(x)$, the preservation of the boundary conditions implies

$$\epsilon(a) = \epsilon(b) = 0. \tag{6.2}$$

Now substitute and expand to first order in $\epsilon(x)$,

$$\begin{aligned}
\delta I[y] &= I[y+\epsilon] - I[y] \\
&= \int_a^b dx\, F(y(x)+\epsilon(x), y'(x)+\epsilon'(x), x) - \int_a^b dx\, F(y(x), y'(x), x) \\
&= \int_a^b dx\, \left(\frac{\partial F}{\partial y(x)} \epsilon(x) + \frac{\partial F}{\partial y'(x)} \epsilon'(x) \right) \\
&= \int_a^b dx\, \left(\frac{\partial F}{\partial y(x)} \epsilon(x) - \frac{d}{dx} \frac{\partial F}{\partial y'(x)} \epsilon(x) \right) \\
&= \int_a^b dx\, \epsilon(x) \left[\frac{\partial F}{\partial y(x)} - \frac{d}{dx} \frac{\partial F}{\partial y'(x)} \right]
\end{aligned}$$

where we have integrated by parts to obtain the penultimate line, using the boundary conditions on ϵ.

Since $\epsilon(x)$ is allowed to vary arbitrarily, this is only zero if the quantity multiplying ϵ is zero at every point x. For example, you can choose a set of ϵ's that are all peaked around a particular value of x. We thus see that the term proportional to ϵ vanishes at each point x, and we get the *Euler–Lagrange equation*

$$\frac{\partial F}{\partial y(x)} - \frac{d}{dx} \frac{\partial F}{\partial y'(x)} = 0. \tag{6.3}$$

Remarks

- we often don't write the dependence on x, but it is implicitly assumed that you understand that this is a "functional equation".
- We use the functional derivative notation
$$\frac{\delta I[y]}{\delta y}$$
for the term in the functional $I[y + \delta y]$ proportional to δy,
$$I[y + \delta y] = I[y] + \int dx\, \delta y(x)\, \frac{\delta I[y]}{\delta y}(x) + \dots \quad .$$
- If the functional is not an integral, e.g.,
$$I[y] = y(0) \quad ,$$
we can turn it into an integral by inserting a delta function. In the case above,
$$I[y] = \int y(x) \delta(x)\, dx.$$

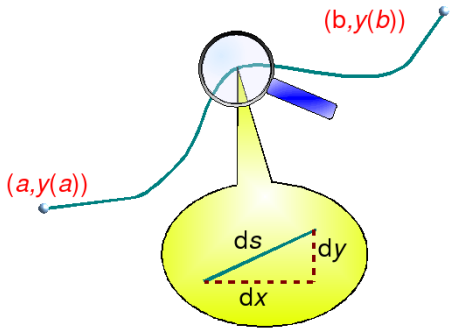

Figure 6.1: The distance between two points along a path connecting two fixed points

- The notations $\frac{\delta I[y]}{\delta y}(x)$ and $\frac{\delta I[y]}{\delta y(x)}$ are used interchangeably.

For a general functional, the equation

$$\frac{\delta I[y]}{\delta y} = 0$$

is called the Euler–Lagrange equation.

Solutions to this equation define stationary points of the functional.

6.3 Special cases with examples: first integrals

Let us look at a few special cases for the functional I defined in (6.1).

6.3.1 Functional of first derivative only

We first consider the case $F(y(x), y'(x), x) = F(y'(x), x)$, and thus independent of y. The Euler–Lagrange equation,

$$\frac{d}{dx}\frac{\partial F}{\partial y'(x)} = 0,$$

has the simple solution

$$\frac{\partial F}{\partial y'(x)} = \text{constant}. \tag{6.4}$$

This equation is called the "first integral" of the problem.

Example 6.2:

Show that the shortest distance between any two fixed points (in 2D space, for simplicity) is along a straight line.

Solution:

We parametrize the curve connecting the two points by $(x, y(x))$ (which assumes each value x only occurs once, and we thus only look at a sensible subclass of paths). The endpoints $(a, y(a))$ and $(b, y(b))$ are fixed. If we take a small step along the line, the distance travelled is

$$(ds)^2 = (dx)^2 + (dy)^2 = (dx)^2[1 + (dy/dx)^2].$$

Thus

$$ds = (1 + y'^2)^{1/2} dx.$$

The total path length is thus the functional

$$L[y] = \int_a^b (1 + y'^2)^{1/2} dx,$$

which is of the form investigated above. Thus

$$\frac{\partial F}{\partial y'(x)} = \frac{y'(x)}{(1 + y'(x)^2)^{1/2}} = k.$$

It is not too hard to solve this equation, by squaring both sides,

$$\begin{aligned} y'^2(x) &= k^2(1 + y'(x)^2) \quad , \\ y'(x) &= \frac{k}{\sqrt{1 - k^2}} = c \quad , \\ y(x) &= cx + d \end{aligned}$$

We can determine c and d from the boundary conditions

$$\begin{aligned} c &= \frac{y(b) - y(a)}{b - a}, \\ d &= \frac{by(a) - ay(b)}{b - a}. \end{aligned}$$

6.3.2 No explicit dependence on x

If $F(y, y', x) = F(y, y')$, independent of x, we proceed in a slightly different way. We combine the Euler–Lagrange equation

$$\frac{\partial F}{\partial y(x)} = \frac{d}{dx} \frac{\partial F}{\partial y'(x)}$$

with an explicit differentiation of F,

$$\frac{dF}{dx} = \frac{\partial F}{\partial y(x)} y'(x) + \frac{\partial F}{\partial y'(x)} y''(x),$$

to find

$$\begin{aligned} \frac{dF}{dx} &= \frac{d}{dx} \left(\frac{\partial F}{\partial y'(x)} \right) y'(x) + \frac{\partial F}{\partial y'(x)} \frac{d}{dx} y'(x) \\ &= \frac{d}{dx} \left(y'(x) \frac{\partial F}{\partial y'(x)} \right). \end{aligned}$$

Combining left-hand and right-hand sides, we find

$$\frac{d}{dx} \left(F - y' \frac{\partial F}{\partial y'(x)} \right) = 0.$$

We thus conclude that for $F[y, y']$ (i.e., no explicit x dependence in the functional) we have the first integral

$$\boxed{F - y' \frac{\partial F}{\partial y'(x)} = \text{constant} \quad .} \tag{6.5}$$

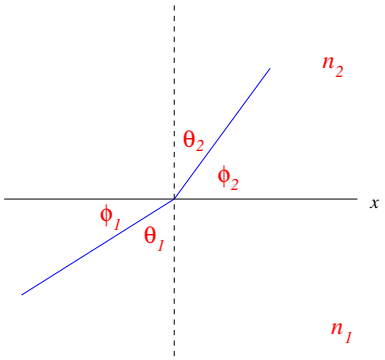

Figure 6.2: Snell's law

Example 6.3:

Fermat's principle of geometrical optics states that light always travels between two points along the path that takes least time, or equivalently which has shortest optical path length (since time is pathlength divided by the speed of light). Show that this implies Snell's law.

Solution:

Following notations as for the shortest path problem above, we find that the travel time of light along an arbitrary path $y(x)$ is

$$\begin{aligned} t[y] &= \int \frac{ds}{v} \\ &= \frac{1}{c}\int n(x,y)ds \\ &= \frac{1}{c}\int n(y)\sqrt{1+y'^2}dx, \end{aligned}$$

or in terms of the optical path

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

We have assumed that $n(x,y) = n(y)$. Its correctness depends on both path and arrangement of the problem.

We now use the result (6.5) from above, and find with $F = n(y(x))\sqrt{1+y'^2}$ that

$$\begin{aligned} \text{constant} &= n(y)\sqrt{1+y'^2} - y'\frac{n(y)y'}{\sqrt{1+y'^2}} \\ &= n(y)\left(\frac{1+y'^2}{\sqrt{1+y'^2}} - \frac{y'^2}{\sqrt{1+y'^2}}\right) \\ &= n(y)\frac{1}{\sqrt{1+y'^2}} \quad . \end{aligned}$$

Thus

$$\boxed{n(y) = \text{const}\sqrt{1+y'^2} \quad .} \tag{6.6}$$

Now consider areas where $n(y)$ is constant. The problem turns into the least distance problem discussed above, and we find that in such an area the optical path becomes a straight line. We now assume two such areas, with index of refraction n_1 below the x axis, and n_2 above, see Fig. 6.2. As usual it is easy to see that $y'(x) = \tan\phi$, and from

$$\sqrt{1+y'^2} = \sqrt{1+\tan^2\phi} = \sec\phi = 1/\cos\phi$$

we conclude from Eq. (6.6) that $n\cos\phi = \text{constant}$. Thus

$$n_1\cos\phi_1 = n_2\cos\phi_2 \quad ,$$

and using $\cos\phi = \cos(\frac{\pi}{2} - \theta) = \sin\theta$ we get

$$\boxed{n_1\sin\theta_1 = n_2\sin\theta_2,}$$

i.e., we have proven Snell's law.

Let's look at one more related problem

Example 6.4:

The brachistochrone is the curve along with a particle slides the fastest between two points under the influence of gravity; think of a bead moving along a metal wire. Given two fixed endpoints, $A = (0,0)$ and a second point B, find the brachistochrone connecting these points.

Solution:

We find for the travel time

$$T = \int_A^B dt = \int_A^B \frac{dt}{ds}ds = \int_A^B \frac{ds}{v},$$

which has to be a minimum. From energy conservation we get

$$\frac{1}{2}mv^2 = mgy, \text{ or } v = \sqrt{2gy},$$

and as before

$$ds = \sqrt{1+y'^2}dx \quad .$$

Taking all of this together

$$T[y] = \int_0^b \left(\frac{1+y'^2}{2gy}\right)^{1/2} dx. \tag{6.7}$$

We now drop the factor $2g$ from the denominator, and minimize

$$I[y] = \int_0^b \left(\frac{1+y'^2}{y}\right)^{1/2} dx.$$

Since $F = \left(\frac{1+y'^2}{y}\right)^{1/2}$ has no explicit x dependence, we find

$$F - \frac{\partial F}{\partial y'}y' = \text{constant},$$

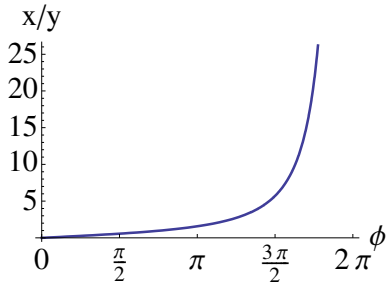

Figure 6.3: x/y as a function of ϕ_0.

i.e.,

$$\begin{aligned}\text{const} &= \frac{1+y'^2}{y} - \frac{1}{\sqrt{y}}\frac{y'}{\sqrt{1+y'^2}y'} \\ &= \frac{1+y'^2}{\sqrt{y(1+y'^2)}} - \frac{y'^2}{\sqrt{y(1+y'^2)}} \\ &= \frac{1}{\sqrt{y(1+y'^2)}} \quad .\end{aligned}$$

Substituting a convenient value for the constant, we find

$$\boxed{y(1+y'^2) = 2R,}$$

which is the equation for a *cycloid*. To solve this, we write $y' = \cot(\phi/2)$, which now leads to

$$1 + y'^2 = 1 + \cos^2(\phi/2)/\sin^2(\phi/2) = 1/\sin^2(\phi/2),$$

and

$$y(\phi) = 2R/(1+y'^2) = 2R\sin^2(\phi/2) = R(1-\cos\phi). \tag{6.8}$$

That would be fine if we knew also $x(\phi)$, so we can represent the curve by a parametric plot! We have from (6.8)

$$\frac{dx}{d\phi} = \frac{1}{dy/dx}\frac{dy}{d\phi} = \tan(\phi/2)2R\sin\phi/2\cos\phi/2 = 2R\sin^2\phi/2 = y.$$

Thus using Eq. (6.8) we get $x = R(\phi - \sin\phi) + C$. Imposing the condition that the curve runs through $(0,0)$, we find

$$\boxed{x = R(\phi - \sin\phi), \qquad y = R(1-\cos\phi).}$$

We determine R and an angle ϕ_0 from the conditions

$$(R(\phi_0 - \sin\phi_0), R(1-\cos\phi_0)) = (b, y(b)).$$

This has multiple solutions. In order to cover all points with positive x/y once, we need to require $0 < \phi < 2\pi$, see Fig. 6.3.

Once we have fixed the range of ϕ, we can then solve for the brachistochrone, see Fig. 6.4 for a few examples.

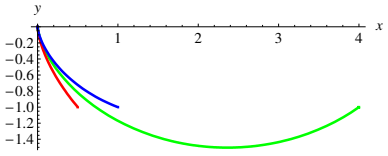

Figure 6.4: A few brachistochrone curves for $y_f = 1$.

So what is the value of the travel time? Substituting the solution into Eq. (6.7) we get

$$\begin{aligned} T &= \int_0^{\phi_0} \left(\frac{2R}{2gy^2}\right)^{1/2} y d\phi \\ &= \phi_0 \sqrt{\frac{R}{g}} \quad . \end{aligned}$$

6.4 Generalizations

6.4.1 Variable end points

So far we have considered

$$\delta I[y] = \delta \int_a^b F(y, y', x) dx = 0,$$

where the value of $y(a)$ and $y(b)$ were fixed. What happens if we allow the value at the endpoints to vary as well?

6.4.2 One endpoint free

Let's look at the simplest case: we once again want to find a function y such that

$$\delta I[y] = \delta \int_a^b dx\, F(y, y', x) = 0 \tag{6.9}$$

where a, b, $y(a)$ are fixed but we allow $y(b)$ to vary.

In the integration by parts we can now no longer show that the boundary terms are zero, so we need to work through the algebra again to see what happens. As before we make the substitution $y(x) \to y(x) + \epsilon(x)$ and expand to first order in ϵ with $\epsilon(a) = 0$, but without a boundary condition for $\epsilon(b)$. Using the techniques employed before, we find

$$\begin{aligned} \delta I &= \left[\epsilon(x) \frac{\partial F}{\partial y'(x)}\right]_a^b + \int_a^b \left[\frac{\partial F}{\partial y(x)} - \frac{d}{dx}\left(\frac{\partial F}{\partial y'(x)}\right)\right] \epsilon(x)\, dx \\ &= \epsilon(b) \frac{\partial F}{\partial y'(x)}\bigg|_{x=b} + \int_a^b \left[\frac{\partial F}{\partial y(x)} - \frac{d}{dx}\left(\frac{\partial F}{\partial y'(x)}\right)\right] \epsilon(x)\, dx, \end{aligned}$$

where we have applied the boundary condition $\epsilon(a) = 0$ in the last line. From the integral we still get the the Euler–Lagrange equation,

$$\frac{\partial F}{\partial y(x)} - \frac{d}{dx}\frac{\partial F}{\partial y'(x)} = 0,$$

but from the boundary term we get an additional equation,

$$\frac{\partial F}{\partial y'}\bigg|_{x=b} = 0. \tag{6.10}$$

Example 6.5:

What is the shortest time for a particle to slide along a frictionless wire under the influence of gravity from $(x, y) = (0, 0)$ to $x = x_f$ for arbitrary y_f? (A variation on the brachistochrone.)

Solution:

From the brachistochrone problem we know that for

$$F(y, y') = \left(1 + y'^2\right)^{1/2} y^{-1/2} \quad ,$$

and that the Euler–Lagrange equation has the first integral

$$[y(1 + y'^2)]^{1/2} = k \quad .$$

The solution is still a cycloid,

$$x = R(\phi - \sin\phi), \qquad y = R(1 - \cos\phi),$$

which indeed passes through $(0, 0)$ for $\phi = 0$. Now for an extremum of the travel time, we have the additional condition

$$\left.\frac{\partial F}{\partial y'}\right|_{x=x_f} = \frac{y'}{\sqrt{y(1 + y'^2)}} = 0.$$

We conclude $y'(x_f) = 0$, i.e., the cycloid is horizontal at $x = x_f$. This occurs when

$$\frac{dy}{d\phi} = R\sin(\phi) = 0,$$

i.e., when $\phi = \pi$. In that case we can find R from

$$x(\phi = \pi) = R\pi = x_f,$$

and thus $R = x_f/\pi$. Finally, $y(x_f) = 2x_f/\pi$.

6.4.3 More than one function: Hamilton's principle

We often encounter functionals of several functions $y_1, y_2, \ldots, y_n$ of the form

$$I[\{y_i\}] = \int_a^b dx\, F(\{y_i(x), y_i'(x)\}, x), \qquad i = 1, 2, \ldots, N. \tag{6.11}$$

We now look for stationary points with respect to all y_i, again keeping the functions at the endpoints fixed. Generalizing the usual technique for partial derivatives to functional ones, i.e., varying each function in turn keeping all others fixed, we find

$$\frac{\delta I}{\delta y_i} = 0.$$

The usual integration-by-parts technique thus leads to N Euler–Lagrange equations,

$$\frac{\partial F}{\partial y_i(x)} - \frac{d}{dx}\frac{\partial F}{\partial y_i'(x)} = 0, \qquad i = 1, 2, \ldots, N. \tag{6.12}$$

Hamilton's principle of least action

An important application in classical dynamics is Hamilton's principle. Suppose we have a dynamical system defined by N "generalized coordinates" $q_i(t)$, $i = 1, 2, \ldots, N$, which fix all spatial positions of a mechanical system at time t.

In standard Newtonian mechanics, where the energy is made up of a kinetic energy T and potential energy V, we can now define an object called the Lagrangian by

$$L(q_i, \dot{q}_i, t) = T(q_i, \dot{q}_i) - V(q_i, t).$$

The left hand-side of this equation is more fundamental than the right-hand one: We can define Lagrangians for many problems, including those where we cannot easily make a separation $E = T + V$.

Hamilton's principle states that the system evolves between the configuration q_i at time t_1 to a new configuration q_i' at time t_2 along a path such that the action S, the integral of L over time, is minimal,

$$\delta S = \delta \int_{t_1}^{t_2} L(q_i, \dot{q}_i, t) dt = 0.$$

Using the Euler–Lagrange equation for the functional $S[q, \dot{q}]$, we find what is usually called *Lagrange's equation of motion*,

$$\frac{\partial L}{\partial q_i(t)} - \frac{d}{dt}\left(\frac{\partial L}{\partial \dot{q}_i(t)}\right) = 0. \tag{6.13}$$

Example 6.6:

Derive Newton's equation of motion for a particle of mass m attached to a spring from the Lagrangian.

Solution:

$$L = T - V = \frac{1}{2} m\dot{x}^2 - \tfrac{1}{2} kx^2 \quad .$$

From (6.13) we find that

$$-kx - \frac{d}{dt}(m\dot{x}) = 0 \quad ,$$

or

$$m\ddot{x} = -kx = -\frac{dV(x)}{dx} \quad .$$

One interesting consequence of our previous discussion of first integrals, is that they carry over to this problem, and will give us *conservation laws*.

First of all, let us look what happens if we are looking at an isolated self-interacting system. This means there are no external forces, and thus there can be no explicit time dependence of the Lagrangian,

$$L = L(q_i, \dot{q}_i).$$

From experience we expect the total energy to be conserved. Can we verify that?

We know from the case of a functional of a single function,

$$I[y] = \int dx\, F(y, y'),$$

that the first integral is

$$F - y'(x)\frac{\partial F}{\partial y'(x)} = \text{constant}.$$

The obvious generalization for this case is

$$L - \sum_i \dot{q}_i \frac{\partial L}{\partial \dot{q}_i(t)} = \text{constant} = -E.$$

The identification with $-E$ comes from looking at standard examples where the kinetic energy is always quadratic in $\dot{q}$, in which case $-\sum_i \dot{q}_i \frac{\partial T}{\partial \dot{q}_i(t)} = -2T$. Since in this case $L = T - V$, we find that $T - V - 2T = -(T + V) = -E$.

Secondly, what happens if a coordinate is missing from L? In that case we get the first integral

$$\frac{\partial L}{\partial \dot{q}_i(t)} = \text{constant}.$$

If we identify $\partial L/\partial \dot{q}_i(t)$ as the "canonical momentum" p_i, we find that p_i is a constant of motion, i.e., it doesn't change.

The form of mechanics based on Lagrangians is more amenable to generalization than the use of the Hamiltonian, but it is not as easy to turn it into quantum mechanics. To show its power let us look at a relativistic charge in an electromagnetic field, where the Lagrangian takes the (at first sight surprising) form

$$L(\mathbf{x}, \dot{\mathbf{x}}, t) = -mc^2\left(1 - \dot{\mathbf{x}}^2/c^2\right)^{1/2} + q\mathbf{A}\cdot\dot{\mathbf{x}} - q\Phi \quad .$$

The first term can be understood by Taylor expansion for small velocities, where we must find $-mc^2 + m\dot{x}^2/2$, which is the right mixture of a potential ($-mc^2$) and kinetic term.

The equations of motion take the form (remembering that $\mathbf{A}$ and Φ depend on $\mathbf{x}(t)$)

$$\frac{d}{dt}\frac{m\dot{x}_i}{\left(1 - \dot{\mathbf{x}}^2/c^2\right)^{1/2}} = q(\nabla_i \mathbf{A})\cdot\dot{\mathbf{x}} - q(\dot{\mathbf{x}}\cdot\nabla)A_i - q\partial_t A_i - q\nabla_i\Phi\,.$$

Defining fields $\mathbf{B} = \nabla\times\mathbf{A}$, $\mathbf{E} = -\nabla\Phi - \partial_t\mathbf{A}$ and a (non-canonical) momentum $\mathbf{p} = m\mathbf{v}/\left(1 - v^2/c^2\right)^{1/2}$, we have

$$\frac{d\mathbf{p}}{dt} = q(\mathbf{v}\times\mathbf{B} + \mathbf{E})\,,$$

which is the usual equation of motion for a charged particle in an electromagnetic field; to verify the last step you will need to show that $\mathbf{v}\times[\nabla\times\mathbf{A}] = \nabla(\mathbf{v}\cdot\mathbf{A}) - (\mathbf{v}\cdot\nabla)\mathbf{A}$. What is the *canonical* momentum of the particle?

6.4.4 More dimensions: field equations

For dynamics in more dimensions $x = x^1, x^2, \ldots, x^N$, we should look at the generalization of the action,

$$S[\phi] = \int_\Omega d\tau\, \Lambda(\phi(x), \partial_\mu\phi(x), x) \tag{6.14}$$

where $d\tau = dx^1 dx^2 \ldots dx^N$ is an infinitesimal volume in N-dimensional space and

$$\phi_{,\mu} \equiv \partial_\mu\phi = \frac{\partial\phi}{\partial x^\mu}, \qquad \mu = 1, 2, \ldots, N. \tag{6.15}$$

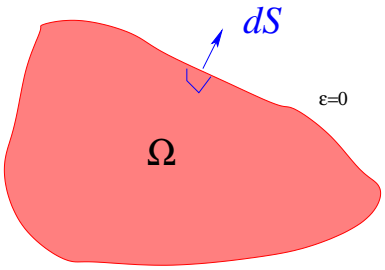

Figure 6.5: The volume Ω and the surface area $d\mathbf{S}$.

As usual, we now look for a minimum of the action. We make the change $\phi(x) \to \phi(x) + \epsilon(x)$, keeping the variations small, but zero on the surface of the region Ω (mathematically, that is sometimes written as $\epsilon(x)|_{\partial\Omega} = 0$), see Fig. 6.5.

Looking for variations to first order in ϵ, we get

$$\begin{aligned}
\delta S &= \int_\Omega \left(\epsilon(x) \frac{\partial \Lambda}{\partial \phi(x)} + \sum_{n=1}^{N} \epsilon_{,\mu} \frac{\partial \Lambda}{\partial \phi_{,\mu}(x)} \right) d\tau \\
&= \int_\Omega \left[\epsilon(x) \frac{\partial \Lambda}{\partial \phi(x)} + \sum_{n=1}^{N} \partial_\mu \left(\epsilon \frac{\partial \Lambda}{\partial \phi_{,\mu}(x)} \right) - \epsilon \sum_{n=1}^{N} \partial_\mu \left(\frac{\partial \Lambda}{\partial \phi_{,\mu}(x)} \right) \right] d\tau \\
&= \int_\Omega \epsilon \left[\frac{\partial \Lambda}{\partial \phi(x)} - \sum_{\mu=1}^{N} \partial_\mu \left(\frac{\partial \Lambda}{\partial \phi_{,\mu}(x)} \right) \right] d\tau + \sum_{\mu=1}^{N} \int_{\partial\Omega} \epsilon \frac{\partial \Lambda}{\partial \phi_{,\mu}(x)} \, dS_\mu \quad .
\end{aligned}$$

where $dS_\mu \equiv \prod_{i \neq \mu} dx^i$. The surface integral vanishes due to the boundary conditions, and requiring $\delta S = 0$, we find the Euler–Lagrange equation,

$$\frac{\partial \Lambda}{\partial \phi} - \sum_\mu \partial_\mu \frac{\partial \Lambda}{\partial \phi_{,\mu}} = 0, \tag{6.16}$$

or, more explicitly:

$$\frac{\partial \Lambda}{\partial \phi(x)} - \sum_\mu \frac{\partial}{\partial x^\mu} \frac{\partial \Lambda}{\partial \partial_\mu \phi(x)} = 0. \tag{6.17}$$

The slightly abstract form discussed above can be illustrated for the case of a 1D continuum field (e.g., a displacement), which depends on both position x and time t. With $\mu = 1$ for x and $\mu = 2$ for t the E-L equations become

$$\frac{\partial \Lambda}{\partial \phi} - \frac{\partial}{\partial t} \frac{\partial \Lambda}{\partial \dot{\phi}} - \frac{\partial}{\partial x} \frac{\partial \Lambda}{\partial \phi'} = 0$$

with

$$\dot{\phi} = \frac{\partial \phi}{\partial t}, \qquad \phi' = \frac{\partial \phi}{\partial x}.$$

For that case the action takes the form

$$S = \int dt \int dx \, \Lambda(\phi, \phi', \dot{\phi}, x, t).$$

Clearly this suggest that $\int dx \, \Lambda$ plays the role of Lagrangian, and we call Λ the *Lagrangian density*.

Example 6.7:

Describe the motion of an elastic stretched string, with fixed endpoints, assuming small deformation, see Fig. 6.6.

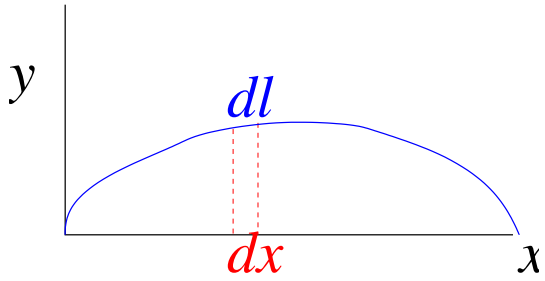

Figure 6.6: The stretched string

Solution:

As ever, we parametrize the position by $y(x,t)$, and assume y to be small. In that case we have

$$dl = \sqrt{1+y'^2}dx \approx \left(1+\frac{1}{2}y'^2\right)dx.$$

The mass density of the string remains almost constant, and we find that the contribution to the kinetic energy between x and $x+dx$ is

$$dK = \frac{1}{2}mv^2 = \frac{1}{2}\rho\dot{y}^2dx \quad .$$

The potential energy in that part of the string is the tension times the stretching,

$$dV = T(dl-dx) = T\frac{1}{2}y'^2dx.$$

We conclude

$$L = \int(dK-dV) = \int\left(\frac{1}{2}\rho\dot{y}^2 - T\frac{1}{2}y'^2\right)dx = \int dx\,\Lambda,$$

and

$$S = \int\int\left(\frac{1}{2}\rho\dot{y}^2 - \frac{1}{2}Ty'^2\right)dx\,dt.$$

Using the previous results with $\phi \to y$, we get

$$\begin{aligned} 0 &= \frac{\partial\Lambda}{\partial y} - \frac{\partial}{\partial t}\frac{\partial\Lambda}{\partial\dot{y}} - \frac{\partial}{\partial x}\frac{\partial\Lambda}{\partial y'} \\ &= -\frac{\partial}{\partial t}\rho\dot{y} - \frac{\partial}{\partial x}(-Ty') \\ &= -\rho\ddot{y} + Ty''. \end{aligned}$$

We thus get the wave equation

$$\frac{1}{c^2}\ddot{y} = y'',$$

with $c^2 = T/\rho$.

Example 6.8:

Find the equations of motion for a freely moving elastic band of length $2\pi l$. For simplicity, assume a two-dimensional world, small stretching, and uniform density.
Discuss the solution to the equations of motion for an almost circular band.

Solution:

Specify the points on the band as $(x(\phi), y(\phi))$, with periodic boundary conditions $x(0) = x(2\pi)$, $y(0) = y(2\pi)$. The local length is $ds = \sqrt{x'^2 + y'^2}\, d\phi$. This needs to be compared to the unstretched band, where $ds = l d\phi$ (but the band does not have to be circular!). For small stretching, the energy for compression or stretching must be given by a form Hook's law, i.e, be proportional to the local stretching or compression squared,

$$dV = \kappa \tfrac{1}{2} \left(\sqrt{x'^2 + y'^2} - l \right)^2 d\phi.$$

At the same time the kinetic energy is given by

$$dT = \rho l \tfrac{1}{2} (\dot{x}^2 + \dot{y}^2) d\phi.$$

Thus,

$$S = \int dt \int_0^{2\pi} d\phi \left[\rho l \tfrac{1}{2} (\dot{x}^2 + \dot{y}^2) - \kappa \tfrac{1}{2} \left(\sqrt{x'^2 + y'^2} - l \right)^2 \right].$$

The EoM are found form a combination of Hamilton's principle and the field problems discussed above,

$$-\rho l \ddot{x} + \kappa \partial_\phi \left(\frac{x'}{\sqrt{x'^2 + y'^2}} (\sqrt{x'^2 + y'^2} - l) \right) = 0 \quad ,$$
$$-\rho l \ddot{y} + \kappa \partial_\phi \left(\frac{y'}{\sqrt{x'^2 + y'^2}} (\sqrt{x'^2 + y'^2} - l) \right) = 0 \quad .$$

If the band is almost circular, we write $(x(\phi), y(\phi)) = (l + \lambda(\phi))(\cos(\phi + \psi(\phi)), \sin(\phi + \psi(\phi)))$, and expand to first order in λ and ψ,

$$-\rho l (\cos(\phi)\ddot{\lambda} - l \sin(\phi)\ddot{\psi}) = \kappa \left(-\cos(\phi)(\lambda + l\psi') - \sin(\phi)(\lambda' + l\psi'') \right)$$
$$-\rho l (\sin(\phi)\ddot{\lambda} + l \cos(\phi)\ddot{\psi}) = \kappa \left(-\sin(\phi)(\lambda + l\psi') + \cos(\phi)(\lambda' + l\psi'') \right)$$

This can be rewritten as

$$\rho l \ddot{\lambda} = -\kappa(\lambda + l\partial_\phi \psi) \quad ,$$
$$\rho l^2 \ddot{\psi} = \kappa(\partial_\phi \lambda + l\partial_{\phi^2} \psi) \quad .$$

This shows the conservation law $\partial_\phi \ddot{\lambda} = -l\ddot{\psi}$.

Thus, it is easy to solve the case when λ is independent of ϕ and $\psi = 0$. Then

$$\ddot{\lambda} = -\frac{\kappa}{\rho l} \lambda \quad ,$$

which describes simple harmonic motion.

Example 6.9:

Show that the Lagrangian density (in 3+1 dimensions)

$$\Lambda = \frac{1}{2} \left[(\partial_t \phi)^2 - (\nabla \phi)^2 - m^2 \phi^2 \right]$$

leads to the Klein–Gordon equation.

Solution:

First note that the first term is the kinetic energy density, so the next two terms can be interpreted as minus the potential energy. There is some ambiguity to this, since we have

$$S = \int dt \int d^3x\Lambda = \int d^4x\Lambda,$$

the action for a *relativistic* (covariant) field theory.

From the Euler–Lagrange equations we find that

$$-m^2\phi - \partial_t\partial_t\phi + \partial_x\partial_x\phi = 0,$$

leading to the Klein–Gordon equation, a slightly modified form of the wave-equation, describing a field with modes with mass m—i.e., a classical description of massive bosons.

6.4.5 Higher derivatives

Occasionally we encounter problems where the functional contains higher than first order derivatives; much what we have said above is of course rather specific to the case of first order derivatives only!

6.5 Constrained variational problems

It is quite common that we have subsidiary conditions on a minimization problem; i.e., we want to know the minimum provided that certain other conditions hold. Let us first analyse this problem for ordinary functions of several variables.

6.5.1 Lagrange multipliers

To find the stationary points of a function $f(\mathbf{x})$ subject to constraints $g_k(\mathbf{x}) = c_k$, $(k = 1, 2, \ldots)$, we can solve an auxiliary problem, which is to find the *unconstrained* stationary points of the modified function

$$F(\mathbf{x}, \lambda_1, \lambda_2, \ldots) = f(\mathbf{x}) - \lambda_1 g_1(\mathbf{x}) - \lambda_2 g_2(\mathbf{x}) - \ldots, \tag{6.18}$$

with respect to $\mathbf{x}$. The parameters $\{\lambda_i\}$ that appear in F are called *Lagrange multipliers*; they are to be regarded as being independent of the variables $\{x_k\}$.

Let's look at a somewhat explicit example. We wish to minimize a function $f(x, y)$ subject to a single constraint $g(x, y) = 0$. We thus need to minimize the modified function

$$F(x, y, \lambda) = f(x, y) - \lambda g(x, y)\,,$$

and find

$$\frac{\partial F}{\partial x} = \frac{\partial f}{\partial x} - \lambda\frac{\partial g}{\partial x} = 0 \qquad \text{and} \qquad \frac{\partial F}{\partial y} = \frac{\partial f}{\partial y} - \lambda\frac{\partial g}{\partial y} = 0\,.$$

From these, we obtain

$$\frac{\partial f}{\partial x} = \lambda\frac{\partial g}{\partial x} \qquad \text{and} \qquad \frac{\partial f}{\partial y} = \lambda\frac{\partial g}{\partial y}\,, \tag{6.19}$$

which shows that that the unconstrained minimum of F is reached when the gradient of the function f is parallel to the gradient of the constraint.

How does this artificial-looking procedure lead to a solution of the original problem, which was to find a *constrained* minimum of $f(x, y)$? To see that it does, suppose that $\delta\mathbf{x}_c$ is an arbitrarily small vector displacement satisfying the constraint, so that $\delta\mathbf{x}_c \cdot \nabla g = 0$ to first order in the displacement. Then, from (6.19), it follows that $\delta\mathbf{x}_c \cdot \nabla f = 0$, which is the condition for f to be stationary along the contour of constant g. We shall use a very similar argument later, for the case of functionals.

Example 6.10:

Find stationary points of $f(x,y)$ under the subsidiary condition $x^2+y^2=1$.

Solution:

Look for stationary points of

$$F = xy - \lambda(x^2+y^2),$$

which are given by the solution(s) of

$$\frac{\partial F}{\partial x} = y - 2\lambda x = 0\,,$$
$$\frac{\partial F}{\partial y} = x - 2\lambda y = 0\,.$$

These two equations give $x^2 = y^2$, or $x = \pm y$; the corresponding values of λ are $\pm 1/2$. By making use of the equation of constraint we then find four solutions, $(x,y) = (\pm 1/\sqrt{2}, \pm 1/\sqrt{2})$.

Note that we could also have solved this problem *without* introducing a Lagrange multiplier, by solving the equation of constraint to obtain $y(x) = \pm\sqrt{1-x^2}$. Inserting this expression into $f(x,y)$ gives

$$f = \pm x\sqrt{1-x^2}\,.$$

Differentiation with respect to x then enables us to locate the stationary points,

$$\frac{df}{dx} = \pm\sqrt{1-x^2} \mp \frac{x^2}{\sqrt{1-x^2}} = \pm\left\{\frac{1-2x^2}{\sqrt{1-x^2}}\right\} = 0\,,$$

which gives $x = \pm 1/\sqrt{2}$ and hence $y = \pm 1/\sqrt{2}$. This is a satisfactory solution to this particular problem, but the method is ugly (it breaks the symmetry between x and y) and it is hard to generalize the method of elimination to functions of several variables with more complicated constraints.

6.5.2 Generalization to functionals

We look for stationary points of $I[y]$ subject to a constraint $J[y] = C$, where I, J are given functionals of $y(x)$ and C is a given constant; there might, of course, be multiple constraints, but we'll return to that generalization later.

We first state the procedure for solving problems of this kind, and then explain why it works. The method is to introduce an *auxiliary functional* containing a Lagrange multiplier λ,

$$K([y],\lambda) = I[y] - \lambda J[y]\,; \tag{6.20}$$

we then solve the *unconstrained* variational problem

$$\delta K = \delta I - \lambda\,\delta J = 0\,.$$

The solution of this problem, $y(x,\lambda)$, depends on the parameter λ, which is chosen so that the constraint $J[y(x,\lambda)] = C$ is satisfied. This last step is sometimes tricky to carry out, and there may be more than one solution for λ. In many problems, however, λ can be eliminated from the equations, and so remains undetermined.

It is worth understanding clearly why this procedure works, so that you can quickly develop generalizations of it when necessary—I find that they are needed quite often:

1. The original problem to be solved is

$$(\delta I)_c = \int \frac{\delta I}{\delta y}\,\delta y_c(x)\,dx = 0\,, \tag{6.21}$$

where the variation $\delta y_c(x)$ satisfies the constraint

$$(\delta J)_c = \int \frac{\delta J}{\delta y}\,\delta y_c(x)\,dx = 0\,, \tag{6.22}$$

but is otherwise arbitrary.

2. The auxiliary problem is to solve

$$\delta K = \int \left\{ \frac{\delta I}{\delta y} - \lambda \frac{\delta J}{\delta y} \right\} \delta y(x)\,dx = 0\,, \tag{6.23}$$

where the variation $\delta y(x)$ is not subject to any constraint; as usual, this leads to the Euler–Lagrange equation

$$\frac{\delta K}{\delta y} = 0, \qquad \text{or} \qquad \frac{\delta I}{\delta y} - \lambda \frac{\delta J}{\delta y} = 0\,.$$

3. To see that this solves the original problem, insert a δy_c satisfying (6.22) into Eq. (6.23):

$$(\delta K)_c = \int \left\{ \frac{\delta I}{\delta y} - \lambda \frac{\delta J}{\delta y} \right\} \delta y_c(x)\,dx = (\delta I)_c - \lambda (\delta J)_c = 0\,;$$

the result is zero, because we've already ensured that the function multiplying $\delta y_c(x)$ is zero. But $(\delta J)_c$ is *also* zero, by virtue of the constraint (6.22); and hence

$$(\delta I)_c = 0\,,$$

which was the original problem to be solved.

The argument given above, and the resulting procedure for solving constrained variational problems, is surprisingly simple. It is worth trying a couple of examples to see how it works out in practice.

Example 6.11:

The isoperimetric problem: Find a closed curve of fixed length L_0 which encloses the maximum area A.

Solution:

Let points on the curve be specified in parametric form $(x(t), y(t))$, where the parameter t varies between 0 and 1. The curve is closed, so $x(0) = x(1)$ and $y(0) = y(1)$. The length of the curve and the enclosed area are given by

$$L = \int_0^1 \left(\dot{x}^2 + \dot{y}^2\right)^{1/2} dt \qquad \text{and} \qquad A = \oint y\,dx = \int_0^1 y\,\dot{x}\,dt\,,$$

where the dots denote differentiation with respect to t. The auxiliary problem is to find stationary points of the functional

$$F([x,y],\lambda) = A[x,y] - \lambda L[x,y] = \int_0^1 \left\{ y\,\dot{x} - \lambda\left(\dot{x}^2 + \dot{y}^2\right)^{1/2} \right\} dt \equiv \int_0^1 f(\dot{x},\dot{y},y)\,dt\,.$$

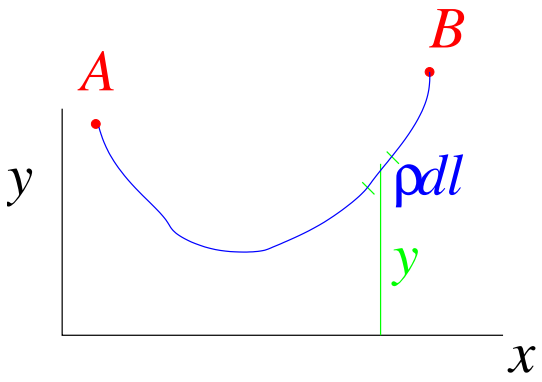

Figure 6.7: The catenary

The function f has no explicit dependence on x, so one integral of the Euler–Lagrange equation for x will be

$$\frac{\partial f}{\partial \dot{x}} = y - \frac{\lambda \dot{x}}{\sqrt{\dot{x}^2 + \dot{y}^2}} = Q\,, \qquad \text{or} \qquad y - Q = \frac{\lambda \dot{x}}{\sqrt{\dot{x}^2 + \dot{y}^2}}\,.$$

The Euler-Lagrange equation for y is

$$\frac{\delta F}{\delta y} = \frac{\partial f}{\partial y} - \frac{d}{dt}\frac{\partial f}{\partial \dot{y}} = \dot{x} + \frac{d}{dt}\frac{\lambda \dot{y}}{\sqrt{\dot{x}^2 + \dot{y}^2}} = 0\,,$$

which can be integrated at once to give

$$x - P = -\frac{\lambda \dot{y}}{\sqrt{\dot{x}^2 + \dot{y}^2}}\,.$$

Dividing each side of this equation for $(x - P)$ by the corresponding sides of the equation for $(y - Q)$ gives

$$\frac{x - P}{y - Q} = -\frac{\dot{y}}{\dot{x}} = -\frac{dy}{dx}\,.$$

The last equation can be integrated to give

$$(x - P)^2 + (y - Q)^2 = R^2\,,$$

which describes a circle of radius R, centred at (P, Q). The constant of integration, R^2, is chosen so that $2\pi R = L_0$.

In this example, the Lagrange multiplier λ was eliminated, so we never had to consider its value explicitly.

Example 6.12:

What is the equilibrium curve for a flexible, inextensible "chain" of length L_0 and density ρ per unit length, when we hang it between two points A and B? (*The catenary*, see Fig. 6.7.)

Solution:

We need to minimize the gravitational potential energy

$$E[y] = \int \rho g\, y\, dl = \rho g \int_a^b y\sqrt{1 + y'^2}\, dx,$$

subject to the constraint of constant length $L[y] = L_0$, with

$$L[y] = \int dl = \int_a^b \sqrt{1+y'^2}\, dx.$$

From here onwards we set $\rho g = 1$; this amounts to a choice of the units for time (or mass) and can have no effect on the solution, which will be a function $y(x)$. The auxiliary problem is to find the unconstrained minimum of $G[y] = E[y] - \lambda L[y]$.

The integrand

$$g(y, y', \lambda) = (y - \lambda)\sqrt{1+y'^2}$$

has no explicit dependence on x, so we can use the first integral,

$$g - y' \frac{\partial g}{\partial y'} = C,$$

or explicitly,

$$(y-\lambda)\sqrt{1+y'^2} - y'(y-\lambda)\frac{y'}{\sqrt{1+y'^2}} = \frac{y-\lambda}{\sqrt{1+y'^2}} = C.$$

which can be rearranged to give

$$\frac{dy}{dx} = \pm\left((y-\lambda)^2/C^2 - 1\right)^{1/2}.$$

This form for the right-hand side suggests that we make the substitution

$$y - \lambda = C\cosh\psi\,,$$

which yields (after using the identity $\cosh^2\psi - 1 = \sinh^2\psi$)

$$\frac{dy}{dx} = C\sinh\psi\,\frac{d\psi}{dx} = \pm\sinh\psi\,.$$

If we absorb the "$\pm$" into the constant C, we then obtain

$$x - x_0 = C\psi\,, \qquad \text{so that} \qquad y = \lambda + C\cosh[(x-x_0)/C]$$

is the shape adopted by the hanging chain. The three constants C, x_0 and λ are determined by the condition that the chain passes through A and B and has length

$$\begin{aligned} L_0 = \int_a^b \left(1+y'^2\right)^{1/2} dx &= \int_a^b \left\{(y-\lambda)/C\right\} dx \\ &= \int_a^b \cosh[(x-x_0)/C]\, dx\,. \end{aligned}$$

The point x_0 is where the curve gets closest to the ground. If $a = -b$ and $y(-b) = y(b) = 0$, then, by symmetry, this lowest point is $x_0 = 0$. In this case we can be more explicit about the relation between L_0 and the remaining constants λ and C:

$$L_0 = \int_{-b}^{b} \cosh[x/C]\, dx = 2C\sinh[b/C] \qquad \text{and} \qquad \lambda = -C\cosh[b/C]\,.$$

A good demonstration can be found on "Catenary: The Hanging Chain" on The Wolfram Demonstrations Project.

6.5.3 Extensions to the method of Lagrange multipliers

The approach used to obtain the method of Lagrange multipliers is easily extended to the case of several constraints $J_a[y] = C_a$. The procedure (which you should verify yourself) is to introduce a Lagrange multiplier λ_a for each of the constraints. The unconstrained auxiliary problem is to find the stationary points of

$$K([y], \{\lambda_a\}) = I[y] - \sum_a \lambda_a J_a[y] \,,$$

which leads to the Euler–Lagrange equation

$$\frac{\delta K}{\delta y} = \frac{\delta I}{\delta y} - \sum_a \lambda_a \frac{\delta J_a}{\delta y} = 0 \,.$$

Once a solution $y(x, \{\lambda_a\})$ has been found, the parameters λ_a must be chosen so that all of the constraints $J_a[y(x, \{\lambda_a\}] = C_a$ are satisfied.

A further generalization covers the case of a family of constraints parametrized by a continuously varying label a. By analogy with the method for discrete constraints, the auxiliary functional takes the form

$$K([y(x)], [\lambda(a)]) = I[y] - \int \lambda(a) J([y], a)\, da \,;$$

the only difference is that the Lagrange multipliers have become a *function*, so that an integral appears in place of the sum. This latter generalization is used very frequently in Lagrangian dynamics, when the coordinates $\{q_i\}$ are related by a constraint

$$\phi(\{q_i(t)\}) = 0 \tag{6.24}$$

which is required to hold for all times t. In principle, the equation of constraint could be solved, so that one of the coordinates could be expressed in terms of the others; but quite often the equation $\phi = 0$ is too hard to solve, or the process of doing that might spoil a neat symmetry of the physical system. The method of Lagrange multipliers avoids both problems, and may provide some additional physical insight.

Suppose that a mechanical system with (unconstrained) Lagrangian $L(\{q_i, \dot{q}_i\})$ is subject to a constraint such as (6.24). We can define a modified action

$$S^*[\{q_i\}] = \int_{t_1}^{t_2} \{L(\{q_i, \dot{q}_i\}) - \lambda(t)\, \phi(\{q_i(t)\})\}\, dt \,,$$

and solve the unconstrained variational problem $\delta S^* = 0$. The Euler–Lagrange equations are

$$\frac{\delta S^*}{\delta q_i} = \frac{\partial L}{\partial q_i} - \frac{d}{dt}\frac{\partial L}{\partial \dot{q}_i} - \lambda(t)\frac{\partial \phi}{\partial q_i} = 0 \,,$$

which can be rearranged to give

$$\frac{d}{dt}\frac{\partial L}{\partial \dot{q}_i} = \frac{\partial L}{\partial q_i} - \lambda(t)\frac{\partial \phi}{\partial q_i} \,. \tag{6.25}$$

Expressed in this way, it is quite clear what the term involving $\lambda(t)$ means physically: it is the *force of constraint* that must be applied to ensure that (6.24) is satisfied.

To give a specific example, consider a pendulum consisting of a mass m attached to the ceiling via a lightweight, rigid rod of length R, which is hinged at the point of support. If θ is the angle that the rod makes with the vertical, and r is the distance of the mass from the point of support, the Lagrangian for the unconstrained problem (i.e., without the rod) is

$$L = \tfrac{1}{2} m\left(\dot{r}^2 + r^2\, \dot{\theta}^2\right) + mgr\cos\theta \,;$$

the equation of constraint is simply $r(t) = R$, or

$$\phi(r(t), \theta(t)) = r(t) - R = 0\,.$$

Plugging L and ϕ into the equations of motion (6.25) then gives

$$m\frac{d}{dt}\left(r^2\frac{d\theta}{dt}\right) = -mgr\sin\theta \quad \text{and} \quad m\frac{d^2r}{dt^2} = mg\cos\theta + mr\left(\frac{d\theta}{dt}\right)^2 - \lambda(t)\,.$$

We see that in this case, $\lambda(t)$ is a force acting radially on the mass: it is, of course, the tension in the rod. In the equation of motion for θ, r can be replaced by the constant R; and, given a solution $\theta(t)$, the second equation yields

$$\lambda(t) = mg\cos\theta + mR\left(\frac{d\theta}{dt}\right)^2$$

as the tension in the rod. You should convince yourself that this last expression is correct.

For another illustration of how a constraint can be imposed by means of a Lagrange-multiplier *function*, we revisit the isoperimetric problem considered earlier in this chapter.

Example 6.13:

The isoperimetric problem (again): Find a closed curve of fixed length L which encloses the maximum area A.

Solution:

Let points on the curve be specified in parametric form $(x(s), y(s))$, where $s \in [0, L]$ is the *arc-length*, measured along the curve. The curve is closed, so $x(0) = x(L)$ and $y(0) = y(L)$. The enclosed area is

$$A = \oint y\,dx = \int_0^L y\,\dot{x}\,ds\,,$$

where this time the dot denotes differentiation with respect to s. The differentials dx, dy and ds are related, as usual, by $dx^2 + dy^2 = ds^2$, which we regard as a constraint on the derivatives $\dot{x}$ and $\dot{y}$,

$$\dot{x}^2 + \dot{y}^2 = 1\,,$$

which must be satisfied at every point on the curve. The unconstrained auxiliary problem is to find stationary points of the functional

$$F([x,y]) = A[x,y] - \int_0^L \lambda(s)\left(\dot{x}^2+\dot{y}^2\right)ds = \int_0^L \left\{y\,\dot{x} - \lambda(s)\left(\dot{x}^2+\dot{y}^2\right)\right\}ds\,.$$

From this, the Euler–Lagrange equations for x and y are

$$\frac{\delta F}{\delta x} = -\dot{y} + \frac{d}{ds}\left\{2\lambda(s)\,\dot{x}\right\} = 0 \qquad \text{and} \qquad \frac{\delta F}{\delta y} = \dot{x} + \frac{d}{ds}\left\{2\lambda(s)\,\dot{y}\right\} = 0\,.$$

Each of these is a total derivative with respect to s, and so can be integrated to give, respectively,

$$y - Q = 2\lambda(s)\,\dot{x} \qquad \text{and} \qquad x - P = -2\lambda(s)\,\dot{y}\,,$$

where P and Q are the constants of integration. Just as in the earlier treatment of this problem, we can eliminate the Lagrange multiplier (though here it is a function), and obtain

$$\frac{x-P}{y-Q} = -\frac{2\lambda(s)\,\dot{y}}{2\lambda(s)\,\dot{x}} = -\frac{\dot{y}}{\dot{x}} = -\frac{dy}{dx}\,;$$

the rest of the solution (the derivation of the equation of a circle) is exactly as before.

6.5.4 Eigenvalue problems

Consider the eigenvalue equation for the function $\psi(x)$

$$L\psi = \lambda\rho\psi\,, \tag{6.26}$$

where L is an Hermitian operator, $\rho(\mathbf{x})$ is a positive, real weight function. We now look for the stationary points of

$$I[u] = \int d\tau\, \psi^* L\psi \tag{6.27}$$

subject to the normalization constraint

$$\int d\tau\, \rho\psi^*\psi = 1. \tag{6.28}$$

We first look for an unconstrained stationary point of

$$J_\lambda[\psi] = \int d\tau\, \psi^* L\psi - \lambda \int d\tau\, \rho\psi^*\psi\,.$$

We get

$$\begin{aligned}\delta J &= \int d\tau\, (\psi^* L\delta\psi + \delta\psi^* L\psi) - \lambda \int d\tau\, \rho\, (\psi^*\delta\psi + (\delta\psi^*)\psi) \\ &= \int d\tau\, (L\psi - \lambda\rho\psi)^*\, \delta\psi + \int d\tau\, \delta\psi^*\, (L\psi - \lambda\rho\psi)\,,\end{aligned}$$

where we have used $L = L^\dagger$.

A key difference with the previous examples is that we have a complex function $\psi = u + iv$, and any variation thus falls into two parts,

$$\begin{aligned}\delta\psi &= \delta u + i\delta v, \\ \delta\psi^* &= \delta u - i\delta v.\end{aligned}$$

The real and imaginary parts δu and δv are independent small functions, i.e., we can vary those independently. It would certainly be nice if we could conclude that the alternative orthogonal combination of these two variations provided by $\delta\psi$ and $\delta\psi^*$ vary independently; for then we could select either of the two terms above, and conclude that each was zero independently.

It is not too hard to persuade ourselves that the final statement, at least, is correct. Under the integral sign we have an expression of the form

$$\begin{aligned}f\,\delta\psi + g\,\delta\psi^* &= f(\delta u + i\delta v) + g(\delta u - i\delta v) \\ &= [f+g]\delta u + i[f-g]\delta v \\ &= 0\,.\end{aligned}$$

The variations δu and δv are independent, so their coefficients $f + g$ and $f - g$ must be zero. From this we can conclude that f and g are also both zero; i.e., the result is exactly the same as if we had regarded $\delta\psi$ and $\delta\psi^*$ as independent quantities.

Given the result of the preceding argument, the function multiplying $\delta\psi^*$ must satisfy

$$L\psi - \lambda\rho\psi = 0,$$

which shows that ψ is an eigenfunction of L. We conclude that the stationary points are the eigenfunctions $u = u_0, u_1, \ldots$ and the corresponding values of λ are the eigenvalues $\lambda_0, \lambda_1, \ldots$.

Now suppose that there is a minimum eigenvalue λ_0. This implies that for a *normalized* ψ, $I[\psi] \geq \lambda_0$. We show below how we can use that to our benefit.

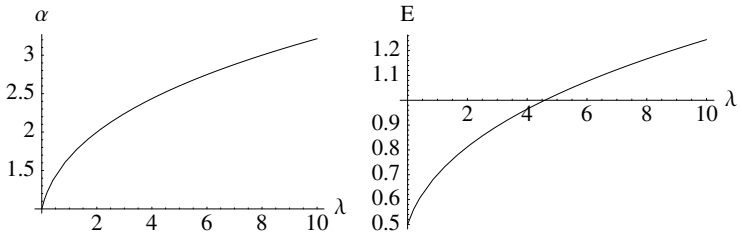

Figure 6.8: The parameter α and the energy E as a function of anharmonicity λ.

6.5.5 The Rayleigh–Ritz method

Suppose the function u_0 gives the minimum of

$$I[u] = \int u^* L u \, d\tau,$$

subject to the constraint

$$\int d\tau \, \rho \, u^* u = 1.$$

Now suppose v_0 gives the unconstrained minimum of

$$K[v] = \frac{\int d\tau \, v^* L v}{\int d\tau \, v^* \rho v}. \tag{6.29}$$

Theorem 6.1. *The unconstrained minimum of $K[v]$ and the constrained minimum of $I[u]$ with the normalization constraint are identical.*

Proof.

$$K[u_0] = \frac{\int d\tau \, {u_0}^* L u_0}{\int d\tau \, u_0^* \rho u_0} = I[u_0] \geq K[v_0].$$

(The last inequality holds if v_0 is the minimum of K). Now find a similar relation for I. Define $N = \int d\tau \, v_0^* \rho v_0$ and $w_0 = v_0/\sqrt{N}$, then

$$I[w_0] = \int w_0^* L w_0 \, d\tau = \frac{1}{N} \int v_0^* L v_0 \, d\tau = K[v_0] \geq I[u_0].$$

Thus $K[v_0] = I[u_0]$, and unless there are degenerate minima, $w_0 = u_0$. □

This technique is very commonly used in quantum mechanics, where we then replace the functional dependence with a parametrized dependence by choosing a set of wave functions depending on set of parameters. In this case $L = H$, $\rho = 1$ and $u = \psi$.

Example 6.14:

Find an approximation to the ground state of the quartic anharmonic oscillator

$$H = \tfrac{1}{2} \left\{ -\frac{d^2}{dx^2} + x^2 + \lambda x^4 \right\},$$

of the form $\psi(x) = \exp(-\alpha x^2/2)$.

Solution:

The normalization integral is

$$\int_{-\infty}^{\infty} \exp(-\alpha x^2) dx = \sqrt{\pi/\alpha}.$$

By differentiating both sides with respect to α, we get two more useful integrals,

$$\int_{-\infty}^{\infty} x^2 \exp(-\alpha x^2) dx = \frac{1}{2\alpha}\sqrt{\pi/\alpha}.$$

$$\int_{-\infty}^{\infty} x^4 \exp(-\alpha x^2) dx = \frac{3}{4\alpha^2}\sqrt{\pi/\alpha}.$$

The expectation value of the Hamiltonian requires the derivative

$$\frac{d^2}{dx^2} \exp(-\alpha x^2/2) = (x^2\alpha^2 - \alpha) \exp(-\alpha x^2/2).$$

Thus the numerator of the variational functional becomes

$$\int_{-\infty}^{\infty} \tfrac{1}{2}(-x^2\alpha^2 + \alpha + x^2 + \lambda x^4) \exp(-\alpha x^2) dx = \sqrt{\pi/\alpha} \left(-\alpha/2 + \alpha + 1/(2\alpha) + 3\lambda/(4\alpha^2)\right)/2.$$

The denominator is simply the normalization integral given earlier; hence,

$$K(\alpha) = \frac{1}{4}\left(\alpha + 1/\alpha + 3\lambda/(2\alpha^2)\right).$$

Minimizing with respect to α, we find

$$1 - 1/\alpha^2 - 3\lambda/\alpha^3 = 0.$$

This equation can be solved in closed form, but is rather complicated. We find that α increases with λ, see Fig. 6.8.

Appendix A

Contour Integration

A.1 The Basics

The key word linked to contour integration is "analyticity" or the absense thereof:

A function is called analytic in a region R in the complex plane iff all the derivatives of the function (1st, 2nd, ...) exist for every point inside R.

This means that the Taylor series

$$f(z) = \sum_{n=0}^{\infty} f^{(n)}(c) \frac{(z-c)^n}{n!} \tag{A.1}$$

exists for every point c inside R.

In most cases we are actually interested in functions that are *not* analytic; if this only happens at isolated points (i.e., we don't consider a "line of singularities", usually called a "cut" or "branch-cut") we can still expand the function in a Laurent series

$$f(z) = \sum_{n=-\infty}^{\infty} f^{(n)}(c) \frac{(z-c)^n}{n!} \tag{A.2}$$

How we obtain the coefficients $f^{(n)}(c)$ from the function is closely linked to the problem of contour integration.

A.2 Contour Integration

Let us look at the effects of integrating the powers of z along a line in the complex plane (note that we implicitely assume that the answer is independent of the position of the line, and only depends on beginning and end!)

$$\int_{z_0}^{z_1} z^n \, dz, \quad n \in \mathbb{Z}. \tag{A.3}$$

We know how to integrate powers, so apart from the case $n = -1$, we get

$$\int_{z_0}^{z_1} z^n \, dz = \left[\frac{1}{n+1} z^{n+1} \right]_{z_0}^{z_1}, \quad n \neq -1, \tag{A.4}$$

$$\int_{z_0}^{z_1} z^{-1} \, dz = [\log z]_{z_0}^{z_1}, \quad n = -1. \tag{A.5}$$

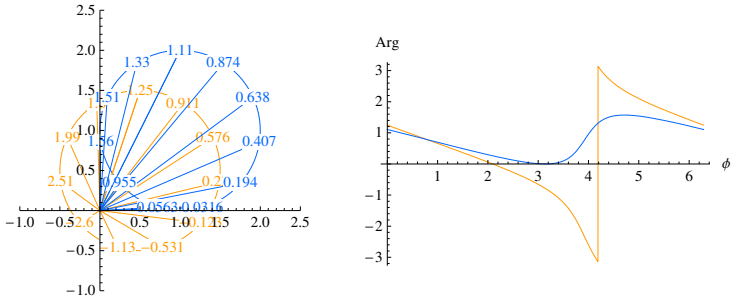

Figure A.1: Two contours: The blue one does not include the origin, the orange one does. The numbers on the left plot show the phase of the relevant complex numbers. These are also graphed in the right panel.

So the first of these integrals is indepdent of the path between begin and end. It thus goes to zero as we look at a closed path, but the second integral actually does depend on the path of integration:

$$\text{Use } z = re^{i\phi}; \log(z) = \log(r) + i\phi. \tag{A.6}$$

We have two options: the contour (the technical word for the closed path) either encloses the origin where the singularity resides or not, see Fig. A.1.

As we move the around the curve, you notice for the blue curve that the phase (the number plotted on the line connecting to the point for which we calculate the phase) gently oscillates up and down, and thus the answer of the contour integral is zero; for the orange curve we see a jump at the negative x-axis. This is due to a convention; in principle we can put this jump along any half-line in the complex plane ending at the origin.

If we move the value at the right of the jump down by 2π (making the function continuous) we realise that the begin and endpoint differ in phase by 2π. Thus for any contour *enclosing the origin* the phase changes by 2π, and thus we expect that

$$\oint z^{-1} dz = \pm 2\pi i \tag{A.7}$$

for a contour enclosing the origin. The sign is positive if we integrate around in the positive sense (anti-clockwise), and negative if we do the integral along a contour that encircles the origin in a clockwise fashion.

If a function $f(z)$ behaves like $\frac{1}{z-c}$ near the point c, we say that the function has a pole at $z = c$.

A.3 Residues

We are now ready to make the general statement:

If a function $f(z)$ has a term $\frac{R}{z-c}$ in its Laurent series around the point c (i.e., it is not analytic in a region around c, but it has an "isolated singularity" at c), then for any contour that encloses *this and only this* pole

$$\oint f(z) dz = \pm 2\pi i R \tag{A.8}$$

Here R is called the residue of f at c, and the sign depends on the orientation of the contour around c.

If multiple singularities are enclosed, we find that (all residues contribute with the same sign, since the contour must enclose them with the same orientation!)

$$\oint f(z)dz = \pm 2\pi i \sum_k R_k \tag{A.9}$$

We can find the residue by expanding $f(z)$ around c; it is often more useful (quicker) to look at the limit

$$\lim_{z\to c}(z-c)f(z) = R. \tag{A.10}$$

This works if there are no higher order singularities, i.e. no terms $b_{-2}/(z-c)^2$, etc. in the Laurent series.

A.4 Example 1: Simplest case

Contour integration is most commonly used to calculate integrals along the real axis, by turning them into complex integrals.

Calculate the integral

$$\int_{-\infty}^{\infty} \frac{1}{1+x^2}\,dx \tag{A.11}$$

We actually know this one: it is $[\arctan(x)]_{-\infty}^{\infty} = \pi$. This is the simplest example of an integral doable by contour integration. Rewrite as a complex integral

$$\int_{-\infty}^{\infty} \frac{1}{1+z^2}\,dz$$

As $|z| \to \infty$, the integral over the half circle $z = Re^{i\phi}$ (R fixed) gives ($dz = d\left(Re^{i\phi}\right) = Re^{i\phi}id\phi$)

$$\int_{-R}^{R} \frac{1}{1+z^2}\,dz = R\int_0^{\pi} \frac{1}{1+R^2e^{2i\phi}}de^{i\phi} \propto \frac{1}{R} \to 0. \tag{A.12}$$

This means we can close of the integral by adding a contour from ∞ to $-\infty$ along a half circle. We easily see that $z^2+1 = (z+i)(z-i)$, and thus has poles in the upper and lower half plane. Only the one in the upper half plane is contained inside the contour, which goes around in positive sense.

The residue is $-\frac{i}{2}$ and thus

$$\int_{-\infty}^{\infty} \frac{1}{1+x^2}\,dx = \int_{-\infty}^{\infty} \frac{1}{1+z^2}\,dz = \oint \frac{1}{1+z^2}dz = -\frac{i}{2}2\pi i = \pi \tag{A.13}$$

as we know should be the case.

Note that in order to work, the ratio of denomiator over numerator should be at least $\frac{1}{R^2}$ for large radius.

A.5 Example 2: Complex exponentials

The most common problem is with complex exponentials (or sines and cosines which can be written as such).

Calculate the integral (which falls slowly for large x!)

$$\int_{-\infty}^{\infty} \frac{e^{ikx}}{i-x}\,dx \tag{A.14}$$

We shall analyse this for $k > 0$.

If we substitute $x = z = Re^{i\phi}$, we find

The problem can be seen on substitution of $z = Re^{i\phi}$, for R fixed (as a bove)

$$\frac{e^{ikx}}{i-x} = \frac{e^{-kR\sin(\phi)}(\cos(kR\cos(\phi)) + i\sin(kR\cos(\phi)))}{-R\cos(\phi) - iR\sin(\phi) + i}$$

For $\sin(\phi) > 0$ the integrand goes to zero very quickly with R, but for ϕ=0 we enter a grey territory, where the integrand decays like $1/R$. If we move the original integral up by just a little bit (ϵ) we are OK, since ϕ doesn't become zero. Thus

$$\int_{-\infty}^{\infty} \frac{e^{ikx}}{i-x}\,dx = \int_{-\infty+i\epsilon}^{\infty+i\epsilon} \frac{e^{ikz}}{i-z}\,dz = \oint \frac{e^{ikz}}{i-z}dz \tag{A.15}$$

The residue is easily seen to be $R = -e^{-k}$, and thus

$$\int_{-\infty}^{\infty} \frac{e^{ikx}}{i-x}\,dx = \int_{-\infty+i\epsilon}^{\infty+i\epsilon} \frac{e^{ikz}}{i-z}\,dz = \oint \frac{e^{ikz}}{i-z}dz = 2\pi i\left(-e^{-k}\right) = -2\pi i\,e^{-k}\ (k>0) \tag{A.16}$$

In the same way we can show that for $k < 0$ we must close the contour in the lower plane (since $k\sin(\phi)$ must be negative)

$$\int_{-\infty}^{\infty} \frac{e^{ikx}}{i-x}\,dx = \int_{-\infty-i\epsilon}^{\infty-i\epsilon} \frac{e^{ikz}}{i-z}\,dz = \oint \frac{e^{ikz}}{i-z}dz = -2\pi i(0) = 0\ (k<0) \tag{A.17}$$

since no pole is enclosed inside the contour.

A.6 Final case: poles on the real axis

The techniques shown above fail if a pole occurs on the real axis, since we don't know what side of the contour it lies! The technique to deal with that is usually based on physics: Determine whether there are physical conditions that must be satisfied on the quantity you wish to evaluate. Decide whether these imply that a pole should contribute (which means we need to move the pole just inside the contour) or whether it should not contribute (move pole just outside the contour). There are even cases where the logical choice is to asign half on the inside and half on the outside. Clearly, the physical background decides which choice to make.