Mathematical Methods

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based on work by

Graham Shaw

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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. I hope they have turned into a reasonably complete guide to the material presented in the course, and in an accurate form!

I would suggest you come back to this reasonably often, 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, and thus 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 I find quite useful is to understand a number of the key principles underlying this work, so that you can derive most results quickly. Combined with practise 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

The course PHYS 20171, Mathematics of Waves and Fields, is a prerequisite for this course. If you feel rusty, have a look at my website for the material for the related 2C1 course (`walet.phy.umist.ac.uk/2C1`)), which may help to refresh your memory.

In addition, the Section on Green Functions requires a simple knowledge of contour integration and the . The latter material has been covered in MATH 20612.

Alternatively, a student who has not attended this course should read Appendix A (about 10 pages) and the first two or three pages of section 3.3 of Matthews 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 `walet.phy.umist.ac.uk/MaMe`, as well as a pdf file (Contour.pdf), and much of the material is also summarised in Appendix A.

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) $\boldsymbol{a}, \boldsymbol{b}, \boldsymbol{c}, \ldots$ with two operations:

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

These must satisfy the following conditions

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

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

Example 2.1:

The space $\mathbb{R}^3$ of vectors $\boldsymbol{r} = \begin{pmatrix} x \\ y \\ z \end{pmatrix} = x\boldsymbol{i} + y\boldsymbol{j} + z\boldsymbol{k}$ 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 $\boldsymbol{a}$ there is only one inverse $-\boldsymbol{a}$.

2.2 Linear independence and basis vectors

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

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

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

This can be used to show that when you pick one of the vectors $\boldsymbol{a}, \boldsymbol{b}, \ldots, \boldsymbol{u}$, it can not be expressed as a sum over the rest. There usually 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 $\boldsymbol{e}_1, \boldsymbol{e}_2, \ldots, \boldsymbol{e}_n$ in an n-dimensional space is said to form a *complete set of basis vectors*, since one can show that any vector $\boldsymbol{x}$ in the space can be expanded in the form

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

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

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):

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

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

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

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

Linear independence of the vectors $\{\boldsymbol{e}_i\}$ 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 highly non-trivial (i.e., quite hard) 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 $\boldsymbol{a}, \boldsymbol{b}$ we can define a scalar product[1] $(\boldsymbol{a}, \boldsymbol{b})$ [the mathematicians' preferred notation for $\boldsymbol{a} \cdot \boldsymbol{b}$], which satisfies:

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

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

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

together with

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

where the equality holds for $\boldsymbol{a} = \boldsymbol{0}$ only.
Note: Mathematically the inner product is a mapping from $V \otimes V \mapsto S$!
Note: In functional spaces we physicists often use the Dirac bra-ket notation $\langle\psi|\phi\rangle$ for (ψ, ϕ) . We can use the inner product to define the norm (a more correct description of the length) of the vector $\boldsymbol{a}$,

$$\|\boldsymbol{a}\| \equiv (\boldsymbol{a}, \boldsymbol{a})^{1/2}.$$

One can define a length without an inner product. A good example is the so-called "1-norm" of a vector, $||\boldsymbol{x}||_1 = \sum_n |x_n|$, 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 $\boldsymbol{a}$ and $\boldsymbol{b}$ are said to be *orthogonal* if $(\boldsymbol{a}, \boldsymbol{b}) = 0$.

Triangle and Cauchy-Schwartz inequality

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

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

From the triangle inequality we can prove the Cauchy Schwartz inequality

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

$$|(\boldsymbol{a}, \boldsymbol{b})| \leq ab.$$

Proof. The proof is simple. Consider $(\boldsymbol{a} + x\boldsymbol{b}, \boldsymbol{a} + x\boldsymbol{b},)$, which is ≥ 0. Minimise this with respect to x, and we find a minimum for $x = -(a, b)/\|\boldsymbol{b}\|^2$. At that point the function takes on the value $a^2 - (a, b)^2/b^2 \geq 0$. Multiply this by b^2 and take the square root at both sides for the desired result. □

Orthogonalisation and Orthogonalisation

There are two ways to turn an arbitrary set of vectors into an orthogonal set–one where every pair of vectors is orthogonal–, or even better orthonormal set–an orthogonal set where each vector has length one.

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

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

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 $\boldsymbol{e}'_m$ is normalised.

A more modern approach (based on extensive use of numerical linear algebra) is based on the construction of the "overlap matrix" (also called norm matrix, which is why we use the symbol) N, with

entries $N_{ij} = (\boldsymbol{e}_i, \boldsymbol{e}_j)$. 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

$$\boldsymbol{e}'^{(i)}_k = (N^{-1/2})_{kl}\boldsymbol{e}^{(i)}_l.$$

For a *real symmetric matrix* M (and similarly for a 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

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

Question: Show that M^a is a symmetric matrix

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

$$(\boldsymbol{e}_i, \boldsymbol{e}_j) = \delta_{ij}. \tag{2.5}$$

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.

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

$$\sum_i (\boldsymbol{e}_i)_a (\boldsymbol{e}_i)_b = \delta_{ab}. \tag{2.6}$$

2.2.2 Questions

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

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]

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

and expand in these functions,

$$f(x) = \int_{-\infty}^{\infty} dk\, \phi_k(x)\tilde{f}(k). \tag{2.7}$$

[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.

[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.

The expansion coefficient is nothing but the Fourier transform,

$$\tilde{f}(k) = \int_{-\infty}^{\infty} dx\, \phi_k^*(x) f(x). \tag{2.8}$$

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 (2.8) into (2.7), which gives the relation

$$f(x) = \int_{-\infty}^{\infty} dk\, \phi_k(x) \int_{-\infty}^{\infty} dx'\, \phi_k^*(x') f(x'), \tag{2.9}$$

which must hold for any $f(x)$. We now swap integrals, and find

$$f(x) = \int_{-\infty}^{\infty} dx' \left[\int_{-\infty}^{\infty} dk\, \phi_k(x) \phi_k^*(x') \right] f(x'). \tag{2.10}$$

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

$$\delta(y) = \frac{1}{2\pi} \int_{-\infty}^{\infty} dz\, e^{iyz}. \tag{2.11}$$

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

From the definition (2.11) 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*.

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

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. (2.5))

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

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

$$\psi(x) = \sum_n c_n \phi_n(x). \tag{2.12}$$

The coefficients c_n can be determined from the orthogonality relation, multiplying (2.12) from the left with ψ_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

$$c_m = (\phi_m, \psi). \tag{2.13}$$

Substituting Eq. (2.13) into Eq. (2.12) we find

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

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 continuous 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. (2.9,2.10). 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.

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.

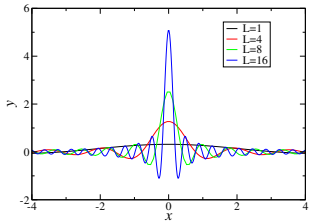

Figure 2.1: A sketch of $\frac{1}{2\pi}\frac{2}{x}\sin(Lx)$ for a few values of L. This function converges to a Dirac delta function

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

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

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

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

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 $a \to 0$.

[5] The δ function is strictly speaking not a function, it is only defined *inside* an integral!

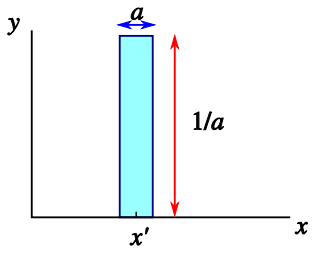

Figure 2.2: A sketch of a piecewise constant function, that in the limit $a \to 0$ gives the Dirac delta function

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,

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

A very useful relation is obtained when we scale the variables in the delta function ($y = ax$)

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

We can interpret this is 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 as argument. Here we need to sum over all zeroes of the function inside the integration inetrval, and the quantity a above becomes the slope at each of the zeroes,

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

where the sum extends over all points x_i in $]a, b[$ where $f(x_i) = 0$.

Example 2.6:

Calculate the integral

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

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

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

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 $\boldsymbol{a}, \boldsymbol{b} \ldots$ in a linear vector space V to give new vectors $L\boldsymbol{a}$, $L\boldsymbol{b}, \ldots$ such that[1]

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

Example 3.1:

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

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

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 $\boldsymbol{f}$ on the vector $\boldsymbol{g}$, $L\boldsymbol{f} = \boldsymbol{g}$, the vector space of $\boldsymbol{f}$'s (the domain) can be different from the vector space of $\boldsymbol{g}$'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 cases we shall assume that the range and codomain coincide.

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

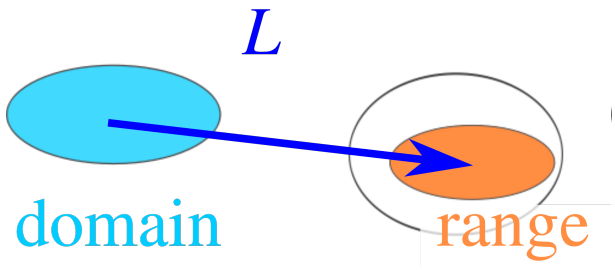

Figure 3.1: The definition of domain, codomain and range

Example 3.2:

1. The operator L: $\mathbb{C}^n \to \mathbb{C}$ defined by $L\boldsymbol{a} = (\boldsymbol{a}, \boldsymbol{b})$ with $\boldsymbol{b}$ 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 $\boldsymbol{\nabla}$ maps from the space of scalar fields ($f(\boldsymbol{x})$ is a real function of 3 variables) to the space of vector fields ($\boldsymbol{\nabla} f(x)$ 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 $\boldsymbol{y} = l\boldsymbol{x}$. Let $\boldsymbol{e}_1, \boldsymbol{e}_2, \ldots$ and $\boldsymbol{u}_1, \boldsymbol{u}_2, \ldots$ be chosen sets of basis vectors in the domain and codomain, respectively, so that

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

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

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

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* transformatio!

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

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

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

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

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

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

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

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

with

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

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,

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

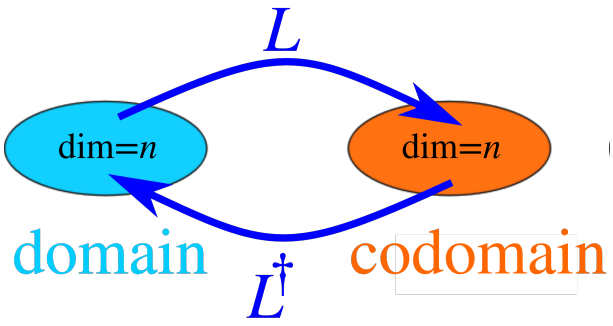

Figure 3.2: The definition of a matrix and its Hermitian conjugate

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

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

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

$$(w, v) = w^\dagger v.$$

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 $\boldsymbol{a}$ and $\boldsymbol{b}$ in the range and domain,
>
> $$(\boldsymbol{a}, M\boldsymbol{b}) = (M^\dagger \boldsymbol{a}, \boldsymbol{b}).$$

Thus, with a little algebra,

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

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 $n \times m$ one.

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 gleamed 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,

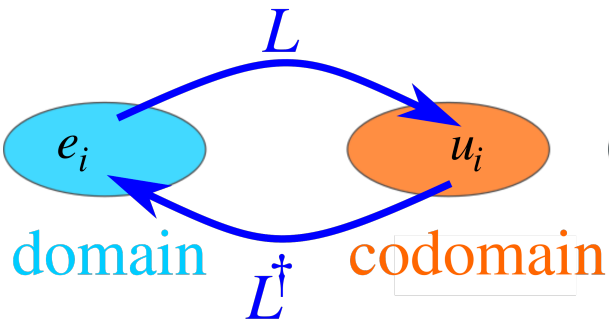

Figure 3.3: The definition of an operator and its Hermitian conjugate

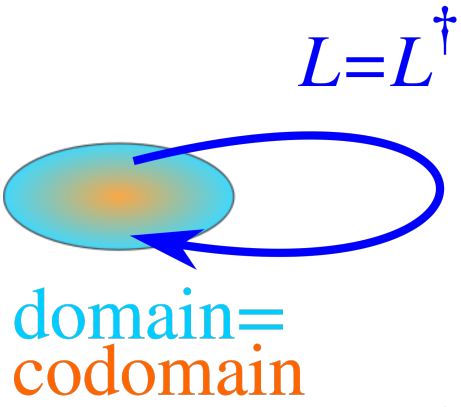

Figure 3.4: A schematic representation of a self-adjoint operator.

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

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

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

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

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

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

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

Positivity of $(\boldsymbol{a}, \boldsymbol{a})$, ($(\boldsymbol{a}, \boldsymbol{a}) \geq 0$ and is only 0 if $\boldsymbol{a} = \boldsymbol{0}$) 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 $L\boldsymbol{b} = \mu \boldsymbol{b}$, 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 $\boldsymbol{a}$ or $L^\dagger = L$ on $\boldsymbol{b}$) for

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

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

This does not apply to the case when we have two different eigenvalues for the same eigenvalue (degeneracy). There is no rule precluding $(\boldsymbol{a}, \boldsymbol{b})$ 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

$$Me = \lambda e.$$

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

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

A little guesswork shows that this can be factorized as

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

The unique eigenvalue 6 has an eigenvector satisfying

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

which has as normalised solution $e_3 = \begin{pmatrix} 1 \\ 1 \\ 1 \end{pmatrix} / \sqrt{3}$. The degenerate eigenspace for $\lambda = 3$ has eigenvectors satisfying

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

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 Gramm-Schmidt procedure to find orthonormal eigenvectors of the form $e_1 = (1,1,-2)/\sqrt{6}$ and $e_2 = (1,-1,0)/\sqrt{2}$. The general eigenvector for eigenvalue 3 is then $ae_1 + be_2$.

This example shows the reality of the eigenfunctions, 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.

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

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

Name	$p(x)$	$q(x)$	$\rho(x)$	$[a,b]$
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}	$(-\infty,\infty)$
Chebychev's equations	$(1-x^2)^{1/2}$	0	$(1-x^2)^{-1/2}$	$[-1,1]$
Bessel's equation	x	$-\nu^2/x$	x	$[0,R]$, R finite.
and many others.				

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

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

where the Wronskian W is defined as

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

In mathematical physics the domain is often delimited by points a and b where $p(a) = p(b) = 0$. If we then add a boundary condition that $w(x)p(x)$ and $w'(x)p(x)$ are finite (or a specific finite number) as $x \to a, b$ for all solutions $w(x)$, the operator is Hermitian.

Note that such boundary conditions forbid "second solutions" in general – 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

$$Lu(x) + \lambda\rho u(x) = 0, \tag{3.10}$$
$$Lv(x) + \lambda\rho v(x) = 0. \tag{3.11}$$

We now multiply (3.10) by $v(x)$ and (3.11) by $u(x)$, and subtract:

$$uLv - vLu = 0$$

or, using the result above

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

Hence

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

i.e.,

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

Since u is known, this is differential equation for v (first order!). 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 component proportionsl to u into the solution, which we already know is allowed. We can also take $c = 1$, since the multiplication with 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 almost always the interval $[a, b]$, on which the Sturm-Liouville operator is defined, is delimited by such special singular points, and $p(a) = p(b) = 0$!

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 Hermitian S-L operators, we state witout 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 $u_n(x) = u_n^*(x)$ apart from a multiplicative constant. 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

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

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

3. The number of nodes in the n-th eigenvector, if the corresponding eigenvalues are ordered as above, is exactly equal to n.

4. Eigenfunctions u, v with $u \neq v$ are orthogonal with weight function $\rho(x)$,

   $$(u, v)_\rho = \int_a^b dx\, \rho(x) u^*(x) v(x) = 0 \quad .$$

5. The eigenfunctions

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

   form a complete basis set of functions on the interval $[a, b]$ satisfying the boundary conditions. (Proof 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 this from the Legendre polynomials discussed in the second year math course (or see http://walet.phy.umist.ac.uk/2C1).

These functions 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

$$\frac{d^2}{dz^2}\psi(z) + (2\lambda - z^2)\psi(z) = 0. \tag{3.12}$$

Functions in $\mathcal{L}^2(\mathbb{R})$ must decay sufficiently fast at infinity: not all solutions to (3.12) 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 (3.12), and find an equation for f,

$$f''(z) - 2zf'(z) + (2\lambda - 1)f(z) = 0. \tag{3.13}$$

This is of Sturm-Liouville form; actually we can multiply if with $p(z) = e^{-z^2}$ to find

$$[\exp(-z^2)f'(z)]' + (2\lambda - 1)\exp(-z^2)f(z) = 0. \tag{3.14}$$

This is a Sturm-Liouville problem, with eigenvalues $2\lambda - 1$. The points $z = \pm\infty$ are singular, since p vanishes. Thus $[a, b]$ is actually $(-\infty, \infty)$, as we would expect.

So how do we tackle Hermite's equation (3.13)? The technique should be familiar: we substitute a Taylor series around $z = 0$,

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

and collect the coefficient of terms containing the same power of z, and equate all these coefficients to zero

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

This recurrence relation can be used to bootstrap our way up from c_0 or c_1. It never terminates, unless $(2\lambda - 1)$ is an even integer. It must terminate to have the correct behaviour at infinity (like a power). 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 call $\lambda = n + 1/2$, with n integer, the first solution is $H_0(z) = 1$, $H_1(z) = z$, $H_2(z) = 1 - z^2$, ... These are orthogonal with respect to the weighted inner product

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

This shows that the eigenfunctions of the Harmonic oscillator are all of the form

$$\psi_n(x) = \exp(-x^2/(2b^2))H_n(x/b)$$

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,

$$\Big[(1-x^2)y'(x)\Big]' + \lambda y(x) = 0. \tag{3.15}$$

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. (3.15) 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

$$(1-2tx+t^2)^{-1/2} = \sum_n t^n P_n(x), \qquad (t \in [-1,1]), \tag{3.16}$$

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. (3.16) satisfy Eq. (3.15).

1. First we differentiate (3.16) w.r.t. to x and t,

$$t(1-2tx+t^2)^{-3/2} = \sum_n t^n P_n'(x), \tag{3.17}$$

$$(x-t)(1-2tx+t^2)^{-3/2} = \sum_n n t^{n-1} P_n(x). \tag{3.18}$$

2. We then replace $(1-2tx+t^2)^{-1/2}$ on the l.h.s. of (3.17) 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

$$P_n(x) = P_{n+1}'(x) - 2xP_n'(x) + P_{n-1}'(x). \tag{3.19}$$

3. Since $(x-t)$ times the l.h.s. of (3.17) equals t times the l.h.s. of (3.18), 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

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

4. Combine (3.19) with (3.20) to find

$$(n+1)P_n(x) = P'_{n+1}(x) - xP'_n(x). \tag{3.21}$$

5. Let n go to $n-1$ in (3.21), and subtract (3.20) 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 (3.20) 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,

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

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

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

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

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

Let us first assume $r_2 > r_1$,

$$\begin{aligned}|\boldsymbol{r}_1 - \boldsymbol{r}_2|^{-1} &= \frac{1}{\sqrt{r_1^2 + r_2^2 - 2r_1 r_2\cos\theta}} \\ &= \frac{1}{r_2\sqrt{(r_1/r_2)^2 + 1 - 2r_1/r_2\cos\theta}} \\ &= \frac{1}{r_2}\sum_n \left(\frac{r_1}{r_2}\right)^n P_n(\cos\theta),\end{aligned} \tag{3.22}$$

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

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

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

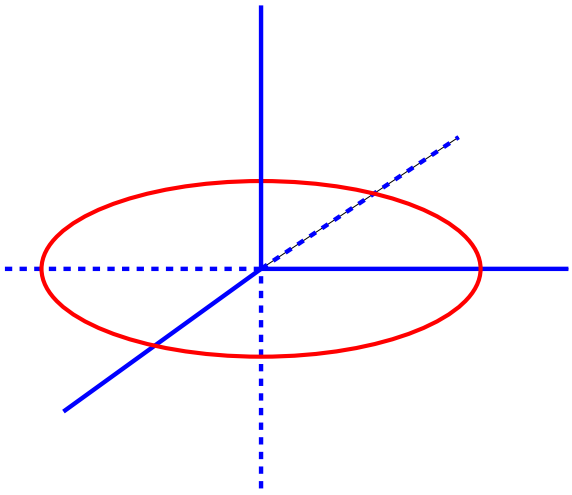

Figure 3.5: A homogeneously charged ring in the xy plane.

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,

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

Substituting the generating function, we find

$$\begin{aligned} \int_{-1}^{1} (1 - 2xt + t^2)^{-1} \, dx &= \frac{1}{t} \ln \left(\frac{1+t}{1-t} \right) \\ &= \frac{1}{t} \sum_{m=1}^{\infty} \frac{1}{m} t^m - \frac{1}{m} (-t)^m \\ &= \sum_{m=2n+1} \frac{2}{2n+1} t^{2n}. \end{aligned} \tag{3.23}$$

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

$$V = \sum_{n=0}^{\infty} c_n \frac{a^n}{r^{n+1}} P_n(\cos\theta). \tag{3.24}$$

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 (3.24)? 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

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

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

$$r^2R''(r) + rR'(r) + \lambda r^2R(r) - m^2R(r) = 0, \tag{3.25}$$

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

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

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

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.

Chapter 4

Green functions

4.1 General properties

The Green 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 hermitian operator 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 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 function, without it ever being made explicit. The problem of interest is the determination of the electrostatic potential $\Phi(\boldsymbol{x})$ for a *static* charge distribution $\rho(\boldsymbol{x})$. From $\boldsymbol{\nabla}\cdot\boldsymbol{E} = \rho/\epsilon_0$ and $\boldsymbol{E} = -\boldsymbol{\nabla}\Phi$ we can easily show that

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

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

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

$$\nabla^2\Phi(\boldsymbol{x}) = -(q/\epsilon_0)\delta^{(3)}(\boldsymbol{x}-\boldsymbol{x}').$$

[The notation $\delta^{(3)}(\boldsymbol{x})$ stands for the 3D δ function $\delta(x)\delta(y)\delta(z)$.] We all know the solution, which is Coulomb's law,

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

In other words, the Green function G which solves

$$\nabla^2 G(\boldsymbol{x},\boldsymbol{x}') = \delta^{(3)}(\boldsymbol{x}-\boldsymbol{x}')$$

is

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

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

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

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

4.1.2 The eigenstate method

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

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

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

$$Lu_n(x) = \lambda_n u_n(x), \tag{4.7}$$

where we have made the assumption that there are no zero eigenvalues.

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,

$$\begin{aligned} u(x) &= \sum_n c_n u_n(x), \\ f(x) &= \sum_n d_n u_n(x). \end{aligned} \tag{4.8}$$

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

Now substitute (4.8) into (4.7) 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

$$0 = c_0\lambda_0 = d_0. \tag{4.9}$$

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

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

Here

$$G(x, x') = c u_0(x) + \sum_{n=1}^{\infty} \frac{1}{\lambda_n} \int u_n(x) u_n(x') \quad ,$$

with

$$c = c_0 / \int f(x)\, dx \quad .$$

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 $f(x) = F(x)/T$,

$$v'' + k^2 v = f(x), \tag{4.10}$$

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

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

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

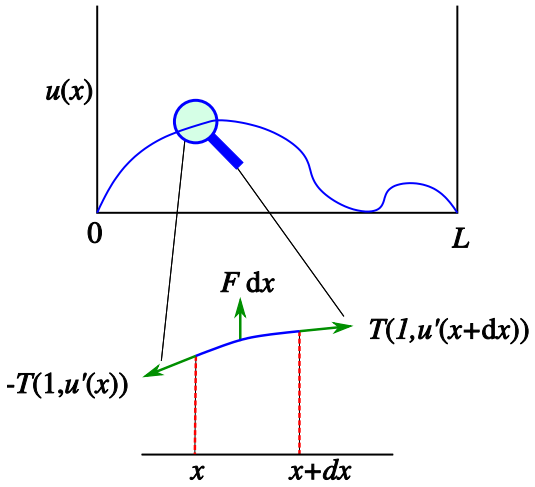

Figure 4.1: The balance of forces in a driven string

If we write this as $v_n'' = (\lambda_n - k^2)v_n$, we recognise a problem of the simple form $y'' = ky$, 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

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

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

In this method for solving second order equations of the form

$$\left[\frac{d^2}{dx^2} + \alpha(x)\frac{d}{dx} + \beta(x)\right] G(x,x') = \delta(x - x')$$

one

(a) solves (4.1.3) 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 $x = x'$, and the discontinuity of the derivative, which is easily shown to be the inverse of the coefficient of the second derivative in the ODE,

$$\frac{d}{dx}G(x' + \epsilon, x') - \frac{d}{dx}G(x' - \epsilon, x') = 1 \quad ,$$

see below for an explanation.

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

$$\left(\frac{d^2}{dx^2}+k^2\right)G(x,x')=\delta(x-x'), \tag{4.11}$$

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

We first solve the problem

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

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 (4.11) over x around x' (where ϵ is a very small number)

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

or

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

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

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

From the form of G derived above, we conclude that

$$\begin{aligned} A(x')\sin kx' &= B(x')\sin k(L-x') \\ -B(x')k\cos k(L-x')-A(x')k\cos kx' &= 1 \end{aligned} \tag{4.12}$$

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

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

Taking this 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 is a common feature on Green functions.

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

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

where ϕ satisfies the time-independent Schrödinger equation

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

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

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

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, $\phi(\boldsymbol{r}) \to e^{ikz}$, 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 spherical waves.

> Spherical waves are solutions to the radial part of the Laplace operator,
>
> $$-\frac{1}{r^2}\frac{d}{dr}r^2\frac{d}{dr}f(r) = k^2 f(r).$$
>
> Solutions are $\frac{e^{\pm ikr}}{r}$. Using the radial part of the momentum operator $\boldsymbol{p}_r = \boldsymbol{e}_r \frac{\hbar}{i}\frac{d}{dr}$, we find that the plus sign in the exponent corresponds to outward travelling ways; 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

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

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 $\phi(\boldsymbol{r}) = e^{ikz} + \chi(\boldsymbol{r})$, we find we have to solve the equation

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

subject to the boundary condition

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

Solve this by the Green's function method,

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

or using translational invariance,

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

Actually, since we know the solution to

$$\nabla^2 G_0(\boldsymbol{r}) = \delta(\boldsymbol{r})$$

is

$$G_0 = -\frac{1}{4\pi}\frac{1}{r} \quad ,$$

we know that the G must approach this solution for $r \downarrow 0$. With the fact that

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

for $r \neq 0$, and that the boundary conditions require a plus sign in the exponent, we conclude that

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

Using Stoke's theorem, it is not hard to show that

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

This also shows we really have a δ function.

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

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

If we also remember how ρ is related to ϕ, we get (the coordinate representation of) the integral equation for scattering,

$$\phi(\boldsymbol{r}) = e^{ikz} + \frac{2m}{\hbar^2}\int d^3r' G(\boldsymbol{r}, \boldsymbol{r}')V(\boldsymbol{r}')\phi(\boldsymbol{r}') \quad . \tag{4.13}$$

This equation is called the *Lipmann-Schwinger* equation.

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 (4.13). This results in the equation

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

For weak potentials we can truncate at first order:

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

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

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

so

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

with

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

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 may have met the equations for the scalar potential Φ and vector potential $\boldsymbol{A}$, which in free space are of the form

$$\Box\Phi = 0, \qquad \Box\boldsymbol{A} = 0, \qquad \text{where } \Box = \frac{1}{c^2}\frac{\partial^2}{\partial t^2} - \boldsymbol{\nabla}^2.$$

These equation are satisfied for the "gauge choice" $\nabla\cdot\boldsymbol{A} = 0$, the Coulomb or radiation gauge.

As usual we can analyse what happens with external charge and current distributions, where the potentials satisfy

$$\Box\Phi = \frac{\rho(\boldsymbol{r},t)}{\epsilon_0}, \qquad \Box\boldsymbol{A} = \mu_0\boldsymbol{j}(\boldsymbol{r},t). \tag{4.14}$$

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

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

The boundary conditions are

1. that the potentials should go to zero far from sources, $G(\boldsymbol{r},t;\boldsymbol{r}',t) \to 0$ as $r \to \infty$.
2. that the effect of a source always occurs after its cause (causality) $G(\boldsymbol{r},t;\boldsymbol{r}',t) = 0$ 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 function only depends on $(\boldsymbol{r}-\boldsymbol{r}')$ and $t-t'$,

$$G(\boldsymbol{r},t;\boldsymbol{r}',t) = G(\boldsymbol{r}-\boldsymbol{r}',t-t') \quad .$$

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

$$\left(\frac{1}{c^2}\frac{\partial^2}{\partial t^2} - \boldsymbol{\nabla}^2\right) G(\boldsymbol{r},t) = \delta(\boldsymbol{r})\delta(t). \tag{4.15}$$

4.3.1 Solution for the Green 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.

$$\begin{aligned}
\tilde{G}(\boldsymbol{k},\omega) &= \int d^3r \int dt\, G(\boldsymbol{r},t)\exp[-i(\boldsymbol{k}\cdot\boldsymbol{r}-\omega t)] \quad , \\
G(\boldsymbol{r},t) &= \int \frac{d^3k}{(2\pi)^3}\int \frac{d\omega}{2\pi}\,\tilde{G}(\boldsymbol{k},\omega)\exp[i(\boldsymbol{k}\cdot\boldsymbol{r}-\omega t)] \quad , \\
\delta(\boldsymbol{r})\delta(t) &= \int \frac{d^3k}{(2\pi)^3}\int \frac{d\omega}{2\pi}\exp[i(\boldsymbol{k}\cdot\boldsymbol{r}-\omega t)] \quad ,
\end{aligned} \tag{4.16}$$

and solve for the Fourier transform $\tilde{G}(\boldsymbol{k},\omega)$ by substituting the second of these relations into Eq. (4.15): This equation becomes

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

If we now equate the integrands, we find that

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

We now substitute $\tilde{G}(\boldsymbol{k},\omega)$ back into (4.16)

$$G(\boldsymbol{r},t) = -c^2\int \frac{d^3k}{(2\pi)^3}\int \frac{d\omega}{2\pi}\,\frac{\exp[i(\boldsymbol{k}\cdot\boldsymbol{r}-\omega t)]}{\omega^2-c^2k^2} \quad . \tag{4.17}$$

Integration over Euler angles

The d^3k part of the integral (4.17) is of the generic form

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

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 $\boldsymbol{r}$, and find

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

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 (4.17) to find

$$G(\boldsymbol{r}, t) = -\frac{c^2}{(2\pi)^2 ir} \int_{-\infty}^\infty kdk \int_{-\infty}^\infty \frac{d\omega}{2\pi} \frac{\exp[i(kr - \omega t)]}{\omega^2 - c^2k^2}. \tag{4.18}$$

We now tackle the ω integral,

$$\int_{-\infty}^\infty \frac{d\omega}{2\pi} \frac{e^{-i\omega t}}{\omega^2 - c^2k^2}. \tag{4.19}$$

The problem with this integrand is that we have poles at $\omega = \pm ck$ on the real axis, and we have to integrand 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,

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

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

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

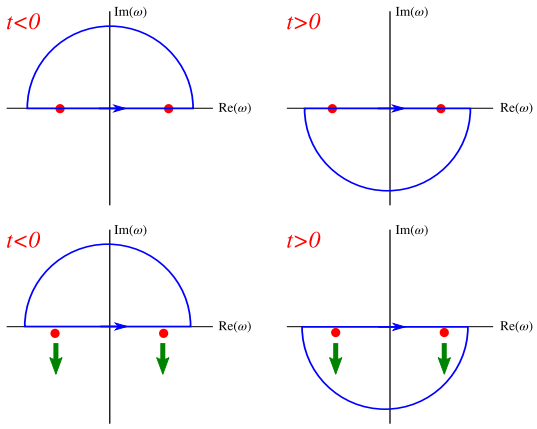

Figure 4.2: The contours used in the ω integral (4.19).

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 (4.18), we find that ($t > 0$!)

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

We discard the second delta function above, since its argument $r + ct > 0$ if $t > 0$, and thus the δ function is always zero.

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

$$G(\boldsymbol{r},t;\boldsymbol{r}',t) = \frac{c}{4\pi|\boldsymbol{r}-\boldsymbol{r}'|}\delta\big(|\boldsymbol{r}-\boldsymbol{r}'| - c(t-t')\big). \tag{4.20}$$

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

Two special cases can be obtained simply:

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

$$\begin{aligned} \Phi(\boldsymbol{x}) &= \int d^3\boldsymbol{r}'dt' \frac{c}{4\pi|\boldsymbol{r}-\boldsymbol{r}'|}\delta\left(|\boldsymbol{r}-\boldsymbol{r}'| - c(t-t')\right)\frac{\rho(\boldsymbol{r}')}{\epsilon_0} \\ &= \int d^3\boldsymbol{r}' \frac{1}{4\pi\epsilon_0|\boldsymbol{r}-\boldsymbol{r}'|}\frac{\rho(\boldsymbol{r}')}{\epsilon_0}, \end{aligned}$$

   using

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

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

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

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

The δ function selects those points on the path followed by the charge that intersect the light-cone with apex $\boldsymbol{r}, t$ at a time $\boldsymbol{s}(t'), t'$.

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

Green functions for wave equations in (2+1) dimensions 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:

$$G^{(2)}(x-x', y-y', t-t') = \int dz'\, G(\boldsymbol{r}, t; \boldsymbol{r}', t') \tag{4.21}$$

for $t > t'$.

This can be checked quite simply. From

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

We find that

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

If we now swap differentiation and integration, we get

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

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

From equation (4.20) we find

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

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

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

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

$$G^{(2)}(\boldsymbol{x}-\boldsymbol{x}',t-t') = \frac{c}{2\pi}\frac{1}{(c^2(t-t')^2-|\boldsymbol{x}-\boldsymbol{x}'|^2)^{1/2}} \tag{4.22}$$

for $t > t'$, where $\boldsymbol{x}$ is a 2-dimensional space vector $\boldsymbol{x} = (x, y)$. 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

Variational calculus

5.1 Functionals and stationary points

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

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

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 5.1:

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	$\pi^3/3$
$\vdots$	$\vdots$

5.2 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

$$I[y] = \int_a^b dx\, F(y(x), y'(x), x) \quad , \tag{5.1}$$

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

$$\epsilon(a) = \epsilon(b) = 0. \tag{5.2}$$

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*

$$\frac{\partial F}{\partial y(x)} - \frac{d}{dx} \frac{\partial F}{\partial y'(x)} = 0. \tag{5.3}$$

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 adding a delta function. In the case above,
$$I[y] = \int y(x)\delta(x)\, dx.$$

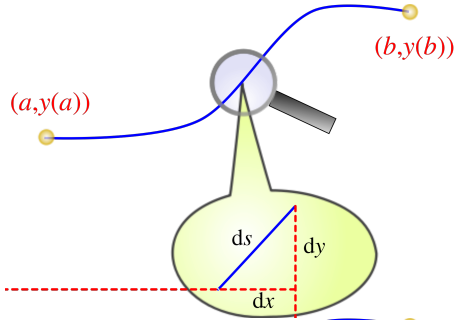

Figure 5.1: The distance between two points along a path connecting two fixed points

- 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.

5.3 Special cases with examples: first integrals

Let us look at a few special cases for the functional I defined in (5.1).

5.3.1 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

$$\frac{\partial F}{\partial y'(x)} = \text{constant}. \tag{5.4}$$

This equation is called the "first integral" of the problem.

Example 5.2:

Show that the shortest distance between any two fixed points (in 2D space, for simplicity) is along a straight line.

Solution:

We parametrise 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

$$\begin{aligned} c &= \frac{y(b) - y(a)}{b - a}, \\ d &= \frac{by(a) - ay(b)}{b - a}. \end{aligned}$$

5.3.2 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

$$\boxed{F - y' \frac{\partial F}{\partial y'(x)} = \text{constant} \quad .} \tag{5.5}$$

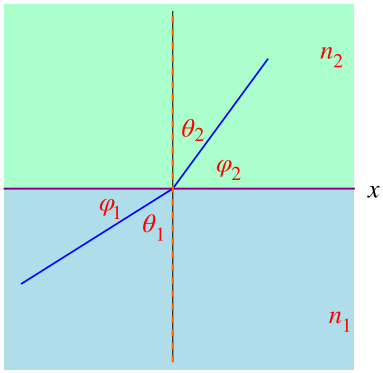

Figure 5.2: Snell's law

Example 5.3:

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 (5.5) 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

$$\boxed{n(y) = \text{const}\sqrt{1+y'^2} \quad .} \tag{5.6}$$

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. 5.2. 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. (5.6) that $n\cos\phi =$ 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 5.4:

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 brachistichrone 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

$$T[y] = \int_0^b \left(\frac{1+y'^2}{2gy}\right)^{1/2} dx. \tag{5.7}$$

We now drop the factor $2g$ from the denominator, and minimise

$$I[y] = \int_0^b \left(\frac{1+y'^2}{y}\right)^{1/2} dx.$$

Since $F = \left(\frac{1+y'^2}{y}\right)^{1/2}$ has no explicit x dependence, we find

$$F - \frac{\partial F}{\partial y'}y' = \text{constant},$$

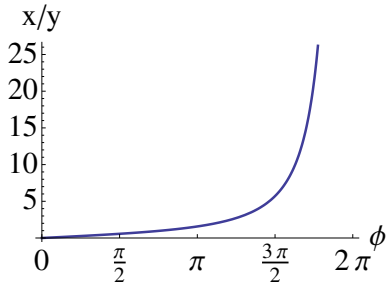

Figure 5.3: x/y as a function of ϕ_0.

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

$$y(\phi) = 2R/(1+y'^2) = 2R\sin^2(\phi/2) = R(1-\cos\phi). \tag{5.8}$$

That would be fine if we knew also $x(\phi)$, so we can represent the curve by a parametric plot! We have from (5.8)

$$\frac{dx}{d\phi} = \frac{1}{dy/dx}\frac{dy}{d\phi} = \tan(\phi/2)2R\sin\phi/2\cos\phi/2 = 2R\sin^2\phi/2 = y.$$

Thus using Eq. (5.8) 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. 5.3.

Once we have fixed the range of ϕ, we can then solve for the brachystochrone, see Fig. 5.4 for a few examples.

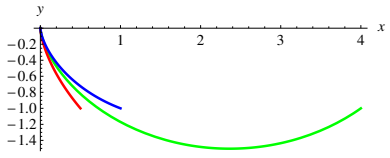

Figure 5.4: A few brachystochrone curves for $y_f = 1$.

So what is the value of the travel time? Substituting the solution into Eq. (5.7) we get

$$\begin{aligned} T &= \int_0^{\phi_0} \left(\frac{2R}{2gy^2}\right)^{1/2} y d\phi \\ &= \phi_0 \sqrt{\frac{R}{g}} \quad . \end{aligned}$$

5.4 Generalisations

5.4.1 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?

5.4.2 One endpoint free

Let's look at the simplest case: we once again want to find a function y such that

$$\delta I[y] = \delta \int_a^b dx\, F(y, y', x) = 0 \tag{5.9}$$

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,

$$\frac{\partial F}{\partial y'}\bigg|_{x=b} = 0. \tag{5.10}$$

Example 5.5:

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, $y(x_f) = 2x_f/\pi$.

5.4.3 More than one function: Hamilton's principle

We often encounter functionals of several functions $y_1, y_2, \ldots, y_n$ of the form

$$I[\{y_i\}] = \int_a^b dx\, F(\{y_i(x), y_i'(x)\}, x), \qquad i = 1, 2, \ldots, N. \tag{5.11}$$

We now look for stationary points with respect to all y_i, again keeping the functions at the endpoints fixed. Generalising 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,

$$\frac{\partial F}{\partial y_i(x)} - \frac{d}{dx}\frac{\partial F}{\partial y_i'(x)} = 0, \qquad i = 1, 2, \ldots, N. \tag{5.12}$$

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 "generalised coordinates" $q_i(t)$, $i = 1, 2, \ldots, N$, which fix all spacial 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, also 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*,

$$\frac{\partial L}{\partial q_i(t)} - \frac{d}{dt}\left(\frac{\partial L}{\partial \dot{q}_i(t)}\right) = 0. \tag{5.13}$$

Example 5.6:

Derive Newton's equation of motion for a particle of mass m attached to a spring from the Lagrangian.

Solution:

$$L = T - V = \frac{1}{2} m\dot{x}^2 - \tfrac{1}{2} k x^2 \quad .$$

From (5.13) 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 generalisation 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 $\frac{\partial L}{\partial \dot{q}_i(t)}$ as the "canonical momentum" p_i, we find that p_i is a constant of motion, i.e., doesn't change.

The form of mechanics based on Lagrangians is more amenable to generalisation 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 fixed external E.M. fields, where the Lagrangian takes the (at first sight surprising) form

$$L(x, \dot{x}, t) = -mc^2 \left(1 - \dot{x}^2/c^2\right)^{1/2} + q\boldsymbol{A} \cdot \dot{\boldsymbol{x}} - q\Phi \quad .$$

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 $\boldsymbol{A}$ and Φ depend on $\boldsymbol{x}$)

$$\frac{d}{dt}\frac{m\dot{x}_i}{(1 - \dot{x}^2/c^2)^{1/2}} = q(\nabla_i \boldsymbol{A}) \cdot \dot{\boldsymbol{x}} q - q\partial_t A_i - q\nabla_i \Phi.$$

With a standard definition of $\boldsymbol{B} = \boldsymbol{\nabla} \times \boldsymbol{A}$ and $\boldsymbol{E} = -\boldsymbol{\nabla}\Phi - \partial_t \boldsymbol{A}$, we have

$$\frac{d}{dt}\boldsymbol{p} = q(\boldsymbol{v} \times \boldsymbol{B} + \boldsymbol{E}).$$

5.4.4 More dimensions: field equations

For dynamics in more dimensions $x = x^1, x^2, \ldots, x^N$, we should look at the generalisation of the action,

$$\mathcal{S}[\phi] = \int_\Omega d\tau\, \mathcal{L}(\phi(x), \partial_\mu \phi(x), x) \tag{5.14}$$

where $d\tau = dx^1 dx^2 \ldots dx^N$ is an infinitesimal volume in N-dimensional space and

$$\phi_{,\mu} \equiv \partial_\mu \phi = \frac{\partial \phi}{\partial x^\mu}, \qquad \mu = 1, 2, \ldots, N. \tag{5.15}$$

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. 5.5.

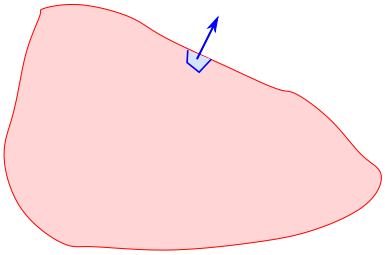

Figure 5.5: The volume Ω and the surface area dS.

Looking for variations to first order in ϵ, we get

$$\begin{aligned}\delta\mathcal{S} &= \int_\Omega \left(\epsilon(x)\frac{\partial\mathcal{L}}{\partial\phi(x)} + \sum_{n=1}^{N}\epsilon_{,\mu}\frac{\partial\mathcal{L}}{\partial\phi_{,\mu}(x)}\right)d\tau \\ &= \int_\Omega \left[\epsilon(x)\frac{\partial\mathcal{L}}{\partial\phi(x)} + \sum_{n=1}^{N}\partial_\mu\left(\epsilon\frac{\partial\mathcal{L}}{\partial\phi_{,\mu}(x)}\right) - \epsilon\sum_{n=1}^{N}\partial_\mu\left(\frac{\partial\mathcal{L}}{\partial\phi_{,\mu}(x)}\right)\right]d\tau \\ &= \int_\Omega \epsilon\left[\frac{\partial\mathcal{L}}{\partial\phi(x)} - \sum_{\mu=1}^{N}\partial_\mu\left(\frac{\partial\mathcal{L}}{\partial\phi_{,\mu}(x)}\right)\right]d\tau + \sum_{\mu=1}^{N}\int_{\partial\Omega}\epsilon\frac{\partial\mathcal{L}}{\partial\phi_{,\mu}(x)}\,dS_\mu \quad .\end{aligned}$$

($dS_\mu = \prod_{i\neq\mu} dx^i = d\tau/dx^\mu$). The surface integral vanishes due to the boundary conditions, and requiring $\delta\mathcal{S} = 0$, we find the Euler-Lagrange equation,

$$\frac{\partial\mathcal{L}}{\partial\phi} - \sum_\mu \partial_\mu\frac{\partial\mathcal{L}}{\partial\phi_\mu} = 0, \tag{5.16}$$

or, more explicitly:

$$\frac{\partial\mathcal{L}}{\partial\phi(x)} - \sum_\mu \frac{\partial}{\partial x^\mu}\frac{\partial\mathcal{L}}{\partial\partial_\mu\phi(x)} = 0. \tag{5.17}$$

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

$$\frac{\partial\mathcal{L}}{\partial\phi} - \frac{\partial}{\partial t}\frac{\partial\mathcal{L}}{\partial\dot{\phi}} - \frac{\partial}{\partial x}\frac{\partial\mathcal{L}}{\partial\phi'} = 0$$

with

$$\dot{\phi} = \frac{\partial\phi}{\partial t}, \qquad \phi' = \frac{\partial\phi}{\partial x}.$$

For that case the action takes the form

$$\mathcal{S} = \int dt \int dx\, \mathcal{L}(\phi, \phi', \dot{\phi}, x, t).$$

Clearly this suggest that $\int dx\,\mathcal{L}$ plays the role of Lagrangian, and we call $\mathcal{L}$ the *Lagrange density*.

Example 5.7:

Describe the motion of an elastic stretched string, with fixed endpoints, assuming small deformation, see Fig. 5.6.

Solution:

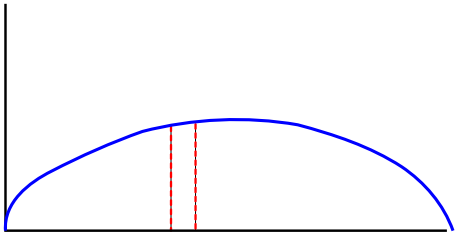

Figure 5.6: The stretched string

As per usual, we parametrise the position by $x, y(x,t)$, 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

$$L = \int (dK - dV) = \int \left(\frac{1}{2}\rho\dot{y}^2 - T\frac{1}{2}y'^2\right)dx = \int dx\,\mathcal{L},$$

and

$$\mathcal{S} = \int\int \left(\frac{1}{2}\rho\dot{y}^2 - \frac{1}{2}Ty'^2\right)dx\,dt.$$

Using the previous results with $\phi \to y$, we get

$$\begin{aligned} 0 &= \frac{\partial\mathcal{L}}{\partial y} - \frac{\partial}{\partial t}\frac{\partial\mathcal{L}}{\partial\dot{y}} - \frac{\partial}{\partial x}\frac{\partial\mathcal{L}}{\partial y'} \\ &= -\frac{\partial}{\partial t}\rho\dot{y} - \frac{\partial}{\partial x}(-Ty') \\ &= -\rho\ddot{y} + Ty''. \end{aligned}$$

We thus get the wave equation

$$\frac{1}{c^2}\ddot{y} = y'',$$

with $c^2 = T/\rho$.

Example 5.8:

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,

$$\mathcal{S} = \int dt \int_0^{2\pi} d\phi \left[\rho l \tfrac{1}{2} (\dot{x}^2 + \dot{y}^2) - \kappa \tfrac{1}{2} \left(\sqrt{x'^2 + y'^2} - l \right)^2 \right].$$

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 5.9:

Show that the Lagrangian density (in 3+1 dimensions)

$$\mathcal{L} = \frac{1}{2} \left[(\partial_t \phi)^2 - (\boldsymbol{\nabla} \phi)^2 - m^2 \phi^2 \right]$$

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 amiguity to this, since we have

$$\mathcal{S} = \int dt \int d^3x \mathcal{L} = \int d^4x \mathcal{L},$$

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.

5.4.5 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!

5.5 Constrained variational problems

It is quite common that we have subsidiary conditions on a minimisation problem, i.e., we want to know the minimum provided that certain other conditions hold. Let us first analyse this problem for ordinary functions first

5.5.1 Lagrange's undetermined multipliers

To find the stationary points of a function $f(\boldsymbol{x})$ subject to constraints $g_k(\boldsymbol{x}) = 0$, $(k = 1, 2, \ldots)$, we can solve an extended problem and find the unconstrained stationary points of the extended functional

$$F(\boldsymbol{x}, \lambda_1, \lambda_2, \ldots) = f(\boldsymbol{x}) - \lambda_1 g_1(\boldsymbol{x}) - \lambda_2 g_2(\boldsymbol{x}) - \ldots, \tag{5.18}$$

w.r.t to $\boldsymbol{x}$ and λ_i.

Let's look at a somewhat explicit example. We wish to minimise a function $f(x, y)$ subject to a single constraint $g(x, y) = 0$. We thus need to minimise the extended function

$$F(x, y, \lambda) = f(x, y) - \lambda g(x, y),$$

and find

$$\begin{aligned}
\frac{\partial F}{\partial x} &= \frac{\partial f}{\partial x} - \lambda \frac{\partial g}{\partial x} = 0 \quad , \\
\frac{\partial F}{\partial y} &= \frac{\partial f}{\partial y} - \lambda \frac{\partial g}{\partial y} = 0 \quad , \\
\frac{\partial F}{\partial \lambda} &= g(x, y) = 0.
\end{aligned}$$

The last line clearly states that the constraint must be implemented. The new terms (proportional to λ) in the first two lines say that a *constrained minimum* is reached when the gradient of the function is parallel to the gradient of the constraint. This says that there is no change in the function, unless we violate our constraint condition–clearly a sensible definition of a stationary point.

Example 5.10:

Find stationary points of $f(x,y)$ under the subsidiary condition $x^2+y^2=1$.

Solution:

Look for stationary points of

$$F = xy - \lambda(x^2+y^2-1),$$

which are given by the solution(s) of

$$\begin{aligned}\frac{\partial F}{\partial x} &= y - 2\lambda x = 0,\\ \frac{\partial F}{\partial y} &= x - 2\lambda y = 0,\\ \frac{\partial F}{\partial \lambda} &= x^2+y^2-1 = 0.\end{aligned}$$

The first two conditions give $x^2=y^2$, and from the constraint we find $(x,y)=(\pm 1/\sqrt{2}, \pm 1/\sqrt{2})$. The values of λ associated with this are $\lambda = \pm 1/2$.

5.5.2 Generalisation to functionals

We look for stationary points of $I[y]$ subject to a constraint $J[y]=C$, (can also be multiple constraints) where I, J are given functionals of $y(x)$ and C is a given constant.

To do this: we solve for the stationary points of an extended funtional,

$$K[y,\lambda] = I[y] - \lambda(J[y]-C) \quad , \tag{5.19}$$

with respect to variations in the function $y(x)$ and λ. We then have

$$\delta K = \delta I - \lambda\,\delta J - d\lambda\,(J[y]-C),$$

which can be dealt with as an unconstrained variational problem. Its solution can be slightly tricky; one way is to solve the problem

$$\delta K = \delta I - \lambda \delta J$$

for fixed λ to find $y(x)$ as a function of λ, and then use the constraint $J[y]=C$ to find the allowed value(s) of λ, and thus the solution.

Example 5.11:

Find a closed curve of fixed length $L = 2\pi l$ which encloses the maximum area A. (The isoperimetric problem, see Fig. 5.7.)

Solution:

Describe the curve in polar coordinates by $(\theta, r(\theta))$, assuming the origin lies within the curve. We then find that

$$\begin{aligned}A[r] &= \int_0^{2\pi} \frac{1}{2} r^2 d\theta,\\ L[r] &= \int dl = \int_0^{2\pi} (r^2 d\theta^2 + dr^2)\\ &= \int_0^{2\pi} \sqrt{r^2 + r'^2}\, d\theta = 2\pi l \quad .\end{aligned}$$

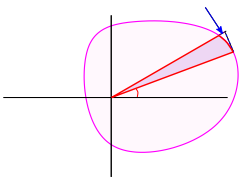

Figure 5.7: The isoperimetric problem.

We now need to find stationary points of

$$I[r,\lambda] = A[r] - \lambda(L[r] - 2\pi l) = \int_0^{2\pi} (r^2/2 - \lambda\sqrt{r^2 + r'^2})d\theta + 2\pi l.$$

Minimising with respect to $r(\theta)$, we find a problem where there is no explicit dependence of the function we usually call "F" on θ, and thus

$$F - r'\frac{\partial F}{\partial r'} = K.$$

Explicitly,

$$\begin{aligned} K &= \frac{1}{2}r^2 - \lambda\sqrt{r^2 + r'^2} - r'\left(-\lambda(-1/2)2r'/\sqrt{r^2 + r'^2}\right) \\ &= \frac{1}{2}r^2 - \lambda\frac{r^2}{\sqrt{r^2 + r'^2}} \quad , \end{aligned} \tag{5.20}$$

together with the constraint

$$L = \int_0^{2\pi} \sqrt{r^2 + r'^2}d\theta = 2\pi l.$$

Unfortunately, this equation is not easy to solve in general, but we can guess one solution: Look at $\lambda = 0$ when we find $r = l$, $K = l^2/2$. This describes a circle through the origin. By translational invariance we see any other circle also satisfies this condition.

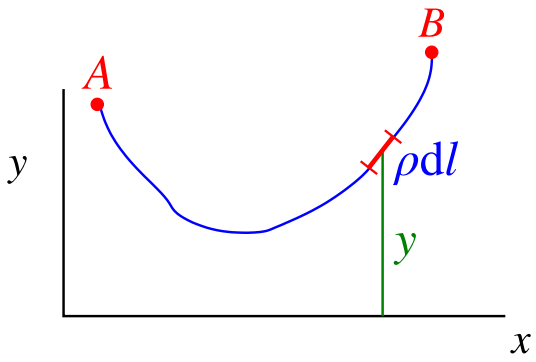

Figure 5.8: The catenary

Example 5.12:

What is the equilibrium curve for a flexible "chain" of length l and density ρ per unit length, when we hang it between two points A and B. (*The catenary*, see Fig. 5.8.)

Solution:

We need to minimise the gravitational potential energy

$$E[y] = \int_a^B \rho dl\, y = \int_a^b \rho g y \sqrt{1+y'^2}dx,$$

subject to the constraint of constant length $L[y] = l$, with

$$L[y] = \int_A^B dl = \int_a^b \sqrt{1+y'^2}dx.$$

Thus we need to find stationary points of $G[y] = E[y] - \lambda(L[y] - l)$.

As usual the variation with respect to y is simple, since the integrand

$$F(y, y', \lambda) = (\rho g y - \lambda)\sqrt{1+y'^2}$$

has no *explicit* dependence on x we can use the first integral,

$$F - y' \frac{\partial F}{\partial y'} = C,$$

or explicitly,

$$(\rho g y - \lambda)\sqrt{1+y'^2} - y'(\rho g y - \lambda)\frac{y'}{\sqrt{1+y'^2}} = \frac{\rho g y - \lambda}{\sqrt{1+y'^2}} = C.$$

This can be solved by making a shift on y,

$$u = y - \lambda/(g\rho), \qquad \alpha = C/(g\rho).$$

The new function u satisfies

$$\begin{aligned} u &= \alpha\sqrt{1+u'^2} && \Longrightarrow \\ u^2/\alpha^2 &= 1+u'^2 && \Longrightarrow \\ u'^2 &= (u^2-\alpha^2)/\alpha^2 && \Longrightarrow \\ \frac{\alpha u'}{\sqrt{u^2-\alpha^2}} &= 1 && \Longrightarrow \\ \int \frac{\alpha du}{\sqrt{u^2-\alpha^2}} &= \int dx \quad . \end{aligned}$$

Now use $u = \alpha\cosh w$, $du = \alpha \sinh w\, dw$ to find

$$\begin{aligned} \int \frac{\alpha^2 \sinh w\, dw}{\alpha \sinh w} &= x && \Longrightarrow \\ \alpha w &= x - x_0 && \Longrightarrow \\ u &= \alpha\cosh((x-x_0)/\alpha) && \Longrightarrow \\ y &= \alpha\cosh((x-x_0)/\alpha) + \lambda/(\rho g) \quad . \end{aligned}$$

The three constants α, x_0 and λ are determined by the condition that line goes through A and B and has length

$$l = \int_a^b \left(1+\alpha^2\sinh^2(x-x_0)/\alpha\right)^{1/2} dx.$$

The point x_0 is where the curve gets closest to the ground. If $y(a) = y(b)$, $x_0 = (a+b)/2$ by symmetry.

A good demonstration can be found on "Catenary: The Hanging Chain" on The Wolfram Demonstrations Project.

5.5.3 Eigenvalue problems

Consider the eigenvalue equation for the function $u(x)$

$$Lu = \lambda\rho u \quad , \tag{5.21}$$

where L is an Hermitian operator, $\rho(\boldsymbol{x})$ is a positive, real weight function. We now look for the stationary points of

$$I[u] = \int d\tau\, u^* Lu \tag{5.22}$$

subject to the normalisation constraint

$$\int d\tau\, \rho u^* u = 1. \tag{5.23}$$

We first look for an unconstrained stationary point of

$$J_\lambda[u] = \int d\tau\, u^* Lu - \lambda\left(\int d\tau\, \rho u^* u - 1\right),$$

and vary λ to obtain a solution that satisfies the constraint. We get

$$\begin{aligned} \delta J &= \int d\tau\, (u^* L\delta u + \delta u^* Lu) - \lambda\int d\tau\rho\, (u^*\delta u + (\delta u^*)u) \\ &= \int d\tau\, (Lu - \lambda\rho u)^*\, \delta u + \int d\tau \delta u^*\, (Lu - \lambda\rho u)\,, \end{aligned}$$

where we have used hermiticity of the operator L.

A key difference with the previous examples is that we have a complex function u, and any variation thus falls into two parts,

$$\delta u = (\Re\delta u) + i(\Im\delta u),$$
$$\delta u^* = (\Re\delta u) - i(\Im\delta u).$$

The real and imaginary parts are independent small functions, i.e., we can vary those independently. In the same way we can conclude that the alternative orthogonal combination of these two variations provided by δu and δu^* vary independently, so we can select either of the two terms above, since they must both be zero independently. The function multiplying δu^* must thus satisfy

$$Lu - \lambda\rho u = 0,$$

which shows u 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 *normalised* u, $I[u] \geq \lambda_0$. We show below how we can use that to our benefit.

5.5.4 The Rayleigh-Ritz method

Suppose the function u_0 gives the minimum of

$$I[u] = \int u^* Lu \, d\tau,$$

subject to the constraint

$$\int d\tau \rho^* u^* u = 1.$$

Now suppose v_0 gives the unconstrained minimum of

$$K[v] = \frac{\int d\tau v^* Lv}{\int d\tau v^* \rho v}. \tag{5.24}$$

Theorem 5.1. *The unconstrained minimum of $K[v]$ and the constrained minimum of $I[u]$ with the normalisation 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 parametrised dependence by choosing a set of wave functions depending on set of parameters. In this case $L = H$, $\rho = 1$ and $u = \psi$.

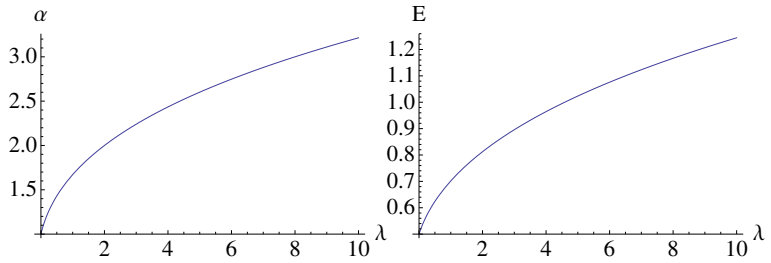

Figure 5.9: The parameter α and the energy E as a function of anharmonicity λ.

Example 5.13:

Find an approximation to the ground state of the quartic anharmonic oscillator

$$H = -\frac{1}{2}\frac{d^2}{dx^2} + \frac{1}{2}x^2 + \lambda/2x^4,$$

of the form $\psi(x) = \exp(-\alpha x^2/2)$.

Solution:

The normalisation integral is

$$\int_{-\infty}^{\infty} \exp(-\alpha x^2)dx = \sqrt{\pi/\alpha}.$$

By differentiating both sides w.r.t. α, we get two more useful integrals,

$$\int_{-\infty}^{\infty} x^2 \exp(-\alpha x^2)dx = \frac{1}{2\alpha}\sqrt{\pi/\alpha}.$$

$$\int_{-\infty}^{\infty} x^4 \exp(-\alpha x^2)dx = \frac{3}{4\alpha^2}\sqrt{\pi/\alpha}.$$

Thus the expectation value of the Hamiltonian requires the derivative

$$\frac{d^2}{dx^2}\exp(-\alpha x^2) = (x^2\alpha^2 - \alpha)\exp(-\alpha x^2).$$

Thus the denominator of the variational functional becomes

$$\int_{-\infty}^{\infty} (-x^2\alpha^2 + \alpha + x^2 + \lambda x^4)/2 \exp(-\alpha x^2)dx = \sqrt{\pi/\alpha}\left(-\alpha/2 + \alpha + 1/(2\alpha) + 3\lambda/(4\alpha^2)\right)/2.$$

And thus

$$K(\alpha) = \frac{1}{4}\left(\alpha + 1/\alpha + 3\lambda/(2\alpha^2)\right).$$

Minimising w.r.t. 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. 5.9.

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

$$\int_{z_0}^{z_1} z^n \, dz = \left[\frac{1}{n+1} z^{n+1} \right]_{z_0}^{z_1}, \quad n \neq -1, \tag{A.4}$$

$$\int_{z_0}^{z_1} z^{-1} \, dz = [\log z]_{z_0}^{z_1}, \quad n = -1. \tag{A.5}$$

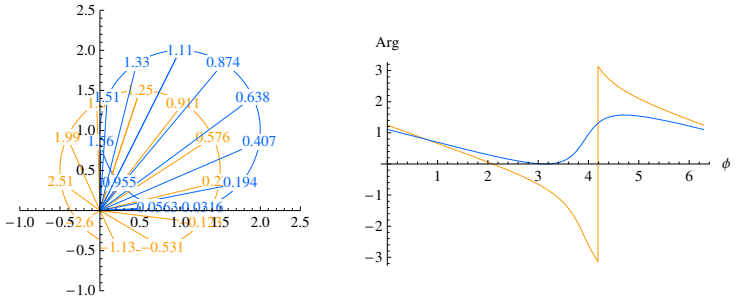

Figure A.1: Two contours: The blue one does not include the origin, the orange one does. The numbers on the left plot show the phase of the relevant complex numbers. These are also graphed in the right panel.

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.