Mathematical Methods

University of Cambridge Part IB Mathematical Tripos

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Abstract: These are the lecture notes for the Mathematical Methods course given to students taking Part IB Maths in Cambridge during Michaelmas Term of 2015. The course aims to provide an introduction to Fourier Series and Fourier Transforms, Sturm–Liouville Theory, and PDEs such as the Laplace, heat and wave equations.

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Preliminaries

Recommended Books

While these notes should contain the material we cover in the lectures, they're very far from a comprehensive treatment and undoubtedly reflect my idiosyncracies in choice of material. So it's a good idea to balance them with a proper textbook. Here are some of the ones I've found useful in preparing the course.

- Arfken, G. and Weber, H., *Mathematical Methods for Physicists*, Academic (2005).
  The single most suitable book for this course. Covers all the core material.
- Boas, M., *Mathematical Methods in the Physical Sciences*, Wiley (2005).
  Also appropriate for this course.
- Mathews, J. and Walker, R. *Mathematical Methods of Physics*, Benjamin Cummins (1970).
- Jeffreys, H. and Jeffreys B. *Methods of Mathematical Physics*, CUP 3rd edition (1999).
  A classic. To be found on the shelves of many generations of mathematical physicists.
- Körner, T. *Fourier Analysis*, Cambridge (1989).
  More advanced, but wonderful. Very engagingly written with a unique blend of mathematical rigour and historical anecdote. I enjoyed reading this a lot when preparing these notes.
- Renardy, M. and Rogers, R. *An Introduction to Partial Differential Equations*, Springer (2004).
  Again more advanced; contains lots of extra material going into further depth in the later parts of this course.

Acknowledgments

Nothing in these lecture notes is original to me. In particular, the notes are based on lecture notes I inherited from Prof R. Jozsa, which were in turn inherited from Prof. C. Caulfield. You can still find Prof. Jozsa's notes here. I've also borrowed heavily from sections of the books listed above. Any errors, major or minor, are of course mine. If you spot one please email me and point it out.

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1 Fourier Series

Many of the most important equations of mathematical physics are *linear*, including

$$\begin{aligned}
&\text{Laplace's equation} && \left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2}\right)\phi(x,y) = 0 \\
&\text{The heat (or diffusion) equation} && \left(\frac{\partial}{\partial t} - K\frac{\partial^2}{\partial x^2}\right)\phi(t,x) = 0 \\
&\text{The wave equation} && \left(\frac{1}{c^2}\frac{\partial^2}{\partial t^2} - \frac{\partial^2}{\partial x^2}\right)\phi(t,x) = 0 \\
&\text{Schrödinger's equation} && \left(\mathrm{i}\hbar\frac{\partial}{\partial t} + \frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} - V(x)\right)\psi(t,x) = 0 \\
&\text{Maxwell's vacuum equations} && \nabla\cdot\mathbf{E} = 0 \qquad \nabla\cdot\mathbf{B} = 0 \\
& && \nabla\times\mathbf{E} = -\frac{1}{c}\frac{\partial\mathbf{B}}{\partial t} \qquad \nabla\times\mathbf{B} = \frac{1}{c}\frac{\partial\mathbf{E}}{\partial t}
\end{aligned}$$

Linearity means that if we are given two solutions ϕ_1 and ϕ_2 of one of these equations – say the wave equation – then $\lambda_1\phi_1 + \lambda_2\phi_2$ is also a solution for arbitrary constants λ_1, λ_2.

With one possible exception, the real reason all these equations are linear is the same: they're approximations. The most common way for linear equations to arise is by slightly perturbing a general system. Whatever the complicated equations governing the dynamics of the underlying theory, if we just look to first order in the small perturbations then we'll find a linear equation essentially by definition[1]. For example, the wave equation will give a good description of ripples on the surface of a still pond, or light travelling through a pane of glass, but don't expect to use it to find out how big a splash you'll make when you bomb into the swimming pool, or if we shine a strong laser at the glass. Similarly, we'll learn how to use the heat equation to tell us about the average jiggling of the atoms in a metal bar when it's being gently warmed somewhere, but if we jiggle them too much then the metal bar will melt.

The possible exception is Schrödinger's equation in Quantum Mechanics. We know of many ways to generalize this equation, such as making it relativistic or passing to Quantum Field Theory, but in each case the analogue of Schrödinger's equation always remains exactly linear. No one knows if there is a fundamental reason for this (though it's certainly built into the principles of Quantum Mechanics at a deep level), or whether our experiments just haven't probed far enough.

In any case, learning to solve linear differential equations such as the above, and their generalizations to higher dimensions, is an important first step in understanding the dynamics of a very wide class of physical (and even biological) systems. Fourier's insight was to take linearity as the key: if we can find a class of simple solutions then we may be able to construct a more general one by taking linear combinations of these.

[1] Often with a source term.

1.1 Vectors

Let's begin by recalling a few facts about vectors that you met last year. A *vector space* over a field F (in this course we'll always take $F = \mathbb{R}$ or $F = \mathbb{C}$) is defined to be a set V together with the operation $+$ of addition, obeying

$$\begin{aligned} \text{commutativity} \qquad & \mathbf{u} + \mathbf{v} = \mathbf{v} + \mathbf{u} \\ \text{associativity} \qquad & \mathbf{u} + (\mathbf{v} + \mathbf{w}) = (\mathbf{u} + \mathbf{v}) + \mathbf{w} \\ \text{identity} \qquad & \exists!\ \mathbf{0} \in V \ s.t.\ \mathbf{0} + \mathbf{u} = \mathbf{u} \end{aligned}$$

for all $\mathbf{u}, \mathbf{v}, \mathbf{w} \in V$, and the operation of multiplication by a scalar $\lambda \in F$ that is

$$\begin{aligned} \text{distributive in } V \qquad & \lambda(\mathbf{u} + \mathbf{v}) = \lambda\mathbf{u} + \lambda\mathbf{v} \\ \text{distributive in } F \qquad & (\lambda + \mu)\mathbf{u} = \lambda\mathbf{u} + \mu\mathbf{u}\ . \end{aligned}$$

It's often useful to give our vector space an *inner product*. This is a choice of map $(\ ,\ ) : V \times V \to F$ that obeys[2]

$$\begin{aligned} \text{conjugate symmetry} \qquad & (\mathbf{u}, \mathbf{v}) = (\mathbf{v}, \mathbf{u})^* \\ \text{linearity} \qquad & (\mathbf{u}, \lambda\mathbf{v}) = \lambda(\mathbf{u}, \mathbf{v}) \\ \text{additivity} \qquad & (\mathbf{u}, \mathbf{v} + \mathbf{w}) = (\mathbf{u}, \mathbf{v}) + (\mathbf{u}, \mathbf{w}) \\ \text{positive-definiteness} \qquad & (\mathbf{u}, \mathbf{u}) \geq 0 \text{ for all } \mathbf{u} \in V, \text{ with equality iff } \mathbf{u} = \mathbf{0}. \end{aligned}$$

Note that *if* our vectors are real, then the property $(\mathbf{u}, \mathbf{v}) = (\mathbf{v}, \mathbf{u})^*$ implies that $(\ ,\ )$ is symmetric in its arguments. In this case, the map $(\ ,\ ) : V \times V \to \mathbb{R}$ is bilinear. If $F = \mathbb{C}$ the map is sometimes called *sesquilinear*.

The inner product on $V \times V$ automatically provides our vector space with a *norm*. We can define the length of a vector $\mathbf{u}$ to be the norm $\sqrt{(\mathbf{u}, \mathbf{u})}$. In the real case, the angle between two vectors is given by

$$\phi = \arccos\left(\frac{(\mathbf{u}, \mathbf{v})}{\sqrt{(\mathbf{u}, \mathbf{u})\,(\mathbf{v}, \mathbf{v})}}\right) \tag{1.1}$$

where the Cauchy-Schwartz inequality $(\mathbf{u}, \mathbf{v})^2 \leq (\mathbf{u}, \mathbf{u})\,(\mathbf{v}, \mathbf{v})$ ensuring that this makes sense.

A set of vectors $\{\mathbf{v}_1, \mathbf{v}_2, \ldots, \mathbf{v}_n\}$ form a *basis* of V if any element $\mathbf{u} \in V$ can be uniquely written as $\mathbf{u} = \sum_{i=1}^{n} \lambda_i \mathbf{v}_i$ for some scalars λ_i. The *dimension* of the vector space is the number of elements of any basis. A basis $\{\mathbf{v}_1, \mathbf{v}_2, \ldots, \mathbf{v}_n\}$ is *orthogonal wrt the inner product* if $(\mathbf{v}_i, \mathbf{v}_j)$ vanishes whenever $i \neq j$, the name coming from (1.1). The basis is *orthonormal* if also the length of each $\mathbf{v}_i$ is 1. If we're given an orthonormal basis, we can use the inner product to explicitly decompose a general into this basis. For example, if

$$\mathbf{u} = \sum_{i=1}^{n} \lambda_i \mathbf{v}_i\,, \tag{1.2}$$

[2]Beware! It's very common for some authors to define the inner product to be linear in the *first* entry, rather than the second as I have done here. I've chosen this way for maximal agreement with your Quantum Mechanics lectures. And because I'm a physicist.

then we have

$$(\mathbf{v}_j, \mathbf{u}) = \left(\mathbf{v}_j, \sum_{i=1}^{n} \lambda_i \mathbf{v}_i \right) = \sum_{i=1}^{n} (\mathbf{v}_j, \lambda_i \mathbf{v}_i) = \sum_{i=1}^{n} \lambda_i (\mathbf{v}_j, \mathbf{v}_i) = \lambda_j \,, \tag{1.3}$$

where we used the additivity and linearity properties of $(\ ,\ )$, as well as orthonormality of the basis. Thus we find $\lambda_j = (\mathbf{v}_j, \mathbf{u})$. For real vectors, λ_j is just the projection of $\mathbf{u}$ onto $\mathbf{v}_j$.

1.2 Spaces of functions as infinite dimensional vector spaces

Consider the set of complex valued functions on some domain Ω. Such a function f can be viewed as a map $f : \Omega \to \mathbb{C}$. The set of all such functions is naturally thought of as a vector space, where vector addition $+$ is just pointwise addition of the functions; that is, for $x \in \Omega$ we have

$$(f + g)(x) = f(x) + g(x) \tag{1.4}$$

where the addition on the rhs is just addition in $\mathbb{C}$. Likewise, we can multiply functions by scalars as

$$(\lambda f)(x) = \lambda\, f(x) \,, \tag{1.5}$$

where again the multiplication is just the usual multiplication in $\mathbb{C}$.

How about the inner product? One possible choice is to take

$$(f, g) \equiv \int_{\Omega} f(x)^*\, g(x)\, \mathrm{d}\mu \tag{1.6}$$

where $\mathrm{d}\mu$ is some choice of integration measure, and where the functions $f(x)$ and $g(x)$ are sufficiently well-behaved that the integral exists. The idea is that this is a simple generalization of the inner product between two finite dimensional vectors: if we think of the different point $x \in \Omega$ as labelling the different 'components' of our functions, then we multiply the 'component' $f(x)$ of f and the 'component' $g(x)$ of g together (after taking an appropriate complex conjugate) and then add them up, *i.e.,* integrate over Ω. The measure $\mathrm{d}\mu$ tells us how much weight to assign to each point of the domain.

As a simple example, if Ω is the interval $[a, b]$, then we may take the measure to be just $\mathrm{d}x$ so that

$$(f, g) = \int_{a}^{b} f(x)^*\, g(x)\, \mathrm{d}x \,. \tag{1.7}$$

As a second example, if Ω is the unit disc D_2 then we may take

$$(f, g) = \int_{r=0}^{1} \int_{\theta=0}^{2\pi} f(r, \theta)^*\, g(r, \theta)\, r \mathrm{d}r\, \mathrm{d}\theta \tag{1.8}$$

with measure $\mathrm{d}\mu = r \mathrm{d}r\, \mathrm{d}\theta$. Later in the course, we'll meet some other measures.

If the domain Ω is bounded, then we may sometimes wish to restrict the class of functions we consider by requiring they satisfy *boundary conditions*. Ideally, we'd like these boundary conditions to preserve the vector space structure in the sense that if f and

g both satisfy the boundary conditions then so too does $\lambda_1 f + \lambda_2 g$. Any such boundary condition must be *homogeneous* (of degree 1) in the function. For example, if $\Omega = [a, b]$ then the boundary conditions $f(a) = 0$, $f(a) = f(b)$ and $f(a) + 7f'(b) = 0$ all preserve the vector space structure, whereas the boundary conditions $f(a) = 1$ or $f(a) + 3f'(b) = 7$ are not.

An important class of functions are *periodic* functions. In the first instance, these may be thought of as maps $f : \mathbb{R} \to \mathbb{C}$ that obey the condition $f(t + T) = f(t)$ for all t (and conventionally we take the smallest such T). Note that this condition is indeed homogeneous. The fixed constant T is called the *period*, while $1/T$ is the *frequency*. Note that f is fully specified once we give its values on $[0, T)$. The basic examples of periodic functions are just the trigonometric functions $\sin \omega t$ and $\cos \omega t$, which each have period $T = 2\pi/\omega$.

If we interpret the variable t as time, then T is the length of time is takes for our function to complete one whole oscillation, while $1/T$ is the number of oscillations per unit time. The constant ω is known as the *angular* frequency. It tells us the number of oscillations that fit in a 2π interval (useful when we're thinking in terms of a map from a circle). Sometimes, we may prefer to think of our function $f(x)$ as being periodic in space rather than time, for example $A \sin kx$. In this case, we call $\lambda \equiv 2\pi/k$ the *wavelength* as it tells us the spatial extent of one complete oscillation. $1/\lambda = k/2\pi$ is called the wavenumber and gives the number of waves per unit length, while the constant k is the angular wavenumber. In practice, we often do not distinguish between frequency/wavenumber and angular frequency/wavenumber, with the terminology being clear from the context.

In what follows below we'll often treat periodic functions as maps $f : S^1 \to \mathbb{C}$ from the circle. To simplify the notation we'll usually parameterize the circle with a coordinate $\theta \in [-\pi, \pi)$. So if you're given a periodic function $f(t)$ whose period is T, you must remember to set $\theta = 2\pi t/T$ and $\mathrm{d}\theta = 2\pi/T \, \mathrm{d}t$ to use the formulæ below!

1.3 Fourier series

The simplest and most frequently occurring complex-valued periodic function is the complex exponential $\mathrm{e}^{\mathrm{i}\theta} = \cos\theta + \mathrm{i}\sin\theta$. This is periodic with period 2π, and so we can view it as a map $\exp : S^1 \to \mathbb{C}$ from the circle described by coordinates θ. By convention, we'll take $\theta \in [-\pi, \pi)$. Integer powers of these exponentials are orthogonal with respect to the inner product[3]

$$(\mathrm{e}^{\mathrm{i}m\theta}, \mathrm{e}^{\mathrm{i}n\theta}) = \int_{-\pi}^{\pi} \mathrm{e}^{-\mathrm{i}m\theta} \, \mathrm{e}^{\mathrm{i}n\theta} \, \mathrm{d}\theta = \int_{-\pi}^{\pi} \mathrm{e}^{\mathrm{i}(n-m)\theta} \, \mathrm{d}\theta = 2\pi \, \delta_{m,n} \tag{1.9}$$

where $m, n \in \mathbb{Z}$ and $\delta_{m,n}$ is the Kronecker δ-symbol defined by

$$\delta_{m,n} = \begin{cases} 1 & \text{when } n = m \\ 0 & \text{else.} \end{cases} \tag{1.10}$$

[3]Recall that the inner product $(\ ,\ )$ on complex functions is *anti*linear in its first slot, which is the origin of the minus sign in the argument of the first exponential.

(To check the integral, note that whenever $m \neq n$ we're just integrating either sin or cos over a complete period. When $m = n$ we're just integrating 1.) Thus the set $\left\{ \frac{1}{\sqrt{2\pi}} \mathrm{e}^{\mathrm{i}n\theta} : n \in \mathbb{Z} \right\}$ form an orthonormal set of complex valued periodic functions.

Fourier's idea was to try to use this set as a basis in which to expand any such periodic function. Given an arbitrary function $f : S^1 \to \mathbb{C}$, we define the *Fourier coefficients* $\hat{f}_n$ of $f(\theta)$ by[4]

$$\hat{f}_n \equiv \frac{1}{2\pi}(\mathrm{e}^{\mathrm{i}n\theta}, f) = \frac{1}{2\pi} \int_{-\pi}^{\pi} \mathrm{e}^{-\mathrm{i}n\theta} f(\theta)\, \mathrm{d}\theta \tag{1.11}$$

for all $n \in \mathbb{Z}$, just as we did in (1.3). Fourier now claimed that

$$f(\theta) \stackrel{?}{=} \sum_{n \in \mathbb{Z}} \hat{f}_n \, \mathrm{e}^{\mathrm{i}n\theta} \tag{1.12}$$

thus expanding f in the basis $\{\mathrm{e}^{\mathrm{i}n\theta}/\sqrt{2\pi}\}$ by analogy with (1.2). This expansion is known as the *Fourier series* of $f(\theta)$. As we'll see later in the course, this idea and its generalizations has proven incredibly useful in any number of problems, from vibrating strings (violins and quantum gravity alike), to learning about the origin of galaxies from fluctuations in the early universe, to the electronic wizardry in your laptop, as well as to vast swathes of functional analysis. But to begin with, no-one believed him.

1.3.1 Reality conditions

As an aside, let me point out a common reformulation of the Fourier series that is relevant if $f(\theta) = f(\theta)^*$ so that f is real-valued (rather than $\mathbb{C}$-valued). In this case, the Fourier coefficients obey $\hat{f}_n^* = \hat{f}_{-n}$. This follows straight from their definition:

$$(\hat{f}_n)^* = \frac{1}{2\pi} \left(\int_{-\pi}^{\pi} \mathrm{e}^{-\mathrm{i}n\theta} \, f(\theta)\, \mathrm{d}\theta \right)^* = \frac{1}{2\pi} \int_{-\pi}^{\pi} \mathrm{e}^{+\mathrm{i}n\theta} \, f(\theta)\, \mathrm{d}\theta = \hat{f}_{-n} \ , \tag{1.13}$$

using the reality of $f(\theta)$. We can use this property to reorganise the Fourier series in terms of standard trigonometric functions, because

$$\begin{aligned} f(\theta) &= \sum_{n \in \mathbb{Z}} \hat{f}_n \, \mathrm{e}^{\mathrm{i}n\theta} \\ &= \hat{f}_0 + \sum_{n=1}^{\infty} \left(\hat{f}_n \, \mathrm{e}^{\mathrm{i}n\theta} + \hat{f}_{-n} \, \mathrm{e}^{-\mathrm{i}n\theta} \right) \\ &= \hat{f}_0 + \sum_{n=1}^{\infty} \left(\hat{f}_n \, \mathrm{e}^{\mathrm{i}n\theta} + \hat{f}_n^* \, \mathrm{e}^{-\mathrm{i}n\theta} \right) \\ &= \hat{f}_0 + \sum_{n=1}^{\infty} a_n \cos n\theta + b_n \sin n\theta \end{aligned} \tag{1.14}$$

[4]Recalling that the orthonormal functions were $\{\mathrm{e}^{\mathrm{i}n\theta}/\sqrt{2\pi}\}$, this definition has an extra factor of $1/\sqrt{2\pi}$ compared to what you might expect. It's just a (common) convention I adopted to make some later formulae look prettier.

where in going to the third line we relabelled $n \to -n$ in the last sum and used $\hat{f}_{-n} = \hat{f}_n^*$ for real f. In going to the final line we've used de Moivre's theorem $\mathrm{e}^{\mathrm{i}n\theta} = \cos n\theta + \mathrm{i}\sin n\theta$ and set $\hat{f}_n = (a_n - \mathrm{i}b_n)/2$ so that

$$a_n \equiv 2\,\mathrm{Re}\,\hat{f}_n \qquad \text{and} \qquad b_n \equiv -2\,\mathrm{Im}\,\hat{f}_n\,. \tag{1.15}$$

Note that the sum in our trigonometric Fourier series runs only over positive integers, but that we now have two sets of Fourier coefficients, a_n and b_n. From the definition of the $\hat{f}_n$s and (1.15) we see that

$$a_n = \frac{1}{\pi}\int_{-\pi}^{\pi} \cos n\theta\, f(\theta)\,\mathrm{d}\theta \qquad \text{and} \qquad b_n = \frac{1}{\pi}\int_{-\pi}^{\pi} \sin n\theta\, f(\theta)\,\mathrm{d}\theta\,, \tag{1.16}$$

so a_n and b_n are the Fourier coefficients we'd find if we use $\sin n\theta$ and $\cos n\theta$ as our basis of periodic functions instead of the complex exponentials.

As we'll see later, the real form of the Fourier series is often useful when we are studying some real physical object (such as a vibrating violin string) and we wish to fix a solution of some linear differential equation to obey appropriate real boundary conditions. Boundary conditions may also mean that it is convenient to consider a function $g(\theta)$ defined not over a whole domain, but just on a half-interval, say $\theta \in [0, \pi]$. We can then construct a function defined throughout $[-\pi, \pi)$ by *extending* the given function $g(\theta)$ either as an even or odd function, so that

$$g(\theta) = \pm g(-\theta) \qquad \text{for } \theta \in [-\pi, 0)\,.$$

For example, if we have the (Dirichlet) boundary condition that $g(0) = 0$ (perhaps because a string is tied to a fixed wall there), then it is natural to extend $g(\theta)$ as an odd function, whereas for Neumann boundary conditions extension as an even function may be more appropriate. As above, if g is extended to be even then the real Fourier series will involve non-vanishing coefficients a_n and $\hat{f}_0$ (for $\cos n\theta$ and the constant). Conversely, if it is extended to be odd then the real Fourier series contains non-vanishing coefficients b_n of $\sin n\theta$ only.

However, it is worth pointing out that, even when we ultimately wish to obtain a real Fourier series, it is usually simpler to work with the complex exponential form during the intermediate steps of a calculation. We then impose the relevant boundary conditions and fix the real form only at the end. One reason for this is that the complex exponentials $\mathrm{e}^{\mathrm{i}n\theta}$ have the beautiful property that differentiation *wrt* θ becomes simply multiplication by $\mathrm{i}n$.

1.4 A first look at convergence

What made people so reluctant to accept (1.12) was that Fourier had made no attempt[5] (at least initially) to show that the infinite sum *converges* and, if it does, whether what it converges to is indeed the original function f.

To investigate this, the first thing we must realise is that when dealing with sequences of functions (rather than just numbers) there are many things we might wish to mean by 'converge'. Let's define $S_n f$ to be the finite sum

$$S_n f \equiv \sum_{k=-n}^{n} \hat{f}_k \, \mathrm{e}^{\mathrm{i}n\theta} \tag{1.17}$$

involving just the chunk of terms 'near the middle' of the Fourier series. (Recall that the coefficients $\hat{f}_k$ were defined in (1.11)). One possible notion of convergence would be to ask that

$$\lim_{n\to\infty} (S_n f - f, S_n f - f) = 0 \tag{1.18}$$

so that as more and more terms are included in the sum, the norm of the difference between the partial Fourier series and the function itself is a sequence of numbers converging to zero. For a finite dimensional vector space, $(\mathbf{u}, \mathbf{u}) = 0$ iff $\mathbf{u} = \mathbf{0}$, the unique zero vector. However, in our infinite dimensional function space, we have

$$(S_n f - f, S_n f - f) = \int_{-\pi}^{\pi} |S_n f(\theta) - f(\theta)|^2 \, \mathrm{d}\theta \,, \tag{1.19}$$

so $S_n f$ may still differ from f by arbitrarily large amounts, provided this only occurs at isolated points (or, better, at sets of measure zero).

A stronger notion of convergence is *pointwise* convergence: we could ask that

$$\lim_{n\to\infty} |f(\theta) - S_n f(\theta)| = 0 \qquad \text{at every point } \theta \in S^1 \,, \tag{1.20}$$

so that the Fourier series converges to f everywhere on its domain. Stronger still is *uniform* convergence, where we ask in addition that the *rate* at which $S_n f$ converges to f is the same everywhere on S^1. More formally, a sequence $\{s_0(\theta), s_1(\theta), \ldots, s_n(\theta), \ldots\}$ converges to $s(\theta)$ pointwise if for each θ and for each $\epsilon > 0$ there exists an integer N such that $|s_N(\theta) - s(\theta)| < \epsilon$. However, the integer N *can depend on* θ *as well as on* ϵ. Only if N is independent of θ is the convergence uniform. You'll learn much more about pointwise and uniform convergence in your Analysis II course.

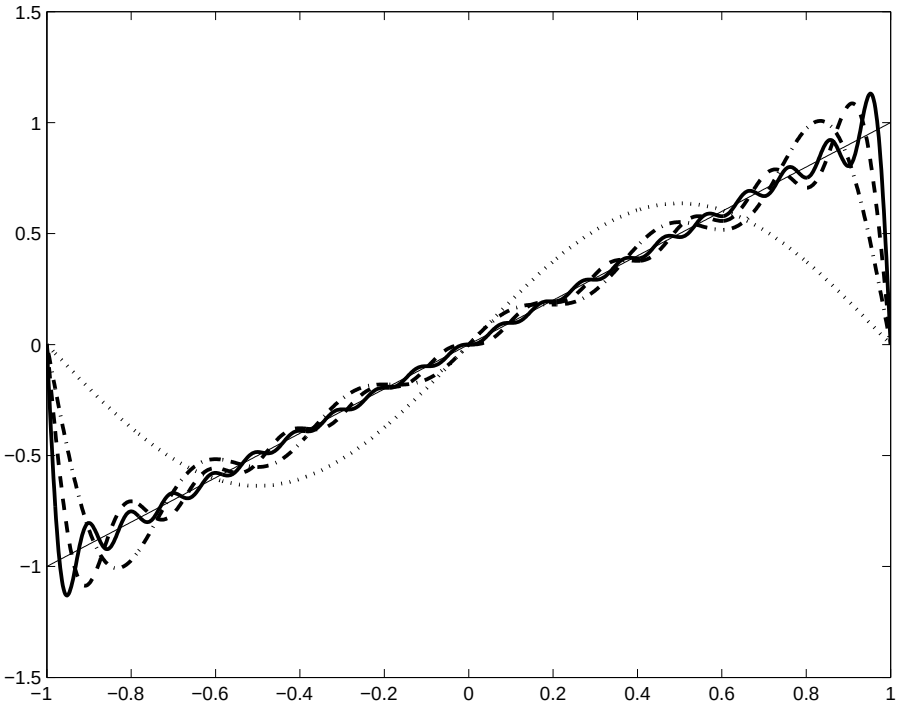


Figure 1. *Plots of the sawtooth function $f(\theta) = \theta$ (thin solid line) together with the partial Fourier sums $S_1 f(\theta)$ (dotted line), $S_5 f(\theta)$ (dot-dashed), $S_{10} f(\theta)$ (dashed) and $S_{20} f(\theta)$ (solid line). Both axes have been rescaled by π.*

1.4.1 Functions with discontinuities

To see why convergence might be a problem, let's examine the behaviour of the Fourier coefficients of functions with sudden jumps. To keep things simple, we'll always assume that our periodic function f has only a finite number of such discontinuities, say at isolated points $\{\theta_1, \theta_2, \ldots, \theta_r\} \in S^1$, and that it jumps by only a finite amount. We meet such functions all the time in everyday life: when you flick on a light switch, the current passing through an average bulb passes very rapidly from zero to about 10^{18} electrons per second (a bit less than half an amp), while wifi networks transmit data via a signal that flickers between 0 and 1 up to a million times a second.

As a first case, consider the *sawtooth function* defined by

$$f(\theta) = \theta \qquad \text{for } \theta \in [-\pi, \pi)\,. \tag{1.21}$$

[5]Fourier believed his methods were good for *arbitrary* periodic functions $f(\theta)$, no matter whether they were smooth, had kinks (*e.g.* $f(\theta) = |\theta|$ for $\theta \in [-\pi, \pi)$ which has a kink at $\theta = 0$), or were even discontinuous (*e.g.* the *sawtooth function* $f(\theta) = \theta$ which is discontinuous at the point $-\pi = \pi$ on the circle). Laplace and Lagrange strongly doubted this claim and, feeling his whole method must be invalid, they blocked Fourier's attempts to publish his theory of heat flow based on using such series. Later, Cauchy claimed to have found a proof that (1.12) does always make sense, but his proof was (fatally) flawed. Dirichlet did manage to prove the validity of the Fourier series for *continuous* functions with bounded continuous derivative, but these conditions are quite restrictive. And as we'll see, they can't easily be relaxed.

This function is discontinuous at $\theta = -\pi$ on S^1, and gets its name because if we think of the function not as a map from a circle but as a map $f : \mathbb{R} \to \mathbb{R}$ that is periodic with period 2π, then the graph looks like the cutting edge of a saw, as in figure 1. Its Fourier coefficients $\hat{f}_n$ are

$$\hat{f}_0 = \frac{1}{2\pi} \int_{-\pi}^{\pi} \theta \, \mathrm{d}\theta = 0 \tag{1.22}$$

when $n = 0$, and

$$\begin{aligned} \hat{f}_n &= \frac{1}{2\pi} \int_{-\pi}^{\pi} \mathrm{e}^{-\mathrm{i}n\theta} \, \theta \, \mathrm{d}\theta = \frac{1}{2\pi\mathrm{i}} \left[-\frac{1}{n} \, \theta \, \mathrm{e}^{-\mathrm{i}n\theta} \right]_{-\pi}^{\pi} + \frac{1}{2\pi\mathrm{i}} \frac{1}{n} \int_{-\pi}^{\pi} \mathrm{e}^{-\mathrm{i}n\theta} \, \mathrm{d}\theta \\ &= \frac{1}{\mathrm{i}n} (-1)^{n+1} \end{aligned} \tag{1.23}$$

when $n \neq 0$. The coefficients here decay rather slowly, like $1/n$. Despite this, as $n \to \infty$ the partial Fourier series

$$S_n f = \sum_{k=-n}^{n} \frac{(-1)^{k+1}}{\mathrm{i}k} \, \mathrm{e}^{\mathrm{i}k\theta} \tag{1.24}$$

do in fact converge on the sawtooth function everywhere except at the discontinuity. Note that since the sawtooth function is real, we can represent it as a trigonometric Fourier series

$$f(\theta) = 2 \sum_{n=1}^{\infty} \frac{(-1)^{n+1}}{n} \sin n\theta \, . \tag{1.25}$$

The fact that $\hat{f}_0$ and all the coefficients of $\cos n\theta$ vanish is exactly as we would expect since $f(-\theta) = -f(\theta)$.

At the discontinuity $\theta = \pi$ the sawtooth function itself is discontinuous. Examining the Fourier series (1.25) we see that since $\sin k\pi = 0$ for any $k \in \mathbb{Z}$, $S_n f(\pi) = S_n f(-\pi) = 0$ for all n, so the Fourier series converges on zero at the location of the discontinuity. The significance of this is that zero is the *average* value of the sawtooth function on either side of the discontinuity.

We now want to show that the behaviour of the Fourier series for the sawtooth is typical for functions with discontinuities. That is, we want to show that if some function $g(\theta)$ jumps, say at $\theta = \pi$, then

$$S_n g(\pi) \to \frac{g(\pi^+) + g(\pi^-)}{2} \qquad \text{where} \qquad g(\pi^\pm) = \lim_{\epsilon \to 0} g(\pi \pm \epsilon) \, , \tag{1.26}$$

or in other words that its Fourier series converges to the average value on either side of the jump, just as we obtained for the sawtooth function. To do so, define

$$G(\theta) \equiv \begin{cases} g(\theta) + \dfrac{g(\pi^+) - g(\pi^-)}{2\pi} \, f(\theta) & \text{for } \theta \neq \pi \\ \dfrac{g(\pi^+) + g(\pi^-)}{2} & \text{at } \theta = \pi \ , \end{cases} \tag{1.27}$$

where $f(\theta)$ is exactly the sawtooth function from above. The point of this definition is that $G(\theta)$ is now continuous at π, because the discontinuity in our function $g(\theta)$ is balanced by the discontinuity of the sawtooth. The Fourier coefficients of G are linear combinations of those of g and those of the sawtooth. Since the Fourier series of the sawtooth converges, S_nG will converge provided S_ng does. But because G is continuous, its Fourier series will now converge to the original function G everywhere. In particular, at $\theta = \pi$ we have $S_nG(\pi) \to G(\pi) = (g(\pi^+) + g(\pi^-))/2$. However,

$$S_nG(\pi) = S_ng(\pi) + \frac{g(\pi^+) - g(\pi^-)}{2\pi} S_nf(\pi) = S_ng(\pi) \tag{1.28}$$

since the Fourier series S_nf of the sawtooth vanishes at $\theta = \pi$. Thus as $n \to \infty$, $S_ng(\pi)$ converges to $(g(\pi^+) + g(\pi^-))/2$, as was to be shown.

1.4.2 Integration *vs.* differentiation

When we first learnt calculus, most people started with differentiation. The differential $\mathrm{d}f/\mathrm{d}x$ has an intuitively clear definition in terms of the difference in the values of f at nearby pointss. Better still, it is easy to apply this rule the some simple functions we were familiar with such as powers or trigonometric functions, and with practice we may have felt confident we could apply it to any given function. Integration, by contrast, is defined as the 'inverse of differentiation' and so (perhaps) seemed a little mysterious. If we want to know the indefinite integral of x for example, we first have to recognize that this is what we'd have obtained if we'd differentiated $x^2/2+c$. But you may have worried about how we would proceed if we'd been asked to integrate say $\ln(1-x)$, where we might not recognize its integral[6]. Indeed, many functions are simply *defined* to be the integral of some other function.

However, if we're not so much interested in an explicit closed-form expression for our function, but just knowing whether the integral or derivative exists, then matters are different. Vastly more functions can be integrated in principle than can be differentiated. This is because integration is a *smoothing* operation. For example, consider the step function

$$\Theta(x) \equiv \begin{cases} 0 & \text{for } x < 0 \\ 1 & \text{for } x \geq 0 \end{cases} \tag{1.29}$$

which is discontinuous at the origin. The derivative of the step function fails to exist here[7] because the gradient of the function becomes infinite. However, it's easy to integrate

$$\int_{-\infty}^{x} \Theta(y)\,\mathrm{d}y = \begin{cases} 0 & \text{for } x < 0 \\ x & \text{for } x \geq 0. \end{cases} \tag{1.30}$$

This functions is now continuous at the origin, though it has a kink there. Integrating further we'd create functions that are always zero on the negative x-axis, but which join

[6] In this case the integral is actually $\mathrm{Li}_2(x)$, known as a dilogarithm. According to the number theorist Don Zagier, it's the only mathematical function with a sense of humour.

[7] At least as a function. Later in the course we'll meet distributions.

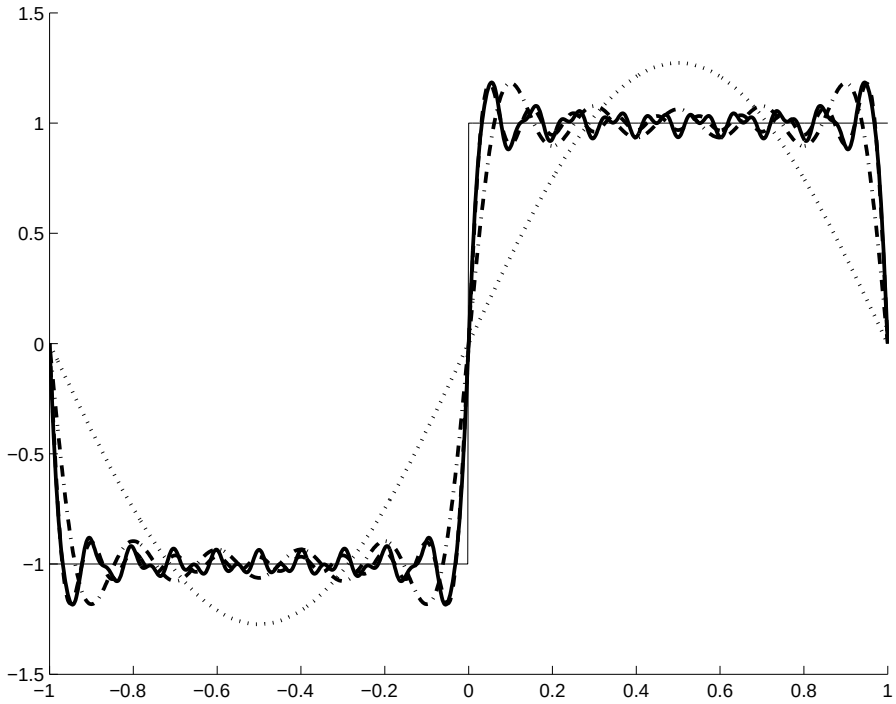


Figure 2. *Plots of the square wave $f(\theta)$ (thin solid line), together with its partial Fourier sums $S_1 f$ (dotted), $S_5 f$ (dot-dashed), $S_{10} f$ (dashed) and $S_{20} f$ (solid). The θ-axis has been rescaled by a factor of π compared to the values in the text.*

at the origin in a smoother and smoother way. Conversely, differentiating these functions will lead to worse and worse behaviour at the origin. Note that none of these functions admit a Taylor series around $x = 0$.

The same is true for Fourier series. Suppose we have a function $f : S^1 \to \mathbb{C}$ whose sequence of partial Fourier series $S_n f$ converge pointwise to f. Then we can define a new sequence $S_n F$ by the integrals

$$\begin{aligned} S_n F &\equiv \int_{-\pi}^{\theta} S_n f(\phi)\, \mathrm{d}\phi \\ &= (\theta - \pi)\hat{f}_0 + \sum_{k=-n}^{-1} \hat{f}_k \, \frac{\mathrm{e}^{\mathrm{i}k\theta} - (-1)^k}{\mathrm{i}k} + \sum_{k=1}^{n} \hat{f}_k \, \frac{\mathrm{e}^{\mathrm{i}k\theta} - (-1)^k}{\mathrm{i}k} \end{aligned} \tag{1.31}$$

This new series is guaranteed converge, because the original one did by assumption and integration has suppressed each coefficient by a further power of k. Even if the original function had jump discontinuities, so that at some discrete points the Fourier series converged to the average value of f on either side of the discontinuity, we've seen that integration produces a continuous function for us, so the new series will converge to $F(\theta) = \int_{-\pi}^{\theta} f(\phi)\, \mathrm{d}\phi$ everywhere.

By contrast, if we differentiate a Fourier series term by term then we *multiply* each coefficient by $\mathrm{i}k$ and this makes convergence worse, perhaps fatally. For example, consider

the *square wave* given by

$$f(\theta) = \begin{cases} -1 & \text{for } -\pi \le \theta < 0 \\ +1 & \text{for } 0 < \theta < \pi \end{cases} \tag{1.32}$$

and shown in figure 2. You can check (*exercise!*) that this has Fourier series

$$f(\theta) = \frac{4}{\pi} \sum_{n=1}^{\infty} \frac{\sin(2n-1)\theta}{2n-1} \tag{1.33}$$

which converges to f everywhere except at the origin, where it converges to zero – the average of the values taken when the origin is approached from the left and from the right. If we formally differentiate term-by-term we obtain the series

$$f'(\theta) \stackrel{?!}{=} \frac{4}{\pi} \sum_{n=1}^{\infty} \cos(2n-1)\theta \tag{1.34}$$

which is divergent. The problem, of course is that $f'(\theta)$ is *not defined* at the origin, so $f'(\theta)$ does not admit a Fourier series. You might think we could get around this by just defining $f'(0) \equiv c$ for some constant c. Perhaps you'd choose $c = 0$, which is the value of both $f'(0^+)$ and $f'(0^-)$? The problem is that this breaks the fundamental rule of calculus, that

$$f(\theta) = f(-\pi) + \int_{-\pi}^{\theta} f'(\phi)\, \mathrm{d}\phi\,,$$

because with any finite value of c the integral on the rhs vanishes. Such a rule would mean we never see f jump!

So when can we safely differentiate a Fourier series term by term? Clearly, it is not enough for $f(\theta)$ itself to have a Fourier series that converges. In fact, there is a theorem that if $f : S^1 \to \mathbb{C}$ is continuous *and* $\sum_{k\in\mathbb{Z}} |k||\hat{f}_k|$ converges, then f is differentiable and the partial sums

$$S_n(f') \equiv \sum_{k=-n}^{n} \mathrm{i}k\, \hat{f}_k\, \mathrm{e}^{\mathrm{i}k\theta}$$

converge uniformly to $f'(\theta)$ as $n \to \infty$. To see this, note that the conditions imply that both f and f' do indeed have Fourier series

$$f(\theta) = \frac{1}{2\pi} \sum_{n\in\mathbb{Z}} \hat{f}_n\, \mathrm{e}^{\mathrm{i}n\theta} \qquad \text{and} \qquad f'(\theta) = \frac{1}{2\pi} \sum_{n\in Z} \hat{\phi}_n\, \mathrm{e}^{\mathrm{i}n\theta} \tag{1.35}$$

with some Fourier coefficients $\hat{f}_n$ and $\hat{\phi}_n$. The Fourier series of f certainly converges if that of f' does. Furthmore, the Fourier coefficients of f' in (1.35) are, by definition,

$$\hat{\phi}_0 = \frac{1}{2\pi} \int_{-\pi}^{\pi} \frac{df}{d\theta}\, \mathrm{d}\theta = 0 \tag{1.36}$$

by periodicity of f, and

$$\hat{\phi}_n = \frac{1}{2\pi} \int_{-\pi}^{\pi} \mathrm{e}^{-\mathrm{i}n\theta}\, \frac{df}{d\theta}\, \mathrm{d}\theta = -\frac{1}{2\pi} \int_{-\pi}^{\pi} f(\theta)\, \frac{d}{d\theta} \mathrm{e}^{-\mathrm{i}n\theta} \mathrm{d}\theta = \mathrm{i}n\hat{f}_n \tag{1.37}$$

for $n \neq 0$, by integration by parts (the boundary term again cancelling by periodicity and continuity). But this is exactly what we would find by differentiating the Fourier series term by term.

1.4.3 The rate of convergence

In fact, the decay of the Fourier coefficients $\hat{f}_n k$ as $k \to \infty$ tells us quite generally about the order of differentiability (smoothness) of the function. The intuition here is that if a function has a very sharp feature – such as a sudden jump, or the cusp at $\theta = 0$ in $\sqrt{|\theta|}$ – then we will need to include a significant amount of very high frequency terms in its Fourier series. Last year, you learned that in relativity, the frequency of a wave is its energy in units of $\hbar$. Thus this same principle of sharp features needing high frequencies drives the construction of particle accelerators such as the LHC at CERN: if you want to things that happen at a very small scale, you need a very powerful microscope.

Let's now quantify these ideas. We will show that if we're given the Fourier coefficients $\hat{f}_k$ of some continuous function, we can read off the order of differentiability of the original f by seeing how quickly these coefficients fall with k. Suppose that $f : S^1 \to \mathbb{C}$ together with its first $m-1$ derivatives are continuous, but that the m^{th} derivative $f^{(m)}$ jumps at some isolated points $\{\theta_1, \theta_2, \ldots, \theta_r\} \in S^1$. We further suppose that all these functions remain finite throughout. Now comes a trick. Integrate by parts to write the Fourier coefficient $\hat{f}_k$ (with $k \neq 0$) as

$$\begin{aligned} \hat{f}_k &= \frac{1}{2\pi} \int_{-\pi}^{\pi} \mathrm{e}^{-\mathrm{i}k\theta} \, f(\theta) \, \mathrm{d}\theta \\ &= \left[-f(\theta) \frac{\mathrm{e}^{-\mathrm{i}k\theta}}{2\pi \mathrm{i} k} \right]_{-\pi}^{\pi} + \frac{1}{2\pi \mathrm{i} k} \int_{-\pi}^{\pi} \mathrm{e}^{-\mathrm{i}k\theta} \, f'(\theta) \, \mathrm{d}\theta \\ &= \frac{1}{2\pi \mathrm{i} k} \int_{-\pi}^{\pi} \mathrm{e}^{-\mathrm{i}k\theta} \, f'(\theta) \, \mathrm{d}\theta \,, \end{aligned} \tag{1.38}$$

where the boundary terms cancel since f is periodic and continuous everywhere on S^1.

If we perform this trick m times then the boundary terms always cancel, since f', f'' up to $f^{(m-1)}$ are continuous. Therefore

$$\hat{f}_k = \frac{1}{2\pi} \frac{1}{(\mathrm{i}k)^m} \int_{-\pi}^{\pi} \mathrm{e}^{-\mathrm{i}k\theta} \, f^{(m)}(\theta) \, \mathrm{d}\theta \,. \tag{1.39}$$

However, if we want to continue with this game, we must be careful because $f^{(m)}$ has discontinuities at $\{\theta_1, \theta_2, \ldots, \theta_r\}$ and its derivative cannot be defined there. To proceed, recall that even though it jumps, $f^{(m)}$ remains finite everywhere by assumption. So the integral (1.39) does not change appreciably if we remove an infinitesimal neighbourhood of each of the discontinuities. For the remaining values of θ, $f^{(m+1)}$ is finite, so we can again

integrate by parts. Putting this together, we have

$$\begin{aligned}\hat{f}_k &= \lim_{\epsilon\to 0}\frac{1}{2\pi}\frac{1}{(\mathrm{i}k)^m}\left[\int_{-\pi}^{\theta_1^-} + \int_{\theta_1^+}^{\theta_2^-} + \cdots + \int_{\theta_r^+}^{\pi} \mathrm{e}^{-\mathrm{i}k\theta}\, f^{(m)}(\theta)\,\mathrm{d}\theta\right] \\ &= \lim_{\epsilon\to 0}\frac{1}{2\pi}\frac{1}{(\mathrm{i}k)^{m+1}}\left[\sum_{s=1}^{r}\left(f^{(m)}(\theta_s^+) - f^{(m)}(\theta_s^-)\right)\mathrm{e}^{-\mathrm{i}k\theta_s} + \int \mathrm{e}^{-\mathrm{i}k\theta}\, f^{(m+1)}(\theta)\,\mathrm{d}\theta\right]\end{aligned} \tag{1.40}$$

where $\theta_s^{\pm} = \theta_s \pm \epsilon$ with $\epsilon > 0$, and where the dangerous neigbourhoods $\theta_s^- < \theta < \theta_s^+$ (for $s = 1, \ldots, r$) are excluded from the final integral. The size $f^{(m)}(\theta_s^+) - f^{(m)}(\theta_s^-)$ of the jumps appear as a boundary term in the final line, terminating the process of integration by parts. By our assumptions, these jumps are finite and $f^{(m+1)}$ is finite everywhere except at the discontinuities of $f^{(m)}$, so the quantity in square brackets is finite. Thus, if we first meet a discontinuity after differentiating a function m times then the Fourier coefficient $\hat{f}_k$ falls as $O(1/k^{m+1})$.

1.5 Fejér's theorem

Sadly, this section is non-examinable, at least for this course. You really shouldn't worry about that in Michaelmas.

Trying to make sense of exactly when Fourier series do converge to the original function has been a major motivation for the development of a large part of Analysis. Much of this is highly technical, but one important and readily understandable theorem in Fourier analysis was proved at the turn of the 20$^{\text{th}}$ century by the Hungarian mathematician Fejér. Instead of asking whether the sequence $S_n f$ converges to f, Fejér asked whether, given all the Fourier coefficients $\hat{f}_n$, the original function $f(\theta)$ could somehow be recovered. His result was that provided $f : S^1 \to \mathbb{C}$ is merely *continuous* then this can be done, with no further assumptions on the smoothness of f. He was nineteen.

Here's an outline of his proof. First, for any sequence $\{s_0, s_1, s_2, \ldots\}$, we construct a new sequence $\{\sigma_0, \sigma_1, \sigma_2, \ldots\}$ where

$$\sigma_n \equiv \frac{1}{n+1}\sum_{m=0}^{n} s_m \tag{1.41}$$

is just the arithmetic mean of the first $n+1$ terms in the original sequence. Césaro noticed that this new sequence may have better convergence properties than the original sequence. The standard example is to take $s_m = (-1)^m$ which clearly does not converge, while

$$|\sigma_n| = \left|\frac{1}{n+1}\sum_{m=0}^{n} s_n\right| = \frac{1}{n+1}\left|\sum_{m=0}^{n} s_m\right| \leq \frac{1}{n+1}$$

which converges to zero as $n \to \infty$.

Fejér realized that this idea could be applied to help the convergence of a Fourier series. From (1.17) and the definition of the Fourier coefficients we have

$$\begin{aligned} S_m f(\theta) &= \frac{1}{2\pi} \sum_{k=-m}^{m} \left[\int_{-\pi}^{\pi} \mathrm{e}^{-\mathrm{i}k\phi} f(\phi)\, \mathrm{d}\phi \right] \mathrm{e}^{\mathrm{i}k\theta} \\ &= \frac{1}{2\pi} \int_{-\pi}^{\pi} f(\phi) \sum_{k=-m}^{m} \mathrm{e}^{\mathrm{i}k(\theta-\phi)}\, \mathrm{d}\phi \\ &= \frac{1}{2\pi} \int_{-\pi}^{\pi} f(\phi)\, D_m(\theta-\phi)\, \mathrm{d}\phi \end{aligned} \tag{1.42}$$

where $D_m(x) = \sum_{k=-m}^{m} \mathrm{e}^{\mathrm{i}kx}$ is known as the *Dirichlet kernel*. Fejér now applied Césaro's idea, setting

$$\sigma_n(f) = \frac{1}{n+1} \sum_{m=0}^{n} S_m f = \frac{1}{2\pi} \int_{-\pi}^{\pi} f(\phi)\, F_n(\theta-\phi)\, \mathrm{d}\phi \tag{1.43}$$

where the *Fejér kernel* $F_n(x) \equiv \frac{1}{n+1} \sum_{m=0}^{n} D_m(x)$. It's a straightforward exercise to show that

$$F_n(x) = \begin{cases} \dfrac{1}{n+1} \dfrac{\sin^2[(n+1)x/2]}{\sin^2[x/2]} & \text{for } x \neq 0 \\ n+1 & \text{when } x = 0\,, \end{cases} \tag{1.44}$$

but I'll skip the proof. To make progress, we first list some important properties of $F_n(x)$. These are *i)* $F_n(x) \geq 0$ everywhere, *ii)* $\frac{1}{2\pi} \int_{-\pi}^{\pi} F_n(\theta)\, \mathrm{d}\theta = 1$, and *iii)* $F_n(x) \to 0$ uniformly outside an arbitrarily small region $[-\delta, \delta]$ around $\theta = 0$. Property *i)* is obvious. Property *ii)* is best seen using the definition of F_n in terms of the Dirichlet kernel:

$$\begin{aligned} \frac{1}{2\pi} \int_{-\pi}^{\pi} F_n(\theta)\, \mathrm{d}\theta &= \frac{1}{2\pi} \int_{-\pi}^{\pi} \left[\frac{1}{n+1} \sum_{m=0}^{n} \sum_{k=-m}^{m} \mathrm{e}^{\mathrm{i}k\theta} \right] \mathrm{d}\theta \\ &= \frac{1}{n+1} \sum_{m=0}^{n} \sum_{k=-m}^{m} \left[\frac{1}{2\pi} \int_{-\pi}^{\pi} \mathrm{e}^{\mathrm{i}k\theta}\, \mathrm{d}\theta \right]. \end{aligned}$$

The integral in square brackets vanishes whenever $k \neq 0$, and gives 1 when $k = 0$. For each value of m, the value $k = 0$ occurs exactly once, so the double sum gives $n+1$ and property *ii)* is proved. Property *iii)* follows since for $\delta \leq |x| \leq \pi$

$$F_n(x) \leq \frac{1}{n+1} \frac{1}{\sin^2[x/2]} \leq \frac{1}{n+1} \frac{1}{\sin^2[\delta/2]} \to 0\,,$$

with convergence being uniform.

The idea of Fejér's proof is that since property *iii)* shows that $F_n(\theta-\phi)$ is concentrated on $\theta = \phi$ as $n \to \infty$, in this limit the integral on the right of (1.43) for $\sigma_n(f)$ receives an appreciable contribution only from a tiny neighbourhood of $\phi = \theta$. Since f is continuous, in this neighbourhood $f(\phi)$ may be approximated by $f(\theta)$, so

$$\sigma_n(f) = \frac{1}{2\pi} \int_{-\pi}^{\pi} f(\phi)\, F_n(\theta-\phi)\, \mathrm{d}\phi \approx \frac{f(\theta)}{2\pi} \int_{-\pi}^{\pi} F_n(\theta-\phi)\, \mathrm{d}\phi = f(\theta)\,, \tag{1.45}$$

using property *ii*) of the Fejér kernel. Thus $|\sigma_n - f(\theta)| \to 0$ uniformly as $n \to \infty$ and so the σ_n converge uniformly on the original function. Once you're seen enough of Analysis II, you might like to fill in the 'epsilonics' to make the idea sketched above into a firm proof. It's actually possible to generalize the proof to allow $f : S^1 \to \mathbb{C}$ to be discontinuous at a finite number of isolated points $\{\theta_1, \theta_2, \ldots, \theta_r\} \in S^1$, provided $\int_{S^1} |f(\theta)|\, \mathrm{d}\theta$ exists[8]. Then $\sigma_n(f)$ converges to the original function at all points $\theta \in S^1$ where $f(\theta)$ *is* continuous.

Fejér assures us that we can recover any continuous function from its Fourier coefficients, but not that the partial Fourier series $S_n f$ itself actually converge when $n \to \infty$. In fact, one can prove that for continuous functions, $S_n f$ does indeed converge to $f(\theta)$ provided $\sum_{n=-\infty}^{\infty} |\hat{f}_n|$ converges. The proof is an application of the Weierstrass M test. Have a go at proving it if you know what this is!

1.6 Pragmatism

To the horror of the analysts, in this course we'll henceforth mostly gloss over these subtle issues of convergence. The emphasis instead will be on seeing how we can actually *use* Fourier series to solve various linear differential equations, very much in the spirit of Fourier's own approach. In partial defense of this position, I say again that in physics, the reason we're interested in these linear equations in the first place is typically because they provide an approximation to a deeper, more complicated underlying system. If we're having to go very far down the Fourier series to get reasonable convergence to our original function, it's likely because some this function has some sharp feature that is in any case unphysical.

As an example, the 'plucked string' function

$$f(\theta) = \frac{\pi}{2} - |\theta| \tag{1.46}$$

for $\theta \in [-\pi, \pi)$ has Fourier coefficients

$$\hat{f}_n = \frac{1}{2\pi} \int_{-\pi}^{\pi} \mathrm{e}^{-\mathrm{i}n\theta} \left(\frac{\pi}{2} - |\theta| \right) \mathrm{d}\theta = \begin{cases} 0 & \text{when } k \text{ is even and } n \neq 0 \\ \dfrac{2}{\pi n^2} & \text{when } n \text{ is odd} \end{cases} \tag{1.47}$$

(*check this as an exercise!*). These fall off like $\sim 1/n^2$, in agreement with the general results of section 1.4.3, since f is continuous but has a discontinuous first derivative, and $S_n f$ converges to $f(\theta)$. If we keep just the first three non-vanishing terms then

$$S_n f = \frac{4}{\pi} \left(\cos\theta + \frac{1}{9} \cos 3\theta + \frac{1}{25} \cos 5\theta + \cdots \right)$$

gives us an approximation to the plucked string that is good to 1 part in 10. But to obtain very high accuracy, we need to keep many millions of terms. The reason such high frequency terms are needed is because we need waves with very rapid oscillations to reproduce the sharp kink in the plucked string. But a real string will not kink precisely;

[8] As a Riemann integral.

the string has some thickness and any attempt to sharpen the kink too far will eventually cause the material to break. In other words, our naive attempt to model the behaviour of our real string by a linear equation breaks down, and the Fourier analysis based on the idea of an infinite dimensional vector space is no longer appropriate.

However, there is a cautionary conclusion to this tail. If you look at figures 1 and 2 you will observe a persistent overshoot – around 18% of the true value – of the Fourier series near the discontinuity. These little blips are known as the *Gibbs-Wilbraham phenomenon* and are explored in more detail in the problems. What is happening is that because the sawtooth and square wave functions have discontinuities, while the Fourier series do converge *pointwise*, they do *not* do so *uniformly*: convergence is slower near the discontinuities. This phenomenon was first discovered by Wilbraham in 1848, but was forgotten as a mathematical curiosity. In the 1890s Michelson constructed a device which could compute Fourier series automatically. When fed the square wave, he noticed the overshoot and assumed the machine was faulty until Gibbs provided the explanation. During WW2, the new British invention of radar was crucial in locating and intercepting Lüftwaffe bombers. The radar pulse sent out was a sawtooth, and engineers were puzzled by the little blips near the edge of each tooth.

1.7 Parseval's identity

When we first introduced the inner product as the integral $(f,g) = \int_\Omega f^* g \, \mathrm{d}\mu$ in (1.6) we treated the value a function takes at each point in its domain Ω as its components, with the norm-squared $(f,f) = \int |f|^2 \, \mathrm{d}\mu$ telling us to add the mod-square of these 'components' over Ω. On the other hand, Fourier has encouraged us to think about expanding a periodic function in terms of the basis $\{\mathrm{e}^{\mathrm{i}n\theta};\ n \in \mathbb{Z}\}$ of orthogonal functions, with the Fourier coefficients $\hat{f}_n$ being the components in this basis. Using this, we have

$$\begin{aligned}(f,f) &\stackrel{?}{=} \int_{-\pi}^{\pi} \left(\sum_{m\in\mathbb{Z}} \hat{f}_m \, \mathrm{e}^{\mathrm{i}m\theta}\right)^* \left(\sum_{n\in\mathbb{Z}} \hat{f}_n \, \mathrm{e}^{\mathrm{i}n\theta}\right) \mathrm{d}\theta \\ &= \int_{-\pi}^{\pi} \sum_{m,n\in\mathbb{Z}} \hat{f}_m^* \hat{f}_n \, \mathrm{e}^{\mathrm{i}(n-m)\theta} \, \mathrm{d}\theta \ \stackrel{?}{=} \sum_{m,n\in\mathbb{Z}} \hat{f}_m^* \hat{f}_n \int_{-\pi}^{\pi} \mathrm{e}^{\mathrm{i}(n-m)\theta} \, \mathrm{d}\theta \,,\end{aligned} \tag{1.48}$$

where I've rather cavalierly exchanged infinite sums and integrals. Using the orthogonality of our basis functions, the norm squared of our function can be written as

$$(f,f) = 2\pi \sum_{n\in\mathbb{Z}} |\hat{f}_n|^2 \,, \tag{1.49}$$

which is known as *Parseval's identity*. Parseval's identity can be viewed as an infinite dimensional version of Pythagoras' theorem: it says that the norm squared f is equal to the sum of the (mod-)squares of its coefficients in the (Fourier) basis of orthogonal functions[9]. (The factor of 2π can be traced to our conventions in the defintion (1.11) of the Fourier coefficients.)

[9] More formally, if we view the Fourier series as a map from a function to the sequence $\{\hat{f}_n\}$, then viewing this sequence as the coefficients of an infinite dimensional vector, Parseval's identity tells us that this map is an *isometry* – meaning it preserves lengths.

Parseval's identity has many uses. For example, suppose that a point x on a vibrating string has velocity $v(x)$ in the transverse direction. Then the total kinetic energy of the string is

$$E = \frac{T}{2}(v,v) = \frac{T}{2}\int_0^L v(x)^2\,\mathrm{d}x\,,$$

where T is the string's tension and L is its length. Decomposing the motion into a Fourier series, Parseval's identity tells us that the total kinetic energy of the string is the sum of kinetic energies stored in all the separate modes of oscillation (the *harmonics* of the string).

Parseval's identity is also good for generating rather pretty identities involving infinite sums of the type beloved by Euler. For example, consider again the sawtooth function $f(\theta) = \theta$ for $\theta \in [-\pi, \pi)$, whose Fourier coefficients we found in (1.23) to be

$$\hat{f}_n = \frac{\mathrm{i}}{n}(-1)^n \text{ for } n \in \mathbb{Z}_{>0} \qquad \text{while} \qquad \hat{f}_0 = 0\,,$$

with $\hat{f}_{-n} = (\hat{f}_n)^*$ since the sawtooth is real. Then Parseval's identity becomes

$$\frac{2\pi^3}{3} = \int_{-\pi}^{\pi}\theta^2\,\mathrm{d}\theta = 2\pi\sum_{n\in\mathbb{Z}}|\hat{f}_n|^2 = 4\pi\sum_{n=1}^{\infty}\frac{1}{n^2}\,,$$

or in other words

$$\frac{\pi^2}{6} = 1 + \frac{1}{4} + \frac{1}{9} + \frac{1}{16} + \cdots\,. \tag{1.50}$$

As an exercise, you might also like to show that

$$\frac{\pi^4}{90} = \sum_{n=1}^{\infty}\frac{1}{n^4}$$

using Parseval's identity for the *integral* of the sawtooth function.

The derivation of Parseval's identity given above is sufficient for your 1B (Methods) exam, but it leaves rather a lot to be desired. You should worry that we said nothing about the convergence of the Fourier series itself, nor about the convergence of resulting sum (1.49). And you should have been more worried still when I exchanged the infinite sums with the integrals. To save our blushes, let's give a more careful derivation.

We first consider the norm-squared (S_nf, S_nf) of the n^{th} partial Fourier sum. This is

$$\begin{aligned}(S_nf, S_nf) &= \int_{-\pi}^{\pi}\left(\sum_{j=-n}^{n}\hat{f}_j\,\mathrm{e}^{\mathrm{i}j\theta}\right)^*\left(\sum_{k=-n}^{n}\hat{f}_k\,\mathrm{e}^{\mathrm{i}k\theta}\right)\mathrm{d}\theta \\ &= \sum_{j,k=-n}^{n}\left(\hat{f}_j^*\,\hat{f}_k\int_{-\pi}^{\pi}\mathrm{e}^{\mathrm{i}(k-j)\theta}\,\mathrm{d}\theta\right) \\ &= 2\pi\sum_{j,k=-n}^{n}\hat{f}_j^*\hat{f}_k\,\delta_{k,j} = 2\pi\sum_{k=-n}^{n}|\hat{f}_k|^2\,.\end{aligned} \tag{1.51}$$

Since the sums are finite here, no convergence worries arise, and it's safe to pull the sums out of the integral. Similarly, the inner product of $S_n f$ with f itself is

$$\begin{aligned}(S_n f, f) &= \int_{-\pi}^{\pi} \left[\sum_{k=-n}^{n} \hat{f}_k^* \, \mathrm{e}^{-\mathrm{i}k\theta} \right] f(\theta) \, \mathrm{d}\theta \\ &= \sum_{k=-n}^{n} \hat{f}_k^* \left[\int_{-\pi}^{\pi} \mathrm{e}^{-\mathrm{i}k\theta} \, f(\theta) \, \mathrm{d}\theta \right] = 2\pi \sum_{k=-n}^{n} |\hat{f}_k|^2 \,,\end{aligned} \tag{1.52}$$

which is clearly real. Thus $(S_n f, S_n f) = (S_n f, f) = (f, S_n f)$. Therefore, the norm-squared of the difference between the partial Fourier sum and the original function is

$$\begin{aligned}(S_n f - f, S_n f - f) &= (S_n f, S_n f) + (f, f) - (S_n f, f) - (f, S_n f) \\ &= (f, f) - 2\pi \sum_{k=-n}^{n} |\hat{f}_k|^2 \,.\end{aligned} \tag{1.53}$$

Now, let's suppose that as $n \to \infty$, the sequence of partial Fourier sums $S_n f$ converges, and further that it converges to f itself everywhere except perhaps at finitely many isolated points (for instance, if f jumps). Then we must have

$$\lim_{n\to\infty} (S_n f - f, S_n f - f) = \lim_{n\to\infty} \int_{-\pi}^{\pi} |S_n f(\theta) - f(\theta)|^2 \, \mathrm{d}\theta = 0 \tag{1.54}$$

because as $n \to \infty$ the integrand itself gets closer and closer to zero everywhere except perhaps at some isolated points. Comparing with the previous expression, we see that $\lim_{n\to\infty} \left[(f, f) - 2\pi \sum_{k=-n}^{n} |\hat{f}_k|^2 \right] = 0$ and so $(f, f) = 2\pi \sum_{k\in\mathbb{Z}} |\hat{f}_k|^2$. Phew!

In fact, though this derivation doesn't show it, Parseval's identity holds in even more general circumstances than we've allowed. But if you want to know about that, I recommend you to read Prof. Körner's *Fourier Analysis* book, or take the Part II course on Topics in Analysis.

2 Sturm–Liouville Theory

So far, we've examined the Fourier decomposition of functions defined on some interval (often scaled to be from $-\pi$ to π). We viewed this expansion as an infinite dimensional analogue of expanding a finite dimensional vector into its components in an orthonormal basis. But this is just the tip of the iceberg. Recalling other games we play in linear algebra, you might well be wondering whether we couldn't have found some other basis in which to expand our functions. You might also wonder whether there shouldn't be some role for *matrices* in this story. If so, read on!

2.1 Self-adjoint matrices

We'll begin by reviewing some facts about matrices. Let V and W be finite dimensional vector spaces (defined, say, over the complex numbers) with $\dim V = n$ and $\dim W = m$. Suppose we have a linear map $M : V \to W$. By linearity, we know what M does to any vector $\mathbf{v} \in V$ if we know what it does to a complete set $\{\mathbf{v}_1, \mathbf{v}_2, \ldots, \mathbf{v}_n\}$ of basis vectors in V. Furthermore, given a basis $\{\mathbf{w}_1, \mathbf{w}_2, \ldots, \mathbf{w}_m\}$ of W we can represent the map M in terms of an $m \times n$ *matrix* $\mathbf{M}$ whose components are

$$\mathbf{M}_{ai} = (\mathbf{w}_a, M\mathbf{v}_i) \qquad \text{for } a = 1, \ldots, m \;\text{ and }\; i = 1, \ldots, n\,, \tag{2.1}$$

where $(\ ,\ )$ is the inner product in W.

We'll be particularly interested in the case $m = n$, when the matrix $\mathbf{M}$ is square and the map M takes $M : V \to W \cong V$ is an isomorphism of vector spaces. For any $n \times n$ matrix M we define it's eigenvalues $\{\lambda_1, \lambda_2, \ldots, \lambda_n\}$ to be the roots of the characteristic equation $P(\lambda) \equiv \det(\mathbf{M} - \lambda\mathbf{I}) = 0$, where $\mathbf{I}$ is the identity matrix. This characteristic equation has degree n and the fundamental theorem of algebra assures us that we'll always be able to find n roots (generically complex, and not necessarily distinct). The *eigenvector* $\mathbf{v_i}$ of $\mathbf{M}$ that corresponds to the eigenvalue λ_i is then defined by $\mathbf{M}\mathbf{v_i} = \lambda_i\mathbf{v_i}$ (at least for non-degenerate eigenvalues).

Given a complex $n \times n$ matrix $\mathbf{M}$, its *Hermitian conjugate* $\mathbf{M}^\dagger$ is defined to be the complex conjugate of the transpose matrix, $\mathbf{M}^\dagger \equiv (\mathbf{M}^{\mathrm{T}})^*$, where the complex conjugation acts on each entry of $\mathbf{M}^{\mathrm{T}}$. A matrix is said to be *Hermitian* or *self-adjoint* if $\mathbf{M}^\dagger = \mathbf{M}$. There's a neater way to define this: since for two vectors we have $(\mathbf{u}, \mathbf{v}) = \mathbf{u}^\dagger \cdot \mathbf{v}$, we see that a matrix $\mathbf{B}$ is the adjoint of a matrix $\mathbf{A}$ iff

$$(\mathbf{Bu}, \mathbf{v}) = (\mathbf{u}, \mathbf{Av}) \tag{2.2}$$

because the vector $(\mathbf{Bu})^\dagger = \mathbf{u}^\dagger\mathbf{B}^\dagger$. The advantages of this definition are that *i*) it does not require that we pick any particular components in which to write the matrix and *ii*) it applies whenever we have a definition of an inner product $(\ ,\ )$.

Self-adjoint matrices have a number of very important properties. Firstly, since

$$\lambda_i(\mathbf{v_i}, \mathbf{v_i}) = (\mathbf{v_i}, \mathbf{Mv_i}) = (\mathbf{Mv_i}, \mathbf{v_i}) = \lambda_i^*(\mathbf{v}_i, \mathbf{v}_i) \tag{2.3}$$

the eigenvalues of a self-adjoint matrix are always real. Secondly, we have

$$\lambda_i(\mathbf{v_j}, \mathbf{v_i}) = (\mathbf{v_j}, \mathbf{M v_i}) = (\mathbf{M v_j}, \mathbf{v_i}) = \lambda_j(\mathbf{v}_j, \mathbf{v}_i) \tag{2.4}$$

or in other words

$$(\lambda_i - \lambda_j)(\mathbf{v}_j, \mathbf{v}_i) = 0 \tag{2.5}$$

so that eigenvectors corresponding to distinct eigenvalues are orthogonal *wrt* the inner product (,). After rescaling the eigenvectors to have unit norm, we can express any $\mathbf{v} \in V$ as a linear combination of the orthonormal set $\{\mathbf{v}_1, \mathbf{v}_2, \ldots, \mathbf{v}_n\}$ of eigenvectors of some self-adjoint $\mathbf{M}$. If $\mathbf{M}$ has degenerate eigenvalues (*i.e.* two or more distinct vectors have the same eigenvalue) then the set of vectors sharing an eigenvalue form a vector subspace of V and we simply choose an orthonormal basis for each of these subspaces. In any case, the important point here is that self-adjoint matrices provide a *natural* way to pick a basis on our vector space.

A self-adjoint matrix $\mathbf{M}$ is non-singular ($\det \mathbf{M} \neq 0$ so that $\mathbf{M}^{-1}$ exists) if and only if all its eigenvalues are non-zero. In this case, we can solve the linear equation $\mathbf{Mu} = \mathbf{f}$ for a fixed vector $\mathbf{f}$ and unknown $\mathbf{u}$. Formally, the solution is $\mathbf{u} = \mathbf{M}^{-1}\mathbf{f}$, but a practical way to determine $\mathbf{u}$ proceeds as follows. Suppose $\{\mathbf{v}_1, \mathbf{v}_2, \ldots, \mathbf{v}_n\}$ is an orthonormal basis of eigenvectors of $\mathbf{M}$. Then we can write

$$\mathbf{f} = \sum_{i=1}^{n} f_i \mathbf{v_i} \qquad \text{and} \qquad \mathbf{u} = \sum_{i=1}^{n} u_i \mathbf{v_i}$$

where $f_i = (\mathbf{v}_i, \mathbf{f})$ *etc.* as before. We will know the vector $\mathbf{u}$ if we can find all its coefficients u_i in the $\{\mathbf{v}_i\}$ basis. But by linearity

$$\mathbf{Mu} = \sum_{i=1}^{n} u_i \, \mathbf{M v}_i = \sum_{i=1}^{n} u_i \lambda_i \mathbf{v}_i \;=\; \mathbf{f} = \sum_{i=1}^{n} f_i \mathbf{v}_i \;, \tag{2.6}$$

and taking the inner product of this equation with $\mathbf{v}_j$ gives

$$\sum_{i=1}^{n} u_i \lambda_i \, (\mathbf{v}_j, \mathbf{v}_i) = u_j \lambda_j \;=\; \sum_{i=1}^{n} f_i (\mathbf{v}_j, \mathbf{v}_i) = f_j \tag{2.7}$$

using the orthonormality of the basis. Provided $\lambda_j \neq 0$ we deduce $u_j = f_j/\lambda_j$ so that

$$\mathbf{u} = \sum_{i=1}^{n} \frac{f_i}{\lambda_i} \mathbf{v}_i \;. \tag{2.8}$$

If $\mathbf{M}$ is singular then either $\mathbf{Mu} = \mathbf{f}$ has no solution or else has a non-unique solution (which it is depends on the choice of $\mathbf{f}$).

2.2 Differential operators

In the previous chapter we learned to think of functions as infinite dimensional vectors. We'd now like to think of the analogue of matrices. Sturm and Liouville realised that these

could be thought of as *linear differential operators* $\mathcal{L}$. This is just a linear combination of derivatives with coefficients that can also be functions of x, *i.e.* $\mathcal{L}$ is a linear differential operator of order p if

$$\mathcal{L} = A_p(x)\frac{d^p}{dx^p} + A_{p-1}(x)\frac{d^{p-1}}{dx^{p-1}} + \cdots + A_1(x)\frac{d}{dx} + A_0(x) \ .$$

When it acts on a (sufficiently smooth) function $y(x)$ it gives us back some other function $\mathcal{L}y(x)$ obtained by differentiating $y(x)$ in the obvious way. This is a linear map between spaces of functions because for two (p-times differentiable) functions $y_{1,2}(x)$ and constants $c_{1,2}$ we have $\mathcal{L}(c_1y_1 + c_2y_2) = c_1\mathcal{L}y_1 + c_2\mathcal{L}y_2$. The analogue of the matrix equation $\mathbf{Mu} = \mathbf{f}$ is then the differential equation $\mathcal{L}y(x) = f(x)$ where we assume that both the coefficient functions $A_p(x), \ldots, A_0(x)$ in $\mathcal{L}$ and the function $f(x)$ are known, and that we wish to find the unknown function $y(x)$.

For most of our applications in mathematical physics, we'll be interested in *second order*[10] linear differential operators[11]

$$\mathcal{L} = P(x)\frac{d^2}{dx^2} + R(x)\frac{d}{dx} - Q(x) \ . \tag{2.9}$$

Recall that for any such operator, the *homogeneous equation* $\mathcal{L}y(x) = 0$ has precisely two non-trivial linearly independent solutions, say $y = y_1(x)$ and $y = y_2(x)$ and the general solution $y(x) = c_1y_1(x) + c_2y_2(x)$ with $c_i \in \mathbb{C}$ is known as the *complementary function*. When dealing with the *inhomogeneous equation* $\mathcal{L}y = f$, we seek any single solution $y(x) = y_p(x)$, and the general solution is then a linear combination

$$y(x) = c_py_p(x) + c_1y_1(x) + c_2y_2(x)$$

of the particular and complementary solutions. In many physical applications, the function f represents a driving force for a system that obeys $\mathcal{L}y(x) = 0$ if left undisturbed.

In the cases (I assume) you've seen up to now, actually *finding* the particular solution required a good deal of either luck or inspired guesswork – you 'noticed' that if you differentiated such-and-such a function you'd get something that looked pretty close to the solution you're after, and perhaps you could then refine this guess to find an exact solution. Sturm–Liouville theory provides a more systematic approach, analogous to solving the matrix equation $\mathbf{Mu} = \mathbf{f}$ above.

2.3 Self-adjoint differential operators

The 2$^{\text{nd}}$-order differential operators considered by Sturm & Liouville take the form

$$\mathcal{L}y \equiv \frac{d}{dx}\left(p(x)\frac{dy}{dx}\right) - q(x)y \, , \tag{2.10}$$

where $p(x)$ is *real* (and once differentiable) and $q(x)$ is real and continuous. This may look to be a tremendous specialization of the general form (2.9), with $R(x)$ restricted to be

[10] It's a beautiful question to ask 'why only second order'? Particularly in quantum theory.

[11] The sign in front of $Q(x)$ is just a convention.

$P'(x)$, but actually this isn't the case. Provided $P(x) \neq 0$, starting from (2.9) we divide through by $P(x)$ to obtain

$$\frac{d^2}{dx^2} + \frac{R(x)}{P(x)}\frac{d}{dx} - \frac{Q(x)}{P(x)} = \mathrm{e}^{-\int_0^x R(t)/P(t)\,\mathrm{d}t}\,\frac{d}{dx}\left(\mathrm{e}^{\int_0^x R(t)/P(t)\,\mathrm{d}t}\,\frac{d}{dx}\right) - \frac{Q(x)}{P(x)} \tag{2.11}$$

Thus setting $p(x)$ to be the integrating factor $p(x) = \exp\left(\int_0^x R(t)/P(t)\,\mathrm{d}t\right)$ and likewise setting $q(x) = Q(x)p(x)/P(x)$, we see that the forms (2.10) and (2.9) are equivalent. However, for most purposes (2.10) will be more convenient.

The beautiful feature of these Sturm–Liouville operators is that they are self-adjoint with respect the inner product

$$(f, g) = \int_a^b f(x)^* g(x)\,\mathrm{d}x\,, \tag{2.12}$$

provided the functions on which they act obey appropriate boundary conditions. To see this, we simply integrate by parts twice:

$$\begin{aligned}
(\mathcal{L}f, g) &= \int_a^b \left[\frac{d}{dx}\left(p(x)\frac{df^*}{dx}\right) - q(x)f^*(x)\right] g(x)\,\mathrm{d}x \\
&= \left[p\,\frac{df^*}{dx}\,g\right]_a^b - \int_a^b p(x)\frac{df^*}{dx}\frac{dg}{dx} - q(x)f(x)^*g(x)\,\mathrm{d}x \\
&= \left[p\,\frac{df^*}{dx}\,g - p\,f^*\frac{dg}{dx}\right]_a^b + \int_a^b f(x)^*\left[\frac{d}{dx}\left(p(x)\frac{dg}{dx}\right) - q(x)\,g(x)\right] \\
&= \left[p(x)\left(\frac{df^*}{dx}\,g - f^*\frac{dg}{dx}\right)\right]_a^b + (f, \mathcal{L}g)
\end{aligned} \tag{2.13}$$

where in the first line we have used fact that p and q are real for a Sturm–Liouville operator. So we see that $(\mathcal{L}f, g) = (f, \mathcal{L}g)$ provided we restrict ourselves to functions which obey the boundary conditions

$$\left[p(x)\left(\frac{df^*}{dx}\,g - f^*\frac{dg}{dx}\right)\right]_a^b = 0\,. \tag{2.14}$$

Examples of such boundary conditions are to require that *all* our functions satisfy

$$\begin{aligned}
b_1 f'(a) + b_2 f(a) &= 0 \\
c_1 f'(b) + c_2 f(b) &= 0\,,
\end{aligned} \tag{2.15}$$

where $b_{1,2}$ and $c_{1,2}$ are constants, not both zero. I emphasize that we must choose the *same* constants for all our functions. These boundary conditions ensure that (2.14) vanishes at each boundary separately. If the function $p(x)$ obeys $p(a) = p(b)$ then we can likewise ask that all our functions are periodic, so that $f(a) = f(b)$ and $f'(a) = f'(b)$; this ensures that the contributions at each boundary cancel in (2.14). Finally, it may sometimes be that $p(a) = p(b) = 0$, though in this case the endpoints of the interval $[a, b]$ are singular points of the differential equation.

2.4 Eigenfunctions and weight functions

Whatever boundary conditions we choose, provided they satisfy (2.14) we have $(\mathcal{L}f, g) = (f, \mathcal{L}g)$ and $\mathcal{L}$ is self-adjoint. Just as in the finite dimensional case of self-adjoint matrices, these self-adjoint differential operators automatically inherit many useful properties.

We start by defining the notion of an *eigenfunction* of our differential operator. It's convenient to do this in a slightly surprising way. A *weight function* $w(x)$ is a real-valued, non-negative function that has at most finitely many zeros on the domain $[a, b]$. A function $y(x)$ is said to be an *eigenfunction of* $\mathcal{L}$ *with eigenvalue* λ *and weight* $w(x)$ if

$$\mathcal{L}y(x) = \lambda w(x) y(x) \tag{2.16}$$

where we note the presence of the weight function on the right hand side. In fact, given such an eigenfunction we can always find a corresponding eigenfunction $\tilde{y}(x)$ with weight function 1 by setting $\tilde{y}(x) = \sqrt{w(x)}\, y(x)$ and replacing $\mathcal{L}y$ by $\frac{1}{\sqrt{w}}\mathcal{L}\left(\frac{\tilde{y}}{\sqrt{w}}\right)$, so the weight function does not really represent anything new, but it's conventional (and will turn out to be convenient) to keep it explicit.

The weight function plays a role in the inner product. We define the *inner product with weight* w to be

$$(f, g)_w \equiv \int_a^b f(x)^* g(x)\, w(x)\, \mathrm{d}x \tag{2.17}$$

so that the measure includes a factor of w. Notice that since w is real

$$(f, g)_w = (f, wg) = (wf, g) \tag{2.18}$$

where the inner products on the *rhs* are the standard ones with measure $\mathrm{d}x$ only. This inner product is again non-degenerate in the sense that $(f, f)_w = 0$ implies $f = 0$ if f is continuous (at least in a neighbourhood of any zeros of $w(x)$). This is because

$$(f, f)_w = \int_a^b |f(x)|^2\, w(x)\, \mathrm{d}x$$

is the integral of a continuous positive function $w(x)|f(x)|^2$. By assumption w has only finitely many zeros on $[a, b]$ while f is continuous, so the integral gives zero if and only if $f(x) = 0$ identically on $[a, b]$.

The first property of Sturm–Liouville operators is that their eigenvalues are always real. The proof is exactly the same as in the finite dimensional case: if $\mathcal{L}f = \lambda w f$ then

$$\lambda\,(f, f)_w = (f, \lambda w f) = (f, \mathcal{L}f) = (\mathcal{L}f, f) = \lambda^*(f, f)_w \tag{2.19}$$

using the self-adjointness of $\mathcal{L}$ and the fact that the inner product $(\ ,\ )$ is *anti*-linear in its first entry. Note that if f has eigenvalue λ, then because the eigenvalues, weight w and coefficients $p(x)$ and $q(x)$ are real

$$\mathcal{L}(f^*) = (\mathcal{L}f)^* = (\lambda w f)^* = \lambda w(x)\, f(x)^* \tag{2.20}$$

so that f^* is also an eigenfunction of $\mathcal{L}$ with the same eigenvalue. Thus, taking Re f and Im f if necessary, we can always choose our eigenfunctions to be real-valued.

Just as in the finite dimensional case, eigenfunctions f_1 and f_2 with distinct eigenvalues, but the *same* weight function, are orthogonal wrt the inner product with weight w, since:

$$\lambda_i(f_j, f_i)_w = (f_j, \mathcal{L}f_i) = (\mathcal{L}f_j, f_i) = \lambda_j(f_j, f_i)_w \tag{2.21}$$

so that if $\lambda_i \neq \lambda_j$ then

$$(f_j, f_i)_w = \int_a^b f_j(x)^* f_i(x)\, w(x)\, \mathrm{d}x = 0\,. \tag{2.22}$$

Thus, exactly as in the finite dimensional case, given a self-adjoint operator $\mathcal{L}$ we can form an orthonormal set $\{Y_1(x), Y_2(x), \ldots\}$ of its eigenfunctions by setting

$$Y_n(x) = y_n(x) \Big/ \sqrt{\int_a^b |y_n|^2\, w\, \mathrm{d}x} \tag{2.23}$$

where $y_n(x)$ is the unnormalised eigenfunction. I emphasize again the presence of the weight function in these orthogonality and normalization conditions.

Finally, after making a particular choice of boundary conditions, one can also show[12] that the eigenvalues form a countably infinite sequence $\lambda_1, \lambda_2, \ldots$, with $|\lambda_n| \to \infty$ as $n \to \infty$, and that the corresponding set of orthonormal eigenfunctions $Y_1(x), Y_2(x), \ldots$ form a *complete* basis for functions on $[a, b]$ satisfying these boundary conditions. That is, any function $f(x)$ on $[a, b]$ that obeys the chosen boundary conditions may be expanded as[13]

$$f(x) = \sum_{n=1}^{\infty} f_n\, Y_n(x)\,, \qquad \text{where} \qquad f_n = \int_a^b Y_n^*(x) f(x)\, w(x)\, \mathrm{d}x = (Y_n, f)_w\,. \tag{2.24}$$

The significant feature here is that the function $f(x)$ is expanded as a *discrete* sum, just as we saw for Fourier series. This is really remarkable, because the definition of the Y_ns – that they be normalised eigenfunctions of $\mathcal{L}$ – involves no hint of discreteness. In fact, we'll see later in the course that the discreteness arises because the domain $[a, b]$ is *compact*, and because of our boundary conditions (2.14).

2.5 Some examples

Let's take a look at some simple examples of the general theory above. The simplest non-trivial case is just to take the domain $[a, b]$ to be $[-L, L]$ and impose the homogeneous boundary conditions that all our functions are periodic *i.e.* $f(-L) = f(L)$ and $f'(-L) = f'(L)$. If we also choose $p(x) = 1$ and $q(x) = 0$ then the Sturm–Liouville operator reduces to

$$\mathcal{L} = \frac{d^2}{dx^2}\,, \tag{2.25}$$

[12] But, sadly, not in this course.

[13] As warned, in this course we will no longer worry about convergence of these infinite sums, although see section 2.8.

which is easily seen to be self-adjoint when acting on functions obeying these boundary conditions. Finally, we choose the weight function to be $w(x) = 1$ identically.

The eigenfunction equation becomes

$$\mathcal{L}y(x) = -\lambda y(x) \tag{2.26}$$

where we've introduced a minus sign for convenience (just by relabelling the eigenvalues). If $\lambda < 0$ then the only solution *that obeys the periodic boundary conditions* is the trivial case $y(x) = 0$. However, if $\lambda \geq 0$ then a basis of solutions is given by

$$y_n(x) = \exp\left(\mathrm{i}\frac{n\pi x}{L}\right) \qquad \text{for} \qquad \lambda_n = \left(\frac{n\pi}{L}\right)^2 \quad \text{with} \quad n \in \mathbb{Z}\,. \tag{2.27}$$

Thus we have recovered the Fourier series of section 1.3 as a special case! Note that these eigenvalues are degenerate, with $\lambda_n = \lambda_{-n}$; as we saw before, whenever $y(x)$ is a complex–valued eigenfunction of a SL operator, then $y^*(x)$ is also an eigenfunction with the same eigenvalue. If instead of asking for the functions to be periodic, we'd asked specifically that $f(-L) = f(L) = 0$, then we would find just the sinusoidal Fourier series which has non-degenerate eigenvalues.

For a more interesting example, suppose we're interested in solving the differential equation[14]

$$\frac{1}{2}H'' - xH' = -\lambda H(x) \qquad \text{for} \qquad x \in \mathbb{R}\,, \tag{2.28}$$

subject to the condition that $H(x)$ behaves like a polynomial as $|x| \to \infty$ (so that in particular $\mathrm{e}^{-x^2/2}H(x) \to 0$ as $|x| \to \infty$). The reason for this strange looking condition will be revealed below.

Equation (2.28) is not yet in Sturm–Liouville form, so we first compute the integrating factor

$$p(x) = -\int_0^x 2t\,\mathrm{d}t = -x^2 \tag{2.29}$$

and rewrite (2.28) as

$$\frac{d}{dx}\left(\mathrm{e}^{-x^2}\frac{dH}{dx}\right) = -2\lambda\,\mathrm{e}^{-x^2}\,H(x) \tag{2.30}$$

(multiply through by $2\mathrm{e}^{-x^2}$ to recover the form (2.28)). This equation is known as *Hermite's equation* and it plays an important role in combinatorics, probability and in the quantum mechanics of a harmonic oscillator. We can now understand the condition that $H(x)$ grows at most polynomially at large $|x|$: in checking self–adjointness of the Sturm–Liouville operator on the unbounded domain $\mathbb{R}$, we do not need to consider boundary terms, but we do need to ensure the integrals

$$\int_{-\infty}^{\infty} f^*\frac{d}{dx}\left(\mathrm{e}^{-x^2}\frac{dg}{dx}\right)\,\mathrm{d}x = \int_{-\infty}^{\infty}\frac{df^*}{dx}\,\mathrm{e}^{-x^2}\,\frac{dg}{dx}\,\mathrm{d}x$$

[14] I'm cheating here by working on an unbounded domain $x \in \mathbb{R}$ rather than $x \in [a, b]$. Much of the theory holds, but notice the rather strange boundary condition we impose. This is just to ensure that the integrals over the entire real axis that arise when we check self-duality of $\mathcal{L}$ are bounded.

actually remain finite! For f and g regular along $\mathbb{R}$ this will be so as long as the integral is suppressed at large $|x|$. This is what our decay condition is designed to ensure.

I'll state without proof that equation (2.30) has non-trivial solutions that are regular for all $x \in \mathbb{R}$ iff the eigenvalue λ is a non-negative integer n, and you can check that these solutions are given by

$$H_n(x) = (-1)^n \, \mathrm{e}^{x^2} \, \frac{d^n}{dx^n} \, \mathrm{e}^{-x^2} \, . \tag{2.31}$$

Carrying out the differentiation in (2.31) we find for example, $H_0(x) = 1$, $H_1(x) = 2x$, $H_2(x) = 4x^2 - 2$ and $H_3(x) = 8x^3 - 12x$. In general $H_n(x)$ is a real polynomial of degree n, known as a *Hermite polynomial*. The Hermite polynomials are orthogonal with respect to the weight function $w(x) = \mathrm{e}^{-x^2}$ and obey the normalization condition

$$(H_m, H_n)_{\mathrm{e}^{-x^2}} = \int_{-\infty}^{\infty} H_m(x) \, H_n(x) \, \mathrm{e}^{-x^2} \, \mathrm{d}x = \delta_{m,n} \, 2^n \sqrt{\pi} \, n! \, , \tag{2.32}$$

where we note the decay condition is again crucial to ensure that this inner product remains finite.

2.6 Inhomogeneous equations and Green's functions

Finally, we return to the infinite dimensional analogue of the inhomogeneous matrix equation $\mathbf{Mu} = \mathbf{f}$ for a self-adjoint matrix $\mathbf{M}$. In the context of Sturm–Liouville differential operators, we seek to solve the inhomogeneous differential equation

$$\mathcal{L}\phi(x) = w(x)F(x) \tag{2.33}$$

where again we choose to include the weight function in the definition of the forcing term on the right hand side. By the remarks above, the functions $\phi(x)$ and $F(x)$ can be expanded in a complete set of eigenfunctions of $\mathcal{L}$. So we suppose that the set $\{Y_1(x), Y_2(x), \ldots\}$ form a complete set of such eigenfunctions with

$$\mathcal{L}Y_n(x) = \lambda_n \, w(x) \, Y_n(x) \qquad \text{and} \qquad (Y_m, Y_n)_w = \delta_{m,n} \tag{2.34}$$

and expand

$$\phi(x) = \sum_{n=1}^{\infty} \phi_n \, Y_n(x) \, , \qquad\qquad F(x) = \sum_{n=1}^{\infty} F_n \, Y_n(x) \, . \tag{2.35}$$

As in the matrix case, it is assumed that the function $F(x)$, and hence the coefficients $F_n = (Y_n, F)_w$ are known, while the coefficients ϕ_n must be found. But again, this can be done exactly in analogy with the finite dimensional case. Since $\mathcal{L}$ is a linear operator we have

$$\begin{aligned} \mathcal{L}\phi &= \sum_{n=1}^{\infty} \phi_n \, \mathcal{L}Y_n = w \sum_{n=1}^{\infty} \phi_n \lambda_n \, Y_n \\ &= wF = w \sum_{n=1}^{\infty} F_n Y_n \end{aligned} \tag{2.36}$$

and taking the inner product with Y_m gives $\phi_m \lambda_m = F_m$. Thus, provided none of the eigenvalues of $\mathcal{L}$ are zero we have found the particular solution

$$\phi_p(x) = \sum_{n=1}^{\infty} \frac{F_n}{\lambda_n} Y_n(x) \,. \tag{2.37}$$

As above, the general solution is now a sum of this particular solution and the complementary function $\phi_c(x)$ satisfying $\mathcal{L}\phi_c = 0$.

It's worth looking a little more closely at the structure of the solution (2.37). Substituting in the definition of the forcing term coefficients F_n and exchanging the sum and integral we have

$$\begin{aligned} \phi_p(x) &= \sum_{n=1}^{\infty} \frac{(Y_n, F)_w}{\lambda_n} Y_n(x) = \sum_{n=1}^{\infty} \left[\frac{1}{\lambda_n} Y_n(x) \int_a^b Y_n^*(t)\, F(t)\, w(t)\, \mathrm{d}t \right] \\ &= \int_a^b G(x,t) f(t)\, \mathrm{d}t \end{aligned} \tag{2.38}$$

where $f(t) = w(t)F(t)$ is the right hand side of the original inhomogeneous equation (2.33) and we've defined the *Green's function*

$$G(x;t) \equiv \sum_{n=1}^{\infty} \frac{Y_n(x) Y_n^*(t)}{\lambda_n} \,. \tag{2.39}$$

The Green's function is a function of two variables $(x,t) \in [a,b] \times [a,b]$. The important point about the Green's function is that it depends on the differential operator $\mathcal{L}$ both through its eigenfunctions and (more subtly) through the boundary conditions we chose to ensure $\mathcal{L}$ is self-adjoint, but it does *not* depend on the forcing function f. Thus if we know the Green's function we can use (2.38) to construct a particular solution of $\mathcal{L}y = f$ for an *arbitrary* forcing term. In this way, the Green's function provides a formal inverse to the differential operator $\mathcal{L}$ in the sense that

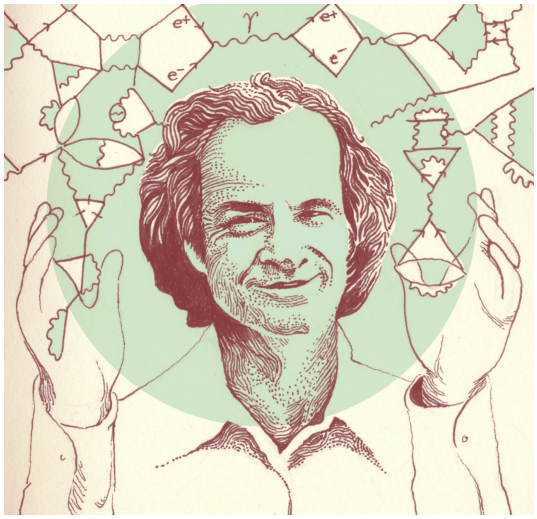
$$\text{if} \qquad \mathcal{L}y(x) = f(x) \qquad \text{then} \qquad y(x) = \int_a^b G(x,t)\, f(t)\, \mathrm{d}t$$

again in analogy with the finite dimensional case where $\mathbf{Mu} = \mathbf{f}$ implies $\mathbf{u} = \mathbf{M}^{-1}\mathbf{f}$ for a non-singular matrix. The notion of a Green's function and the associated integral operator as an inverse of $\mathcal{L}$ is very important. We'll meet it again later in many more general contexts. One of them is depicted here[15]:

2.7 Parseval's identity II

Recall that Pythagoras' theorem says that the length squared of a vector is the sum of the (mod-)squared of its components in *any* orthonormal basis. In the case of the Fourier basis, we obtained an infinite dimensional version of this in equation (1.49). We now establish

[15] I stole this picture from Hannah Wilson Illustration, as you'll quickly discover if, like me, you google Feynman diagrams.



a version of Parseval's identity in this more general context of the weighted inner product $(\ ,\ )_w$.

Let $\{Y_1(x), Y_2(x), \ldots\}$ be a complete set of functions that are orthonormal with respect to some weight function $w(x)$, so that $(Y_m, Y_n)_w = \delta_{m,n}$. Then expanding

$$f(x) = \sum_{n=1}^{\infty} f_n\, Y_n(x) \qquad \text{with} \qquad f_n = (Y_n, f)_w$$

as in (2.24) we have

$$\begin{aligned}(f,f)_w &= \int_a^b \left[\sum_{m=1}^{\infty} f_m^*\, Y_m^*(x)\right]\left[\sum_{n=1}^{\infty} f_n\, Y_n(x)\right] w(x)\,\mathrm{d}x \\ &= \sum_{n,m} f_m^*\, f_n\, (Y_m, Y_n)_w = \sum_{n=1}^{\infty} |f_n|^2\,.\end{aligned} \tag{2.40}$$

This is Parseval's identity for the case of the inner product with weight w.

2.8 Least squares approximation

In the real world, our computers have finite power and memory, and we typically don't have the resources to handle a very large number of eigenfunctions. So in practical applications, it's important to know how accurately we can represent a function by expanding it in just a limited, incomplete set of eigenfunctions. Suppose we consider the *finite* sum

$$g(x) \equiv \sum_{i=1}^{n} c_i\, Y_i(x) \tag{2.41}$$

that just includes some finite number n of the eigenfunctions, for *some* constants c_i. We ask how we should choose these constants if we want g to represent a given function $f(x)$

as closely as possible. One notion of what we mean by 'closely' is to ask that the distance between g and f should be minimized in the $(\ ,\ )_w$ norm, or in other words that

$$(f-g, f-g)_w = \int_a^b |f-g|^2 \; w(x)\,\mathrm{d}x$$

should be made as small as possible by varying the c_is. Using the definition (2.41) of $g(x)$ and the expansion (2.24) of f we have

$$\begin{aligned} \frac{\partial}{\partial c_k}(f-g, f-g)_w &= \frac{\partial}{\partial c_k}\left[(f,f) - (g,f) - (f,g) + (g,g)\right] \\ &= -\frac{\partial}{\partial c_k}\left[\sum_{i=1}^{n} c_i^* f_i + f_i^* c_i - |c_i|^2\right] \\ &= -f_k^* + c_k^* \end{aligned} \tag{2.42}$$

and likewise

$$\frac{\partial}{\partial c_k^*}(f-g, f-g)_w = -f_k + c_k\,, \tag{2.43}$$

where the evaluation of (g,g) uses Parseval's identity. These derivatives vanish iff $c_k = f_k$, and since

$$\frac{\partial^2}{\partial c_j\,\partial c_k}(f-g, f-g)_w = 0 = \frac{\partial^2}{\partial c_j^*\,\partial c_k^*}\,, \qquad \text{while} \qquad \frac{\partial^2}{\partial c_j\,\partial c_k^*}(f-g, f-g)_w = \delta_{j,k} \geq 0$$

the extremum is indeed a minimum. Therefore, if we wish to approximate a function $f(x)$ by representing it as a linear combination of just a few eigenfunctions of some Sturm–Liouville operator, the best we can do is to choose the coefficients $c_k = (Y_k, f)_w$ exactly as in its true expansion. This is also an important first step in checking that the expansion (2.24) of $f(x)$ does indeed converge on the original function as the number of included terms tends to infinity.

3 Laplace's Equation

In the previous chapter, we learnt that there are a set of orthogonal functions associated to *any* second order self-adjoint operator $\mathcal{L}$, with the sines and cosines (or complex exponentials) of Fourier series arising just as the simplest case $\mathcal{L} = -d^2/dx^2$. While this is true, the important – or at least commonly occurring – such functions arise not from Sturm–Liouville operators with randomly chosen (real) coefficient functions $p(x)$ and $q(x)$, but from those SL operators that have some special geometric significance. This is what we'll investigate over the next few chapters.

We'll start by considering Laplace's equation,

$$\nabla^2\psi \equiv \sum_{i=1}^{d} \frac{\partial^2}{\partial x_i^2}\psi = 0 \tag{3.1}$$

where d is the number of spatial dimensions. The Laplace equation is one of the most fundamental differential equations in all of mathematics, pure as well as applied. A function $\psi : M \to \mathbb{R}$ obeying $\nabla^2\psi = 0$ is called *harmonic*, and harmonic analysis is a huge area of study (particularly when M is a smooth manifold or a compact group). In theoretical physics, Laplace's equation is ubiquitous throughout both electromagnetism and gravity. In particular, whenever we have a *conservative* force $\mathbf{F} = -\nabla\psi$ obeying Gauss' law that the flux of the force through any closed surface is proportional to the net charge contained within that surface, then in empty space ψ satisfies Laplace's equation. In this context, ψ is known as a *potential* for the force. If that wasn't enough, Laplace's equation also arises as a limiting case of both the heat and wave equations, $\partial\psi/\partial t = K\nabla^2\psi$ and $\partial^2\psi/\partial t^2 = c^2\nabla^2\psi$, when ψ is independent of time.

We'll meet some of these applications later, but for now we'll concentrate just on solving Laplace's equation everywhere within a bounded domain $\Omega \subset \mathbb{R}^d$ subject to some condition on the behaviour of our solution at the boundary $\partial\Omega$ of our domain. In the case of *Dirichlet* boundary conditions, we require that our solution takes some pre-determined shape on the boundary. So in this case we're given a function $f : \partial\Omega \to \mathbb{R}$ and we require that

$$\psi(\mathbf{x}) = f(\mathbf{x}) \qquad \text{at each point } \mathbf{x} \in \partial\Omega\,. \tag{3.2}$$

If we can find such a solution, then it must be unique, because if ψ_1 and ψ_2 both obey Laplace's equation in Ω and $\psi_1|_{\partial\Omega} = \psi_2|_{\partial\Omega} = f$, then setting $\delta\psi \equiv \psi_1 - \psi_2$ and integrating by parts we have

$$0 = \int_\Omega \delta\psi\,\nabla^2\delta\psi\,\mathrm{d}V = -\int_\Omega (\nabla\delta\psi)\cdot(\nabla\delta\psi)\;\mathrm{d}V + \int_{\partial\Omega} \delta\psi\,\mathbf{n}\cdot(\nabla\delta\psi)\,\mathrm{d}S\,. \tag{3.3}$$

The boundary term vanishes because $\delta\psi|_{\partial\Omega} = 0$ by assumption. The *rhs* is thus the integral of a non–negative quantity $(\nabla\delta\psi)\cdot(\nabla\delta\psi)$, and so the only way the integral can be zero is for $\nabla\delta\psi = 0$ throughout Ω. Hence $\delta\psi = const.$ Finally, since $\delta\psi$ vanishes on the boundary, this constant must be zero so that $\psi_1 = \psi_2$ everywhere and our solution is unique.

The other case to consider is that of *Neumann* boundary conditions. Here, we instead require that the normal derivative $\partial\psi/\partial n = \mathbf{n}\cdot\nabla\psi$ takes some specific form on the boundary. That is, we are given a function $g : \partial\Omega \to \mathbb{R}$ and we ask that

$$\mathbf{n}\cdot\nabla\psi(\mathbf{x}) = g(\mathbf{x}) \qquad \text{at each point } \mathbf{x}\in\partial\Omega\,, \tag{3.4}$$

where $\mathbf{n}$ is the *outward* normal. Notice that the same uniqueness argument as above still shows that $\delta\psi = const.$, but that now the boundary conditions no longer force this constant to vanish. Thus imposing Neumann boundary conditions determines our solution only up to the addition of a constant.

3.1 Laplace's equation on a disc

In two dimensions, a powerful method for solving Laplace's equation is based on the fact that we can think of $\mathbb{R}^2$ as the complex plane $\mathbb{C}$. For $(x,y)\in\mathbb{R}^2$ we introduce $z = x + \mathrm{i}y$ and $\bar z = x - \mathrm{i}y$, whereupon Laplace's equation becomes

$$\frac{\partial^2\psi}{\partial z\,\partial\bar z} = 0\,. \tag{3.5}$$

The general solution of this is $\psi(x,y) = \phi(z) + \chi(\bar z)$ where $\phi(z)$ is holomorphic (*i.e.* $\partial\phi/\partial\bar z = 0$) and $\chi(\bar z)$ is antiholomorphic ($\partial\chi/\partial z = 0$).

Suppose that we wish to solve Laplace's equation inside the unit disc $|z|\le 1$, subject to the condition that ψ is regular throughout this disc and obeys $\psi = f(\theta)$ on the boundary of the disc, where $f(\theta)$ is some choice of function $f : S^1\to\mathbb{C}$ that we assume is sufficiently well–behaved that its Fourier expansion exists. Noting that when $|z| = 1$ we can write $\mathrm{e}^{\mathrm{i}n\theta}$ both as z^n and $\bar z^{-n}$, this Fourier expansion is

$$f(\theta) = \sum_{n\in\mathbb{Z}} \hat f_n\,\mathrm{e}^{\mathrm{i}n\theta} = \hat f_0 \;+\; \sum_{n=1}^{\infty}\hat f_n\,z^n\Big|_{|z|=1} \;+\; \sum_{n=1}^{\infty}\hat f_{-n}\,\bar z^n\Big|_{|z|=1}\,. \tag{3.6}$$

The advantage of writing the Fourier series in this second form is that it may now be extended throughout the unit disc; since no negative powers of z or $\bar z$ arise, the extended function remains finite throughout the disc. Furthermore, the extension of the *rhs* is manifestly of the form of the sum of a holomorphic and an antiholomorphic function (the constant $\hat f_0$, being both holomorphic and antiholomorphic, may be included with either). Therefore we find our desired solution to be

$$\begin{aligned}\psi(x,y) &= \hat f_0 + \sum_{n=1}^{\infty}\Big(\hat f_n\,z^n + \hat f_{-n}\,\bar z^n\Big)\\ &= \hat f_0 + \sum_{n=1}^{\infty}\Big(\hat f_n\,\mathrm{e}^{\mathrm{i}n\theta} + \hat f_{-n}\,\mathrm{e}^{-\mathrm{i}n\theta}\Big)\,r^n\,.\end{aligned} \tag{3.7}$$

Note that since $r\le 1$ everywhere on the unit disc, this expansion will certainly converge throughout the domain whenever the Fourier expansion of the boundary function $f(\theta)$ converges.

If instead we'd asked for a solution just in the annulus $a \leq |z| \leq b$, then we would require information about the behaviour of ψ at each boundary in order to decide how to split up the sum into holomorphic and antiholomorphic pieces. You'll learn much more about the isomorphism $\mathbb{R}^2 \cong \mathbb{C}$ in both the Complex Methods and Complex Analysis courses next term. The amazing power of complex analyticity is one of the true jewels of mathematics.

3.2 Separation of variables

The use of complex variables is very pretty, but beyond two dimensions it isn't generically available[16]. Suppose Ω is the three dimensional region

$$\Omega = \{(x, y, z) \in \mathbb{R}^3 \ : \ \ 0 \leq x \leq a, \ \ 0 \leq y \leq b, \ \ z \geq 0 \} \tag{3.8}$$

and that we wish to find a function $\psi : \Omega \to \mathbb{R}$ that obeys Laplace's equation $\nabla^2 \psi = 0$ throughout the interior of Ω, and that satisfies the Dirichlet boundary conditions

$$\begin{aligned} &\psi(0, y, z) = 0 && \psi(a, y, z) = 0 \\ &\psi(x, 0, z) = 0 && \psi(x, b, z) = 0 \\ &\psi(x, y, 0) = f(x, y) && \psi(x, y, z) \to 0 \text{ as } z \to \infty \end{aligned} \tag{3.9}$$

for some given function $f : [0, a] \times [0, b] \to \mathbb{R}$.

The fundamental idea that allows us to make progress is to assume that ψ takes the form

$$\psi(x, y) = X(x)Y(y)Z(z) \, . \tag{3.10}$$

This is known as *separation of variables*. Inserting this ansatz into Laplace's equation we find $0 = \nabla^2 \psi = Y(y)Z(z)X''(x) + X(x)Z(z)Y''(y) + X(x)Y(y)Z''(z)$, where the primes denote differentiation with respect to the arguments. At any point $(x, y, z) \in \Omega$ where $\psi \neq 0$, we can divide Laplace's equation by ψ to find

$$\frac{X''(x)}{X(x)} + \frac{Y''(y)}{Y(y)} + \frac{Z''(z)}{Z(z)} = 0 \, . \tag{3.11}$$

The key point is that each ratio here depends on only one of the variables, and a different one in each case. So in order for the equation to hold as we move around in Ω, it must be that they are each constant. For example, we could choose to move out along the x-direction while staying at constant y and z. The terms Y''/Y and Z''/Z cannot change along this path, because they don't depend on x. But then since $X''/X = -Y''/Y - Z''/Z$ it must be that X''/X is also independent of x and hence constant. Arguing similarly for the other terms, we have

$$X'' = -\lambda X \, , \qquad\qquad Y'' = -\mu Y \, , \qquad\qquad Z'' = (\lambda + \mu) Z \tag{3.12}$$

[16] In fact, there is a version in four dimensions, which is one way of viewing what Penrose's twistor theory is about. And no, it doesn't have much to do with quaternions.

for some constants λ and μ[17]. Note that the final constant here is not independent because they must all sum to zero by Laplace's equation.

These equations are simple to solve. If $\lambda < 0$ there are no solutions obeying the boundary conditions. When $\lambda \geq 0$ then $X(x) = a\sin(\sqrt{\lambda}x) + b\cos(\sqrt{\lambda}x)$ solves $X'' = \lambda X$ and similarly $Y(y) = c\sin(\sqrt{\mu}y) + d\cos(\sqrt{\mu}y)$ while $Z = re^{-z\sqrt{\lambda+\mu}} + s\,e^{+z\sqrt{\lambda+\mu}}$. Thus, after relabelling the constants,

$$\psi(x,y,z) = A\left(\sin(\sqrt{\lambda}x) + B\cos(\sqrt{\lambda}x)\right)\left(\sin(\sqrt{\mu}y) + C\cos(\sqrt{\mu}y)\ \right)\left(e^{-z\sqrt{\lambda+\mu}} + D\,e^{+z\sqrt{\lambda+\mu}}\right) \tag{3.13}$$

is a solution of Laplace's equation for arbitrary λ and μ. We will assume ψ does not vanish everywhere, so that $A \neq 0$.

We must now try to impose the boundary conditions. We'll begin with the homogeneous ones (*i.e.* those that don't involve $f(x,y)$.) The condition $\psi(0,y,z) = 0$ tells us that $B = 0$. The condition $\psi(a,y,z) = 0$ now tells us that $\sqrt{\lambda} = n\pi/a$ for[18] $n \in \mathbb{Z}^*$, or in other words that λ must take one of the values

$$\lambda_n \equiv \frac{n^2\pi^2}{a^2}\,, \qquad n = 1,2,3,\ldots\,. \tag{3.14}$$

Likewise, the boundary condition $\psi(x,0,z) = 0$ tells us that $C = 0$ while the condition $\psi(x,b,z) = 0$ restricts μ to be

$$\mu_m \equiv \frac{m^2\pi^2}{b^2}\,, \qquad m = 1,2,3,\ldots\,. \tag{3.15}$$

The condition that ψ falls to zero as $z \to +\infty$ immediately tells us that $D = 0$.

At this point, we have a family of solutions

$$\psi_{n,m}(x,y,z) \equiv \sin\left(\frac{n\pi x}{a}\right)\sin\left(\frac{m\pi y}{b}\right)\exp\left(-\pi z\sqrt{\frac{n^2}{a^2}+\frac{m^2}{b^2}}\right) \tag{3.16}$$

labelled by the pair of integers (n,m), all of which obey the boundary conditions we've so far considered. Since Laplace's equation is linear and the boundary conditions we've so far imposed are homogeneous, any linear combination of these solutions is also a solution. Thus our general solution is

$$\psi(x,y) = \sum_{n,m=1}^{\infty} A_{n,m}\sin\left(\frac{n\pi x}{a}\right)\sin\left(\frac{m\pi y}{b}\right)\exp\left(-\pi z\sqrt{\frac{n^2}{a^2}+\frac{m^2}{b^2}}\right) \tag{3.17}$$

for some constants $A_{n,m}$.

The final step is to try to choose the $A_{n,m}$ so as to obey the final boundary condition. Setting $z = 0$ we require $\psi(x,y,0) = \sum_{m,n=1}^{\infty} A_{n,m}\sin\left(\frac{n\pi x}{a}\right)\sin\left(\frac{m\pi y}{b}\right)$ to equal the given function $f(x,y)$, or in other words that

$$f(x,y) = \sum_{m,n=1}^{\infty} A_{n,m}\sin\left(\frac{n\pi x}{a}\right)\sin\left(\frac{m\pi y}{b}\right)\,, \tag{3.18}$$

[17]The signs here are purely for later convenience with the given boundary conditions: check for yourself that nothing changes at the end of the day if you don't include them.

[18]Here $\mathbb{Z}^*$ denotes the non-zero integers $\{\cdots, -2, -1, +1, +2, \ldots\}$.

This looks just like a Fourier (sine) series expansion – in both x and y – for the boundary function $f(x,y)$! Using orthogonality relations

$$\int_0^a \sin\left(\frac{m\pi x}{a}\right)\sin\left(\frac{n\pi x}{a}\right)\mathrm{d}x = \frac{a}{2}\delta_{m,n} \tag{3.19}$$

we see that the constants $A_{n,m}$ are fixed to be

$$A_{n,m} = \frac{4}{ab}\int_{[0,a]\times[0,b]} \sin\left(\frac{n\pi x}{a}\right)\sin\left(\frac{m\pi y}{b}\right)\; f(x,y)\;\mathrm{d}x\,\mathrm{d}y \tag{3.20}$$

in equation (3.17). We note (in passing!) that the function $f(x,y)$ should be smooth enough so that this Fourier series both converges and is (at least) twice differentiable, so that it does indeed define a solution of the Laplace equation.

As a simple example, suppose $f(x,y) = 1$. Then we have

$$A_{n,m} = \frac{4}{ab}\int_{[0,a]\times[0,b]} \sin\left(\frac{n\pi x}{a}\right)\sin\left(\frac{m\pi y}{b}\right)\mathrm{d}x\,\mathrm{d}y = \begin{cases} \dfrac{16}{\pi^2}\dfrac{1}{mn} & \text{if } n \text{ and } m \text{ are both odd,} \\ 0 & \text{otherwise.} \end{cases} \tag{3.21}$$

Therefore, the solution satisfying these boundary conditions is

$$\psi(x,y,z) = \frac{16}{\pi^2}\sum_{k=1}^{\infty}\sum_{\ell=1}^{\infty}\frac{\sin\left[\frac{(2k-1)\pi x}{a}\right]}{(2k-1)}\,\frac{\sin\left[\frac{(2\ell-1)\pi y}{b}\right]}{(2\ell-1)}\,\exp\left[-s_{k,\ell}\,\pi z\right] \tag{3.22}$$

where $s_{k,\ell}^2 = \frac{(2k-1)^2}{a^2} + \frac{(2\ell-1)^2}{b^2}$. We see that at fixed z, the function $\psi(x,y,z)$ is larger near the middle of the region $[0,a]\times[0,b]$, and that for large z the lowest harmonics – where k and ℓ are small – dominate.

Note that in this example, we obtained a Fourier sine series because of the homogeneous Dirichlet boundary conditions on x and y. If instead we'd imposed Neumann boundary conditions $\partial\psi/\partial x = 0$ at $y = 0, b$ and $\partial\psi/\partial y = 0$ at $x = 0, a$, then we would instead find Fourier *co*sine series. Finally if, instead of allowing our domain Ω to extend to infinity in the z direction, we had imposed a boundary conditon $\psi(x,y,c) = g(x,y)$ at some finite location $z = c$, then both the positive and negative exponential terms in the function $Z(z)$ would contribute.

To summarize, the method of separation of variables starts by writing ψ as a product of functions that depend only on one variable each. We use this ansatz to reduce Laplace's PDE to a system of ODEs that depend on a number of constants (here λ and μ). Since Laplace's equation was a second order linear equation, these ODEs will always be of Sturm–Liouville type; the constants will appear as eigenvalues of the SL equation and the equations will be solved by the eigenfunctions of the SL operator. After solving these SL equations, we use the homogeneous boundary conditions to impose restrictions on the possible values of the eigenvalues. The solution for a fixed permissible choice of the eigenvalues is known as a *normal mode* of the system. By linearity, the general solution is a linear combination of these normal modes. The final step is to use the inhomogeneous boundary conditions to determine which linear combination we should take; this will require using the orthogonality property of the eigenfunctions of the SL operator.

3.3 The Laplacian in spherical polar coordinates

In the previous example, our Sturm–Liouville equations were of the form $X'' = -\lambda X$, and we were led to the *Fourier* expansion of $f(x, y)$ on the boundary $z = 0$. This occurred because the domain of that example was a (non-compact) rectangular cuboid, and it was natural to treat this using Cartesian coordinates. We're now going to consider Laplace's equation in spherical polar coordinates. Separation of variables now leads to a more interesting SL equation with a non–constant coefficient function $p(x)$.

Recall that a point $p \in \mathbb{R}^3$ with position vector $\mathbf{r}$ may be described in terms of polar coordinates (r, θ, ϕ). The radial coordinate $r = |\mathbf{r}|$ is the distance of point p from the origin. In particular $r \geq 0$. Whenever $r > 0$ we define θ to be the angle that $\mathbf{r}$ makes with the (chosen) positive z axis, and take $0 \leq \theta \leq \pi$. Finally, whenever $r > 0$ and $0 < \theta < \pi$ we define ϕ to be the angle that the projection of $\mathbf{r}$ into the plane $z = 0$ makes with the positive x axis, measured counterclockwise. Thus $0 \leq \phi < 2\pi$. It follows from the above that

$$x = r\,\sin\theta\,\cos\phi\,, \qquad y = r\,\sin\theta\,\sin\phi\,, \qquad z = r\,\cos\theta \tag{3.23}$$

and hence that the volume element is

$$\mathrm{d}V = \mathrm{d}x\,\mathrm{d}y\,\mathrm{d}z = r^2\sin\theta\,\mathrm{d}r\,\mathrm{d}\theta\,\mathrm{d}\phi \tag{3.24}$$

in spherical polar coordinates.

The Laplacian operator becomes

$$\nabla^2 = \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right) + \frac{1}{r^2\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right) + \frac{1}{r^2\sin^2\theta}\frac{\partial^2}{\partial\phi^2} \tag{3.25}$$

as you check by the chain rule. In this course, for simplicity, we'll restrict attention to axisymmetric situations where all our functions are assumed independent of the angle ϕ. In these circumstances we can omit the final term in the Laplacian (3.25), but you can read about the more general situation in *e.g.* Arfken & Weber or Boas' books.

We now seek solutions of Laplace's equation $\nabla^2\psi(r,\theta) = 0$ in the interior of the spherical domain $\Omega = \{(r,\theta,\phi) \in \mathbb{R}^3 \;:\; r \leq a\}$ for some constant a, where we'll demand that our solution remains finite everywhere in Ω. Once again we separate variables by writing $\psi(r,\theta) = R(r)\Theta(\theta)$ and by our now standard argument find that Laplace's equation is equivalent to the system of ordinary differential equations

$$\begin{aligned} \frac{d}{d\theta}\left(\sin\theta\,\frac{d\Theta}{d\theta}\right) + \lambda\sin\theta\,\Theta = 0 \\ \frac{d}{dr}\left(r^2\frac{dR}{dr}\right) - \lambda R = 0 \end{aligned} \tag{3.26}$$

where $\lambda \in \mathbb{R}$ is our separation constant. Each of these equations is of Sturm–Liouville type. Let's examine them in more detail.

3.3.1 Legendre polynomials

We'll start with the angular equation. We can simplify its form with the substitution $x = \cos\theta$, although note that this x is nothing to do with our original Cartesian coordinate in $\mathbb{R}^3$. Since $0 \le \theta \le \pi$ we have $-1 \le x \le 1$ and

$$\frac{d}{d\theta} = -\sin\theta \frac{d}{dx}\,.$$

Therefore the angular part of Laplace's equation becomes

$$-\sin\theta \frac{d}{dx}\left[\sin\theta\left(-\sin\theta\frac{d\Theta}{dx}\right)\right] + \lambda\sin\theta\,\Theta = 0\,, \tag{3.27}$$

or in other words

$$\frac{d}{dx}\left[(1-x^2)\frac{d\Theta}{dx}\right] = -\lambda\Theta\,. \tag{3.28}$$

This is known as *Legendre's equation*. It is a standard Sturm–Liouville eigenfunction problem on $\Omega = [-1,1]$, with coefficient functions $p(x) = (1-x^2)$ and $q(x) = 0$, and where the weight function $w(x) = 1$. When we checked in chapter 2 whether a Sturm–Liouville operator $\mathcal{L}$ on the domain $[-1,1]$ was self–adjoint, we met the condition

$$(f, \mathcal{L}g) = (\mathcal{L}f, g) + \left[p(x)(f^{*\prime}g - f^*g')\right]_{-1}^{1}\,.$$

In the case of Legendre's equation we see that $p(x) = 0$ at $x = \pm 1$, so the boundary condition required for self–adjointness is simply that the functions and their derivatives remain *regular* on $\partial\Omega$.

Let's now look for a regular solution of (3.28) throughout the interior of Ω that obeys the boundary condition that it remains regular on $\partial\Omega$. We seek a power series solution to (3.28) of the form $\Theta(x) = \sum_{n=0}^{\infty} a_n\, x^n$, where only non–negative powers of x appear since we want the solution to be regular at the origin. Substituting this into (3.28) gives

$$0 = (1-x^2)\sum_{n=2}^{\infty} a_n\, n(n-1)x^{n-2} - 2\sum_{n=1}^{\infty} a_n\, nx^n + \lambda\sum_{n=0}^{\infty} x^n \tag{3.29}$$

which must hold it must hold for each power of x separately as it must hold throughout the open set $x \in (-1,1)$. This implies that the coefficients must obey the recursion relation

$$0 = a_{n+2}(n+2)(n+1) - a_n\, n(n-1) - 2a_n\, n + \lambda a_n\,,$$

or equivalently

$$a_{n+2} = \left[\frac{n(n+1)-\lambda}{(n+1)(n+2)}\right] a_n\,. \tag{3.30}$$

The recursion relation relates a_{n+2} to a_n, so we can pick a_0 and a_1 freely and write

$$\Theta(x) = a_0\Theta_0(x) + a_1\Theta_1(x)\,, \tag{3.31}$$

where

$$\begin{aligned}\Theta_0(x) &= 1 + \frac{(-\lambda)}{2!}x^2 + \frac{(-\lambda)(6-\lambda)}{4!}x^4 + \frac{(-\lambda)(6-\lambda)(20-\lambda)}{6!}x^6 + \cdots \\ \Theta_1(x) &= x + \frac{(2-\lambda)}{3!}x^3 + \frac{(2-\lambda)(12-\lambda)}{5!}x^5 + \cdots .\end{aligned} \tag{3.32}$$

Note that $\Theta_0(-x) = \Theta_0(x)$ while $\Theta_1(-x) = -\Theta_1(x)$. Thus, for any value of λ, we've found two independent solutions of Legendre's second order equation.

We now consider the boundary conditions. The recurrence relation (3.30) shows that as n becomes large

$$\frac{a_{n+2}}{a_n} = 1 - \frac{2}{n} + \frac{4-\lambda}{n^2} . \tag{3.33}$$

Thus, by the ratio test the series will always converge for $|x| < 1$. However, *for generic values of* λ the series diverges at $x = \pm 1$, violating our boundary condition[19]. The only way to avoid this divergence is if the power series for $\Theta(x)$ somehow *terminates*. Looking back at the recurrence relation, this will occur iff λ takes the form

$$\lambda = \ell(\ell+1) \qquad \text{for } \ell \in \mathbb{Z}_{\geq 0} . \tag{3.34}$$

Only for these eigenvalues will (both) the series we found in (3.32) terminate, leaving us with a $\Theta(x)$ that is polynomial of degree ℓ. The situation is exactly analogous to our familiar sines and cosines. For any $\lambda \in \mathbb{R}$, we can solve $y'' = -\lambda y$ on $[-1, 1]$ as $y = A\sin\sqrt{\lambda}x + B\cos\sqrt{\lambda}x$, but if we impose the boundary condition $y(-1) = y(1)$ then the eigenvalue must be restricted to $\lambda = (2\pi n)^2$ for some $n \in \mathbb{Z}$.

The polynomials we've found are known as *Legendre polynomials of order* ℓ, and denoted by $P_\ell(x)$. One can show using the series (3.32) that the first four Legendre polynomials are given by

$$P_0(x) = 1 , \qquad P_1(x) = x , \qquad P_2(x) = \frac{1}{2}(3x^2 - 1) , \qquad P_3(x) = \frac{1}{2}(5x^3 - 3x) .$$

where we've fixed the overall factor by requiring $P_\ell(1) = 1$. You can find plots of the first few Legendre polynomials in figure 3. It turns out that they can be usefully represented as

$$P_\ell(x) = \frac{1}{2^\ell \ell!}\frac{d^\ell}{dx^\ell}(x^2 - 1)^\ell , \tag{3.35}$$

which is known as *Rodrigues' formula*. The numerical prefactor ensures that $P_\ell(1) = 1$; to see this use Leibnitz' rule to compute

$$\begin{aligned}P_\ell(x) &= \frac{1}{2^\ell \ell!}\frac{d^\ell}{dx^\ell}(x^2-1)^\ell = \frac{1}{2^\ell \ell!}\frac{d^\ell}{dx^\ell}\Big[(x-1)^\ell(x+1)^\ell\Big] \\ &= \frac{1}{2^\ell \ell!}\Big[\ell!(x+1)^\ell + \text{terms proportional to } (x-1)\Big]\end{aligned} \tag{3.36}$$

[19] Since $\lim_{n\to\infty}\frac{a_{n+2}}{a_n} = 1$, the ratio test is inconclusive and we must examine the higher order terms. Gauss' test for convergence states that if the ratio of successive coefficients behaves at large n like $1 + \frac{h}{n} + \frac{C_n}{n^2}$ with C_n bounded and $h < 1$ then the series will diverge. So the infinite series $\Theta_0(x)$ and $\Theta_1(x)$ do indeed diverge at $x = \pm 1$. A proof of Gauss' test can be found here.

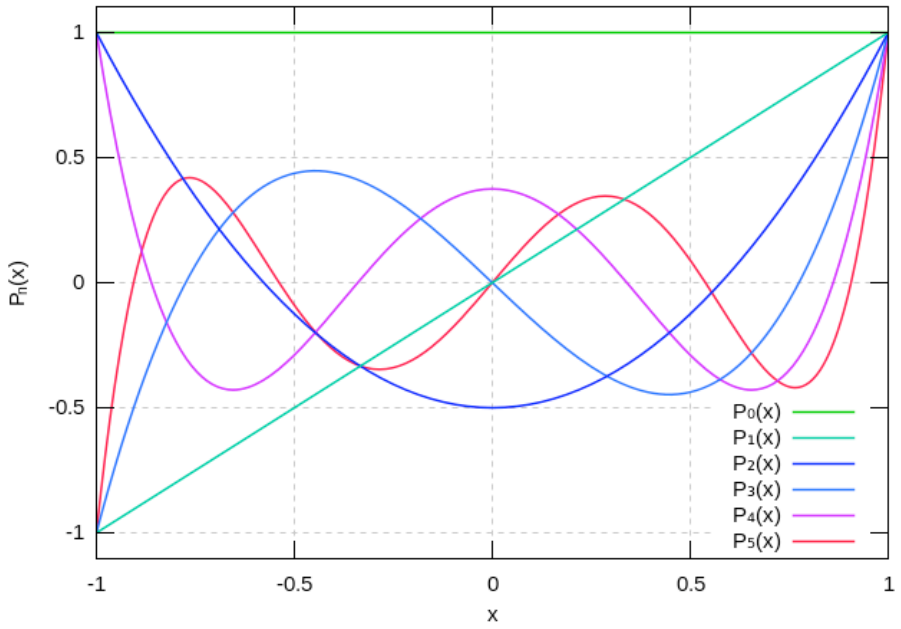


Figure 3. *Plots of the first five Legendre polynomials $P_\ell(x)$ for $x \in [-1,1]$. Note that $P_\ell(x)$ is even (odd) if ℓ is even (odd), that $P_\ell(1) = 1$, and that $P_\ell(x)$ has ℓ real roots in between $x = -1$ and 1.*

and evaluate at $x = 1$. Notice also that since $(x^2-1)^\ell$ is a polynomial in x of degree 2ℓ containing only even powers of x, $P_\ell(x)$ is a polynomial of degree ℓ that is an even (odd) function of x when ℓ is even (odd), in agreement with the expectation from our recurrence relation.

The Legendre polynomials $P_\ell(x)$ are the basic orthogonal polynomials on $[-1,1]$ with weight function $w(x) = 1$. They have many beautiful properties. To prove some of them, it is helpful to first note that if $\ell \geq r \geq 0$ then $(d^r/dx^r)(x^2-1)^\ell = (x^2-1)^{\ell-r}\, Q_{\ell,r}(x)$ where $Q_{\ell,r}(x)$ is some polynomial of degree r. This follows by induction: it is true when $r = 0$, and assuming it is true for some r then differentiating $r+1$ times

$$\begin{aligned}\frac{d^{r+1}}{dx^{r+1}}(x^2-1)^\ell &= \frac{d}{dx}\left[(x^2-1)^{\ell-r}\, Q_{\ell,r}\right] \\ &= (x^2-1)^{\ell-r-1}\left[2x(\ell-r)Q_{\ell,r}(x) + (x^2-1)Q'_{\ell,r}(x)\right] .\end{aligned}$$

If $Q_{\ell,r}(x)$ is a polynomial of degree r then $Q'_{\ell,r}(x)$ is a polynomial of degree $r-1$ and the content of the square brackets is a polynomial of degree $r+1$. Thus the claim holds at $r+1$. A consequence of this lemma is that

$$\frac{d^r}{dx^r}(x^2-1)^\ell \Big|_{x=\pm 1} = 0 \tag{3.37}$$

whenever $r < \ell$ (but $r \geq 0$). This fact is useful in showing that functions $P_\ell(x)$ defined in (3.35) are orthogonal for different values of ℓ. Explicitly, in considering $\int_{-1}^{1} P_m(x)\, P_\ell(x)\, \mathrm{d}x$ for $m \neq \ell$ then without loss of generality we can assume that $m < \ell$. Then repeatedly

integrating by parts $m+1$ times we have

$$\begin{aligned} 2^{\ell+m}\ell!\,m!\int_{-1}^{1} P_m(x)\,P_\ell(x)\,\mathrm{d}x &= \int_{-1}^{1} P_m(x)\,\frac{d^\ell}{dx^\ell}(x^2-1)^\ell\,\mathrm{d}x \\ &= \left[P_m(x)\,\frac{d^{\ell-1}}{dx^{\ell-1}}(x^2-1)^\ell\right]_{-1}^{1} - \int_{-1}^{1}\frac{d}{dx}P_m(x)\,\frac{d^{\ell-1}}{dx^{\ell-1}}(x^2-1)^\ell\,\mathrm{d}x \\ &= -\int_{-1}^{1}\frac{d^{m+1}}{dx^{m+1}}P_m(x)\,\frac{d^{\ell-m-1}}{dx^{\ell-m-1}}(x^2-1)^\ell\,\mathrm{d}x \\ &= 0 \end{aligned} \tag{3.38}$$

where in performing the integrations by parts we note that all the boundary terms vanish by our lemma (3.37), and in going to the final line we use the fact that $P_m(x)$ is a polynomial of degree m. Thus Legendre polynomials with different eigenvalues are indeed orthogonal on $[-1,1]$ in agreement with the general results of Sturm–Liouville theory.

To fix the normalization we similarly note that

$$\begin{aligned} 2^{2\ell}(\ell!)^2\int_{-1}^{1} P_\ell(x)\,P_\ell(x)\,\mathrm{d}x &= \int_{-1}^{1} P_\ell(x)\,\frac{d^\ell}{dx^\ell}(x^2-1)^\ell\,\mathrm{d}x \\ &= -\int_{-1}^{1}(x^2-1)^\ell\,\frac{d^\ell}{dx^\ell}P_\ell(x)\,\mathrm{d}x = -\int_{-1}^{1}(x^2-1)^\ell\,\frac{d^{2\ell}}{dx^{2\ell}}(x^2-1)^\ell\,\mathrm{d}x \end{aligned} \tag{3.39}$$

The only term in $(x^2-1)^\ell$ that survives being differentiated 2ℓ times is the highest power $x^{2\ell}$ and since $(d^r/dx^r)x^r = r!$ we have

$$2^{2\ell}(\ell!)^2\int_{-1}^{1} P_\ell(x)\,P_\ell(x)\,\mathrm{d}x = (2\ell)!\int_{-1}^{1}(x^2-1)^\ell\,\mathrm{d}x \equiv (2\ell)!\,I_\ell\,. \tag{3.40}$$

Yet again integrating by parts we find that for $\ell > 0$

$$\begin{aligned} I_\ell \equiv \int_{-1}^{1}(x^2-1)^\ell\,\mathrm{d}x &= \Big[x(x^2-1)^\ell\Big]_{-1}^{1} - 2\ell\int_{-1}^{1}x^2(x^2-1)^{\ell-1}\,\mathrm{d}x \\ &= -2\ell\,I_\ell + 2\ell\,I_{\ell-1}\,, \end{aligned} \tag{3.41}$$

or in other words $I_\ell = \frac{2\ell}{2\ell+1}I_{\ell-1}$. Since $I_0 = 2$ we find inductively that

$$I_\ell = (-1)^\ell\frac{2^{\ell+1}\ell!}{\prod_{r=0}^{\ell}(2r+1)}\,.$$

Using this in equation (3.39) gives finally

$$\int_{-1}^{1} P_m(x)\,P_\ell(x)\,\mathrm{d}x = \frac{2}{2\ell+1}\,\delta_{m,\ell} \tag{3.42}$$

as the orthogonality relations among the Legendre polynomials.

Any degree ℓ polynomial has ℓ complex roots, but in fact all ℓ roots of $P_\ell(x)$ are real, and remarkably they all lie in $x \in (-1,1)$. To see this, assume for a contradiction that it's false. Then $P_\ell(x)$ has only $k < \ell$ real roots in between -1 and 1. Suppose these are

at points $x_1, x_2, \ldots, x_k$ and construct the polynomial $Q_k(x) \equiv \prod_{r=1}^{k}(x - x_r)$. Then for $x \in [-1, 1]$ the product $P_\ell(x)\, Q_k(x)$ is either always positive or always negative, because by our assumptions $P_\ell(x)$ and $Q_k(x)$ change sign simultaneously. Thus, on the one hand

$$\int_{-1}^{1} P_\ell(x)\, Q_k(x)\, \mathrm{d}x \;\neq\; 0$$

since the integrand always has definite sign. On the other hand, we can always expand as $Q_k(x) = \sum_{r=0}^{k} \hat{Q}_r P_r(x)$ in a basis of Legendre polynomials. Since $k < \ell$ by assumption each term in this sum is orthogonal to $P_\ell(x)$, so the above integral must vanish, giving a contradiction.

The Legendre polynomials have many other curious properties, some of which you will explore in the problem sets and many of which are explained in Arfken & Weber or in Boas. I recommend that you browse through a few of these, but the most important thing to remember is simply that the Legendre polynomials are the solutions of Legendre's equation (3.28) with eigenvalue $\lambda = \ell(\ell+1)$ for $\ell \in \mathbb{Z}_{\geq 0}$. By standard SL theory they form a complete set of orthogonal functions on $x \in [-1, 1]$ or equivalently on $\theta \in [0, \pi]$ where $x = \cos\theta$.

3.3.2 The Cosmic Microwave Background

In 1964, Arno Penzias and Robert Wilson were trying to clean their radio telescope of various pigeon droppings. They were hoping this was the cause of an annoying background noise that was stymying their attempts to measure weak radio waves bouncing off various satellite balloons NASA had launched into the upper atmosphere. But the noise did not go away. They asked around their friends and colleagues to find out if anyone had a clue what could be causing this mysterious microwave background, that seemed to be come evenly from all directions and constant in time.

One of them recalled a recent paper of Dicke, Peebles and Wilkinson which predicted that, had the Universe started in a hot, dense state then some radiation from that time should be around now and would be redshifted down to microwave frequencies. This Cosmic Microwave Background would be, to excellent approximation, homogeneous and isotropic and provided the perfect explanation for the blackbody spectrum of temperature $\sim$ 3K measured by Penzias and Wilson.

The discovery and measurement of the CMB is one of the key pieces of evidence we have for the Big Bang. But it's not completely isotropic. The CMB anisotropies were first measured by the COBE satellite in the early 1990s and have been intensively studied by many telescopes ever since. The best one to date is the Planck satellite – orbiting right now – which has a strong Cambridge involvement. These satellites produce detailed maps of the CMB, a (low resolution) example being shown in figure 4.

To understand what these pictures are trying to tell us, we need to process it a little. Cosmologists are particularly interested in the two–point function

$$C(\theta) \equiv \big\langle \frac{\delta T}{T}(\hat{\mathbf{r}}_1) \frac{\delta T}{T}(\hat{\mathbf{r}}_2) \big\rangle$$

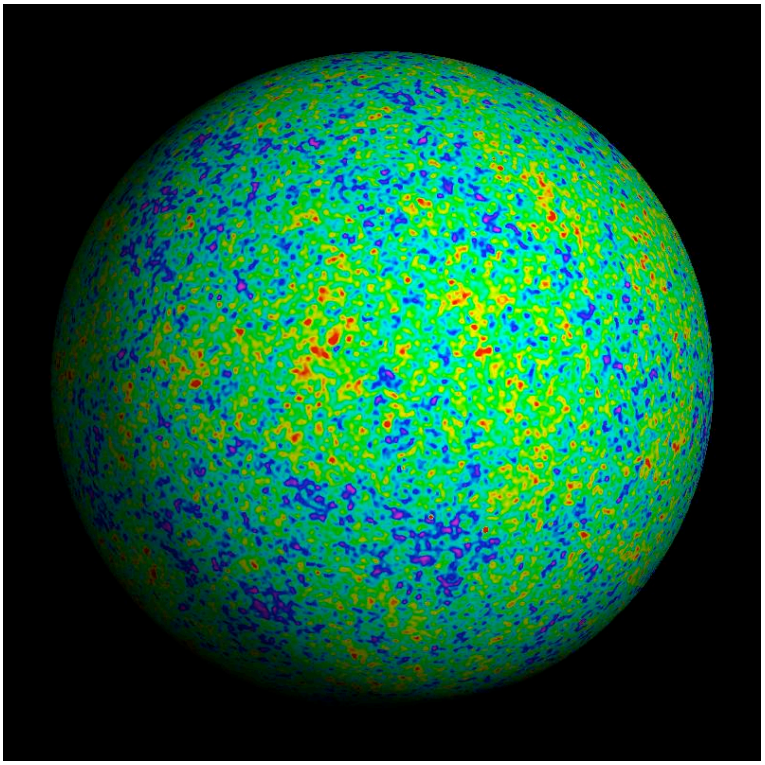


Figure 4. *A map of the CMB, produced by the WMAP satellite. The picture depicts fluctuations around the average temperature $T = 2.725K$ in different directions in the sky, with red and yellow being hotspots while blue and purple are cold. The fluctuations are very small, with $\delta T/T \sim 10^{-5}$.*

defined as the temperature difference of the CMB when looking out in different directions $\hat{\mathbf{r}}_1$ and $\hat{\mathbf{r}}_2$ with $\hat{\mathbf{r}}_1 \cdot \hat{\mathbf{r}}_2 = \cos\theta$, averaged over all points on the sky. The resulting function depends on $\theta \in [0, \pi]$ and so you can expand it in Legendre polynomials as

$$C(\theta) = \frac{1}{4\pi} \sum_{\ell=0}^{\infty} (2\ell + 1)\, C_\ell\, P_\ell(\cos\theta)\,. \tag{3.43}$$

If you do this you'll find the graph shown in figure 3.3.2. The peaks and troughs of this graph contain a vast wealth of information about the history of the very early universe. If you want to know more, take the Part II Cosmology course.

3.3.3 Laplace's equation on the sphere

After this long interlude, let's return to our problem of finding the general regular, axisymmetric solution to Laplace's equation $\nabla^2\psi = 0$ on the spherical domain $\Omega = \{r \leq a\} \subset \mathbb{R}^3$. Using separation of variables we found $\psi(r, \theta) = R(r)\,\Theta(\theta)$ where R and Θ obey the odes (3.26). We've just seen that for a regular solution, we require the separation constant $\lambda = \ell(\ell + 1)$ for $\ell \in \mathbb{Z}_{\geq}$ and that in this case $\Theta = P_\ell(\cos\theta)$. Notice that regularity at $x = \pm 1$, necessary for self–adjointness of the Sturm–Liouville operator in Legendre's equation, amounts to regularity of Θ at $\theta = 0$ and π, or in other words along the z-axis of our

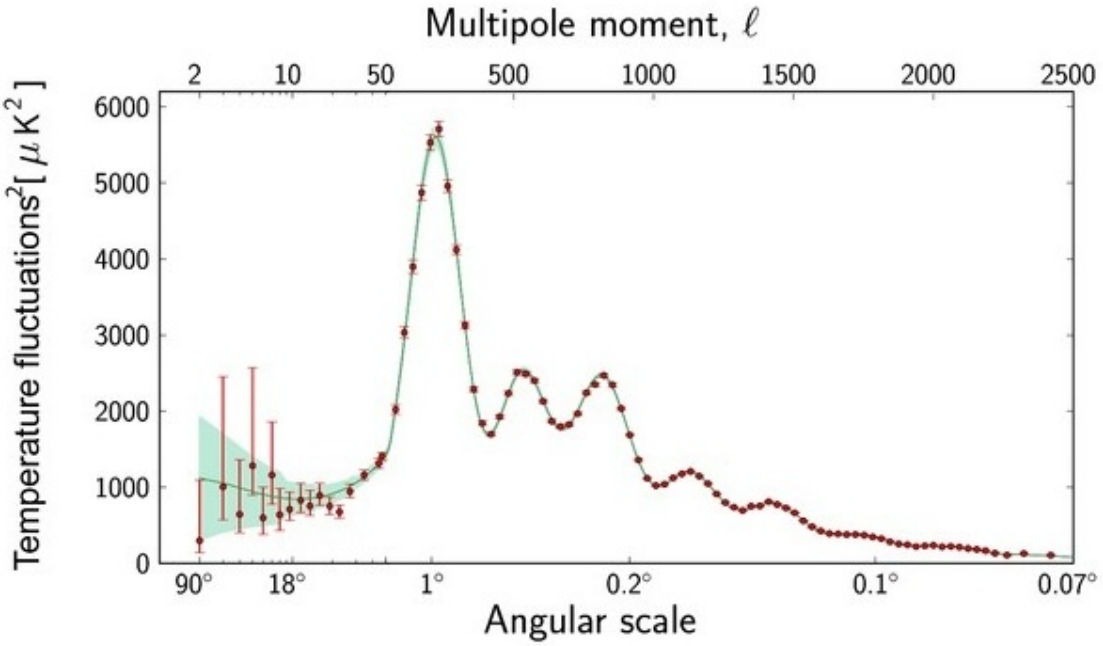


Figure 5. *The CMB power spectrum $|C_\ell|^2$ plotted against ℓ (called the multipole moment).*

original problem in $\mathbb{R}^3$. If we want a solution regular everywhere in the interior of $r \leq a$ then it certainly needs to be regular along the z-axis!

The remaining equation to consider is the radial equation, which with $\lambda = \ell(\ell+1)$ becomes

$$(r^2 R_\ell')' = \ell(\ell+1) R \,. \tag{3.44}$$

Trying a solution of the form $R(r) \propto r^\alpha$ for some power α we learn that

$$\alpha(\alpha+1) = \ell(\ell+1) \tag{3.45}$$

whose roots are $\alpha = \ell$ and $\alpha = -(\ell+1)$. Thus our general solution takes the form

$$\psi(r,\theta) = \sum_{\ell=0}^{\infty} \left(A_\ell \, r^\ell + \frac{B_\ell}{r^{\ell+1}} \right) P_\ell(\cos\theta) \tag{3.46}$$

where for each ℓ the A_ℓ and B_ℓ are (generically complex) constants. Note that we're now treating the Legendre polynomials as functions of θ; they are polynomials in $\cos\theta$. Since we require the solution to be regular everywhere inside $r = a$, we must set $B_\ell = 0$ for all ℓ. (If we were interested in solving Laplace's equation everywhere *outside* the sphere $r = a$, then for regularity as $r \to \infty$ we'd need $A_\ell = 0$ for $\ell > 0$. And, of course, if we wish for a regular solution valid inside the spherical shell $a \leq r \leq b$ then both the A_ℓ and B_ℓ can generically be present.)

As always, to pin down the remaining constants A_ℓ we must impose some boundary condition at $r = a$. For example, if we demand that $\psi(a,\theta) = f(\theta)$ for some axisymmetric

function f on the sphere, then by the general results of Sturm–Liouville theory f has an expansion in terms of the Legendre polynomials as

$$f(\theta) = \sum_{\ell=0}^{\infty} F_\ell \, P_\ell(\cos\theta) \qquad \text{where} \qquad F_\ell = \frac{2\ell+1}{2} \int_{-\pi}^{\pi} P_\ell(\theta)\, f(\theta)\, \sin\theta \, \mathrm{d}\theta \,.$$

Note the presence of the factor $(2\ell+1)/2$ in front of the integral; this comes from the normalization condition (3.39) of the Legendre polynomials. Laplace's equation is thus solved by

$$\psi(r,\theta) = \sum_{\ell=0}^{\infty} F_\ell \left(\frac{r}{a}\right)^\ell P_\ell(\cos\theta) \,. \tag{3.47}$$

with the choice $A_\ell = F_\ell \, a^{-\ell}$ ensuring that our boundary condition $\psi(a,\theta) = f(\theta)$ is met.

3.3.4 Multipole expansions

Consider the function

$$\frac{1}{|\mathbf{r}-\mathbf{k}|} = \frac{1}{\sqrt{1+r^2-2r\cos\theta}} \,. \tag{3.48}$$

where $\mathbf{k}$ is a unit vector in the z-direction. You can check (exercise!) that this function satisfied Laplace's equation for all $\mathbf{r} \neq \mathbf{k}$ and that in particular it is regular at the origin $\mathbf{r} = \mathbf{0}$. So from what we've said above, it must be possible to expand it in terms of Legendre polynomials. That is, we must have

$$\frac{1}{|\mathbf{r}-\mathbf{k}|} = \sum_{\ell=0}^{\infty} a_\ell \, r^\ell \, P_\ell(\cos\theta) \tag{3.49}$$

for some coefficients a_ℓ. It's simple to determine these coefficients: Set $\theta = 0$ in equation (3.48) so that $\mathbf{r}$ also points along the z-axis, and Taylor expand to find

$$\frac{1}{\sqrt{1+r^2-2r}} = \frac{1}{1-r} = \sum_{\ell=0}^{\infty} r^\ell \qquad \text{whenever } r < 1 \,. \tag{3.50}$$

If we recall that $P_\ell(1) = 1$ for all ℓ, then this is compatible with the expansion (3.49) iff $a_\ell = 1$, showing that

$$\frac{1}{|\mathbf{r}-\mathbf{k}|} = \sum_{\ell=0}^{\infty} r^\ell P_\ell(\cos\theta) \tag{3.51}$$

at general locations $\mathbf{r}$. More generally, for any vector $\mathbf{r}'$ we have

$$\frac{1}{|\mathbf{r}-\mathbf{r}'|} = \frac{1}{r'} \sum_{\ell=0}^{\infty} \left(\frac{r}{r'}\right)^\ell P_\ell(\hat{\mathbf{r}}\cdot\hat{\mathbf{r}}') \tag{3.52}$$

whenever $r' > r$. This is known as the *multipole expansion*, with the $\ell = 0$ term known as the *monopole* term and the $\ell = 1$ term known as the *dipole*. In electrostatics, q times the *monopole* term $1/r'$ is the potential experienced at $\mathbf{r}'$ due to a point charge q at the origin. The *dipole* term $r/(r')^2 \cos\theta = \mathbf{r}\cdot\mathbf{r}'/(r')^3$ is likewise proportional to the potential experienced at $\mathbf{r}'$ due to two charges $\pm a$ placed at a separation $\mathbf{r}$ from eachother.

3.4 Laplace's equation in cylindrical polar coordinates

The final case we'll consider in this course is problems with cylindrical symmetry. Here, separation of variables leads to a SL equation that has a non–constant weight function as well as a non–constant SL coefficient function $p(x)$.

Recall that in cylindrical polar coordinates $(x, y, z) = (r\cos\theta, r\sin\theta, z)$ the Laplacian operator

$$\nabla^2 = \frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial}{\partial r}\right) + \frac{1}{r^2}\frac{\partial^2}{\partial\theta^2} + \frac{\partial^2}{\partial z^2}\,. \tag{3.53}$$

Suppose we're interested in solving Laplace's equation $\nabla^2\psi = 0$ on the cylinder $\Omega = \{(r,\theta,z) \in \mathbb{R}^3 \;:\; r \le a\,,\; z \ge 0\}$, subject to the Dirichlet boundary conditions that $\psi(\mathbf{r})$ is single valued and finite throughout Ω and decays as $z \to \infty$. We also assume that ψ vanishes on the curved edge $r = a$ of the cylinder, but that $\psi(r,\theta,0) = f(r,\theta)$ for some given function f on the base of the cylinder.

Again we try separating variables by writing $\psi = R(r)\Theta(\theta)Z(z)$, learning that

$$\left(\frac{R''}{R} + \frac{1}{r}\frac{R'}{R}\right) + \frac{1}{r^2}\frac{\Theta''}{\Theta} + \frac{Z''}{Z} = 0 \tag{3.54}$$

wherever $\psi \neq 0$. We now argue that since Z''/Z depends only on z but cannot vary as z is changed with (r,θ) held fixed, in fact $Z''/Z = \mu$ for some constant μ. This being so, we can now multiply (3.54) through by r^2 and notice that by the same argument, $\Theta''/\Theta = -\lambda$ must also be constant. Therefore, in cylindrical coordinates Laplace's equation reduces to the system of ODEs

$$\begin{aligned} \Theta'' &= -\lambda\Theta \qquad\qquad Z'' = \mu Z \\ 0 &= r^2R'' + rR' + (\mu r^2 - \lambda)R \end{aligned} \tag{3.55}$$

If we want $\psi(\mathbf{r})$ to be single valued, then we must have $\Theta(\theta + 2\pi) = \Theta(\theta)$, so λ must be one of the values $\lambda_n \equiv n^2$ for $n \in \mathbb{Z}$, whereupon we have the usual solution

$$\Theta(\theta) = \Theta_n(\theta) \equiv a_n \sin n\theta + b_n \cos n\theta\,. \tag{3.56}$$

(Note that if $\lambda = 0$ then the equation $\Theta'' = 0$ is solved by $\Theta = a_0\theta + b_0$. Periodicity requires $a_0 = 0$ and the remaining constant term is just what we'd find by putting $n = 0$ in (3.56).) The equation for $Z(z)$ is equally straightforward. If $\mu < 0$ we'd again find solutions in terms of sines and cosines, but let's suppose that $\mu > 0$ and that we require $\psi(\mathbf{r}) \to 0$ as $z \to \infty$. Then the only possibilities are $Z(z) = Z_\mu(z) \equiv c_\mu \exp\left(-z\sqrt{\mu}\right)$ for some $\mu \in \mathbb{R}^+$, where c_μ is a constant.

3.4.1 Bessel functions

We now turn to the radial equation. Multiplying this through by r and noting that $rR'' + R' = (rR')'$ we obtain the standard Sturm–Liouville form

$$\frac{d}{dr}\left(r\frac{dR}{dr}\right) - \frac{n^2}{r}R = -\mu r R \tag{3.57}$$

where the SL coefficients are $p(r) = r$ and $q(r) = -\lambda_n/r = -n^2/r$, while the weight function

$$w(r) = r \tag{3.58}$$

multiplies the eigenvalue $-\mu$. We can actually eliminate μ from this equation by introducing the rescaled radial coordinate[20] $x = r\sqrt{\mu}$ whereupon we find

$$x^2\frac{d^2R}{dx^2} + x\frac{dR}{dx} + (x^2 - n^2)R = 0 \tag{3.59}$$

This equation is known as *Bessel's equation of order n*. As with any second order ODE, this equation has two linearly independent solutions. They're denoted $J_n(x)$ and $Y_n(x)$ and are respectively known as *Bessel functions of the first (second) kind, or order n*, or often just 'Bessel functions' for short. The first few Bessel functions are plotted in figures 6–7. You should think of them as analogues of sines and cosines for the radial equation (3.59) instead of for the Cartesian equation $X'' = -\lambda X$.

Bessel functions of the first kind $J_n(x)$ are *regular* at the origin $x = 0$, and in fact all but $J_0(x)$ actually vanish at the origin. By contrast, the Bessel functions of the second kind $Y_n(x)$ are *singular* at the origin. This property means that if we are interested in solutions to Laplace's equation that are well–behaved within some radius r_0, then the Y_n functions cannot arise. On the other hand, if we're interested not in a solid cylinder, but in a cylindrical shell $r_0 \le r \le r_1$ then both types of Bessel functions generically do occur.

In the eighteenth century, winters were long and there was no Facebook, so people spent their time working out all sorts of properties of these Bessel functions. Here are some of the more prominent ones, none of which I'm going to prove and none of which I expect you to remember:

– Using the Frobenius method of power series, one can show

$$J_n(x) = \left(\frac{x}{2}\right)^n \sum_{k=0}^{\infty} \frac{(-1)^k}{k!(k+n)!}\left(\frac{x}{2}\right)^{2k}$$

whenever n is a non-negative integer. In fact Bessel's equation is of Sturm–Liouville type even if $n \in \mathbb{R}$ rather than $n \in \mathbb{Z}$. This formula still holds provided we replace the factorials by Gamma functions as $k!(k+n)! \rightsquigarrow \Gamma(k+1)\,\Gamma(k+n+1)$.

[20] This x of course has nothing to do with a Cartesian coordinate on the original $\mathbb{R}^3$.

– At small x, one finds

$$J_n(x) = \frac{1}{n!}\left(\frac{x}{2}\right)^n + O(x^{n+2}) \qquad \text{when } n \in \mathbb{Z}_{\geq 0}.$$
$$Y_0(x) = O(\ln x)$$
$$Y_n(x) = O(x^{-n}) \qquad \text{when } n \in \mathbb{Z}_{\geq 0}.$$

– At large x, the asymptotic behaviour of the Bessel functions is

$$J_n(x) = \left(\frac{2}{\pi x}\right)^{1/2} \cos\left[x - \frac{n\pi}{2} - \frac{\pi}{4}\right] + O(x^{-3/2})$$
$$Y_n(x) = \left(\frac{2}{\pi x}\right)^{1/2} \sin\left[x - \frac{n\pi}{2} - \frac{\pi}{4}\right] + O(x^{-3/2})$$

In particular, this shows that both $J_n(x)$ and $Y_n(x)$ have an infinite number of zeros and turning points. If we recall that $x = \sqrt{\mu}r$, where r was the radial coordinate in Laplace's equation, then we see that the location of these zeros in the radial direction of $\mathbb{R}^3$ depends on the eigenvalue μ.

You can find derivations of these and many more properties of Bessel functions in the books by Arfken & Weber or by Boas that I recommended earlier. As with the Legendre polynomials, I recommend you take a look through some of these, but again the most important fact about the n^{th} order Bessel functions are simply that they are eigenfunctions of a Sturm–Liouville operator that arises from the Laplacian in cylindrical polar coordinates when the angular equation $\Theta'' = -n^2\Theta$ has eigenvalue n^2.

3.4.2 Boundary value problems in cylindrical coordinates

Armed with the Bessel functions, we now return to our boundary value problem. We've found

$$\psi_{\mu,n}(r,\theta,\phi) = (a_n \sin n\theta + b_n \cos n\theta)\, \mathrm{e}^{-z\sqrt{\mu}}\, (J_n(r\sqrt{\mu}) + B_n Y_n(r\sqrt{\mu}))$$

for $n \in \mathbb{Z}_{\geq 0}$ and $\mu \in \mathbb{R}^+$ provides a solution of Laplace's equation that decays as $z \to +\infty$. Since we want the solution to be regular throughout the cylinder, in particular along the z-axis, we must set $B_n = 0$. The boundary condition that $\psi(\mathbf{r}) = 0$ at $r = a$ requires $J_n(a\sqrt{\mu}) = 0$. Thus, for any given n, this fixes μ to be one of the values

$$\sqrt{\mu} = \frac{k_{ni}}{a} \qquad \text{for } i = 1, 2, 3, \ldots \tag{3.60}$$

where i labels the roots $J_n(k_{ni}) = 0$ of the n^{th} Bessel function. This is just like we found for the sinusoidal case: the homogeneous boundary conditions fix the allowed eigenvalues. Since we've so far imposed only the homogeneous boundary conditions, we can consider an arbitrary linear combination of these normal modes. Relabelling constants, we have

$$\psi(r,\theta,z) = \sum_{n=0}^{\infty}\sum_{i=1}^{\infty} (A_{ni} \sin n\theta + B_{ni} \cos n\theta)\, J_n(k_{ni} r/a)\, \mathrm{e}^{-k_{ni} z/a} \tag{3.61}$$

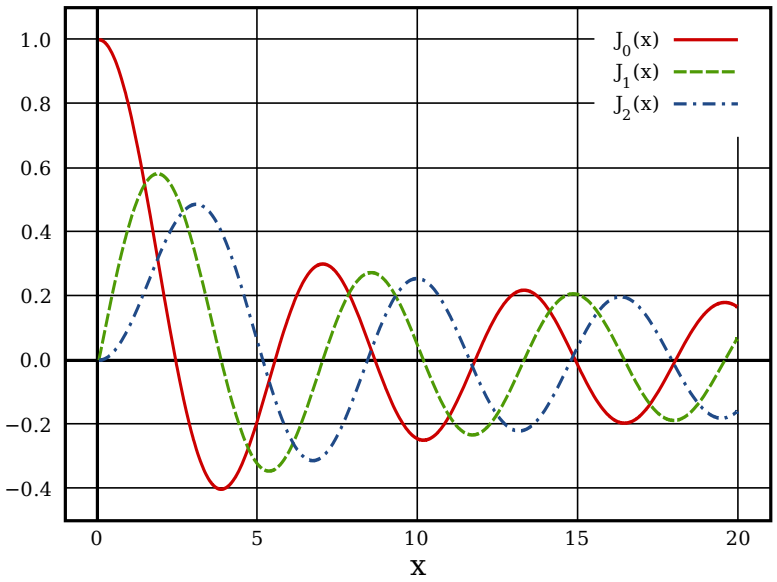


Figure 6. *Plots of some Bessel functions of the first kind $J_n(x)$, for order $n = 0, 1, 2$. The location of the first zero in $x > 0$ increases as the order of the Bessel function increases, and $J_n(x)$ is falling as it passes through this zero. Note that the zeros are not evenly spaced. $J_0(0) = 1$ while all other $J_n(x)$ vanish at the origin.*

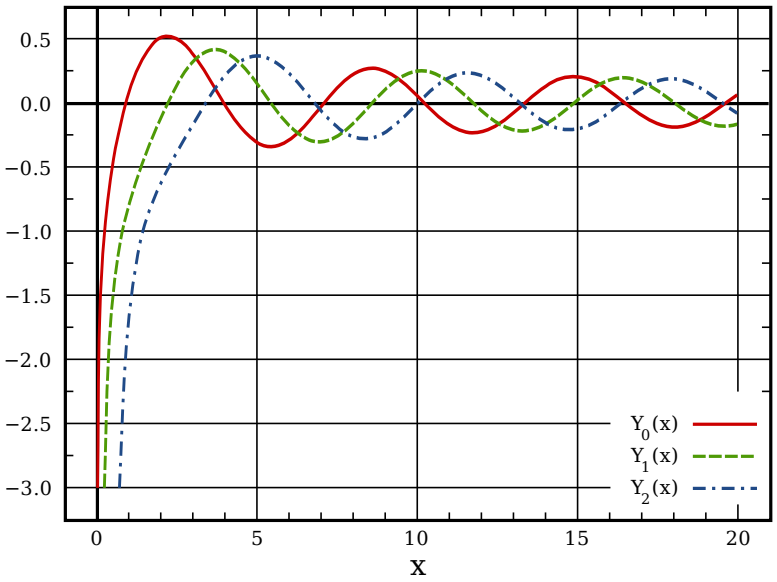


Figure 7. *Plots of some Bessel functions of the second kind $Y_n(x)$, for order $n = 0, 1, 2$. Again, the location of the first zero increases as the order of the Bessel function, but now $Y_n(x)$ rises as it passes through zero. All the $Y_n(x)$ are singular at the origin.*

as our general solution.

The final step is to fix the constants A_{ni} and B_{ni} by imposing the inhomogeneous

boundary condition $\psi(r,\theta,0) = f(r,\theta)$ when $z = 0$. Again, this is done using the Sturm–Liouville orthogonality conditions

$$\int_0^a J_n(k_{mj}r/a)\, J_n(k_{ni}r/a)\, r\,\mathrm{d}r = \frac{a^2}{2}\,\delta_{i,j}\left[J_n'(k_{ni})\right]^2 = \frac{a^2}{2}\,\delta_{i,j}\left[J_{n+1}(k_{ni})\right]^2 \tag{3.62}$$

for the Bessel functions. There are two things to note about this orthogonality relation. First, in (3.58) we identified the weight function in Bessel's equation as $w(r) = r$; it appears here. The second point note is that the Bessel functions $J_n(k_{ni}r)$ satisfy orthogonality relations *for each fixed n, but between different values i, j of the index labelling the roots.* You'll derive this relation in the problems sheets, and it's just what we need here. We can use the orthogonality relations

$$\frac{1}{\pi}\int_{-\pi}^{\pi} \sin m\theta\, \sin n\theta\,\mathrm{d}\theta = \delta_{m,n}\,,\quad \frac{1}{\pi}\int_{-\pi}^{\pi} \cos m\theta\, \cos n\theta\,\mathrm{d}\theta = \delta_{m,n}\,,\quad \frac{1}{\pi}\int_{-\pi}^{\pi} \sin m\theta\, \cos n\theta\,\mathrm{d}\theta = 0$$

among the trigonometric functions to fix a value of the n index, determining which order of Bessel function we're considering. For example, setting $z = 0$ and integrating (3.61) against $\cos m\theta$ gives

$$\frac{1}{\pi}\int_{-\pi}^{\pi} \cos m\theta\, f(r,\theta)\,\mathrm{d}\theta = \sum_{i=1}^{\infty} B_{mi}\, J_m(k_{mi}r/a) \tag{3.63}$$

involving only the m^{th} order Bessel function of the first kind, but with k_{mi} still summed over all the roots. The orthogonality condition (3.62) for the Bessel functions then gives

$$B_{mj} = \frac{2}{\pi a^2}\frac{1}{[J_m'(k_{mj})]^2}\int_0^a \left[J_m(k_{mj}r/a)\int_{-\pi}^{\pi}\cos m\theta\, f(r,\theta)\,\mathrm{d}\theta\right] r\,\mathrm{d}r \tag{3.64}$$

which fixes the constants B_{mj} in terms of the function f in the boundary condition. The B_{mj} are determined similarly.

As an example, let's suppose $f(r,\theta) = C$, a constant. Since this is in particular independent of θ, we see immediately from (**??**) that $B_{mj} = 0$ whenever $m \neq 0$. (The A_{mj} are similarly all zero.) The only non-zero coefficients are thus B_{0j}, multiplying a function with trivial angular dependence. These are

$$B_{0j} = \frac{2C}{a^2}\frac{1}{[J_1(k_{0j})]^2}\int_0^a J_0(k_{0j}r/a)\, r\,\mathrm{d}r = \frac{2C}{k_{0j}}\frac{1}{J_1(k_{0j})} \tag{3.65}$$

where the second equality is something you'll prove in the problem sets.

4 The Heat Equation

Our next equation of study is the heat equation. In the first instance, this acts on functions Φ defined on a domain of the form $\Omega \times [0, \infty)$, where we think of Ω as 'space' and the half–line $[0, \infty)$ as 'time after an initial event'. The equation is

$$\frac{\partial \Phi}{\partial t} = K \nabla^2 \Phi \tag{4.1}$$

where ∇^2 is the Laplacian operator on Ω and K is a real, positive constant known as the *diffusion constant*. For example, in the simplest case of one dimension where $\Omega = [a, b]$ the equation becomes just $\partial\Phi/\partial t = K\, \partial^2\Phi/\partial x^2$ where $x \in [a, b]$.

The heat equation genuinely is one of my favourite equations. It's range of applications is utterly mind–boggling. As the name suggests, it was originally constructed by Fourier in trying to understand how heat flows through a body from a hotter region to a cooler one, but it goes far, far beyond this. It describes the transport of any quantity that diffuses (*i.e.*, spreads out) as a consequence of spatial gradients in its concentration, such as drops of dye in water. The heat equation was used by Black and Scholes to model the behaviour of the stock market, and it underlies Turing's explanation of how the cheetah got its spots and the zebra its stripes. In pure maths, it plays a starring role in the derivation of the Atiyah–Singer index theorem relating topology to geometry, while a modification of the heat equation known as Ricci flow was used by Perelman to affirm the Poincaré conjecture, giving him chance to decline a Fields Medal. And, in the guise of something called *renormalization*, it's the best answer we have to the questions 'why can we understand physics at all?' or 'why is the Universe comprehensible?'[21]. Let's get started!

4.1 The fundamental solution

The first important property of the heat equation is that the total amount of heat is conserved. That is, if Φ solves the heat equation on $\Omega \times [0, \infty)$, then by differentiating under the integral sign

$$\frac{d}{dt}\left(\int_\Omega \Phi \, \mathrm{d}V\right) = \int_\Omega \frac{\partial \Phi}{\partial t} \, \mathrm{d}V = K \int_\Omega \nabla^2 \Phi \, \mathrm{d}V = K \int_{\partial\Omega} \mathbf{n} \cdot \nabla \Phi \, \mathrm{d}S \,, \tag{4.2}$$

where $\mathbf{n}$ is the outward normal to the boundary $\partial\Omega$ of the spatial region. In particular, if $\mathbf{n} \cdot \nabla\Phi|_{\partial\Omega} = 0$, which says that no heat flows out of our region, then

$$\frac{d}{dt}\left(\int_\Omega \Phi \, \mathrm{d}V\right) = 0 \tag{4.3}$$

and the total amount of heat in Ω is conserved. The heat equation moves heat around, but it doesn't just get 'lost'. (Notice that if Ω were non–compact, we'd have to demand that $|\nabla\Phi|$ decays sufficiently quickly as we move out to infinity in the spatial directions for these integrals to be well–defined.)

[21] Sadly, I won't be able to explain this to you in this course. But come to the Part III AQFT course and be amazed...

The second property we'll mention is that if $\Phi(x,t)$ solves the heat equation for (x,t) in $\mathbb{R}^n \times [0,\infty)$, then so too do the translated function

$$\Phi_1(x,t) \equiv \Phi(x - x_0, t - t_0)$$

and the rescaled function

$$\Phi_2(x,t) \equiv A\,\Phi(\lambda x, \lambda^2 t)\,,$$

where A, λ and t_0 are real constants and where $x_0 \in \mathbb{R}^n$. The proof of this is an easy exercise that I'll leave to you. Let's try to choose the constant A so that the total amount of heat in the solution Φ_2 is the same as in our original solution Φ. We have

$$\int_{\mathbb{R}^n} \Phi_2 \,\mathrm{d}^n x = A \int_{\mathbb{R}^n} \Phi(\lambda x, \lambda^2 t)\,\mathrm{d}^n x = A\,\lambda^{-n} \int_{\mathbb{R}^n} \Phi(y, \lambda^2 t)\,\mathrm{d}^n y \tag{4.4}$$

where $y = \lambda x$. If we choose $A = \lambda^n$ then the total heat in Φ_2 at time t will be the same as the total heat in Φ at time $\lambda^2 t$. But the total heat is conserved, so they are the same at all times.

The rescaling property is useful because it says there is nothing really new about the time variable t compared to the spatial variables. In other words, although $\Phi(x,t)$ looks as though it depends on n spatial variables and one time variable, we can always rescale so as to eliminate one of these variables. In particular, in 1+1 dimensions the heat equation becomes simply

$$\frac{\partial \Phi}{\partial t} = K \frac{\partial^2 \Phi}{\partial x^2} \tag{4.5}$$

and, choosing $\lambda = 1/\sqrt{Kt}$ nothing is really lost by considering solutions of the form

$$\Phi(x,t) = \frac{1}{\sqrt{Kt}} F(x/\sqrt{Kt}, 1) = \frac{1}{\sqrt{Kt}} F(\eta) \tag{4.6}$$

where we have introduced the *similarity variable*

$$\eta \equiv \frac{x}{\sqrt{Kt}}\,. \tag{4.7}$$

The similarity variable is a dimensionless parameter that is invariant under further rescalings $(x,t) \to (\lambda x, \lambda^2 t)$. We'll see that it characterizes the linear–time spread of heat.

Plugging the form (4.6) into the heat equation we obtain

$$\begin{aligned} \frac{\partial \Phi}{\partial t} &= -\frac{1}{2} \frac{1}{\sqrt{Kt^3}} F(\eta) + \frac{1}{\sqrt{Kt}} \frac{\partial \eta}{\partial t} F'(\eta) = -\frac{1}{2} \frac{1}{\sqrt{Kt^3}} (F + \eta F') \\ K \frac{\partial^2 \Phi}{\partial x^2} &= \sqrt{\frac{K}{t}} \frac{\partial}{\partial x} \left(\frac{\partial \eta}{\partial x} F' \right) = \frac{1}{t} \frac{\partial \eta}{\partial x} F'' = \frac{1}{\sqrt{Kt^3}} F'' \end{aligned} \tag{4.8}$$

so the heat equation pde reduces to the ode

$$0 = 2F'' + \eta F' + F\,. \tag{4.9}$$

Noting that the *rhs* of this equation is $(2F' + \eta F)'$ we see that $2F' + \eta F = D$ for some constant D. We can set D to zero by requiring that our solution obeys $F'(0) = 0$, and

one then finds $F(\eta) = Ce^{-\eta^2/4}$ for some further constant C. It is standard to fix this new constant by normalizing the total amount of heat to be 1. We have[22]

$$1 = \int_{-\infty}^{\infty} \Phi(x,t)\,dx = \frac{C}{\sqrt{Kt}} \int_{-\infty}^{\infty} e^{-x^2/4Kt}\,dx = 2C \int_{-\infty}^{\infty} e^{-u^2}\,du = 2C\sqrt{\pi}\,. \tag{4.10}$$

Therefore our normalized solution is

$$\Phi(x,t) = G(x,t) \equiv \frac{1}{\sqrt{4\pi Kt}} \exp\left(-\frac{x^2}{4Kt}\right) \tag{4.11}$$

It follows from the translation argument above that

$$G(x-x_0, t-t_0) = \frac{1}{\sqrt{4\pi K(t-t_0)}} \exp\left(-\frac{(x-x_0)^2}{4K(t-t_0)}\right) \tag{4.12}$$

also solves the (1+1)–dimensional heat equation. This class of solutions is known as the *heat kernel*, or sometimes as the *fundamental solutions* of the heat equation. It is also straightforward to show (or just to verify) that

$$\Gamma(\mathbf{x}-\mathbf{x}_0, t-t_0) \equiv \frac{1}{(4\pi K(t-t_0))^{n/2}} \exp\left(-\frac{|\mathbf{x}-\mathbf{x}_0|^2}{4K(t-t_0)}\right) \tag{4.13}$$

is the fundamental soluton of the heat equation in $n+1$ dimensions, $\mathbb{R}^n \times (t_0, \infty)$.

The heat kernel is a Gaussian centred on x_0. The rms width (standard deviation) of the Gaussian is $\sqrt{2K(t-t_0)}$ while the height of the peak at $x = x_0$ is $1/\sqrt{4\pi K(t-t_0)}$. This means that as $t \to \infty$ this fundamental solution becomes flatter and flatter, with its value at any fixed $x \in \Omega$ approaching zero exponentially rapidly. On the other hand, if we trace the behaviour of the fundamental solution backwards in time then as t approaches the initial time t_0 from above, the Gaussian becomes more and more sharply peaked near its centre x_0, and the height of the curve tends to infinity. The actual limit at $t = t_0$ is known as the *Dirac δ–function*, though it's not really a function at all. We'll meet it again in detail later. Plots of the heat kernel in 1+1 dimensions for various fixed times can be found in figure 8.

We have obtained the heat kernel as a solution to the heat equation within the domain $\mathbb{R}^n \times [0, \infty)$ without imposing any particular boundary conditions. However, one use of the heat kernel is as any early time approximation to heat flow problems in an *arbitrary* finite domain Ω near to interior points $x \in \Omega$ where the initial concentration of heat $\Phi(x, 0)$ has a sharp, highly localized spike. Intuitively, this is because it takes some time for this strongly localized interior profile to 'feel the influence' of the boundary conditions. For example, we may be interested in the effect of a sudden blast of heat perhaps coming from a blowtorch that is suddenly turned on, then immediately extinguished. at the centre of a furnace. The spread of heat is constrained by the boundary condition that it cannot penetrate the thick brick walls of the furnace, but at very short times this is irrelevant.

[22]The final integral can be performed by a trick: Let $I = \int_{\mathbb{R}} e^{-u^2}\,du$. Then

$$I^2 = \int_{\mathbb{R}^2} e^{-(u^2+v^2)}\,du\,dv = 2\pi \int_0^{\infty} e^{-r^2} r\,dr = \pi\,[-e^{-r^2}]_0^{\infty} = \pi\,.$$

Therefore $I = \sqrt{\pi}$, with the positive square root taken because I is the integral of a non–negative function.

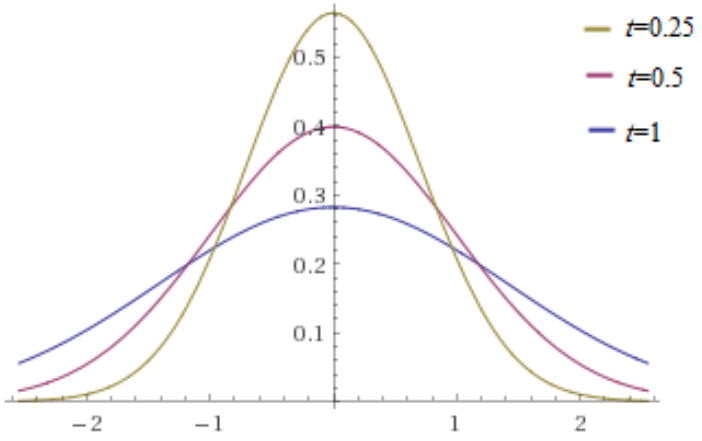


Figure 8. *Plots of the heat kernel* (4.11) *in one space and one time dimension, drawn at successive times $t > t_0 = 0$. For simplicity we have set $K = 1$. The curve is a Gaussian whose height increases without bound as $t \to 0^+$. Since the total heat is conserved, the area under the graph is constant, and equal to 1 by our normalization condition.*

4.2 Heat flow as a smoothing operation

The smoothing we observed in the fundamental solution – moving from a sharp spike to a flat line as $t \to \infty$ – is the generic behaviour of functions under heat flow, and is in accordance with our intuition that heat flows from hotter places to cooler ones. This smoothing property is one of the most important properties of the heat equation. Let's see it more generally.

First, we note that if $\psi : \Omega \to \mathbb{C}$ is an eigenfunction of the Laplacian (with weight 1) so that $\nabla^2\psi = -\lambda\psi$ for some constant λ, then provided ψ obeys suitable conditions on $\partial\Omega$, the eigenvalue λ is non-negative. This follows because

$$-\lambda \int_\Omega |\psi|^2 \, \mathrm{d}V = \int_\Omega \psi^* \, \nabla^2\psi \, \mathrm{d}V = \int_{\partial\Omega} \psi^* \, \nabla\psi \cdot \mathrm{d}\mathbf{S} - \int_\Omega \nabla\psi^* \cdot \nabla\psi \, \mathrm{d}V \tag{4.14}$$

where $\mathrm{d}V = \mathrm{d}x_1 \, \mathrm{d}x_2 \cdots \mathrm{d}x_d$ is the standard measure on Ω. Since both $\int_\Omega |\psi|^2 \, \mathrm{d}V$ and $\int_\Omega |\nabla\psi|^2 \, \mathrm{d}V$ are the integrals of non-negative functions, we see that provided the boundary term vanishes

$$\lambda = \frac{\int_\Omega |\nabla\psi|^2 \, \mathrm{d}V}{\int_\Omega |\psi|^2 \, \mathrm{d}V} \geq 0 \, . \tag{4.15}$$

In particular all the eigenvalues of a Laplacian on a closed, compact space (so that $\partial\Omega = \emptyset$) are non-negative.

Now, suppose a certain function $\Phi : \Omega \times [0, \infty) \to \mathbb{C}$ evolves in time according to the heat equation $\partial\Phi/\partial t = \nabla^2\Phi$, where ∇^2 is the Laplacian on the closed, compact space Ω and $t \in [0, \infty)$ denotes the time. To reduce clutter, we've also set the diffusion constant to unity. If Φ looks initially like some function $f : \Omega \to \mathbb{C}$, so that $\Phi(\mathbf{x}, 0) = f(\mathbf{x})$, then at finite later times t we have (somewhat formally)

$$\Phi(\mathbf{x}, t) = \exp\left(t\nabla^2\right) \Phi(\mathbf{x}, 0) \, . \tag{4.16}$$

But given a basis $\{\psi_I\}$ of eigenstates of ∇^2 on Ω, we can expand f in this basis as

$$\Phi(\mathbf{x}, 0) = f(\mathbf{x}) = \sum_I c_I \, \psi_I(\mathbf{x}) \tag{4.17}$$

for some coefficients c_I. (When $\dim \Omega > 1$ the index 'I' really stands for a whole collection of indices, each one of which is being summed over. For example, if $\Omega = T^2 = S^1 \times S^1$ then we will have two indices, each denoting the Fourier components around one of the circles. The sum over I is supposed to indicate a sum over all values of each of these indices, with independent coefficients.) Finally, if $\nabla^2 \psi_I = -\lambda_I \psi_I$ then inserting this into equation (4.16) and using the linearity of the Laplacian gives

$$\begin{aligned} \Phi(\mathbf{x}, t) &= \exp\left(t\nabla^2\right) \left[\sum_I c_I \, \psi_I\right] = \sum_I c_I \, \mathrm{e}^{-\lambda_I t} \, \psi_I(\mathbf{x}) \\ &\equiv \sum_I c_I(t) \, \psi_I(\mathbf{x}) \, . \end{aligned} \tag{4.18}$$

In the final line I've introduced the *time–dependent coefficients* $c_I(t) \equiv \mathrm{e}^{-\lambda_I t} c_I$. Thus, since the eigenvalues are non-negative, the coefficients decay exponentially with time. We saw earlier[23] that the rate at which the coefficients in an eigenfunction expansion decay as one goes out to very high eigenvalues tells us something about the smoothness of the function we're expanding. The important observation is under evolution by the heat equation, that coefficients of eigenfunctions corresponding to the largest values of $|\lambda_I|$ decay most rapidly. Thus, in accordance with our intuition, heat flow *smooths* our function in accordance with our intuition. In fact, the smoothing is so effective that a function that is discontinuous at $t = 0$ becomes continuous for all $t > 0$ if it evolves by the heat equation.

Not only does Φ become smoother, it's also easy to see that the norm of Φ over Ω decreases rapidly. At a fixed time $t \geq 0$ we have

$$\begin{aligned} (\Phi, \Phi) &= \int_\Omega \Phi^* \, \Phi \, \mathrm{d}V = \sum_{I,J} \left[c_I^*(t) \, c_J(t) \int_\Omega \psi_I^*(\mathbf{x}) \, \psi_J(\mathbf{x}) \, \mathrm{d}V \right] \\ &= \sum_I |c_I(t)|^2 \leq \sum_I |c_I(0)|^2 \end{aligned} \tag{4.19}$$

using orthonormality of the eigenfunctions ψ_I.

Incidentally, I hope you now see the reason I've emphasized that the time variable t in the heat equation takes values on the half–line $[0, \infty)$ rather than $t \in \mathbb{R}$. If we try to follow heat flow backwards in time, then the convergence of our series becomes exponentially *worse*, with the eigenfunctions having greater and greater $|\lambda_I|$ rapidly becoming more and more important. In fact, if we start from a generic smooth function and trace its evolution back in time, then it's a theorem that we'll arrive at an arbitrarily badly singular function in finite time. Setting the diffusion constant to 1 for simplicity, we sometimes say that

[23] We saw this just in the special case of Fourier series in one dimension, but something similar is true quite generally.

the operators $e^{t\nabla^2}$ form a *semigroup*, because for t_1 and t_2 both ≥ 0 we have the group multiplication law

$$e^{(t_1+t_2)\nabla^2} = e^{t_1\nabla^2}\ e^{t_2\nabla^2}$$

while setting $t = 0$ gives the identity operator. However, we're not allowed to consider heat flow for negative times because we'd meet too singular functions, so the inverse operators do not exist and heat flow is a one–way street.

The fact that evolution via the heat equation smears out sharp features can be both a blessing and a curse, as the following two examples illustrate:

4.2.1 The transatlantic cable

In 1858 the first telegraph cable was laid under the Atlantic, with Great Britain and the United States both looking forward to the benefits this new form of communication could bring to trade and governance. The first message to be sent was a 98 word greeting from Queen Victoria to President Buchanan. The British telegraph operators dutifully tapped out the message in Morse code and sent it on its way. But by the time the signal made landfall in Newfoundland, it had degraded so as to be barely detectable, let alone readable. What went wrong? Because seawater is a much better conductor than air, the signal traveling along the submerged cable obeyed the heat equation, not the wave equation[24] as it would for an overland telegraph wire. The form of the fundamental solution of equation (4.11) shows that an initially sharp spike traveling along a (one–dimensional!) cable of length L in accordance with the heat equation will emerge as a broad pulse spread over a time $T \sim L^2$. The precise dots and dashes of Morse code had been smeared out so much that it took the American engineers 16 hours to decipher the message.

Desperate to please his employers, the chief engineer tried to make the signal more distinct by increasing the voltage to 2000V. This promptly fried the cable's protective cover somewhere in the mid Atlantic, destroying the cable. The chief engineer was sacked. Following the advice of his replacement, a further cable was laid with thicker insulation and higher quality copper wire (thus increasing the conductivity K). It was driven at low voltage with a sensitive 'mirror galvanometer' used to detect the incoming signal. The new cable was a resounding success.

The first engineer's name was Wildman Whitehouse – you've never heard of him. His replacement William Thomson was rewarded with the title of Lord Kelvin, grew an impressive beard and became very wealthy.

4.2.2 The Atiyah–Singer index theorem

The index theorem of Atiyah & Singer provides a fundamental link between topological information about a (closed, compact) space Ω to local information, such as how curved the space is near some point. A beautiful proof of this theorem was provided by Atiyah & Bott. Their proof uses properties we know about the heat equation.

The point is that under heat flow, a function spreads out and ultimately smears itself all over the compact space Ω, giving us access to global information about the topology

[24] We'll see in the next chapter that signals propagating via the wave equation preserves their integrity.

of Ω. More specifically, if we follow the behaviour of some $\Phi(\mathbf{x}, t)$ under heat flow right through to arbitarily late times, then from equation (4.18) we find

$$\lim_{t\to\infty} \Phi(\mathbf{x}, t) = \lim_{t\to\infty} \sum_I c_I \, \mathrm{e}^{-t\lambda_I} \, \psi_I(\mathbf{x}) = \sum_{I\,:\,\lambda_I=0} c_I \, \psi_I(\mathbf{x}) \,, \tag{4.20}$$

where the final sum is over only those eigenfunctions of the Laplacian whose eigenvalues are zero. This always includes the constant function, but on a manifold with interesting topology there may be non–trivial functions that nonetheless have zero eigenvalue[25]. However, if at $t = 0$ we choose Φ to have support just inside some small compact region $R \subset \Omega$, then for early times Φ remains exponentially small outside R.

Heat flow from $t = 0$ to $t \to \infty$ thus provides a natural link between local and global properties of Ω. The idea of Atiyah & Bott was to find a quantity – known as the "index of a Dirac operator" – that can be proved to be *independent* of time and track it during heat flow. At early times one finds the index can be computed in terms of local, geometric information while at late times it depends only on topological properties of Ω.

4.3 Brownian motion and the existence of atoms

The fact that heat always flows from a hotter to a cooler body – just the smoothing property we examined above – posed a challenge to the Newtonian, mechanical view of the world. According to the hypothesis that matter is fundamentally made up of atoms (dating back in some form to the ancient Greeks), heat is simply the kinetic energy of these atoms as they jiggle around. The problem is that at the microscopic level, Newton's laws of motion are time reversible: for forces such as electromagnetism, gravity, or collisions between hard particles, $\mathbf{F} = m\mathbf{a}$ is invariant under the replacement $t \mapsto -t$. Philosophers such as Mach and chemists such as Ostwald thought that this microscopic time reversibility was incompatible with the macroscopic arrow of time inherent in heat flow, and concluded that atoms did not exist.

Einstein realized that the apparently random motion of small dust particles observed by the botanist Robert Brown must be due to their random collisions with water molecules. To construct a one–dimensional model of this problem, assume that our dust particle is jostled at regular time intervals Δt. We let $p(y)$ be the probability that the dust particle moves through a displacement y at each time step, with $\int_{-\infty}^{\infty} p(y)\,\mathrm{d}y = 1$. The key assumption is that $p(y)$ is *independent of which time step we're considering.* That is, the process is memoryless – the probability $p(y)$ does not depend on the previous motion of the particle. This is also known as a *Markov process.* We further assume that $p(y)$ is homogeneous, so that it does not depend on the actual location of the dust particle. Finally, we'll assume that $p(y)$ is an even function of y so that the mean value $\langle y \rangle$ is zero. This just means that there is no preference for the particle to drift either to the left or right; it's easy to drop this final assumption.

[25] To come clean, I'll admit that Φ should really be something more general than a 'function' here, and we need to be careful about what we mean by the Laplacian in this more general context. Believe it or not, the case relevant to the Atiyah–Singer index theorem is where Φ is the quantum mechanical wavefunction describing a type of relativistic electron.

If we now let $P(x,t)$ be the probability density that the dust particle is located at some position $x \in \mathbb{R}$ at time t, then we have

$$P(x;t+\Delta t) = \int_{-\infty}^{\infty} p(y)\, P(x-y;t)\, \mathrm{d}y\,. \tag{4.21}$$

This equation says that the probability the particle is located at x at time $t+\Delta t$ is the product of the probability it was some amount y away at the previous time interval, times the probability it stepped through exactly y, for any choice of y. Expanding $P(x-y;t)$ as a Taylor series in y we have

$$\begin{aligned} P(x;t+\Delta t) &= \int_{-\infty}^{\infty} p(y) \left(P(x;t) - y\frac{\partial P}{\partial x}(x;t) + \frac{1}{2}y^2 \frac{\partial^2 P}{\partial x^2}(x;t) + \cdots \right) \mathrm{d}y \\ &= \sum_{r=0}^{\infty} \frac{\langle y^r \rangle}{r!} \frac{\partial^r P}{\partial x^r}(x;t) \end{aligned} \tag{4.22}$$

where by $\langle y^r \rangle$ we mean simply the average value $\int_{-\infty}^{\infty} y^r\, p(y)\, \mathrm{d}y$ of y^r. By our assumption, $\langle y \rangle = 0$. Furthermore, if the motion of the particle is small so that $p(y)$ is concentrated near $y = 0$, then $\langle y^r \rangle$ will drop rapidly as r increases. Keeping only the leading non–trivial term we have

$$P(x;t+\Delta t) - P(x;t) = \frac{1}{2}\langle y^2 \rangle \frac{\partial^2 P}{\partial x^2}(x;t)\,. \tag{4.23}$$

In the limit of small time steps $\Delta t \to 0$ we find that $P(x,t)$ satisfies the heat equation

$$\frac{\partial P}{\partial t} = K \frac{\partial^2 P}{\partial x^2} \tag{4.24}$$

where the diffusion constant K can be identified as $\langle y^2 \rangle / 2\Delta t$.

THIS SECTION NEEDS MORE WORK!! NOT YET RELATED TO EXISTENCE OF ATOMS

4.4 Boundary conditions and uniqueness

Let $M \equiv \Omega \times [0,T]$ where $\Omega \subset \mathbb{R}^n$ is a compact domain with boundary $\partial\Omega$, and where $[0,T)$ is the time direction. We'd now like to check whether there is a unique solution to the heat equation $\partial\psi/\partial t = K\nabla^2\psi$ in the interior of M that obeys the Dirichlet conditions

$$\begin{aligned} \psi|_{\Omega\times\{0\}} &= f(x) \qquad && \text{(initial condition)} \\ \psi|_{\partial\Omega\times[0,T]} &= g(x,t) \qquad && \text{(boundary condition)} \end{aligned} \tag{4.25}$$

for some given functions $f : \Omega \to \mathbb{R}$ and $g : \partial\Omega \times [0,T] \to \mathbb{R}$.

As in the case of Laplace's equation, suppose on the contrary that ψ_1 and ψ_2 are two such solutions, each obeying the boundary conditions (4.25). Then if $\delta\psi \equiv \psi_1 - \psi_2$ we have

$$0 = \int_\Omega \delta\psi \left(\frac{\partial \delta\psi}{\partial t} - K\nabla^2 \delta\psi \right) \mathrm{d}V \tag{4.26}$$

where the integral is over the spatial region Ω at some arbitrary fixed time t. Hence differentiating the integral with respect to time we have

$$\begin{aligned}\frac{1}{2}\frac{d}{dt}\int_\Omega \delta\psi^2\,\mathrm{d}V &= \int_\Omega \delta\psi\,\frac{\partial\delta\psi}{\partial t} = K\int_\Omega \delta\psi\,\nabla^2\delta\psi \\ &= -K\int_\Omega (\nabla\delta\psi)\cdot(\nabla\delta\psi)\,\mathrm{d}V + K\int_{\partial\Omega}\delta\psi\,\nabla\delta\psi\,\cdot\mathrm{d}\mathbf{S}\end{aligned} \tag{4.27}$$

The boundary term vanishes since ψ_1 and ψ_2 agree on $\partial\Omega$ at all times, and the remaining term is $-K$ times the integral of a non–negative function. Therefore

$$\frac{d}{dt}\left(\int_\Omega \delta\psi^2\,\mathrm{d}V\right) \le 0\,. \tag{4.28}$$

The quantity $E(t) \equiv \int_\Omega \delta\psi^2\,\mathrm{d}V$ is the integral of a non–negative function, which by (4.28) can never increase. Since $E(0) = 0$ by our initial conditions, we must have $E(t) = 0$ at all times t for which the heat equation holds. This is only possible if $\delta\psi = 0$ everywhere in Ω and at all times $t \in [0, T]$, so that the solutions ψ_1 and ψ_2 agree everywhere in M.

There's an important caveat to the above argument: Compactness of Ω in all spatial directions is important. If, for example, we replaced the compact region Ω by the semi–infinite bar $\{(x, y, z) \in \mathbb{R}^3 \,:\, 0 \le x \le a\,,\ 0 \le y \le b\,,\ z \ge 0\}$ then our argument above might be invalid, because it could be that the integrals over the spatial region now *diverge*. This is not just a technical nicety: it's really true that, when Ω has non–compact directions, solutions to the heat equation are *not* unique unless we impose a limit of the rate of growth of ψ as we head out towards infinity in Ω. In the case of the semi–infinite bar, the correct limit turns out to be $|\psi| \le A\mathrm{e}^{\lambda|z|^2}$ as $z \to \infty$, for some constants A and λ, although I won't prove that here.

4.5 Heat conduction in a plane medium

After the above, rather formal, considerations, in the next few sections we'll return to actually solving the heat equation in the presence of boundary and initial conditions.

One of Fourier's original motivations for introducing his series was to study the problem of heat flow through a plane medium. In particular, he wanted to study how the temperature Θ of the soil at a depth $x \ge 0$ beneath the surface was affected by the regular heating and cooling of the daily cycle. For simplicity, we'll assume that the earth is flat and that ground level may be represented by the plane $x = 0$. If the sun's rays strike the earth evenly, then the problem may be modeled by the heat equation

$$\frac{\partial\Theta}{\partial t}(x,t) = K\frac{\partial^2\Theta}{\partial x^2}(x,t) \tag{4.29}$$

in 1+1 dimensions, where K is the thermal diffusivity of the soil. The boundary conditions are that the temperature decays to a constant as $x \to +\infty$ (deep under the surface of the earth) and that at $x = 0$ the temperature oscillates both daily and annually as

$$\Theta(0,t) = \Theta_0 + A\cos(2\pi t/t_\mathrm{D}) + B\cos(2\pi t/t_\mathrm{Y}) \tag{4.30}$$

where $t_{\rm D}$ is the length of one day, and $t_{\rm Y}$ the length of one year in whatever units we're using to measure time. The constants A and B govern the size of the daily and annual variation around the average temperature Θ_0.

We again separate variables, writing $\Theta = T(t)X(x)$, and discover that the heat equation (4.29) becomes

$$T' = \lambda T\,, \qquad\qquad X'' = \frac{\lambda}{K} X \tag{4.31}$$

for some constant λ. Noting that we want oscillatory behaviour in time, with an eye on the boundary condition at $x = 0$ we set $\lambda = \mathrm{i}\omega$ with $\omega \in \mathbb{R}$. The heat equation is then solved by

$$\Theta = \Theta_\omega \equiv \mathrm{e}^{\mathrm{i}\omega t}\left(a_\omega\,\mathrm{e}^{-x\sqrt{\mathrm{i}\omega/K}} + b_\omega\,\mathrm{e}^{x\sqrt{\mathrm{i}\omega/K}}\right) \tag{4.32}$$

for some choice of ω and constants a_ω, b_ω. By linearity, we can add solutions with different values of the separation constant ω. Since $\sqrt{\mathrm{i}\omega} = (1+\mathrm{i})\sqrt{|\omega|/2}$ for $\omega > 0$ and $\sqrt{\mathrm{i}\omega} = (\mathrm{i}-1)\sqrt{|\omega|/2}$ for $\omega < 0$, the boundary condition that Θ decays to a constant as $x \to +\infty$ shows that we must take $b_\omega = 0$ when $\omega > 0$ and $a_\omega = 0$ when $\omega < 0$. Writing the boundary condition at $x = 0$ as

$$\Theta(0,t) = \Theta_0 + \frac{A}{2}\left(\mathrm{e}^{\mathrm{i}\omega_{\rm D} t} + \mathrm{e}^{-\mathrm{i}\omega_{\rm D} t}\right) + \frac{B}{2}\left(\mathrm{e}^{\mathrm{i}\omega_{\rm Y} t} + \mathrm{e}^{-\mathrm{i}\omega_{\rm Y} t}\right) \tag{4.33}$$

we see that we should choose $a_\omega = b_\omega = 0$ for all ω except

$$\omega = \pm\omega_{\rm D} \equiv \pm 2\pi/t_{\rm D}\,, \qquad \omega = \pm\omega_{\rm Y} \equiv \pm 2\pi/t_{\rm Y}\,, \qquad \text{and} \qquad \omega = 0\,.$$

The case $\omega = 0$ just gives the constant Θ_0. For the remaining cases we have

$$a_{\omega_{\rm D}} = b_{-\omega_{\rm D}} = \frac{A}{2}\,, \qquad a_{\omega_{\rm Y}} = b_{-\omega_{\rm Y}} = \frac{B}{2} \tag{4.34}$$

so that the general solution obeying the boundary condition becomes

$$\begin{aligned}\Theta(x,t) \;=\; \Theta_0 \;+\; & A\exp\left(-\sqrt{\frac{\omega_{\rm D}}{2K}}\,x\right)\cos\left(\omega_{\rm D} t - \sqrt{\frac{\omega_{\rm D}}{2K}}\,x\right) \\ & +\; B\exp\left(-\sqrt{\frac{\omega_{\rm Y}}{2K}}\,x\right)\cos\left(\omega_{\rm D} t - \sqrt{\frac{\omega_{\rm Y}}{2K}}\,x\right)\,.\end{aligned} \tag{4.35}$$

It is a worthwhile exercise to check that this does indeed obey the heat equation (4.29).

The solution we've found tells us how the temperature of the soil at a depth x and time t responds to the sun's warmth. Examining it, we see that both temperature variations decay exponentially rapidly with increasing depth, so that the diurnal and annual cycles have little effect on the temperature Θ_0 deep underground. Note however that the fall–off of the higher frequency, daily variation is far more rapid than that of the annual variation.

We also see there is a depth–dependent phase delay of $(\omega_{\rm D}/K)^{1/2}\,x$ for the daily, and $(\omega_{\rm Y}/K)^{1/2}\,x$ for the annual temperature variation. Thus, at some depths beneath the surface of the earth the temperature can be completely out of step with that on the surface. The depth at which this occurs depends on the heat conductivity K of the soil, but for reasonable soil types one finds that at a depth of around 2 to 3 metres, the ground is warmer in winter and cooler in summer. That's why it's a good idea to store food and wine in cellars.

4.6 Steady heat conduction in a finite rod

As a small variation of this problem, suppose we have a bar of length $2L$. We'll look for a function ψ that solves the heat equation $\partial\psi/\partial t = K\partial^2\psi/\partial x^2$ everywhere inside the domain $[-L, L] \times [0, \infty)$ and subject to the initial condition

$$\psi(x, 0) = \Theta(x) \equiv \begin{cases} 1 & 0 < x \leq L \\ 0 & -L \leq x < 0\,, \end{cases} \tag{4.36}$$

as well as the boundary condition

$$\psi(L, t) = 1\,, \qquad\qquad \psi(-L, t) = 0 \tag{4.37}$$

so that each end of the bar is kept at a (different) fixed temperature for all time.

The most important thing to note about this example is that *neither the initial nor the boundary condition is homogeneous*. Thus if we try to seperate variables immediately, we'll find there are no homogeneous boundary conditions to impose, and we will not find any constraint on the allowed separation constants. To get around this, we first look for *any particular* solution ψ_s of the wave equation that obeys the boundary condition (4.37), but not necessarily the initial condition (4.36). Any other solution obeying the same boundary conditions will differ from this one by a solution ϕ obeying the homogeneous boundary conditions

$$\phi(-L, t) = 0\,, \qquad\qquad \phi(L, t) = 0 \tag{4.38}$$

and so may be found via separation of variables.

To keep our lives simple, we can look for a particular solution $\phi_s(x)$ that is independent of time – known as a *steady state* solution. Since the time–independent heat equation becomes $\phi_s''(x) = 0$ we have $\phi_s(x) = ax + b$ and to satisfy the boundary condition (4.37) we must choose the constants so that

$$\phi_s(x) = \frac{x + L}{2L}\,. \tag{4.39}$$

We now look for a function $\phi(x, t) = \psi(x, t) - \phi_s(x)$ obeying the heat equation subject to the conditions

$$\begin{aligned} \phi(\pm L, t) &= 0 && (\textit{homogeneous} \text{ boundary condition}) \\ \phi(x, 0) &= \Theta(x) - \frac{x + L}{2L} && (\text{adjusted initial condition}) \end{aligned} \tag{4.40}$$

that reflect the effect of our particular solution.

We now proceed as usual. Write $\phi(x, t) = X(x)T(t)$ and find

$$T' = -K\lambda T\,, \qquad\qquad X'' = -\lambda X \tag{4.41}$$

for some separation constant $\lambda \in \mathbb{R}$. We can solve these as

$$X(x)T(t) = \left[a\,\sin(\sqrt{\lambda}x) + b\,\cos(\sqrt{\lambda}x)\right] \mathrm{e}^{-K\lambda t}\,.$$

The initial condition $\phi(x,0) = \Theta(x) - (x+L)/2L$ is an *odd* function, so we anticipate that we can set $b = 0$. The homogeneous boundary conditions $\phi(\pm L, 0) = 0$ shows that the general solution is then

$$\psi(x,t) = \sum_{n=1}^{\infty} a_n \sin\left(\frac{n\pi x}{L}\right) \mathrm{e}^{-Kt\sqrt{n\pi/L}}\,. \tag{4.42}$$

The last step is to choose the coefficients a_n so as to obey the inhomogeneous initial condition. This will be achieved if we set

$$a_n = \frac{1}{L}\int_{-L}^{L} \sin\frac{n\pi x}{L}\,\left[\Theta(x) - \frac{x+L}{2L}\right]\,\mathrm{d}x = \frac{1}{n\pi}\,, \tag{4.43}$$

where the last equality requires a short calculation (*please check!*). Finally therefore, the solution to the heat equation obeying the original boundary conditions (4.36)-(4.37) is

$$\psi(x,t) = \frac{x+L}{2L} + \frac{1}{\pi}\sum_{n=1}^{\infty}\frac{1}{n}\,\sin\frac{n\pi x}{L}\,\mathrm{e}^{-Kt\sqrt{n\pi/L}}\,. \tag{4.44}$$

Note once more that the convergence of this infinite sum improves rapidly as t increases, and that

$$\lim_{t\to+\infty}\psi(x,t) = \phi_s(x) \tag{4.45}$$

so that $\phi_s(x)$ does indeed emerge as the late time equilibrium solution of our problem.

4.7 Cooling of a uniform sphere

At the end of the nineteenth century, one of the most apparently serious problems faced by Darwinian evolution was that the evolutionary process was so slow that the Earth had not been around for long enough for the observed diversity of life to have arisen. The main proponent of this argument was Kelvin (again) whose argument was as follows.

Kelvin knew the temperature at which rock melts (typically in the range 1000 ± 300°C for most types of rock) and it seemed reasonable to assume that life could not have been present at the time when the whole surface of the earth was molten magma. He also knew from Fourier's results of section 4.5 that, while the temperature of the surface of the Earth undergoes wide daily and annual variations, the sun's influence diminishes rapidly once one heads more than a few hundred metres down into the ground. He thus felt justified in ignoring the sun's influence and took as a boundary condition that the temperature at the surface of the Earth was zero, appropriate for outer space.

The stage was set. If Kelvin could determine how long it would take a sphere, initially heated uniformly to around 1000°C, to cool into outer space so as to form a temperature gradient near its surface of the size then observed, then this time would set an upper limit on the time available for evolution.

Let's make the rough assumption that the Earth is a homogeneous ball of radius R formed from rock with thermal diffusivity K. Under our homogeneity assumptions we expect the solution to be spherically symmetric, so we let $\Theta(r,t)$ denote the temperature

at a radius r from the centre of the Earth, at time t. The behaviour of Θ will be governed by the heat equation

$$\frac{\partial\Theta}{\partial t} = K\nabla^2\phi = K\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial\Theta}{\partial r}\right). \tag{4.46}$$

We want to solve this equation inside the Earth, subject to the initial condition and boundary condition

$$\begin{aligned} \Theta(r,0) &= \Theta_0 \qquad && \text{for all } r < R \\ \Theta(R,t) &= 0 && \text{for all } t > 0\,, \end{aligned} \tag{4.47}$$

where Θ_0 is the temperature of molten rock.

We can solve this using our standard method of separation of variables. Making the usual ansatz $\Theta(r,t) = R(r)T(t)$ the heat equation reduces to the two o.d.e.s

$$\frac{d}{dr}\left(r^2\frac{dR}{dr}\right) = -\lambda^2 r^2 R\,, \qquad \frac{dT}{dt} = -\lambda^2 KT \tag{4.48}$$

for some separation constant λ. The second equation is uniquely solved by $T = A_\lambda\,\mathrm{e}^{-\lambda^2 Kt}$ for some constant A_λ, whereas the radial equation is solved by

$$R(r) = B_\lambda\frac{\sin(\lambda r)}{r} + C_\lambda\frac{\cos(\lambda r)}{r}\,. \tag{4.49}$$

(One way to convince yourself of this is to substitute in $S(r) \equiv r\,R(r)$ whereupon the radial equation reduces to $S'' = -\lambda^2 S$.) We insist that our solution remains regular at $r = 0$ and so we set $C_\lambda = 0$. The boundary condition that $\Theta(R,t) = 0$ then forces

$$\lambda = \frac{n\pi}{R}\,, \qquad n \in \mathbb{Z} \tag{4.50}$$

so our general solution obeying this boundary condition is

$$\Theta(r,t) = \frac{1}{r}\sum_{n\in\mathbb{Z}} A_n \sin\left(\frac{n\pi r}{R}\right)\exp\left(-\frac{n^2\pi^2}{r^2}Kt\right). \tag{4.51}$$

We must now choose the separation constants A_n to enforce the inhomogeneous initial condition $\Theta(r,0) = \Theta_0$. Setting $t = 0$ and multiplying through by r we have

$$r\Theta_0 = \sum_{n\in\mathbb{Z}} A_n \sin\left(\frac{n\pi r}{R}\right) \tag{4.52}$$

and therefore

$$A_n = \Theta_0\int_0^R \sin\left(\frac{n\pi r}{R}\right) r\,\mathrm{d}r = (-1)^{n+1}\frac{\Theta_0 R}{n\pi} \tag{4.53}$$

as follows from integration by parts. Thus our solution at all times is

$$\Theta(r,t) = \frac{\Theta_0 R}{\pi r}\sum_{n\in\mathbb{Z}}(-1)^{n+1}\frac{1}{n}\sin\left(\frac{n\pi r}{R}\right)\exp\left(-\frac{n^2\pi^2}{r^2}Kt\right) \qquad \text{for } r \le R. \tag{4.54}$$

Incidentally, this solution would be valid for arbitrarily large values of r in some fictitious problem where the Earth extends forever, but with $r = R$ held fixed at zero temperature.

In the real situation, the thermal diffusivity K abruptly changes at the surface of the Earth from its value for rock to its value for air, then empty space (where $K = 0$). Thus we do not believe our solution for $r > R$. However, within the Earth's surface the solution (4.54) is good: we have found *a* solution that satisfies both the boundary and initial conditions and our uniqueness theorem guarantees it is the only one.

Miners had long reported the presence of the geothermal gradient – a temperature increase of around 25°C/km as one moves deeper underground – and Kelvin used this information to fix a timescale. From the solution (4.54) we find

$$\left.\frac{\partial\Theta}{\partial r}\right|_{r=R} = -\frac{\Theta_0}{R}\sum_{n\in\mathbb{Z}}\exp\left(-\frac{n^2\pi^2}{R^2}Kt\right) \tag{4.55}$$

where the minus sign indicates the fact that Θ increases as we head towards the centre of the Earth. To go further, notice that the very fact that the rocks do indeed get considerably hotter as one goes deeper – we still have volcano eruptions! – suggests that the Earth's age is not so very great that the exponential term has yet had much effect, since if it had then $\Theta(r,t)$ would itself be vanishingly small. But if $Kt/R^2 \ll 1$ (actually true in our case) then we may approximate

$$\sum_{n\in\mathbb{Z}}\exp\left(-\frac{n^2\pi^2}{R^2}Kt\right) \approx \int_{-\infty}^{\infty}\exp\left(-\frac{x^2\pi^2}{R^2}Kt\right)\,\mathrm{d}x = \sqrt{\frac{R^2}{\pi Kt}}$$

Combining all the pieces we find that there will be a geothermal gradient of order G at a time of order

$$t_0 \sim \frac{\Theta_0^2}{G^2}\frac{1}{\pi K}\,. \tag{4.56}$$

Plugging in his numbers, Kelvin found that it would have taken the Earth not more than 100 million years to cool from its molten beginnings to the present temperature. This, Darwin knew, was not nearly enough time for the current diversity of species to have evolved by natural selection.

Darwin was tremendously worried by Kelvin's conclusions, more than by any other argument proposed against his Theory of Evolution. Kelvin's mathematics was impeccable, so what's going on? We now know that radioactivity – a source of energy unknown to Kelvin – primarily from Uranium deposits deep under the Earth's mantle is responsible for heating the Earth from within. This extra source of heat generation was unaccounted for in the calculation above, and has kept our planet warm for $4\frac{1}{2}$ billion years. Evolution reigns triumphant.

5 The Wave Equation

Waves are extremely common in the physical world. Examples include surface disturbance of a body of fluid, vibration of string instruments and pressure perturbations in air that convey sound. In all these cases, if the amplitude of the disturbance is sufficiently small, the perturbation variable $\phi(\mathbf{x}, t)$ characterising the disturbance will satisfy the *wave equation*:

$$\frac{\partial^2 \phi}{\partial t^2} = c^2 \nabla^2 \phi \tag{5.1}$$

where c is the (phase) speed of propagation of maxima and minima of a sinusoidal wave form. In these examples, extra non-linear terms will need to be introduced if the disturbance becomes large, and the wave equation is only a kind of lowest order approximation. This is entirely analogous to the behaviour of a point particle in mechanics, that is trapped in a local minimum of some potential function and performing *small* motions: regardless of the overall form of the potential, to lowest order approximation (e.g. in Taylor series expansion) any (suitably differentiable) function appears quadratic around a local minimum, and the particle will thus execute *simple harmonic motion* if the amplitude is small. But the wave equation also has genuinely fundamental significance in other areas: for example in electromagnetic theory, Maxwell's equations imply the the electromagnetic potentials must satisfy the wave equation in regions free of sources, and this lead to the understanding of (classical) light as an electromagnetic phenomenon – a truly awesome discovery at the time.

5.1 Vibrations of a uniform string

To bring the discussion down to earth, let's think of the example of a violin string of length L. So we take the spatial region Ω to just be the interval $[0, L]$ with $x \in [0, L]$ denoting the location along the string.

We'll start by illustrating the physical origin of the wave equation in this example. Consider a small transverse oscillation of our string with ends fixed at $x = 0$ and $x = L$. To keep things simple, let's assume that the string is uniform with constant mass per unit length μ and is perfectly elastic. That's pretty much true of a well–made violin string. We'll also assume that the string only performs small transverse oscillations $\phi(x, t)$, so that we only need to work to first order in ϕ. Consider a small element δs of string between x (point A) and $x + \delta x$ (point B) having mass $\mu \delta x$. Let θ_A, θ_B be the angles at the ends and let T_A, T_B be the outward pointing tangential tension forces acting on δs. Since the motion is transverse, the total force along the string is zero so

$$T_A \cos\theta_A = T_B \cos\theta_B = T = \text{constant}\,. \tag{5.2}$$

In the transverse direction, Newton's second law gives

$$\mu \delta x \frac{\partial^2 \phi}{\partial t^2} = T_B \sin\theta_B - T_A \sin\theta_A \tag{5.3}$$

Dividing through by the quantities in equation (5.2) gives

$$\frac{\mu \delta x}{T} \frac{\partial^2 \phi}{\partial t^2} = \frac{T_B \sin\theta_B}{T_B \cos\theta_B} - \frac{T_A \sin\theta_A}{T_A \cos\theta_A} = \tan\theta_B - \tan\theta_A\,. \tag{5.4}$$

Now

$$\tan\theta_B - \tan\theta_A = \left.\frac{\partial\phi}{\partial x}\right|_B - \left.\frac{\partial\phi}{\partial x}\right|_A \approx \frac{\partial^2\phi}{\partial x^2}\,\delta x\,,$$

so that after dividing through by $\mu\,\delta x/T$, equation (5.4) becomes

$$\frac{\partial^2\phi}{\partial t^2} = c^2\frac{\partial^2\phi}{\partial x^2}\,, \qquad \text{where } c^2 = T/\mu. \tag{5.5}$$

Thus we have derived the wave equation in 1+1 dimensions. The constant c has units of a velocity and is called the *phase speed*. Note that from the role of Newton's law in the above derivation, for a unique solution (in addition to the BCs of fixed endpoints $\phi(0,t) = \phi(L,t) = 0$ for all t) we would expect to have to provide both the initial position $\phi(x,0)$ and the initial velocity $\partial\phi/\partial t(x,0)$ for $0 < x < L$ of all points along the string. We'll say more about uniqueness in section 5.2.

We now wish to solve the 1+1 dimensional wave equation subject to the boundary conditions

$$\phi(0,t) = \phi(L,t) = 0 \tag{5.6}$$

and initial conditions

$$\phi(x,0) = f(x)\,, \qquad \frac{\partial\phi}{\partial t}(x,0) = g(x) \tag{5.7}$$

for some given functions f and g, representing the string's initial shape and velocity. Separation of variables $\phi(x,t) = X(x)T(t)$ leads to the o.d.e.s

$$X'' = -\lambda\,X \qquad\qquad T'' = -c^2\lambda\,T \tag{5.8}$$

in terms of a separation constant λ. These are solved by sines and cosines, and the boundary conditions $\phi(0,t) = \phi(L,t) = 0$ enforce require that

$$\lambda = \frac{n^2\pi^2}{L^2} \qquad \text{for some } n \in \mathbb{N}. \tag{5.9}$$

Consequently our individual solution is

$$\phi_n(x,t) = \sin\frac{n\pi x}{L}\,\left[A_n\cos\frac{n\pi ct}{L} + B_n\sin\frac{n\pi ct}{L}\right] \tag{5.10}$$

which, for a fixed value of n is known as a *normal mode* of the oscillation. In particular, the lowest non–trivial value $n = 1$ is known as the *fundamental mode*. We see that all the frequencies of oscillation $\omega_n = n\pi c/L$ are integer multiples of the fundamental frequency ω_1.

Summing over possible separation constants, the general solution is a sum over the normal modes

$$\phi(x,t) = \sum_{n=1}^{\infty}\sin\frac{n\pi x}{L}\,\left[A_n\cos\frac{n\pi ct}{L} + B_n\sin\frac{n\pi ct}{L}\right]. \tag{5.11}$$

As usual, the constants A_n and B_n are fixed by the inhomogeneous initial conditions to be

$$A_n = \frac{2}{L}\int_0^L \sin\frac{n\pi x}{L}\, f(x)\,\mathrm{d}x\ , \qquad\qquad B_n = \frac{2}{n\pi c}\int_0^L \sin\frac{n\pi x}{L}\, g(x)\,\mathrm{d}x\,. \tag{5.12}$$

For example, if we pluck the string, pulling it back to height h in the middle and releasing it from rest, then we have the initial conditions

$$f(x) = \begin{cases} 2hx/L & 0 \le x \le L/2 \\ 2h(L-x)/L & L/2 \le x/leqL \end{cases}$$

while $g(x) = 0$. We computed the Fourier coefficients of this plucked string function $f(x)$ in the problem sets, finding

$$\hat{f}_n = \begin{cases} (-1)^{(n+1)/2}\dfrac{8h}{n^2\pi^2} & \text{when } n \text{ is odd} \\ 0 & \text{else.} \end{cases} \tag{5.13}$$

Using this result we have

$$\phi(x,t) = \frac{8h}{\pi^2}\sum_{n=1}^{\infty}\frac{(-1)^{n+1}}{(2n-1)^2}\,\sin\left[\frac{(2n-1)\pi x}{L}\right]\sin\frac{n\pi ct}{L}\,. \tag{5.14}$$

It's a good idea to check that this does indeed satisfy the wave equation, boundary conditions and initial conditions.

5.2 Energetics and uniqueness

It will be helpful to derive an expression for the energy contained in the string's motion. Since the string has mass per unit length μ, its total kinetic energy at time t is

$$K(t) = \frac{1}{2}\int_0^L \mu\left(\frac{\partial\phi}{\partial t}\right)^2\,\mathrm{d}x\,. \tag{5.15}$$

The string is under tension, so it will also have some potential energy whenever its profile is non–constant. Considering a small element δs of the string we have

$$T\times(\text{extension}) = T(\delta s - \delta x) = T\left[\sqrt{1+\left(\frac{\partial\phi}{\partial x}\right)^2}\ -\ 1\right]\delta x \tag{5.16}$$

and integrating this along the length of the string gives a potential energy contribution at time t

$$V(t) = T\int_0^L\left[\sqrt{1+\left(\frac{\partial\phi}{\partial x}\right)^2}\ -\ 1\right]\mathrm{d}x \approx \frac{T}{2}\int_0^L\left(\frac{\partial\phi}{\partial x}\right)^2\mathrm{d}x\,. \tag{5.17}$$

In the final approximation we used the fact that the oscillations are small. Using the fact that $c^2 = T/\mu$ we see that the total energy of the string is

$$E(t) = \frac{\mu}{2}\int_0^L\left[\left(\frac{\partial\phi}{\partial t}\right)^2 + c^2\left(\frac{\partial\phi}{\partial x}\right)^2\right]\mathrm{d}x\,. \tag{5.18}$$

It's a useful exercise to evaluate this energy function for the explicit solution (5.11). You should find that the kinetic and potential energies are

$$\begin{aligned} K(t) &= \frac{\mu\pi^2 c^2}{4L}\sum_{n=1}^{\infty} n^2 \left[A_n \sin\left(\frac{n\pi ct}{L}\right) - B_n \cos\left(\frac{n\pi ct}{L}\right)\right]^2 \\ V(t) &= \frac{\mu\pi^2 c^2}{4L}\sum_{n=1}^{\infty} n^2 \left[A_n \cos\left(\frac{n\pi ct}{L}\right) + B_n \sin\left(\frac{n\pi ct}{L}\right)\right]^2 \end{aligned} \tag{5.19}$$

so that the total energy is

$$E(t) = \frac{\mu^2 c^2 \pi^2}{4L}\sum_{n=1}^{\infty} n^2 \left(A_n^2 + B_n^2\right). \tag{5.20}$$

Notice in particular that this total energy is independent of time; just like in simple harmonic motion, PE and KE are continuously inter–converted during the motion so that the total energy is conserved. Also notice that, in accordance with our intuition, given two modes with equal amplitudes the higher mode has the higher energy. Finally, recall that the period of oscillation (*i.e.* the period of the fundamental mode) is

$$T = \frac{2\pi}{\omega} = 2\pi\frac{L}{\pi c} = \frac{2L}{c}. \tag{5.21}$$

and we can average over a period to get

$$\overline{K} = \frac{c}{2L}\int_0^{\frac{2L}{c}} K(t)\,\mathrm{d}t = \overline{V} = \frac{c}{2L}\int_0^{\frac{2L}{c}} V(t)\mathrm{d}t = \frac{E}{2}\,, \tag{5.22}$$

so there is an *equipartition of energy* between average potential and kinetic energies.

The energy provides a good way to prove uniqueness of solutions to the wave equation in general, provided they are subject to appropriate boundary and initial conditions. To see this, let $M \cong \Omega \times [0,\infty)$ and let $\phi : M \to \mathbb{R}$ be a solution of the wave equation[26] in the interior of M, that obeys the conditions

$$\begin{aligned} &\phi|_{\Omega\times\{0\}} = f(x) && \text{(initial condition on } \phi \text{ itself)} \\ &\partial_t\phi|_{\Omega\times\{0\}} = g(x) && \text{(initial condition on time derivative of } \phi) \\ &\phi|_{\partial\Omega\times(0,\infty)} = h(x) && \text{(Dirichlet boundary condition at } \partial\Omega) \end{aligned} \tag{5.23}$$

Notice that, as above, we have two initial conditions: at time $t = 0$ we prescribe the values both of ϕ itself and its first time derivative everywhere over space Ω. We also impose Dirichlet boundary conditions at the boundary of our compact region Ω that hold for all times.

Absorbing a factor of μ into the scaling of ϕ, we define the *energy* $E_\phi(t)$ of this wave at time $t \in (0,\infty)$ to be the integral

$$E_\phi(t) \equiv \frac{1}{2}\int_\Omega \left(\frac{\partial\phi}{\partial t}\frac{\partial\phi}{\partial t} + c^2\nabla\phi\cdot\nabla\phi\right)\mathrm{d}V \tag{5.24}$$

[26]For simplicity, I'll only consider real–valued functions here. What I say generalizes to complex–valued waves easily – have a go!

over the spatial region Ω. This is a natural generalization of the energy of our violin string, involving a kinetic term involving the rate $\partial_t\phi$ at which each point in Ω is oscillating, and a potential term involving the tension due to spatial gradients in the wave. Differentiating under the integral and using the fact that partial derivatives commute one finds

$$\begin{aligned}\frac{dE_\phi}{dt} &= \int_\Omega \left[\frac{\partial\phi}{\partial t}\frac{\partial^2\phi}{\partial t^2} + c^2\nabla\left(\frac{\partial\phi}{\partial t}\right)\cdot\nabla\phi\right]\,\mathrm{d}V \\ &= \int_\Omega \frac{\partial\phi}{\partial t}\left[\frac{\partial^2\phi}{\partial t^2} - c^2\nabla^2\phi\right]\,\mathrm{d}V + c^2\int_{\partial\Omega}\frac{\partial\phi}{\partial t}(\mathbf{n}\cdot\nabla\phi)\,\mathrm{d}S \\ &= c^2\int_{\partial\Omega}\frac{\partial\phi}{\partial t}\,\mathbf{n}\cdot\nabla\phi\,\mathrm{d}S\end{aligned} \tag{5.25}$$

where in going to the second line we integrate by parts in the spatial variables, and in going to the last line we used the fact that ϕ solves the wave equation. Thus, if either $\mathbf{n}\cdot\nabla\phi|_{\partial\Omega} = 0$ or $\partial_t\phi|_{\partial\Omega} = 0$ so that no energy is flowing out of the region Ω, then evolution via the wave equation preserves $E_\phi(t)$.

Now we're ready for our uniqueness theorem. Suppose ϕ_1 and ϕ_2 are two solutions of the wave equation inside M that each obey the boundary conditions (5.23). Then $\psi \equiv \phi_1 - \phi_2$ solves the wave equation subject to

$$\psi|_{\Omega\times\{0\}} = \partial_t\psi|_{\Omega\times\{0\}} = \psi|_{\partial\Omega\times(0,\infty)} = 0\,. \tag{5.26}$$

In particular, the fact that $\psi|_{\partial\Omega} = 0$ for all times means that $\partial_t\psi|_{\partial\Omega} = 0$ so that $dE_\psi/dt = 0$ and therefore that

$$E_\psi(t) = \frac{1}{2}\int_\Omega\left(\frac{\partial\psi}{\partial t}\frac{\partial\psi}{\partial t} + c^2\nabla\psi\cdot\nabla\psi\right)\,\mathrm{d}V$$

remains constant. But since both $\partial_t\psi$ and ψ itself vanish throughout Ω at $t = 0$, evaluating this integral at the initial time gives

$$E_\psi(t) = E_\psi(0) = 0\,. \tag{5.27}$$

Finally, since $E(t)$ is the integral of a sum of non–negative quantities, the only way for $E(t)$ to vanish is if $\partial_t\psi$ and $\nabla\psi$ each vanish separately throughout Ω at all times. Thus ψ is constant on $\Omega\times[0,\infty)$ and since the initial value of ψ is zero, ψ is everywhere zero. Hence our two solutions ϕ_1 and ϕ_2 are in fact the same.

This result is useful: it says that if we manage to find a solution satisfying boundary and initial conditions as in (5.23) by any means (*e.g.* separation of variables), then we've found the only solution and we're done. As usual, if we replace the Dirichlet condition on the boundary of the spatial region Ω by a Neumann condition $\mathbf{n}\cdot\nabla\phi|_{\partial\Omega} = h(x)$ the uniqueness argument goes through unchanged up to the last step, where we conclude that our two solutions can differ at most by a constant.

5.3 Vibrations of a circular membrane

For our next example, we'll consider the vibrations of a circular drum. Let's take Ω to be the unit disc $\{(r,\theta)\in\mathbb{R}^2\ :\ r\le 1\}$ and write the wave equation in cylindrical coordinates

as

$$\frac{1}{c^2}\frac{\partial^2\phi}{\partial t^2} = \nabla^2\phi = \frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial\phi}{\partial r}\right) + \frac{1}{r^2}\frac{\partial^2\phi}{\partial\theta^2} \tag{5.28}$$

We'll suppose the drum's membrane it held fast at the boundary, so $\phi|_{r=1} = 0$ for all times t. Writing $\phi(r,\theta,t) = R(r)\,\Theta(\theta)\,T(t)$ we find

$$T'' = -c^2\lambda\,T\ , \qquad \Theta'' = -\mu\,\Theta\ , \qquad r(rR')' + (r^2\lambda - \mu)R = 0 \tag{5.29}$$

The T and Θ equations have the usual sinusoidal and cosinusoidal solutions, and to ensure our solution is single–valued as $\theta \to \theta + 2\pi$ we must take $\mu = m^2$ for some $m \in \mathbb{N}$. The radial equation becomes $r(rR')' + (r^2\lambda - m^2)R = 0$, which is Bessel's equation of order m. As in section 3.4.1, the solutions are

$$R(r) = a_m J_m\left(\sqrt{\lambda}r\right) + b_m Y_m\left(\sqrt{\lambda}r\right) \tag{5.30}$$

where we take $b_m = 0$ to ensure regularity at the origin. To satisfy the boundary condition at $r = 1$, we must choose the separation constant λ to be one of the

$$\lambda = k_{mi}^2 \qquad \text{where } J_m(k_{mi}) = 0 \tag{5.31}$$

so that k_{mi} is the i^{th} root of the m^{th} Bessel function $J_m(r)$.

Combining the pieces, we have the general solution

$$\begin{aligned}\phi(r,\theta,t) = &\sum_{i=1}^{\infty}\left[A_{0i}\sin(k_{0i}ct) + C_{0i}\cos(k_{0i}ct)\right]J_0(k_{0i}r)\\ &+\sum_{m=1}^{\infty}\sum_{i=1}^{\infty}\left[A_{mi}\cos m\theta + B_{mi}\sin m\theta\right]\,\sin(k_{mi}ct)\,J_m(k_{mi}r)\\ &+\sum_{m=1}^{\infty}\sum_{i=1}^{\infty}\left[C_{mi}\cos m\theta + D_{mi}\sin m\theta\right]\,\cos(k_{mi}ct)\,J_m(k_{mi}r)\end{aligned} \tag{5.32}$$

which is admittedly a bit of a mouthful. Pictures of some of the normal modes of oscillation can be seen in figure 9. If the drum's surface has initial profile and velocity

$$\phi(r,\theta,0) = f(r,\theta) \qquad \partial_t\phi(r,\theta,0) = g(r,\theta) \tag{5.33}$$

then the constants $\{A_{mi}, B_{mi}, C_{mi}, D_{mi}\}$ may be fixed by expanding both f and g in Fourier series in θ and Bessel functions in r. We recall that the Bessel functions of order m obey a Sturm–Liouville differential equation and are thus orthogonal for different values of k_{mi}. Explicitly,

$$\int_0^1 J_m(k_{mi}r)\,J_m(k_{mj})\,r\,\mathrm{d}r = \frac{1}{2}\delta_{ij}\,\left[J_{m+1}(k_{mi})\right]^2 \tag{5.34}$$

as you showed in one of the problems.

As an example, suppose that the drum is initially quiet with $\phi = 0$ but at $t = 0$ is suddenly struck in the centre, so that

$$\phi(r,\theta,0) = 0\,, \qquad \partial_t\phi(r,\theta,0) = g(r)\,, \tag{5.35}$$

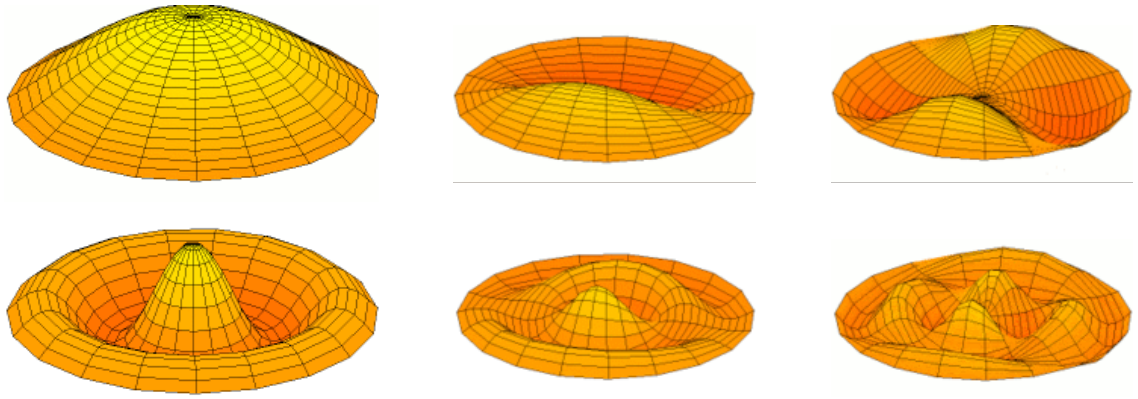


Figure 9. *Various normal modes of oscillation of a circular drum. In the left column the modes* $(m, i) = (0, 1)$ *and* $(0, 3)$ *are shown, the middle column shows the modes* $(m, i) = (1, 1)$ *and* $(1, 3)$ *and the right column shows the modes* $(m, i) = (2, 1)$ *and* $(2, 3)$. *These figures are taken from this Wikipedia page, where you can find animated versions.*

where the initial velocity is a function of r only. The solution is then also independent of the angle θ and the only non–vanishing constants are A_{0i}. (The C_{0i} must vanish since we need $\phi|_{t=0} = 0$. The general solution (5.32) reduces to

$$\phi(r, \theta, t) = \sum_{i=1}^{\infty} A_{0i} \sin(k_{0i} c t)\, J_0(k_{0i} r) \tag{5.36}$$

where the remaining constants A_{0i} are given by

$$A_{0i} = \frac{2}{c k_{0i}} \frac{1}{[J_1(k_{0i})]^2} \int_0^1 J_0(k_{0i} r)\, g(r)\, r \, \mathrm{d}r \,. \tag{5.37}$$

Interestingly, the fundamental frequency for a drum of general radius a is $k_{01} c/a \sim 4.8 c/a$, which is higher than the fundamental frequency $\pi c/a$ of a string of length a. Also, the fundamental response of the drum is just a Bessel function, so our ears experience these functions rather frequently even if they seem unfamiliar to our brains.

5.4 Can one hear the shape of a drum?

I'm sure you can spot my non–examinable sections by now, but just in case: this is one.

We've seen that the normal modes of a violin string oscillate at frequencies that are integer multiples of the fundamental frequency $\pi c/L$ and it's easy to see that the fundamental frequencies of a rectangular membrane with sides of lengths L_1 and L_2 will be $c\pi\sqrt{m^2/L_1^2 + n^2/L_2^2}$ for $m, n \in \mathbb{N}$ if the membrane is held fast along its four edges. (If this isn't clear to you – *work it out!*) On the other hand, for a circular membrane of radius a the frequencies of the normal modes are $k_{mi} c/a$ where k_{mi} are the irregularly spaced roots of the m^{th} Bessel functions. Given a membrane of an arbitrary shape, fixed in place around its boundary, it can be a difficult problem to determine exactly what the normal modes are, particularly in higher dimensions.

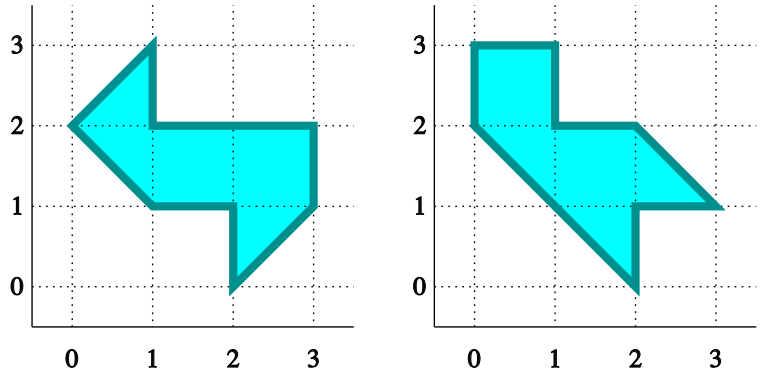


Figure 10. *These two shapes, constructed by Gordon, Webb & Wolpert following a method of Sunada, share all their eigenvalues of the Laplacian, so perfect drums made in these shapes would sound identical. Both polygons have the same area and same perimeter.*

In 1966, Mark Kac turned the question around. Instead of asking "Given a membrae, can we find its frequencies of oscillation?" he asked instead "Suppose we are given the complete set $\{\omega_I\}$ of frequencies of the normal modes of oscillation of some membrane, where I takes values in some indexing set. Can we use these to work out the domain $\Omega \subset \mathbb{R}^n$ spanned by the membrane?". More poetically, the question can be phrased "Can one hear the shape of a drum?".

As put, the answer to this question is "No". In other words, we now know that there do exist two different shapes all of whose eigenvalues of the Laplacian coincide. Such shapes are said to be *isospectral*. The first example to be found was, remarkably enough, in sixteen (!) dimensions and these two 16-dimensional isospectral shapes each turn out to play an important rôle in modern string theory: They're each responsible for one of the two weakly–coupled heterotic string theories, one of which was found by Prof. Michael Green here in Cambridge, together with Prof. John Schwarz in Caltech. The fact that they are isospectral is in fact important for consistency of the two theories. Later, more and more examples of isospectral shapes were found; the simplest known pair in two spatial dimensions is shown in figure 10.

Not being put off by this negative result, people then asked whether the question could be answered 'yes' under special conditions. For example, it's known that if the membrane is *convex*[27] and has boundary specified by a real–analytic function, then one can hear its shape. More generally, you might wonder exactly how much information about Ω can be retrieved from knowing all the frequencies ω_I. For example, Weyl showed that the total area $A(\Omega)$ of the surface of a drum is given by

$$A(\Omega) = 4\pi^2 \lim_{\lambda_0 \to \infty} \frac{N(\lambda_0)}{\lambda_0}\,, \tag{5.38}$$

where $N(\lambda_0)$ is the number of eigenfrequencies less than the scale λ_0. Thus the area is related to the asymptotic growth of the number of eigenvalues. Weyl also generalized this

[27] A region $\Omega \subset \mathbb{R}^n$ is convex if, given any pair of points $x_1, x_2 \in \Omega$ the straight line segment joining x_1 to x_2 is also entirely contained in Ω.

formula to $n+1$ dimensions, and conjectured that the subleading terms in this limit were related to the perimeter of the drum (or the volume of $\partial\Omega$ in higher dimensions).

The whole field of studying the geometry of some Ω by studying its eigenfrequencies is known as *spectral geometry*. You can take a course on it in Part III.

5.5 Wave reflection and transmission

If the medium through which the wave is propagating has spatially varying properties, then the properties of the wave will change too, with for example the possibility of partial reflection at an interface.

Suppose we have an (infinite) string with density $\mu = \mu_-$ for $x < 0$ and $\mu = \mu_+$ for $x > 0$ and consider small transverse deflections. Resolving forces horizontally as before, we see that the tension τ must remain constant (even with density variations) and so the wave speed $c_\pm \equiv \sqrt{\tau/\mu_\pm}$ differs on either side of $x = 0$. Consider an incident wave propagating to the right from $x = -\infty$. The most general form is

$$\phi_I(x,t) = A_I \cos[\omega(t - x/c_-) + \xi_I] \tag{5.39}$$

with frequency ω, amplitude A_I and phase shift ξ_I; the subscript I denotes that this is the "incident" wave. It is convenient to represent such waves in terms of a complex exponential

$$\phi_I(x,t) = \mathrm{Re}\left(I \exp\left[\mathrm{i}\omega\left(t - x/c_-\right)\right]\right) , \tag{5.40}$$

where Re denotes the real part. Here, we've introduced the complex number I whose modulus is the amplitude A_I and whose phase is the phase shift ξ_I of (5.39). Again, the use of the capital letter I reminds us that this is the incident wave; we'll soon meet complex numbers R and T denoting the "reflected" and "transmitted" waves. If necessary, we'll use lowercase r and i to denote the real and imaginary parts of these quantities, so that $I = I_r + \mathrm{i}I_i$ for example.

On arrival at $x = 0$ some of the incident wave will be *transmitted* and so continue to propagate to the right into $x > 0$, while some will be *reflected* and so propagate back to the left. Both of these waves may have different amplitudes and phases than those of the incident wave. However, they must have the same frequencies if the string is to stay together at all times (in particular at the point $x = 0$). Using subscripts T for "transmitted" and R for "reflected" we write

$$\begin{aligned} \phi_T(x,t) &= \mathrm{Re}\left(T \exp\left[\mathrm{i}\omega\left(t - \frac{x}{c_+}\right)\right]\right) \\ \phi_R(x,t) &= \mathrm{Re}\left(R \exp\left[\mathrm{i}\omega\left(t + \frac{x}{c_-}\right)\right]\right) \end{aligned} \tag{5.41}$$

The complex coefficients T and R define the new amplitudes and phases via their moduli and arguments. These coefficients are determined by the following physical matching conditions at $x = 0$:

– We assume the string does not break, so the displacement at $x = 0$ must be continuous *for all time*. That is,

$$\phi_I|_{x=0^-} + \phi_R|_{x=0^-} = \phi_T|_{x=0^+} \ .$$

Using the fact that if $\mathrm{Re}\left(A\mathrm{e}^{\mathrm{i}\omega t}\right) = \mathrm{Re}\left(B\mathrm{e}^{\mathrm{i}\omega t}\right)$ for all t then $A = B$ as complex numbers, we get

$$I + R = T \,. \tag{5.42}$$

– The point $x = 0$ has no inertia (compare with a different situation in probs. 2!) and thus the total vertical force at $x = 0$ vanishes. Hence

$$\tau \left.\frac{\partial\phi}{\partial x}\right|_{x=0^-} = \tau \left.\frac{\partial\phi}{\partial x}\right|_{x=0^+} ,$$

or in other words

$$\frac{R}{c_-} - \frac{I}{c_-} = -\frac{T}{c_+} \,. \tag{5.43}$$

Equations (5.42) & (5.43) suffice to fix the two complex numbers R and T in terms of I. Solving we get

$$R = \left(\frac{c_+ - c_-}{c_+ + c_-}\right) I \qquad \text{and} \qquad T = \left(\frac{2c_+}{c_+ + c_-}\right) I \,. \tag{5.44}$$

This solution has several interesting properties. Firstly, we see that $R_i/R_r = T_i/T_r = I_i/I_r$ so there is a simple relationship between the phases of the waves. Secondly, if $\mu_+ = \mu_-$ so that $c_+ = c_-$, we find that $R = 0$ and $T = I$ as expected: in the absence of any change in μ, the wave travels on unhindered. On the other hand, if the string to the right is very much heavier so that $\mu_+ \gg \mu_-$, then $c_+ \ll c_-$ and we find $T \sim 0$. As expected, almost all the wave is reflected. Note however that the reflected wave has phase shift π compared to the incident wave, since $R \approx -I$. Finally, if the string to the right $x > 0$ is very much lighter $\mu_+ \ll \mu_-$, then $c_+ \gg c_-$ and we find $T \sim 2I$ and $R \sim I$. In this case there is no phase shift, and we get a large amplitude of disturbance to the right. However most of the energy is still reflected (as the mass is very low on the right) so in both the asymmetrical limiting cases, most of the energy is reflected.

6 Generalized Functions

We've used separation of variables to solve various important second–order partial differential equations inside a compact domain $\Omega \subset \mathbb{R}^n$. But our approach should leave you with many questions. The method started by finding a particular solution of the form $\phi(\mathbf{x}) = X(x)Y(z)\cdots$, and then using the homogeneous boundary conditions to constrain (quantize) the allowed values of the separation constants that occur in such a solution. So far so good. We then used linearity of the p.d.e. to claim that a more general solution would be given by summing our particular solutions over all possible allowed values of the separation constants, with coefficients that were fixed by the boundary and/or initial conditions.

The trouble is that, generically, our boundary conditions required that we include an *infinite* number of terms in the sum. We should first of all worry about whether such an infinite sum converges everywhere within Ω, or for all times. But even if it does, can we be sure whether it converges to an actual solution of the differential equation we started with? That is, while each term in the infinite sum certainly obeys the p.d.e., perhaps the infinite sum itself does not: we've seen in chapter 1 that Fourier series sometimes converge to non–differentiable or even non–continuous functions and that term–by–term differentiation of a Fourier series makes convergence worse. And suppose we find the function our series converges to indeed is not twice differentiable. Should we worry? Could there be some sense in which we should still allow these non–differentiable solutions? But, if we do, can we be sure that we've really found the general solution to our problem? The uniqueness theorems we obtained in previous chapters always involved showing that the *integral* of some non-negative quantity was zero, and then concluding that the quantity itself must be zero. This might fail if, say, our series solution differs from the 'true' solution just on a set of measure zero.

You can certainly understand why mathematicians such as Laplace were so reluctant to accept Fourier's methods. Quite remarkably, the most fruitful way forward has turned out not to be to restrict Fourier to situations where everything converges to sufficiently differentiable functions that our concerns are eased, but rather to be *to generalize the very notion of a function itself* with the aim of finding the right class of object where Fourier's method always makes sense. *Generalized functions* were introduced in mathematics by Sobolev and Schwartz. They're designed to fulfill an apparently mutually contradictory pair of requirements: They are sufficiently well–behaved that they're infinitely differentiable and thus have a chance to satisfy partial differential equations, yet at the same time they can be arbitrarily singular – neither smooth, nor differentiable, nor continuous, nor even *finite* – if interpreted naively as 'ordinary functions'. Generalized functions have become a key tool in much of p.d.e. theory, and form a huge part of analysis.

If this formal theory is not your cup of tea, there's yet another reason to be interested in generalized functions. When we come to study inhomogeneous (driven) equations such as Poisson's equation $\nabla^2\phi = \rho$, physics considerations suggest that we'll be interested in cases where the source ρ is not a smooth function. For example, ρ might represent the charge density in some region Ω, and we may only have point–like charges. The total

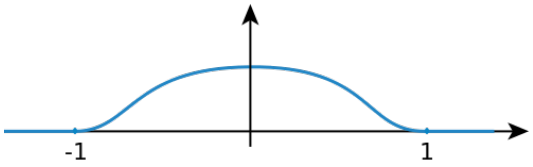


Figure 11. *The bump function $\Psi(x)$ is an example of a smooth test function with compact support.*

charge $Q = \int_\Omega \rho \, \mathrm{d}V$ is thus finite, but ρ vanishes everywhere except at finitely many points. Generalized functions will allow us to handle p.d.e.s with such singular source terms. In fact, the most famous generalized function was discovered in physics by Dirac before the analysts cottoned on, and generalized functions are often known as *distributions*, as a nod to the charge distribution example which inspired them.

6.1 Test functions and distributions

Non–examinable again!

To define a distribution, we must first choose a class of *test functions*. For $\Omega \subseteq \mathbb{R}^n$, the simplest class of test functions are infinitely smooth functions $\phi \in C^\infty(\Omega)$ that have compact support. That is, there exists a compact set $K \subset \Omega$ such that $\phi(x) = 0$ whenever $x \notin K$. A simple example of a test function in one dimension is

$$\Psi(x) \equiv \begin{cases} \mathrm{e}^{-1/(1-x^2)} & \text{when } |x| < 1 \\ 0 & \text{else} \end{cases} \tag{6.1}$$

which is shown in figure 11, but any infinitely smooth function with compact support will do. We let $\mathcal{D}(\Omega)$ denote the space of all such test functions.

Having chosen our class of test functions, we now define a distribution T to be a linear map $T : \mathcal{D}(\Omega) \to \mathbb{R}$, given by

$$T : \phi \mapsto T[\phi] \tag{6.2}$$

for $\phi \in \mathcal{D}(\Omega)$. The square bracket notation in $T[\phi]$ reminds us that T is not a function on Ω itself, but rather is a function *on the infinite dimensional space of test functions* on Ω.

The space of distributions with test functions in $\mathcal{D}(\Omega)$ is denoted $\mathcal{D}'(\Omega)$. It's again an infinite dimensional vector space, because we can add two distributions T_1 and T_2 together, defining the distribution $(T_1 + T_2)$ by

$$(T_1 + T_2)[\phi] \equiv T_1[\phi] + T_2[\phi] \tag{6.3}$$

for all $\phi \in \mathcal{D}(\Omega)$. Similarly, we can multiply a distribution by a constant, defining the distribution (cT) by

$$(cT_1)[\phi] \equiv c\, T_1[\phi] \tag{6.4}$$

for all $\phi \in \mathcal{D}(\Omega)$, and $c \in \mathbb{R}$. The multiplication on the *rhs* here is just the standard multiplication in $\mathbb{R}$. Finally, notice that while we can multiply distributions by smooth functions – if $\psi \in C^\infty(\Omega)$ and $T \in \mathcal{D}'(\Omega)$ then define the distribution (ψT) by $(\psi T)[\phi] := T[\psi\phi]$

using multiplication in $C^\infty(\Omega)$ – in general *there is no way to multiply two distributions together*.

The simplest type of distribution is just an ordinary function $f : \Omega \to \mathbb{R}$ that is locally integrable, meaning that its integral over any compact set converges[28]. To treat f as a distribution we must say how it acts on any test function $\phi \in \mathcal{D}(\Omega)$. To do so, we choose to define

$$f[\phi] := (f, \phi) = \int_\Omega f(x)\, \phi(x)\, \mathrm{d}V\,, \tag{6.5}$$

which is just the inner product of f with ϕ. This integral is guaranteed to be well–defined even when Ω is non–compact (say, the whole of $\mathbb{R}^n$) since ϕ has compact support and f is locally integrable. In particular, note that unlike the test functions, we do *not* require f itself to have compact support. Also notice that (6.5) certainly gives a *linear* map from $\mathcal{D}(\Omega)$ to $\mathbb{R}$, since if ϕ_1 and ϕ_2 are two test functions and c_1, c_2 are constants then

$$\begin{aligned} T_f[c_1\phi_1 + c_2\phi_2] &= (f, c_1\phi_1 + c_2\phi_2) = c_1(f, \phi_1) + c_2(f, \phi_2) \\ &= c_1 T_f[\phi_1] + c_2 T_f[\phi_2] \end{aligned} \tag{6.6}$$

by the linearity of the inner product in its second entry. Thus, in the case where the generalized function is just an ordinary function, the map $T_f : \mathcal{D}(\Omega) \to \mathbb{R}$ just corresponds to the usual inner product between functions.

By far the most important example of a generalized function that is not a function is the *Dirac delta*, written just δ. It is defined by

$$\delta[\phi] := \phi(0) \tag{6.7}$$

for all $\phi \in \mathcal{D}(\Omega)$, where 0 is the origin in $\mathbb{R}^n$. Note again that δ is indeed a linear map $\delta : \mathcal{D}(\Omega) \to \mathbb{R}$, with $\delta[c_1\phi_1 + c_2\phi_2] = c_1\phi_1(0) + c_2\phi_2(0)$, where the addition on the left is in the space of test functions, while the addition on the right is just addition in $\mathbb{R}$.

By analogy with the case where the generalized function is itself a function, it's often convenient to abuse notation and write

$$T[\phi] \stackrel{?!}{=} (T, \phi) = \int_\Omega T(x)\, \phi(x)\, \mathrm{d}V \tag{6.8}$$

even for general distributions. However, for a general distribution *the object $T(x)$ is not a function – i.e.*, there is no sense in which $T : \Omega \to \mathbb{R}$ – and to specify which distribution we're talking about, we have to give a separate definition of what value $T[\phi]$ actually takes. For example, it's common to write

$$\delta[\phi] = \int_\Omega \delta(x)\, \phi(x)\, \mathrm{d}V \tag{6.9}$$

for some object $\delta(x)$. However, $\delta(x)$ can't possibly be a genuine function, for if (6.9) is to be compatible with (6.7) for arbitrary test functions ϕ we need $\delta(x) = 0$ whenever $x \neq 0$.

[28] Thus, in one dimension, a function $1/x^2$ with a non–integrable singularity at $x = 0$ does not qualify as a distribution.

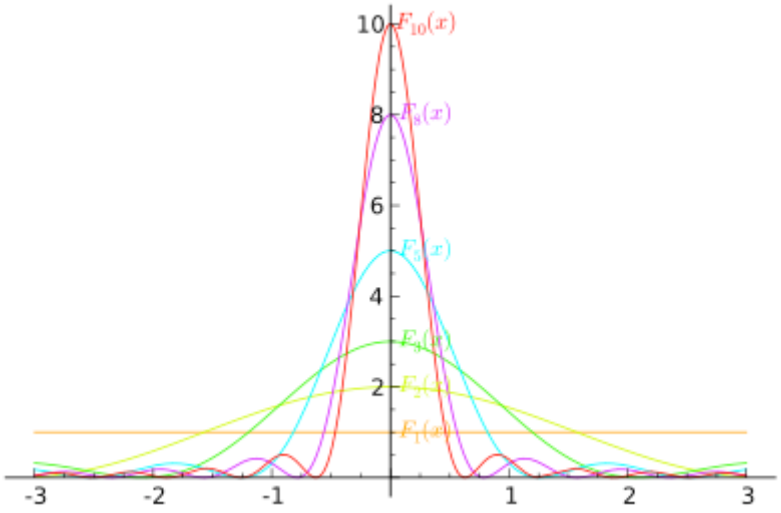


Figure 12. *The Fejér kernels $F_n(x)$ for $n = 1, 2, 3, 5, 8$ and 10. The limiting value of these kernels as $n \to \infty$ can be thought of as the Dirac δ-function.*

If not, we could get a non–zero value for our integral by choosing a test function whose support lies only in some small compact set away from the origin, in conflict with (6.7). On the other hand, if $\delta(x)$ does indeed vanish everywhere except at one point, the integral (6.9) cannot give the finite answer $\phi(0)$ if $\delta(x)$ takes any finite value at $x = 0$. So it isn't a genuine function in the sense of being a map from $\Omega \to \mathbb{R}$. Just to confuse you, $\delta(x)$ is ubiquitously known as the "Dirac δ-function".

One reason this abusive notation is convenient is that distributions can arise as the limit of a sequence of integrals of usual functions. For example, for any finite $n \in \mathbb{N}$ the function

$$F_n(x) = \begin{cases} \dfrac{1}{n+1} \dfrac{\sin^2[(n+1)x/2]}{\sin^2[x/2]} & \text{for } x \neq 0 \\ n+1 & \text{when } x = 0 \end{cases} \tag{6.10}$$

(which you may recognize as a Fejér kernel) is a perfectly respectable, finite and everywhere continuous function. In particular, for any finite n the integral $\int_{\mathbb{R}} F_n(x)\phi(x)\,\mathrm{d}x$ of the Fejér kernel times our compactly supported test function is well-defined. Now, as n increases, the $F_n(x)$ are increasingly concentrated around $x = 0$ as you can see from figure 12. Whilst the limiting value $\lim_{n\to\infty} F_n(x)$ of this sequence of functions does not exist (in particular, $\lim_{n\to\infty}(n+1)$ does not exist), the limiting value of the *integrals* is perfectly finite, and in fact

$$\lim_{n\to\infty} \int_{\mathbb{R}} F_n(x)\,\phi(x)\,\mathrm{d}x = \phi(0) \tag{6.11}$$

as we showed in section 1.5. Thus the Fejér kernels $\{F_n(x)\}$ form a sequence of functions whose limit can be understood as a distribution, which in this case we recognise as the Dirac δ-function.

The functions $F_n(x)$ are far from unique in having the Dirac δ as a limiting case. Other examples include the family of Gaussians (4.11) $G_n(x) = ne^{-n^2x^2}/\sqrt{\pi}$, or the sinc functions

$S_n(x) = \sin(nx)/(\pi x)$, or the so–called 'top hat function'

$$P_n(x) = \begin{cases} \dfrac{n}{2} & \text{for } |x| < \dfrac{1}{n} \\ 0 & \text{otherwise,} \end{cases} \tag{6.12}$$

or any other sequence of functions each member of which has total area is 1, and which become increasingly spiked around the origin.

6.1.1 Differentiation of distributions

Now comes the magic. In order to use distributions in differential equations, we need to know what it means to differentiate them. In the case that our generalized function is just an ordinary function f, in one dimension we would have

$$T_{f'}[\phi] = (f', \phi) = \int_\Omega f'(x)\,\phi(x)\,\mathrm{d}x = -\int_\Omega f(x)\,\phi'(x)\,\mathrm{d}x = -(f, \phi') = -T_f[\phi'] \tag{6.13}$$

where the boundary term vanishes since ϕ had compact support inside Ω. For a generalized function T, we now *define*

$$T'[\phi] \equiv -T[\phi'] \qquad \text{for all } \phi \in \mathcal{D}(\Omega)\,. \tag{6.14}$$

Again, the idea here is that if we think of our distribution as coming from the limit of a sequence of integrals involving only 'ordinary' functions, by (6.13) this relation will hold for every member of the sequence, and so it will hold for the limiting value of the integrals. The definition also means that, provided we know what the distribution T does to all test functions, we also know what the distribution T' does.

As an example, consider again the Dirac δ defined by $\delta[\phi] = \phi(0)$. The derivative of the δ-function is given by (6.14) as

$$\delta'[\phi] = -\delta[\phi'] = -\phi'(0) \tag{6.15}$$

and so evaluates (minus) the derivative of test function at the origin. In turn, the Heaviside step function

$$\Theta(x) \equiv \begin{cases} 1 & \text{when } x > 0 \\ 0 & \text{when } x \le 0\,. \end{cases} \tag{6.16}$$

is a function, whose integral over any compact set converges, so $\Theta(x)$ also defines a generalized function on $\mathbb{R}$ by $\Theta[\phi] = \int_{-\infty}^{\infty} \Theta(x)\phi(x)\,\mathrm{d}x = \int_0^\infty \phi(x)\,\mathrm{d}x$ which converges since ϕ has compact support. But while $\Theta(x)$ is patently not differentiable (or even continuous) as a function, it is perfectly differentiable if treated as a distribution. We have

$$\begin{aligned} \Theta'[\phi] &= -\Theta[\phi'] = -\int_{-\infty}^{\infty} \Theta(x)\,\frac{\partial\phi}{\partial x}\,\mathrm{d}x \\ &= -\int_0^\infty \frac{\partial\phi}{\partial x}\,\mathrm{d}x = \phi(0) - \phi(\infty) = \phi(0)\,, \end{aligned} \tag{6.17}$$

using the fact that ϕ has compact support. Since $\Theta'[\phi] = \phi(0) = \delta[\phi]$ holds for any test function ϕ, we can identify Θ' as the distribution δ.

We define higher derivatives of distributions similarly: since ϕ is infinitely differentiable we have

$$T^{(n)}[\phi] \equiv (-1)^n\, T[\phi^{(n)}] \tag{6.18}$$

and again this is determined once we know what T itself does. For example, all higher derivatives of the Dirac δ are given by

$$\delta^{(n)}[\phi] = (-1)^n\, \delta[\phi^{(n)}] = (-1)^n\, \phi^{(n)}(0)\,, \tag{6.19}$$

and the *rhs* makes sense since the test function $\phi(x)$ was infinitely differentiable. Notice that this definition pulls off a really remarkable trick: we've managed to define *all* the derivatives of an object such as δ that at first sight seems impossibly non–differentiable. Even more, our definition means that distributions inherit the excellent differentiability properties of the infinitely smooth test functions!

The excellent differentiability of distributions also allows us to make sense of divergent Fourier series. Let's recall from section 1.4.1 that the sawtooth function $f(x) = x$ for $x \in [-\pi, \pi)$ has Fourier series

$$2\sum_{n=1}^{\infty} \frac{(-1)^{n+1}}{n}\, \sin nx\,.$$

The Fourier coefficients decay only as $1/n$, so while this series does in fact converge to $f(x)$ everywhere in $(-\pi, \pi)$, and converge to 0 at $x = -\pi$, convergence is very slow. Differentiating the series term–by–term leads to the series

$$2\sum_{n=1}^{\infty}(-1)^{n+1}\, \cos nx \;=\; \cos x - \cos 2x + \cos 3x - \cdots \tag{6.20}$$

which certainly diverges as a function.

If we view the sawtooth function as a 2π-periodic function on $\mathbb{R}$ then for any $x \in \mathbb{R}$ we have

$$2\sum_{n=1}^{\infty} \frac{(-1)^{n+1}}{n}\, \sin nx \;=\; x + 2\pi \sum_{n=1}^{\infty} \Theta(x - n\pi) - 2\pi \sum_{n=0}^{\infty} \Theta(-x - \pi n) \tag{6.21}$$

where the step functions provide the jumps in the sawtooth. Differentiating this expression term–by–term gives

$$2\sum_{n=1}^{\infty}(-1)^{n+1}\, \cos nx \;=\; 1 + 2\pi \sum_{n\in\mathbb{Z}} \delta(x - n\pi) \tag{6.22}$$

which gives meaning to the non–convergent sum as a distribution: The sawtooth function has a constant gradient everywhere except at $x = n\pi$ for $n \in \mathbb{Z}$, where it has a δ-function spike.

6.2 Properties of the Dirac δ

Since the Dirac δ is such an important distribution, it'll be worth our while examining it in somewhat greater detail. We first establish several properties that will come in handy later. These are easiest to obtain if one uses the integral expression (6.9) and manipulates the object $\delta(x)$ *as if* it were a genuine function. Such manipulations can be made rigorous in the deeper theory of distributions, but we'll content ourselves in this Methods course with what follows.

– Since $\delta(x)$ vanishes whenever $x \neq 0$ we can write

$$\delta[\phi] = \int_a^b \delta(x)\,\phi(x)\,\mathrm{d}x$$

where $[a, b]$ is any interval containing the point $x = 0$. If $0 \notin [a, b]$ then the integral is zero.

– If $f : \Omega \to \mathbb{R}$ is continuous in a neighbourhood of the origin $0 \in \Omega$, then the distribution $(f\delta)$ obeys

$$(f\delta)[\phi] = \delta[f\phi] = f(0)\phi(0) = f(0) \times \delta[\phi] \tag{6.23}$$

in accordance with our rule for multiplying distributions by smooth functions. In terms of the Dirac δ-'function' $\delta(x)$ we write this as $f(x)\,\delta(x) = f(0)\,\delta(x)$ using the idea that $\delta(x)$ vanishes whenever $x \neq 0$.

– For any $c \in \mathbb{R}$,

$$\int_{\mathbb{R}} \delta(cx)\,\phi(x)\,\mathrm{d}x = \frac{1}{|c|}\int_{\mathbb{R}} \delta(y)\,\phi(y/c)\,\mathrm{d}y = \frac{1}{|c|}\phi(0)\,, \tag{6.24}$$

so we write $\delta(cx) = \delta(x)/|c|$.

– For any point $a \in \mathbb{R}$ we can define a translated Dirac δ by $\delta_a[\phi] = \phi(a)$. In terms of the δ-function, this is

$$\phi(a) = \int_{\mathbb{R}} \delta(y)\,\phi(y + a)\,\mathrm{d}y = \phi(a)\int_{\mathbb{R}} \delta(x - a)\,\phi(x)\,\mathrm{d}x \tag{6.25}$$

so that translating the δ-function shifts the point at which the test function is evaluated.

– For any continuously differentiable function $f : \Omega \to \mathbb{R}$ we have that $\delta(f(x))$ zero everywhere except at the zeros of f, so that an integral involving $\delta(f(x))$ times a test function receives no contributions outside an arbitrarily small neighbourhood of the zeros of f. In particular, if f has only simple zeros at points $\{x_1, x_2, \ldots, x_n\} \in \Omega$ then

$$\int_{\mathbb{R}} \delta(f(x))\,\phi(x)\,\mathrm{d}x = \sum_{i=1}^{n} \int_{x_i^-}^{x_i^+} \delta(f(x))\,\phi(x)\,\mathrm{d}x\,. \tag{6.26}$$

Using the fact that $f(x) \approx (x - x_i)\, f'(x_i)$ when x is near the root x_i, we have

$$\begin{aligned} \int_{\mathbb{R}} \delta(f(x))\, \phi(x)\, \mathrm{d}x &= \sum_{i=1}^{n} \left[\frac{1}{|f'(x_i)|} \int_{x_i^-}^{x_i^+} \delta(x - x_i)\, \phi(x)\, \mathrm{d}x \right] \\ &= \sum_{i : f(x_i)=0} \frac{\phi(x_i)}{|f'(x_i)|}\,, \end{aligned} \tag{6.27}$$

where the first equality used equation (6.24) and the second (6.25). For example, if $f(x) = x^2 - b^2$ then

$$\int_{\mathbb{R}} \delta(x^2 - b^2)\, \phi(x)\, \mathrm{d}x = \frac{1}{2|b|} \left[\phi(b) + \phi(-b) \right]\,. \tag{6.28}$$

The previous two results (6.24) & (6.25) can be understood as special cases of this one.

In all these expressions, the important point is that the integral is *localized* to an arbitrarily small neighbourhood of the zeros of the argument of the δ-function.

In physics the δ-function models *point sources* in a continuum. For example, suppose we have a unit point charge at $x = 0$ (in one dimension). Then its charge density $\rho(x)$ should satisfy $\rho(x) = 0$ for $x \neq 0$ and total charge $Q = \int \rho(x) = 1$. These are exactly the properties of the δ-function, so we set $\rho(x) = \delta(x)$ and the physical intuition is well modelled by the sequence in, say, (6.12).

In mechanics, δ-functions model *impulses*. Suppose a particle traveling with momentum $p = mv$ in one dimension. Newton's law gives $dp/dt = F$, so

$$p(t_2) - p(t_1) = \int_{t_1}^{t_2} F\, \mathrm{d}t\,.$$

If the particle is suddenly struck by a hammer at $t = 0$ then we might imagine that the force acts only over a vanishingly small time Δt with $|\Delta t| < 2\epsilon$ for some small ϵ, and yet results in a *finite* momentum change, say C. Then $\int_{-\epsilon}^{\epsilon} F\, \mathrm{d}t = \Delta p$ while F is nonzero only very near $t = 0$. In the limit of vanishing time interval Δt, $F(t) = C\, \delta(t)$ models the impulsive force. The δ-function was originally introduced by P.A.M. Dirac in the 1930s from considerations of position and momentum in quantum mechanics.

6.2.1 Eigenfunction expansion of the δ-function

Let's compute the Fourier series of the Dirac δ-function. We first imagine that $\delta(x)$ is a distribution defined for x in the interval $[-L, L]$, and then formally write

$$\delta(x) = \sum_{n \in \mathbb{Z}} \hat{\delta}_n\, \mathrm{e}^{\mathrm{i}n\pi x/L} \qquad \text{with} \qquad \hat{\delta}_n = \frac{1}{2L} \int_{-L}^{L} \mathrm{e}^{-\mathrm{i}n\pi x/L}\, \delta(x)\,. \tag{6.29}$$

From the definition (6.7) we see that $\hat{\delta}_n = 1/2L$ for all n, so we find

$$\delta(x) = \frac{1}{2L} \sum_{n \in \mathbb{Z}} \mathrm{e}^{\mathrm{i}n\pi x/L}\,. \tag{6.30}$$

What can this result possibly mean? On the one hand, the *lhs* is an object that doesn't really exist as a function, whereas on the right hand side we have a series that clearly diverges! The point is that this series *does* converge, but as a distribution and not as a function. To see what this means, we let

$$S_N\delta(x) \equiv \frac{1}{2L}\sum_{n=-N}^{N} \mathrm{e}^{\mathrm{i}n\pi x/L} \tag{6.31}$$

be the partial Fourier sum. Then for any infinitely smooth test function ϕ with compact support inside $[-L, L]$, we have

$$\begin{aligned}\lim_{N\to\infty}\int_{-L}^{L} S_N\delta(x)\,\phi(x)\,\mathrm{d}x \;&=\; \lim_{N\to\infty}\;\frac{1}{2L}\int_{-L}^{L}\left[\sum_{n=-N}^{N}\mathrm{e}^{\mathrm{i}n\pi/L}\,\phi(x)\,\mathrm{d}x\right]\\ &= \lim_{N\to\infty}\sum_{n=-N}^{N}\left[\frac{1}{2L}\int_{-L}^{L}\mathrm{e}^{\mathrm{i}n\pi/L}\,\phi(x)\,\mathrm{d}x\right] \;=\; \lim_{N\to\infty}\sum_{n=-N}^{N}\hat\phi_{-n}\,.\end{aligned} \tag{6.32}$$

In the second equality we exchanged the finite sum and the integral. In the third equality we recognize the integral as the Fourier coefficient ϕ_{-n} of our test function. Now, the final sum in equation (6.32) is just the partial Fourier series of $\phi(x)$, evaluated at $x = 0$. Since the test function is everywhere smooth, its Fourier series converges everywhere. In particular, convergence at the origin means we have

$$\lim_{N\to\infty}\int_{-L}^{L} S_N\delta(x)\,\phi(x)\,\mathrm{d}x = \phi(0)\,. \tag{6.33}$$

Thus the partial sum $\frac{1}{2L}\sum_{n=-N}^{N}\mathrm{e}^{\mathrm{i}\pi x/L}$ does indeed converge to the Dirac δ-distribution as $N\to\infty$.

Of course, there's nothing particularly special about expanding the Dirac δ-function in a Fourier series; any other basis of orthogonal functions will do just as well. For $n\in\mathbb{Z}$ let $\{Y_n(x)\}$ be a complete set of orthonormal eigenfunctions of a Sturm–Liouville operator on the domain $[a, b]$, with weight function $w(x)$. For $\xi\in(a, b)$, the Dirac δ-function $\delta(x-\xi)$ is zero for the boundary points $x = a$ or $x = b$, and so the Sturm–Liouville operator will be self–adjoint. We thus expect to be able to expand

$$\delta(x-\xi) = \sum_{n\in\mathbb{Z}} c_n\,Y_n(x) \tag{6.34}$$

where the coefficient c_n is given by

$$c_n = \int_a^b Y_n^*(x)\,\delta(x-\xi)\,w(x)\,\mathrm{d}x = Y_n^*(\xi)\,w(\xi) \tag{6.35}$$

again from the definition of the δ-function. Using the fact that $\delta(x-\xi) = [w(x)/w(\xi)]\times\delta(x-\xi)$ we can write

$$\delta(x-\xi) = w(\xi)\sum_{n\in\mathbb{Z}} Y_n^*(\xi)\,Y_n(x) = w(x)\sum_{n\in\mathbb{Z}} Y_n^*(\xi)\,Y_n(x)\,. \tag{6.36}$$

This expansion is consistent with the sampling property, since if $g(x) = \sum_{m\in\mathbb{Z}}^{\infty} d_m\, Y_m(x)$ then, again exchanging the sums and integrals,

$$\begin{aligned}\int_a^b g^*(x)\,\delta(x-\xi)\,\mathrm{d}x &= \sum_{m,n\in\mathbb{Z}} \left[Y_n^*(\xi)\, d_m^* \int_a^b w(x)\, Y_m^*(x)\, Y_n(x)\,\mathrm{d}x \right] \\ &= \sum_{m\in\mathbb{Z}} d_m^* Y_m^*(\xi) = g^*(\xi)\end{aligned} \tag{6.37}$$

using the orthonormality of the Sturm–Liouville eigenfunctions.

We'll soon see that the eigenfunction expansion of the δ-function is intimately related to the eigenfunction expansion of the Green's function that we introduced in section 2.6. Our next task is to develop a theory of Green's functions for solving inhomogeneous ODEs.

6.3 Schwartz functions and tempered distributions

Non–examinable, yet again

The definition of distributions depends on a choice of class of test functions. Above, we considered test functions that are infinitely smooth and have compact support. These requirements ensured in particular that the integral in (6.5) was well–defined, and that the integration by parts in (6.13) received no boundary terms. Well–definedness and absence of boundary terms would be retained if we relax our requirement that test functions have compact support to the requirement simply that it decays sufficiently rapidly as $|x| \to \infty$.

We define a *Schwartz function* $\psi : \mathbb{R} \to \mathbb{C}$ to be an infinitely smooth function with the property that

$$\sup_{x\in\mathbb{R}} \left| x^m\, \psi^{(n)}(x) \right| < \infty \qquad \text{for all } m, n \in \mathbb{N}. \tag{6.38}$$

Thus both ψ and all its derivatives are bounded, and in particular vanish faster than any inverse power at infinity. A simple example of a Schwartz function is $\psi(x) = p(x)\,\mathrm{e}^{-x^2}$ with $p(x)$ any polynomial. We denote the space of Schwartz functions on Ω by $\mathcal{S}(\Omega)$ and, because of their excellent asymptotic properties, we can use Schwartz functions as our test functions in defining distributions. Note that any compactly supported test function $\phi \in \mathcal{D}(\Omega)$ certainly obeys the Schwartz conditions (6.38), so $\mathcal{D}(\Omega) \subset \mathcal{S}(\Omega)$ (and in fact one can show that $\mathcal{D}(\Omega)$ is dense in $\mathcal{S}(\Omega)$).

Just as we did with distributions and compactly supported test functions, we now define *tempered distributions* to be linear maps $T : \mathcal{S} \to \mathbb{R}$, and we write the space of tempered distributions as $\mathcal{S}'(\Omega)$. Now however $\mathcal{S}'(\Omega) \subset \mathcal{D}'(\Omega)$ so that there are fewer tempered distributions than distributions. For example, in order for even an *ordinary* function $g : \Omega \to \mathbb{R}$ to be admissible as a tempered distribution we'd need to require that

$$\lim_{|x|\to\infty} x^{-n}\, g(x) = 0 \qquad \text{for } \textit{some } n \in \mathbb{N}, \tag{6.39}$$

because the integral $(g, \psi) = \int_{\mathbb{R}} g(x)\,\psi(x)\,\mathrm{d}x$ will only exist if the good behaviour of ψ is not ruined by that of g. Thus the functions $x^3 + x$, e^{-x^2}, $\sin x$ and $x \ln|x|$ are all good tempered distributions, but the functions $1/x^2$ and e^{-x} are not. (*Exercise:* Show that the Dirac δ distribution is also a tempered distribution.)

Properties of tempered distributions may be obtained in exactly the same way as for distributions with compactly supported test functions. In particular, if $\psi \in \mathcal{S}(|\Omega)$ and $T : \mathcal{S}(\Omega) \to \mathbb{C}$ is a tempered distribution with $T : \psi \mapsto T[\psi]$, then the n^{th} derivative $T^{(n)}[\psi] := (-1)^n T[\psi^{(n)}]$ just as before. Tempered distributions come into their own in conjunction with Fourier transforms: The Fourier transform of a Schwartz function is again a Schwartz function, and this fact allows us to define the Fourier transform of any tempered distribution.

7 Green's Functions for Ordinary Differential Equations

One of the most important applications of the δ-function is as a means to develop a systematic theory of Green's functions for ODEs. Consider a general linear second–order differential operator $\mathcal{L}$ on $[a, b]$ (which may be $\pm\infty$, respectively). We write

$$\mathcal{L}y(x) = \alpha(x)\frac{d^2}{dx^2}y + \beta(x)\frac{d}{dx}y + \gamma(x)y = f(x)\,, \tag{7.1}$$

where α, β, γ are continuous functions on $[a, b]$, and α is nonzero (except perhaps at a finite number of isolated points). We also require the forcing term $f(x)$ to be bounded in $[a, b]$. We now define the *Green's function* $G(x; \xi)$ of $\mathcal{L}$ to be the unique solution to the problem

$$\mathcal{L}G = \delta(x - \xi) \tag{7.2}$$

that satisfies homogeneous boundary conditions[29] $G(a; \xi) = G(b; \xi) = 0$.

The importance of the Green's function comes from the fact that, given our solution $G(x, \xi)$ to equation (7.2), we can immediately solve the more general problem $\mathcal{L}y(x) = f(x)$ of (7.1) for an arbitrary forcing term $f(x)$ by writing

$$y(x) = \int_a^b G(x; \xi)\, f(\xi)\, \mathrm{d}\xi\,. \tag{7.3}$$

To see that it does indeed solve (7.1), we compute

$$\begin{aligned} \mathcal{L}y(x) &= \mathcal{L}\left[\int_a^b G(x, \xi)\, f(\xi)\, \mathrm{d}\xi\right] = \int_a^b \left[\mathcal{L}G(x, \xi)\right]\, f(\xi)\, \mathrm{d}\xi \\ &= \int_a^b \delta(x - \xi)\, f(\xi)\, \mathrm{d}\xi = f(x)\,, \end{aligned} \tag{7.4}$$

since the Green's function is the only thing that depends on x. We also note that the solution (7.3) constructed this way obeys $y(a) = y(b) = 0$ as a direct consequence of these conditions on the Green's function.

The important point is that G depends on $\mathcal{L}$, but *not* on the forcing term $f(x)$. Once G is known, we will be able write down the solution to $\mathcal{L}y = f$ for an *arbitrary* force term. To put this differently, asking for a solution to the differential equation $\mathcal{L}y = f$ is asking to invert the differential operator $\mathcal{L}$, and we might formally write $y(x) = \mathcal{L}^{-1}f(x)$. Equation (7.3) shows what is meant by the inverse of the differential operator $\mathcal{L}$ is integration with the Green's function as the integral kernel.

7.1 Construction of the Green's function

We now give a constructive means for determining the Green's function. (We'll see later how this compares to the eigenfunction expansion for inverting Sturm–Liouville operators that we gave in 2.6.)

[29] Other homogeneous boundary conditions are also possible, but for clarity will will treat only the simplest case $G(a, \xi) = G(b, \xi) = 0$ here.

Our construction relies on the fact that whenever $x \neq \xi$, $\mathcal{L}G = 0$. Thus, both for $x < \xi$ and $x > \xi$ we can express G in terms of solutions of the homogeneous equation. Let us suppose that $\{y_1, y_2\}$ are a basis of linearly independent solutions to the second–order homogeneous problem $\mathcal{L}y = 0$ on $[a, b]$. We define this basis by requiring that $y_1(a) = 0$ whereas $y_2(b) = 0$. That is, each of $y_{1,2}$ obeys *one* of the homogeneous boundary conditions. On $[a, \xi)$ the Green's function obeys $\mathcal{L}G = 0$ and $G(a, \xi) = 0$. But any homogeneous solution to $\mathcal{L}y = 0$ obeying $y(a) = 0$ must be proportional to $y_1(x)$, with a proportionality constant that is independent of x. Thus we set

$$G(x, \xi) = A(\xi)\, y_1(x) \qquad \text{for } x \in [a, \xi)\,. \tag{7.5}$$

Similarly, on $(\xi, b]$ the Green's function must be proportional to $y_2(x)$ and so we set

$$G(x, \xi) = B(\xi)\, y_2(x) \qquad \text{for } x \in 9\xi, b]\,. \tag{7.6}$$

Note that the coefficient functions $A(\xi)$ and $B(\xi)$ may depend on the point ξ, but must be independent of x.

This construction gives us families of Green's function for $x \in [a, b] - \{\xi\}$, in terms of the functions A and B. We must now determine how these two solutions are to be joined together at $x = \xi$. Suppose first that $G(x, \xi)$ was discontinuous at $x = \xi$, with the discontinuity modelled by a step function. Then $\partial_x G \propto \delta(x - \xi)$ and consequently $\partial_x^2 G \propto \delta'(x-\xi)$. However, the form of equation (7.2) shows that $\mathcal{L}G$ involves no generalized functions beyond $\delta(x - \xi)$, and in particular contains no derivatives of δ-functions. Thus we conclude that $G(x, \xi)$ must be continuous throughout $[a, b]$ and in particular at $x = \xi$.

However, integrating equation (7.2) over an infinitesimal neighbourhood of $x = \xi$ we learn that

$$\int_{\xi-\epsilon}^{\xi+\epsilon} \left[\alpha(x)\frac{\partial^2 G}{\partial x^2}\,\mathrm{d}x + \beta(x)\frac{\partial G}{\partial x}\,\mathrm{d}x + \gamma(x)G\right]\mathrm{d}x = \int_{\xi-\epsilon}^{\xi+\epsilon} \delta(x - \xi)\,\mathrm{d}x = 1\,. \tag{7.7}$$

We have already seen that $G(x, \xi)$ is continuous, and all three coefficient functions α, β, γ are bounded by assumption, so the final term on the *lhs* contributes zero as we make the integration region infinitesimally thin. Also, since G is continuous, $\partial_x G$ must be bounded so the term $\beta\partial_x G$ also cannot contribute as the integration region shrinks to zero size. Finally, since α is continuous we have

$$\lim_{\epsilon\to 0^+} \int_{\xi-\epsilon}^{\xi+\epsilon} \alpha(x)\frac{\partial^2 G}{\partial x^2}\,\mathrm{d}x = \alpha(\xi)\left[\left.\frac{\partial G}{\partial x}\right|_{x=\xi^+} - \left.\frac{\partial G}{\partial x}\right|_{x=\xi^-}\right]. \tag{7.8}$$

To summarize, we must glue the Green's functions (7.5) & (7.6) according to the conditions

$$\begin{aligned} G(x, \xi)|_{x=\xi^-} &= G(x, \xi)|_{x=\xi^+} && \text{continuity} \\ \left.\frac{\partial G}{\partial x}\right|_{x=\xi^-} - \left.\frac{\partial G}{\partial x}\right|_{x=\xi^-} &= \frac{1}{\alpha(\xi)} && \text{jump in derivative.} \end{aligned} \tag{7.9}$$

In terms of (7.5) & (7.6) these conditions become

$$A(\xi)\, y_1(\xi) = B(\xi)\, y_2(\xi) \qquad \text{and} \qquad A(\xi)\, y_1'(\xi) - B(\xi)\, y_2'(\xi) = \frac{1}{\alpha(\xi)}\,. \tag{7.10}$$

These are two linear equations for A and B, determining them to be

$$A(\xi) = \frac{y_2(\xi)}{\alpha(\xi)W(\xi)} \qquad \text{and} \qquad B(\xi) = \frac{y_1(\xi)}{\alpha(\xi)W(\xi)}\,, \tag{7.11}$$

where

$$W(x) \equiv y_1 y_2' - y_2 y_1' \tag{7.12}$$

is known as the *Wronskian* of y_1 and y_2. Note that the Wronskian is evaluated at $x = \xi$ in equation (7.11).

To conclude, we have found that the solution $G(x,\xi)$ of $\mathcal{L}G = \delta(x-\xi)$ obeying $G(a,\xi) = G(b,\xi) = 0$ is given by

$$\begin{aligned} G(x;\xi) &= \begin{cases} \dfrac{y_1(x)y_2(\xi)}{\alpha(\xi)W(\xi)} & a \le x < \xi \\ \dfrac{y_2(x)y_1(\xi)}{\alpha(\xi)W(\xi)} & \xi < x \le b \end{cases} \\ &= \frac{1}{\alpha(\xi)W(\xi)}\left[\Theta(\xi - x)\, y_1(x)y_2(\xi) + \Theta(x-\xi)\, y_2(x)y_1(\xi)\right] \end{aligned} \tag{7.13}$$

where Θ is again the step function. Hence the solution to $\mathcal{L}y = f$ is

$$\begin{aligned} y(x) &= \int_a^b G(x;\xi)\, f(\xi)\,\mathrm{d}\xi \\ &= y_2(x)\int_a^x \frac{y_1(\xi)}{\alpha(\xi)W(\xi)} f(\xi)\,\mathrm{d}\xi + y_1(x)\int_x^b \frac{y_2(\xi)}{\alpha(\xi)W(\xi)} f(\xi)\,\mathrm{d}\xi\,. \end{aligned} \tag{7.14}$$

The integral over ξ here is separated at x into two parts, (i) $\int_a^x$ and (ii) $\int_x^b$. In the range of (i) we have $\xi < x$ so the *second* line of equation (7.13) for $G(x;\xi)$ applies, even though this expression incorporates the boundary condition at $x = b$. For (ii) we have $x > \xi$ so we use the $G(x;\xi)$ expression from the *first* line of equation (7.13) that incorporates the boundary condition at $x = a$.

As an example of the use of Green's functions, suppose we wish to solve the forced problem

$$\mathcal{L}y = -y'' - y = f(x) \tag{7.15}$$

on the interval $[0,1]$, subject to the boundary conditions $y(0) = y(1) = 0$. We follow our procedure above. The general homogeneous solution is $c_1 \sin x + c_2 \cos x$ so we can take $y_1(x) = \sin x$ and $y_2(x) = \sin(1-x)$ as our homogeneous solutions satisfying the boundary conditions at $x = 0$ and $x = 1$, respectively. Then

$$G(x;\xi) = \begin{cases} A(\xi)\sin x & 0 \le x < \xi \\ B(\xi)\sin(1-x) & \xi < x \le 1\,. \end{cases} \tag{7.16}$$

Applying the continuity condition we get

$$A\sin\xi = B\sin(1-\xi) \tag{7.17}$$

while the jump condition gives

$$B(-\cos(1-\xi)) - A\cos\xi = -1\,. \tag{7.18}$$

where we note that $\alpha = -1$. Solving these two equations for A and B gives the Green's function

$$G(x;\xi) = \frac{1}{\sin 1}\left[\Theta(\xi - x)\,\sin(1-\xi)\sin x + \Theta(x-\xi)\,\sin(1-x)\sin\xi\right] \tag{7.19}$$

Using this Green's function we are immediately able to write down the complete solution to $-y'' - y = f(x)$ with $y(0) = y(1) = 0$ as

$$y(x) = \frac{\sin(1-x)}{\sin 1}\int_0^x f(\xi)\,\sin\xi\,\mathrm{d}\xi + \frac{\sin x}{\sin 1}\int_x^1 f(\xi)\,\sin(1-\xi)\,\mathrm{d}\xi. \tag{7.20}$$

where again only the *second* term for G in (7.19) contributes in the first integration region where $\xi > x$, while only the *first* term for G contributes to the integral over the region $\xi < x$.

7.2 Physical interpretation of the Green's function

We can think of the expression

$$y(x) = \int_a^b G(x;\xi)\,f(\xi)\,\mathrm{d}\xi \tag{7.21}$$

as a 'summation' (or integral) of individual point source effects, each of strength $f(\xi)$, with $G(x;\xi)$ describing the effect at x of a unit point source placed at ξ.

To illustrate this with a physical example, consider again the wave equation for a horizontal elastic string with ends fixed at $x = 0, L$. If $y(x,t)$ represents the small vertical displacement transverse to the string, we found that $T\partial_x^2 y = \mu\,\partial_t^2 y$. Also including the effect of gravity acting in the vertical direction leads to

$$T\frac{\partial^2 y}{\partial x^2} - \mu g = \mu\frac{\partial^2 y}{\partial t^2} \tag{7.22}$$

for $x \in [0, L]$ with $y(0) = y(L) = 0$. Here, T is the constant tension in the string and μ is the mass density per unit length, which may vary with x.

When the string is at rest, its profile obeys the steady state equation

$$\frac{\partial^2 y}{\partial x^2} = \frac{\mu(x)g}{T}\,, \tag{7.23}$$

whose solution describes the shape of a (non–uniform) string hanging under gravity. We'll be interested in these steady state solutions. We consider three cases. Firstly, suppose μ is a (non–zero) constant then equation (7.23) is easily integrated and we find the parabolic shape

$$y(x) = \frac{\mu g}{2T}\,x(x-L)\,. \tag{7.24}$$

that obeys $y(0) = y(L) = 0$.

In the second case, suppose instead that the string itself is very light, but that it has a metal bead attached at a point $x = \xi$. We treat the bead as a point mass m, and assume it is not too heavy. To find its location, let θ_1 and θ_2 be the angles the string makes on either side of the bead. Resolving forces vertically, the equilibrium condition is

$$mg = T(\sin\theta_1 + \sin\theta_2) \approx T(\tan\theta_1 + \tan\theta_2) \tag{7.25}$$

where the small angle approximation $\sin\theta \approx \tan\theta$ will hold provided the mass m is sufficiently small. (Note also that $y < 0$ since the bead pulls the string down.) Thus the point mass is located at $(x, y) = (\xi, y(\xi))$ where

$$y(\xi) = \frac{mg}{T}\frac{\xi(\xi - L)}{L}\,. \tag{7.26}$$

Since the string is effectively massless on either side of the bead, gravity does not act there, so the only force felt by the string at $x \neq \xi$ is the (tangential) tension. Thus the string must be straight either side of the point mass and so

$$y(x) = \frac{mg}{T} \times \begin{cases} \dfrac{x(\xi - L)}{L} & \text{for } 0 \le x < \xi, \\ \dfrac{\xi(x - L)}{L} & \text{for } \xi < x \le L \end{cases} \tag{7.27}$$

gives the steady–state shape of this string.

We obtained this answer from physical principles; let's now rederive it using the Green's function. For the case of a point mass at $x = \xi$, we take the mass density to be $\mu(x) = m\,\delta(x - \xi)$ so that the steady–state equation becomes

$$\frac{\partial^2 y}{\partial x^2} = \frac{mg}{T}\,\delta(x - \xi)\,. \tag{7.28}$$

The differential operator $\partial^2/\partial x^2$ is a (very simple) self–adjoint operator and the *rhs* is a forcing term. We look for a Green's function $G(x, \xi)$ that obeys

$$\frac{\partial^2 G}{\partial x^2} = \delta(x - \xi) \tag{7.29}$$

subject to the boundary conditions $G(0, \xi) = G(L, \xi) = 0$. Following our usual procedure, we have the general solutions

$$\begin{aligned} G(x, \xi) &= A(\xi)x + B(\xi) && \text{when } \ 0 \le x < \xi, \\ G(x, \xi) &= C(\xi)(1 - x) + D(\xi) && \text{when } \ \xi < x \le L \end{aligned} \tag{7.30}$$

on either side of the point mass. The boundary conditions at 0 and L enforce $B(\xi) = D(\xi) = 0$, and continuity (the string does not break!) at $x = \xi$ fixed $C(\xi) = A(\xi)\xi/(\xi - L)$. Finally, the jump condition on the derivative (with $\alpha = 1$) gives $A(\xi) = (\xi - L)/L$. Thus our Green's function is

$$G(x, \xi) = \begin{cases} \dfrac{x(\xi - L)}{L} & \text{for } \ 0 \le x < \xi, \\ \dfrac{\xi(x - L)}{L} & \text{for } \ \xi < x \le L. \end{cases} \tag{7.31}$$

Rescaling this Green's function by mg/T gives exact agreement with the string profile in (7.27).

For our final case, we now imagine that we have several point masses m_i at positions $x_i \in [0, L]$. We can simply sum the solutions to obtain

$$y(x) = \sum_i G(x, x_i)\, \frac{m_i\, g}{T}\,. \tag{7.32}$$

To take the continuum limit we can imagine there are a large number of masses m_i placed at equal intervals $x_i = iL/N$ along the string, with $i \in \{1, 2, \ldots, N-1\}$. Setting $m_i = \mu(\xi_i)\Delta\xi$ where $\xi_i = i\Delta\xi = iL/N$, then by Riemann's definition of integrals, as $N \to \infty$ equation (7.32) becomes

$$y(x) = \int_0^L G(x, \xi)\, \frac{g\, \mu(\xi)}{T}\, \mathrm{d}\xi\,. \tag{7.33}$$

If μ is constant this function reproduces the parabolic result of case 1, as you should check by direct integration. (*Exercise!* – take care with the limits of integration.)

7.3 Green's functions for inhomogeneous boundary conditions

Our construction of the solution to the forced problem relied on the Green's function obeying *homogeneous* boundary conditions. This is because the integral in equation (7.3) represents a "continuous superposition" of solutions for individual values of ξ. In order to treat problems with inhomogeneous boundary conditions using Green's functions, we must proceed as follows.

First, find *any* particular solution $y_p(x)$ to the *homogeneous* equation $\mathcal{L}y = 0$ that satisfies the *in*homgeneous boundary conditions. This step is usually easy because we're not looking for the most general solution, just any simple solution. Since the differential operator $\mathcal{L}$ is linear, the general solution of $\mathcal{L}y = f$ obeying inhomogeneous boundary conditions is simply

$$y(x) = y_p(x) + \int_a^b G(x, \xi)\, f(\xi)\, \mathrm{d}\xi\,, \tag{7.34}$$

where the term involving the Green's function ensures that $\mathcal{L}y$ indeed equals the forcing term $f(x)$, but does not disturb the boundary values.

As an example, suppose again we wish to solve $-y'' - y = f(x)$, but now with inhomogeneous boundary conditions $y(0) = 0$ and $y(1) = 1$. We already have the Green's function solution to the homogeneous problem in (7.20), so we simply need to find a solution to the homogeneous equation $-y'' - y = 0$ that obeys the boundary conditions. The general solution of this homogeneous equation $c_1 \cos x + c_2 \sin x$ and the inhomogeneous boundary conditions require $c_1 = 0$ and $c_2 = 1/\sin 1$. Therefore $y_p(x) = \sin x / \sin 1$ is the desired particular solution and the general solution is

$$y(x) = \frac{\sin x}{\sin 1} + \frac{\sin(1-x)}{\sin 1} \int_0^x f(\xi)\, \sin\xi\, \mathrm{d}\xi + \frac{\sin x}{\sin 1} \int_x^1 f(\xi)\, \sin(1-\xi)\, \mathrm{d}\xi \tag{7.35}$$

using the result (7.20).

7.4 Equivalence of eigenfunction expansion of $G(x;\xi)$

For self–adjoint differential operators, we have now discovered two different expressions for the Green's function with homogeneous boundary conditions. On the one hand, we have

$$G(x,\xi) = \frac{1}{\alpha(\xi)W(\xi)}\left[\Theta(\xi - x)\, y_1(x)y_2(\xi) + \Theta(x-\xi)\, y_2(x)y_1(\xi)\right] \tag{7.36}$$

as in equation (7.13). On the other hand, in section 2.6 we showed that the Green's function for a self–adjoint operator could be written as

$$G(x,\xi) = \sum_{n=1}^{\infty} \frac{1}{\lambda_n}\, Y_n(x)\, Y_n^*(\xi) \tag{7.37}$$

in terms of the eigenfunctions $\{Y_n(x)\}$ and eigenvalues $\{\lambda_n\}$ of the Sturm–Liouville operator.

Incidentally, we derived (7.37) in section 2.6 without any mention of δ-functions, but it may also be quickly derived using the eigenfunction expansion

$$\delta(x-\xi) = w(x) \sum_{n\in\mathbb{Z}}^{\infty} Y_n(x)\, Y_n^*(\xi) \tag{7.38}$$

as in equation (6.36). Viewing ξ as a parameter we can write an eigenfunction expansion of the Green's function as

$$G(x,\xi) = \sum_{n\in\mathbb{Z}} \hat{G}_n(\xi)\, Y_n(x)\,. \tag{7.39}$$

Applying the self–adjoint operator $\mathcal{L}$ we have

$$\mathcal{L}G = \sum_{n\in Z} \hat{G}_n(\xi)\, \mathcal{L}Y_n(x) = w(x) \sum_{n\in\mathbb{Z}} \hat{G}_n(\xi)\, \lambda_n\, Y_n(x) \tag{7.40}$$

and for this to agree with $\delta(x-\xi)$, so that the expansion (7.39) obeys the defining equation $\mathcal{L}G = \delta(x-\xi)$ for the Green's function, we need

$$\hat{G}_n(\xi) = \frac{1}{\lambda_n}\, Y_n^*(\xi) \tag{7.41}$$

as can be checked by multiplying both sides of $w(x)\sum_{n\in\mathbb{Z}} \hat{G}_n(\xi)\,\lambda_n\, Y_n(x) = \delta(x-\xi)$ by $Y_m^*(x)$, integrating from a to b and using the orthogonality of the Sturm–Liouville eigenfunctions with weight function w. Thus we have recovered the eigenfunction expansion (7.37) of the Green's function. Note that the expression (7.37) requires that all eigenvalues λ_n be *non–zero*. This means that the homogeneous equation $\mathcal{L}y = 0$ — which is the eigenfunction equation when $\lambda = 0$ — should have no non–trivial solutions satisfying the boundary conditions. The existence of such solutions would certainly be problematic for the concept of a Green's function: If such solutions exist, then the inhomogeneous equation $\mathcal{L}y = f$ does not have a unique solution, because if y is any solution then so too is $y + y_0$. The operator $\mathcal{L}$ is thus not invertible, and the Green's function cannot exist. This is just the infinite

dimensional analogue of the familiar situation of a system of linear equations $\mathbf{M}\,\mathbf{u} = \mathbf{f}$ with non–invertible coefficient matrix $\mathbf{M}$. Indeed a matrix is non–invertible iff it has nontrivial eigenvectors with eigenvalue zero.

Since the Green's function is the *unique* solution to $\mathcal{L}G(x,\xi) = \delta(x-\xi)$ that obeys $G(a,\xi) = G(b,\xi) = 0$, it must be that the two expressions (7.36) and (7.37) are the same. To see that this is true, we first notice that for a self–adjoint operator (in Sturm–Liouville form) the first two coefficient functions in

$$\mathcal{L} = \alpha(x)\frac{\partial^2}{\partial x^2} + \beta(x)\frac{\partial}{\partial x} + \gamma(x)$$

are related by $\beta = d\alpha/dx$. In this case, the denominator $\alpha(\xi)W(\xi)$ in equation (**??**) for the Green's function is necessarily a (non–zero) *constant*. To show this, note that

$$\begin{aligned}\frac{d}{dx}(\alpha W) = \alpha' W + \alpha W &= \beta(y_1 y_2' - y_2 y_1') + \alpha(y_1 y_2'' - y_2 y_1'') \\ &= y_1 \mathcal{L} y_2 - y_2 \mathcal{L} y_1 = 0\,.\end{aligned} \tag{7.42}$$

Being constant, $\alpha(x)W(x)$ is independent of where we evaluate it and in particular is independent of ξ. We thus set $\alpha(x)W(x) = c$ and rewrite equation (7.36) as

$$G(x,\xi) = \frac{1}{c}\left[\Theta(\xi - x)\, y_1(x) y_2(\xi) + \Theta(x-\xi)\, y_2(x) y_1(\xi)\right]\,. \tag{7.43}$$

Like the eigenfunction expansion, this expression is now symmetric under exchange of x and ξ, so that $G(x;\xi) = G(\xi;x)$.

Going further in general requires a rather tedious procedure of expanding the step functions and solutions $y_1(x)$ and $y_2(x)$ (which we recall obey $y_1(a) = y_2(b) = 0$) in terms of the eigenfunctions. Instead, we'll content ourselves with an example and for lack of imagination we again take $\mathcal{L}y = -y'' - y$ on $[a,b] = [0,1]$, with boundary conditions $y(0) = y(1) = 0$. The normalized eigenfunctions and corresponding eigenvalues are easily calculated to be

$$Y_n(x) = \sqrt{2}\sin n\pi x \qquad\qquad \text{with}\;\; \lambda_n = n^2\pi^2 - 1 \tag{7.44}$$

and the Green's function is given in terms of these eigenfunctions by

$$G(x,\xi) = 2\sum_{n=1}^{\infty} \frac{\sin n\pi x\, \sin n\pi\xi}{n^2\pi^2 - 1}\,. \tag{7.45}$$

On the other hand, in a previous example we constructed the expression

$$G(x,\xi) = \frac{1}{\sin 1}\left[\Theta(x-\xi)\, \sin(1-x)\, \sin\xi + \Theta(\xi - x)\, \sin x\, \sin(1-\xi)\right] \tag{7.46}$$

using homogeneous solutions. Standard trigonometric addition formulæ for $\sin(1-x)$ allow us to write this as

$$G(x,\xi) = \Theta(x-\xi)\, \cos x\, \sin\xi\, + \Theta(\xi - x)\, \sin x\, \cos\xi - \cot 1\, \sin x\, \sin\xi\,. \tag{7.47}$$

Viewing x as the independent variable and ξ as a parameter, we expand this function as a Fourier sine series

$$\Theta(x-\xi)\,\cos x\,\sin\xi\,+\Theta(\xi-x)\,\sin x\,\cos\xi-\cot 1\,\sin x\,\sin\xi=\sum_{n=1}^{\infty}\hat{g}_n(\xi)\,\sin n\pi x\,. \quad (7.48)$$

As usual, the Fourier coefficients are given by

$$\hat{g}_n(\xi)=2\int_0^1 \sin n\pi x\,[\Theta(x-\xi)\,\cos x\,\sin\xi\,+\Theta(\xi-x)\,\sin x\,\cos\xi-\cot 1\,\sin x\,\sin\xi]\,\mathrm{d}x \quad (7.49)$$

and a direct (though rather tedious calculation — try it as an exercise if you really must) gives

$$\hat{g}_n(\xi)=\frac{2\sin n\pi\xi}{n^2\pi^2-1}\,. \quad (7.50)$$

Comparing this to the eigenfunction expansion (7.45) we see that the two expressions for the Green's function agree, as expected.

7.5 Application of Green's functions to initial value problems

Green's functions can also be used to solve initial value problems. Let's take the independent variable to be time t, and suppose we wish to find the function $y:[t_0,\infty)\to\mathbb{R}$ that obeys the differential equation

$$\mathcal{L}y=f(t) \quad (7.51)$$

subject to the initial conditions $y(t_0)=0$ and $y'(t_0)=0$. The method for construction of the Green's function in this initial value problem is similar to the previous method in the case of a boundary value problem. As before, we want to find G such that $\mathcal{L}G=\delta(t-\tau)$, so that for each value of τ, the Green's function $G(t,\tau)$ will solve the homogeneous equation $\mathcal{L}G=0$ whenever $t\neq\tau$. We proceed as follows

- Construct G for $t_0\le t<\tau$ as a general solution of the homogeneous equation, so $G=Ay_1(t)+By_2(t)$. Here $\{y_1(t),y_2(t)\}$ is *any* basis of linearly independent homogeneous solutions.

- In contrast to the boundary value problem, we now apply *both* initial conditions to this solution. That is, we enforce

$$\begin{aligned} Ay_1(t_0)+By_2(t_0)&=0\,,\\ Ay_1'(t_0)+By_2'(t_0)&=0\,. \end{aligned} \quad (7.52)$$

  This pair of linear equations for A and B can be written as

$$\begin{pmatrix} y_1(t_0) & y_2(t_0)\\ y_1'(t_0) & y_2'(t_0)\end{pmatrix}\begin{pmatrix}A\\B\end{pmatrix}=0 \quad (7.53)$$

  and since y_1 and y_2 are linearly independent, the determinant of the matrix (the Wronskian) is non-zero. Thus the only way to impose both initial conditions is to set $A=B=0$. This implies that $G(t,\tau)=0$ identically whenever $t\in[a,\tau)$!

– For $t > \tau$, again construct the Green's function as a general solution of the homogeneous equation, so $G = Cy_1(t) + Dy_2(t)$.

– Finally, we apply the continuity and jump conditions at $t = \tau$. Since $G = 0$ for $t < \tau$ we obtain

$$\begin{aligned} Cy_1(\tau) + Dy_2(\tau) &= 0 \\ Cy_1'(\tau) + Dy_2'(\tau) &= \frac{1}{\alpha(\tau)} \end{aligned} \tag{7.54}$$

where, as usual, $\alpha(t)$ is the coefficient of the second derivative in the differential operator $\mathcal{L}$. These simultaneous equations determine $C(\tau)$ and $D(\tau)$, thus completing the construction of the Green's function $G(t;\tau)$.

We can again use our Green's function to solve the forced problem (7.51) as

$$y(t) = \int_{t_0}^{\infty} G(t,\tau)\, f(\tau)\, \mathrm{d}\tau = \int_{t_0}^{t} G(t,\tau)\, f(\tau)\, \mathrm{d}\tau\,. \tag{7.55}$$

Here, in the second equality we have used the fact that $G(t,\tau)$ vanishes for $\tau > t$. This equation shows that the solution obeys a *causality condition*: the value of y at time t depends only on the behaviour of the forcing function for *earlier* times $\tau \in [t_0, t]$.

As an example, consider the problem

$$\frac{d^2y}{dt^2} + y = f(t),\ y(0) = y'(0) = 0 \tag{7.56}$$

with initial conditions $y(0) = y'(0) = 0$. Following our procedure above we get

$$G(t,\tau) = \Theta(t-\tau)\left[C(\tau)\,\cos(t-\tau) + D(\tau)\,\sin(t-\tau)\right]\,, \tag{7.57}$$

where we've chosen the basis of linearly independent solutions to be $\{\cos(t-\tau), \sin(t-\tau)\}$ purely because they make it easy to impose the initial conditions. Continuity demands that $G(\tau,\tau) = 0$, so $C(\tau) = 0$. The jump condition (with $\alpha(\tau) = 1$ then enforces $D(\tau) = 1$. Therefore, the Green's function is

$$G(t,\tau) = \Theta(t-\tau)\,\sin(t-\tau) \tag{7.58}$$

and the general solution to $\mathcal{L}y = f(t)$ obeying $y(0) = y'(0) = 0$ is

$$y(t) = \int_0^t \sin(t-\tau)\, f(\tau)\, \mathrm{d}\tau\,. \tag{7.59}$$

Again, we see that this solution knows about what the forcing function was doing only at earlier times.

7.6 Higher order differential operators

We briefly mention that there is a natural generalization of Green's functions to higher order differential operators (and indeed to PDEs, as we shall see in the last part of the course). If $\mathcal{L}$ is a n^{th}-order ODE on $[a, b]$, with $n > 2$ then the general solution to the forced differential equation $\mathcal{L}y = f(x)$ obeying the homogeneous boundary conditions $y(a) = y(b) = 0$ is again given by

$$y(x) = \int_a^b G(x;\xi)\, f(\xi)\, \mathrm{d}\xi\,, \tag{7.60}$$

where G still obeys $\mathcal{L}G = \delta(x - \xi)$ subject to homogeneous boundary conditions $G(a, \xi) = G(b, \xi) = 0$, but where now both G and its first $n - 2$ derivatives are continuous at $x = \xi$, while

$$\left.\frac{\partial^{(n-1)}G}{\partial x^{(n-1)}}\right|_{x=x^+} - \left.\frac{\partial^{(n-1)}G}{\partial x^{(n-1)}}\right|_{x=x^-} = \frac{1}{\alpha(\xi)} \tag{7.61}$$

where we again assume that $\alpha(x)$ is the coefficient function of the highest derivative in $\mathcal{L}$. An example can be found on problem sheet 3.

8 Fourier Transforms

Given a (sufficiently well behaved) function $f : S^1 \to \mathbb{C}$, or equivalently a periodic function on the real line, we've seen that we can represent f as a Fourier series

$$f(x) = \frac{1}{2L} \sum_{n \in \mathbb{Z}} \hat{f}_n \, \mathrm{e}^{\mathrm{i}n\pi x/L} \tag{8.1}$$

where the period is $2L$. In this chapter we'll extend these ideas to non-periodic functions $f : \mathbb{R} \to \mathbb{C}$. This extension, which is again due to Fourier, is one of the most important ideas in all Applied Mathematics (and a great deal of Pure). In one form or other it is at the heart of all spectroscopy (from crystallography to understanding the structure of proteins in your DNA), to the definition of a particle in Quantum Field Theory, to all image processing done by the Nvidia graphics chip in your iPad, not to mention Harmonic Analysis and a large chunk of Representation Theory.

To get started, recall that in the periodic case, the information about our function was stored in its list of Fourier coefficients $\hat{f}_n$, defined by

$$\hat{f}_n = \frac{1}{2\pi} \int_{-\pi}^{\pi} \mathrm{e}^{-\mathrm{i}nx} \, f(x) \, \mathrm{d}x \tag{8.2}$$

for $n \in \mathbb{Z}$. For a (non-periodic) function $f : \mathbb{R} \to \mathbb{C}$, we likewise define the *Fourier transform* $\tilde{f}(k)$ of $f(x)$ to be[30]

$$\tilde{f}(k) := \int_{-\infty}^{\infty} \mathrm{e}^{-\mathrm{i}kx} \, f(x) \, \mathrm{d}x \, . \tag{8.3}$$

The Fourier transform is an example of a linear transform, producing an output function $\tilde{f}(k)$ from the input $f(x)$. We'll sometimes use the notation $\tilde{f} = \mathcal{F}[f]$, where the $\mathcal{F}$ on the *rhs* is to be viewed as the operation of 'taking the Fourier transform', *i.e.* performing the integral in (8.3).

8.1 Simple properties of Fourier transforms

The Fourier transform has a number of elementary properties. For any constants $c_1, c_2 \in \mathbb{C}$ and integrable functions f, g the Fourier transform is linear, obeying

$$\mathcal{F}[c_1 f + c_2 g] = c_1 \mathcal{F}[f] + c_2 \mathcal{F}[g] \, .$$

By changing variables in the integral, it is also readily verified that it obeys

$$\begin{aligned} \text{translation} \qquad & \mathcal{F}[f(x-a)] = \mathrm{e}^{-\mathrm{i}ka} \tilde{f}(k) \\ \text{re-phasing} \qquad & \mathcal{F}[\mathrm{e}^{\mathrm{i}\ell x} f(x)] = \tilde{f}(k-\ell) \\ \text{scaling} \qquad & \mathcal{F}[f(cx)] = \frac{1}{|c|} \tilde{f}(k/c) \, . \end{aligned}$$

[30] Be warned! Various authors use a factor of $1/2\pi$ or $1/\sqrt{2\pi}$ instead. The choice you make here is purely conventional, but affects the corresponding choice you make in the Fourier inversion theorem of section 8.2.

Furthermore, if we define the *convolution*[31] $f * g$ of two functions to be the integral

$$f * g(x) = \int_{-\infty}^{\infty} f(x-y)\, g(y)\, \mathrm{d}y \tag{8.4}$$

then, provided f and g are sufficiently well–behaved for us to change the order of integration, the Fourier transform is

$$\begin{aligned}\mathcal{F}[f * g(x)] &= \int_{-\infty}^{\infty} \mathrm{e}^{-\mathrm{i}kx} \left[\int_{-\infty}^{\infty} f(x-y)\, g(y)\, \mathrm{d}y\right] \mathrm{d}x = \int_{\mathbb{R}^2} \mathrm{e}^{-\mathrm{i}k(x-y)}\, f(x-y)\, \mathrm{e}^{-\mathrm{i}ky}\, g(y)\, \mathrm{d}x\, \mathrm{d}y \\ &= \int_{-\infty}^{\infty} \mathrm{e}^{-\mathrm{i}ku}\, f(u)\, \mathrm{d}u \int_{-\infty}^{\infty} \mathrm{e}^{-\mathrm{i}ky}\, g(y)\, \mathrm{d}y = \mathcal{F}[f]\, \mathcal{F}[g]\,.\end{aligned} \tag{8.5}$$

In other words, the Fourier transform of a convolution of two functions is the product of their Fourier transforms.

By far the most useful property of the Fourier transform comes from the fact that the Fourier transform 'turns differentiation into multiplication'. Specifically, the Fourier transform of the derivative f' of a (smooth, integrable) function f is given by

$$\mathcal{F}[f'(x)] = \int_{-\infty}^{\infty} \mathrm{e}^{-\mathrm{i}kx}\, f'(x)\, \mathrm{d}x = -\int_{-\infty}^{\infty} \left(\frac{d}{dx}\mathrm{e}^{-\mathrm{i}kx}\right) f(x)\, \mathrm{d}x = \mathrm{i}k\tilde{f}(k) \tag{8.6}$$

where we note that the assumption that $f(x)$ was integrable means that in particular it must decay as $|x| \to \infty$, so there is no boundary term. Notice also that, as a sort of converse, if $\tilde{f}(k) = \mathcal{F}[f(x)]$ then the Fourier transform of $xf(x)$ is given by

$$\mathcal{F}[xf(x)] = \int_{-\infty}^{\infty} \mathrm{e}^{-\mathrm{i}kx}\, xf(x)\, \mathrm{d}x = \mathrm{i}\frac{d}{dk}\int_{-\infty}^{\infty} \mathrm{e}^{-\mathrm{i}kx}\, f(x)\, \mathrm{d}x = \mathrm{i}\tilde{f}'(k) \tag{8.7}$$

provided $xf(x)$ is itself integrable (and thus $\tilde{f}$ is differentiable) so that we can justify differentiating under the integral sign.

The fact that differentiation *wrt* x becomes multiplication by $\mathrm{i}k$ is important because it allows us to take the Fourier transform of a differential equation. Suppose

$$\mathcal{L}(\partial) = \sum_{r=0}^{p} c_r \frac{d^r}{dx^r}$$

is a differential operator with constant coefficients $c_r \in \mathbb{C}$. Then if $y : \mathbb{R} \to \mathbb{C}$ has Fourier transform $\tilde{y}$, the Fourier transform of $\mathcal{L}y$ is

$$\mathcal{F}[\mathcal{L}(\partial)y] = \mathcal{L}(\mathrm{i}k)\tilde{y}(k) \tag{8.8}$$

where the differential operator $\mathcal{L}(\partial)$ has been replaced by muliplication by the polynomial

$$\mathcal{L}(\mathrm{i}k) = \sum_{r=0}^{p} c_r (\mathrm{i}k)^r\,.$$

[31] Convolution is 'Faltung' in German, which picturesquely describes the way in which the functions are combined — the graph of g is ßipped (or folded) about the variable vertical line $u = x/2$ and then integrated against f.

(We've also assumed that all the Fourier integrals we meet converge). Thus, if y obeys some differential equation $\mathcal{L}(\partial)y(x) = f(x)$ on $\mathbb{R}$, then we have simply

$$\tilde{y}(k) = \tilde{f}(k)/\mathcal{L}(\mathrm{i}k) \tag{8.9}$$

in terms of the Fourier transforms.

The power of this approach becomes most apparent in higher dimensions. For example, consider the pde

$$\nabla^2\phi(\mathbf{x}) - m^2\phi(\mathbf{x}) = -\rho(\mathbf{x}) \tag{8.10}$$

for $\phi : \mathbb{R}^n \to \mathbb{C}$, where ∇^2 is the n-dimensional Laplacian. Defining the Fourier transform for (appropriately integrable) functions on $\mathbb{R}^n$ by the obvious generalization

$$\mathcal{F}[\phi(\mathbf{x})] = \tilde{\phi}(\mathbf{k}) = \int_{\mathbb{R}^n} \mathrm{e}^{-\mathrm{i}\mathbf{k}\cdot\mathbf{x}}\, \phi(\mathbf{x})\, \mathrm{d}^n x\,, \tag{8.11}$$

our pde becomes simply

$$\tilde{\phi}(\mathbf{k}) = \frac{\tilde{\rho}(\mathbf{k})}{|\mathbf{k}|^2 + m^2} \tag{8.12}$$

in terms of Fourier transforms.

8.2 The Fourier inversion theorem

We've just seen that linear differential equations can often become essentially trivial after a Fourier transform. However, if we are to make use of this result we need to be able to reconstruct the original function from knowledge of its Fourier transform. Recall that in the periodic case, we were able to represent

$$f(x) = \sum_{n\in\mathbb{Z}} \hat{f}_n\, \mathrm{e}^{2\pi\mathrm{i}nx/L} \tag{8.13}$$

for sufficiently smooth functions (or more generally, distributions) $f : S^1 \to \mathbb{C}$ with period L. To extend this to the non–periodic case, let's imagine trying to taking a limit of (8.13) where the period $L \to \infty$. We define $\Delta k \equiv 2\pi/L$ and note that the coefficients in (8.13) are

$$\hat{f}_n = \frac{1}{L}\int_{-L/2}^{L/2} \mathrm{e}^{-\mathrm{i}n\Delta k y}\, f(y)\, \mathrm{d}y = \frac{\Delta k}{2\pi}\int_{-L/2}^{L/2} \mathrm{e}^{-\mathrm{i}n\Delta k y}\, f(y)\, \mathrm{d}y \tag{8.14}$$

For this integral to exist in the limit $L \to \infty$ we should require that $\int_{\mathbb{R}} |f(y)|$ exists, but in that case the $1/L$ factor implies that for each n, $\hat{f}_n \to 0$ too. Nevertheless, for any finite L we can substitute (8.14) into (8.13) to obtain

$$f(x) = \sum_{n\in\mathbb{Z}} \left(\frac{\Delta k}{2\pi}\int_{-L/2}^{L/2} \mathrm{e}^{\mathrm{i}n\Delta k(x-y)}\, f(y)\, \mathrm{d}y \right) \tag{8.15}$$

Now recall the Riemann sum definition of the integral of a function g: As $\Delta k \to 0$ we have

$$\lim_{\Delta k\to 0} \sum_{n\in\mathbb{Z}} \Delta k\, g(n\Delta k) = \int_{\mathbb{R}} g(k)\, \mathrm{d}k \tag{8.16}$$

with k becoming a continuous variable. For (8.15) we take[32]

$$g(n\Delta k) = \frac{\mathrm{e}^{\mathrm{i}n\Delta kx}}{2\pi} \int_{-L/2}^{L/2} \mathrm{e}^{\mathrm{i}n\Delta ky}\, f(y)\,\mathrm{d}y \tag{8.17}$$

with y being viewed as a parameter. Thus, letting $L \to \infty$ we get

$$f(x) = \frac{1}{2\pi} \int_{-\infty}^{\infty} \mathrm{e}^{\mathrm{i}kx} \left[\int_{\mathbb{R}} \mathrm{e}^{-\mathrm{i}ky}\, f(y)\,\mathrm{d}y \right] \mathrm{d}x = \frac{1}{2\pi} \int_{\infty}^{\infty} \mathrm{e}^{\mathrm{i}kx}\, \tilde{f}(k)\,\mathrm{d}k\,. \tag{8.18}$$

This result is known as the *Fourier inversion theorem*; if the manipulations above can be made rigorous, then the function $f(x)$ itself can be expressed in terms of an integral of the Fourier transformed function $\tilde{f}(k)$. In line with our earlier notation, we sometimes write $f(x) = \mathcal{F}^{-1}[\tilde{f}(k)]$ where the *rhs* is just shorthand for the integral in (8.18).

Notice that the inverse Fourier transform looks almost identical to the Fourier transform itself — the only difference is the sign in the exponent and the factor of $1/2\pi$. In particular, replacing x by $-x$ in (8.18) we have the *duality* property

$$\tilde{f}(k) = \mathcal{F}[f(x)] \qquad \Leftrightarrow \qquad f(-x) = \frac{1}{2\pi}\mathcal{F}[\tilde{f}(k)]\,. \tag{8.19}$$

This observation is very useful: if we recognize some specific function g as being the Fourier transform of some function f, then we can immediately write down the Fourier transform of g itself in terms of f. For example, we saw in equation (8.5) that $\mathcal{F}[f*g(x)] = \tilde{f}(k)\,\tilde{g}(k)$. It now follows that

$$\mathcal{F}[f(x)\,g(x)] = \frac{1}{2\pi} \int \tilde{f}(k-\ell)\,\tilde{g}(\ell)\,\mathrm{d}\ell = \frac{1}{2\pi}\tilde{f} * \tilde{g}(k) \tag{8.20}$$

so that the Fourier transform of a product of two functions is the convolution of their individual Fourier transforms.

The Fourier inversion theorem allows us, in principle, to complete the problem of finding the solution to a linear differential equation. We saw in (8.9) that if $\mathcal{L}(\partial)y(x) = f(x)$ then $\tilde{y}(k) = \tilde{f}(k)/\mathcal{L}(\mathrm{i}k)$ where $\mathcal{L}(\mathrm{i}k)$ is a polynomial in k. Provided the *rhs* is integrable so that the Fourier inversion theorem holds, we have now

$$y(x) = \frac{1}{2\pi} \int_{-\infty}^{\infty} \mathrm{e}^{\mathrm{i}kx}\, \frac{\tilde{f}(k)}{\mathcal{L}(\mathrm{i}k)}\,\mathrm{d}k\,. \tag{8.21}$$

As an example, the pde $\nabla^2\phi - m^2\phi = -\rho$ on $\mathbb{R}^n$ is solved by

$$\phi(\mathbf{x}) = \frac{1}{(2\pi)^n} \int_{\mathbb{R}^n} \frac{\mathrm{e}^{\mathrm{i}\mathbf{k}\cdot\mathbf{x}}\, \tilde{\rho}(\mathbf{k})}{|\mathbf{k}|^2 + m^2}\,\mathrm{d}^n k\,. \tag{8.22}$$

Furthermore, from the result (8.20) that the Fourier transform of a product of functions is the convolution of the Fourier transforms, we see that our result will involve a convolution of the forcing term $f(x)$ with the inverse Fourier transform of the rational function $1/\mathcal{L}(\mathrm{i}k)$.

[32] The function g in (8.17) itself changes as $\Delta k \sim 1/L \to 0$, because the integral in its definition is taken over $[-L/2, L/2]$. However, it has a well defined limit $g_{\Delta k}(n\Delta k) \to g_0(k) = \int_{-\infty}^{\infty} \mathrm{e}^{-\mathrm{i}ky}\, f(y)\,\mathrm{d}y$ and so the limit of (8.15) is still as given in (8.18).

In practice, the final step of actually carrying out the integrals in the inverse Fourier transform can often be quite tricky. We'll look at a few simple examples where we can guess the answer in section 8.4, but the inverse Fourier transform is usually best done with the aid of techniques from Complex Analysis that you'll meet next term.

8.2.1 Parseval's theorem for Fourier transforms

A further important feature of the Fourier transform is that it preserves the (L^2) inner product of two functions – just as we saw for Fourier series. To see this, suppose $f, g : \mathbb{R}^n \to \mathbb{C}$ and sufficiently well–behaved that the Fourier transforms $\tilde{f}$ and $\tilde{g}$, exist and that they can themselves be represented in terms of $\tilde{f}$ and $\tilde{g}$ using the Fourier inversion theorem. Then

$$\begin{aligned}(f,g) &= \int_{\mathbb{R}^n} f^*(x)\, g(x)\, \mathrm{d}^n x = \int_{\mathbb{R}^n} f^*(x) \left[\frac{1}{2\pi}\int_{\mathbb{R}^n} \mathrm{e}^{\mathrm{i}k\cdot x}\, \tilde{g}(k)\, \mathrm{d}^n k\right] \mathrm{d}^n x \\ &= \frac{1}{2\pi}\int_{\mathbb{R}^n} \tilde{g}(k) \left[\int_{\mathbb{R}^n} \mathrm{e}^{\mathrm{i}k\cdot x}\, f^*(x)\, \mathrm{d}^n x\right] \mathrm{d}^n k \\ &= \frac{1}{2\pi}\int_{\mathbb{R}^n} \tilde{g}(k) \left[\int_{\mathbb{R}^n} \mathrm{e}^{-\mathrm{i}k\cdot x}\, f(x)\, \mathrm{d}^n x\right]^* \mathrm{d}^n k = \frac{1}{2\pi}\int_{\mathbb{R}^n} \tilde{g}(k)\, \tilde{f}(k)^*\, \mathrm{d}^n k \\ &= \frac{1}{2\pi}(\tilde{f},\tilde{g})\,,\end{aligned} \tag{8.23}$$

where in going to the second line we changed the order of the integrals — this step is justified since we've assumed that f and $\tilde{g}$ are both absolutely integrable on $\mathbb{R}^n$ in order for the Fourier transforms and inverse Fourier transforms to exist.

As a special case, if $f = g$ then we obtain

$$(f,f) = \frac{1}{2\pi}(\tilde{f},\tilde{f}) \tag{8.24}$$

so that the L^2-norm of a Fourier transform agrees with the L^2-norm the original function, up to a factor of $\sqrt{2\pi}$.[33] This is Parseval's theorem in the context of non–periodic functions.

8.3 The Fourier transform of Schwartz functions and tempered distributions

This section is again non–examinable, though you will need to know the results of subsection 8.3.1.

In this section we'll give a more careful discussion of when the Fourier transform exists, and when the manipulations in the above derivation of the Fourier inversion theorem can be made rigorous.

The first question we should ask is 'for what type of object does the Fourier transform make sense?'. To get started, suppose that $f : \mathbb{R} \to \mathbb{C}$ is Riemann integrable on every interval $[a,b]$ and that $\int_{-\infty}^{\infty} |f(x)|\, \mathrm{d}x$ exists. Then whenever k is real, we have

$$|\tilde{f}(k)| = \left|\int_{-\infty}^{\infty} \mathrm{e}^{-\mathrm{i}kx}\, f(x)\, \mathrm{d}x\right| \leq \int_{-\infty}^{\infty} |\mathrm{e}^{-\mathrm{i}kx}\, f(x)|\, \mathrm{d}x = \int_{-\infty}^{\infty} |f(x)|\, \mathrm{d}x \tag{8.25}$$

[33] Some authors choose to include factors of $1/\sqrt{2\pi}$ in their definition of the Fourier transform to avoid this factor here.

which converges by our assumptions on f. In fact, it's straightforward to show that with these assumptions on f, $\tilde{f}(k)$ is in fact everywhere *continuous* (I recommend this as an excercise if you like Analysis). However, even if $\int_{\mathbb{R}} |f(x)|\,\mathrm{d}x$ exists, it can often be that $\int_{\mathbb{R}} |\tilde{f}(k)|\,\mathrm{d}k$ diverges. For example, suppose $f(x)$ is the 'top hat function'

$$f(x) = \begin{cases} 1 & |x| \leq 1 \\ 0 & \text{else}\,. \end{cases} \tag{8.26}$$

This is certainly integrable, and indeed we readily compute the Fourier transform to be

$$\tilde{f}(k) = \int_{-\infty}^{\infty} \mathrm{e}^{-\mathrm{i}kx}\, f(x)\,\mathrm{d}x = \frac{1}{2\pi}\int_{-1}^{1} \mathrm{e}^{-\mathrm{i}kx}\,\mathrm{d}x = 2\,\frac{\sin k}{k}\,. \tag{8.27}$$

The problem is that $\tilde{f}(k)$ is now not integrable, since

$$\begin{aligned} \int_{-(N+1)\pi}^{(N+1)\pi} |\tilde{f}(k)|\mathrm{d}k &\geq \sum_{n=0}^{N} \int_{(n+\frac{1}{4})\pi}^{(n+\frac{3}{4})\pi} |\tilde{f}(k)|\mathrm{d}k \geq \sum_{n=0}^{N} \int_{(n+\frac{1}{4})\pi}^{(n+\frac{3}{4})\pi} \frac{1}{\sqrt{2}k}\mathrm{d}k \\ &\geq \sum_{n=0}^{N} \frac{\pi/2}{\sqrt{2}(n+1)\pi} = \frac{1}{2\sqrt{2}} \sum_{n=0}^{N} \frac{1}{n+1} \end{aligned} \tag{8.28}$$

which diverges as $N \to \infty$. But if taking the Fourier transform of an integrable function $f(x)$ can lead to a function $\tilde{f}(k)$ that is not itself integrable, how do we make sense of the Fourier inversion theorem?

Recall from section 6.3 that a *Schwartz function* ψ is an infinitely smooth function obeying

$$\sup_{x\in\mathbb{R}}\; x^m\,\psi^{(n)}(x) < \infty \qquad \text{for all } m, n \in \mathbb{N}. \tag{8.29}$$

so that in particular ψ decay rapidly as $|x| \to \infty$. As before,

$$|\tilde{\psi}(k)| = \left| \int_{-\infty}^{\infty} \mathrm{e}^{-\mathrm{i}kx}\,\psi(x)\,\mathrm{d}x \right| \leq \int_{-\infty}^{\infty} \left|\mathrm{e}^{-\mathrm{i}kx}\,\psi(x)\right| \mathrm{d}x = \int_{-\infty}^{\infty} |\psi(x)|\,\mathrm{d}x < \infty \tag{8.30}$$

and so that $\tilde{\psi}(k)$ is bounded for all $k \in \mathbb{R}$. What is more, since all the functions $x^m\psi^{(n)}(x)$ of involving monomials times derivatives of a Schwartz function are themselves infinitely smooth and bounded, their Fourier transforms also exist. Explicitly, we have

$$\tilde{\psi}^{(m)}(k) = \frac{d^m}{dk^m}\int_{-\infty}^{\infty} \mathrm{e}^{-\mathrm{i}kx}\,\psi(x)\,\mathrm{d}x = \mathcal{F}[(-\mathrm{i}x)^m\psi(x)] \tag{8.31}$$

where we are justified in differentiating under the integral since $x^m\psi(x)$ is indeed integrable as $\psi(x)$ is a Schwartz function. In particular, since $\mathcal{F}[x^m\psi(x)]$ is bounded for all $k \in \mathbb{R}$, all the derivatives of $\tilde{\psi}$ exist and are bounded, so $\tilde{\psi}$ is infinitely smooth. Likewise

$$k^n\tilde{\psi}(k) = \mathrm{i}^n \int_{-\infty}^{\infty} \frac{d^n\mathrm{e}^{-\mathrm{i}kx}}{dx^n}\,\psi(x)\,\mathrm{d}x = (-\mathrm{i})^n \int_{-\infty}^{\infty} \mathrm{e}^{-\mathrm{i}kx}\,\psi^{(n)}(x)\,\mathrm{d}x = (-\mathrm{i})^n\mathcal{F}[\psi^{(n)}(x)] \tag{8.32}$$

which is again bounded for all $k \in \mathbb{R}$. Combining these results shows that the Fourier transform $\tilde{\psi}(k)$ of a Schwartz function $\psi(x)$ is again a Schwartz function. Thus, the Fourier transform is a map $\mathcal{F} : \mathcal{S}(\mathbb{R}) \to \mathcal{S}(\mathbb{R})$, and by iterating the duality (8.19) four times we find the map

$$\frac{1}{(2\pi)^4}\,\mathcal{F}^4 : \mathcal{S}(\mathbb{R}) \to \mathcal{S}(\mathbb{R}) \tag{8.33}$$

is actually the identity: Up to a numerical factor, taking the (forwards) Fourier transform of a Schwartz function four times in succession just reproduces the Schwartz function.

To go further and define Fourier transforms for more general objects, less well–behaved than Schwartz functions, we first note that if $\phi, \psi \in \mathcal{S}(\mathbb{R})$ then the derivation of (8.23) is sound and

$$(\mathcal{F}\phi, \mathcal{F}\psi) = 2\pi(\phi, \psi)\,. \tag{8.34}$$

Since $\mathcal{F} \circ \mathcal{F}^{-1} = 1$ for Schwartz functions, we can equivalently write this result as $(\mathcal{F}\phi, \tilde{\psi}) = 2\pi(\phi, \mathcal{F}^{-1}\tilde{\psi})$, or just

$$(\mathcal{F}\phi, \chi) = 2\pi(\phi, \mathcal{F}^{-1}\chi)\,, \tag{8.35}$$

where χ is again some Schwartz function. Now we recall from chapter 6 that we can treat $\phi \in \mathcal{S}(\mathbb{R})$ as a special case of a tempered distribution $T_\phi \in \mathcal{S}'(\mathbb{R})$, which acts on a test function ψ via $T_\phi[\psi] = (\phi, \psi)$. In the case that $T \in \mathcal{S}'(\mathbb{R})$ is a more general tempered distribution, we similarly define its Fourier transform $\mathcal{F}T$ by

$$\mathcal{F}T[\chi] = 2\pi\, T[\mathcal{F}^{-1}\chi] \tag{8.36}$$

so as to agree with (8.35) in the restricted case. On the *lhs* here we have the Fourier transformed distribution $\mathcal{F}T$ acting on some test function $\chi \in \mathcal{S}(\mathbb{R})$, whilst on the *rhs* we have the original distribution T acting on the inverse Fourier transform of χ. Again, this definition will be compatible with the idea of obtaining tempered distributions as the limit of a sequence of test functions.

Let's now see how this definition works in practice.

8.3.1 Fourier transform of the Dirac δ

We've seen that, if we want to solve a driven pde $\mathcal{L}y(x) = f(x)$ then its often useful to first construct a Green's function $G(x, \xi)$ obeying $\mathcal{L}G(x, \xi) = \delta(x - \xi)$. Thus, if we wish to use Fourier transforms to solve such equations, we'll need to understand the Fourier transform of distributions such as the δ-function.

In this case, it's easy to obtain the transform naively using the heuristic object $\delta(x)$. We simply compute

$$\mathcal{F}[\delta(x)] = \int_{-\infty}^{\infty} \mathrm{e}^{-\mathrm{i}kx}\,\delta(x)\,\mathrm{d}x = 1\,. \tag{8.37}$$

Let's repeat this using our general definition for Fourier transforms of distributions. According to (8.36), for any test (Schwartz) function ϕ we have

$$\mathcal{F}\delta[\phi] = 2\pi\,\delta[\mathcal{F}^{-1}\phi] \tag{8.38}$$

and using the definition of the Dirac δ acting on $\mathcal{F}^{-1}\phi$ (thought of as a function of x), we obtain

$$2\pi\,\delta[\mathcal{F}^{-1}\phi] = 2\pi\,\delta\left[\frac{1}{2\pi}\int_{-\infty}^{\infty} \mathrm{e}^{\mathrm{i}kx}\,\phi(k)\,\mathrm{d}k\right] = \int_{-\infty}^{\infty}\phi(k)\,\mathrm{d}k = (1,\phi) \tag{8.39}$$

extracting the value of $\mathcal{F}^{-1}\phi$ at $x = 0$. The net result is just the inner product of the test function ϕ with the constant function 1. Recalling the definition of distributions that also happen to be ordinary functions, we see that the Fourier transform of the Dirac δ is just 1!

The Fourier inversion theorem assures us that the Fourier transform of 1 itself should be 2π times a δ-function. However, this claim is not obvious, since it's far from clear what we should make of the integral $\int_{-\infty}^{\infty}\mathrm{e}^{-\mathrm{i}kx}\,\mathrm{d}x$. To make progress, we treat 1 as a tempered distribution T_1. Then according to (8.36), the transformed distribution $\mathcal{F}T_1$ is determined by

$$\mathcal{F}T_1[\psi] = 2\pi\,T_1[\mathcal{F}^{-1}\psi] = 2\pi\,(1,\mathcal{F}^{-1}\psi) \tag{8.40}$$

where the second equality recognizes that T_1 is the distribution associated to an ordinary function, 1. Thus, to understand the Fourier transform of 1 we only need take the inverse Fourier transform of a Schwartz function ψ, which is always well–defined. Comparing with (8.38) we have indeed

$$\mathcal{F}T_1[\psi] = 2\pi\,(1,\mathcal{F}^{-1}\psi) = 2\pi\,\delta[\mathcal{F}^{-1}\psi]\,. \tag{8.41}$$

Thus, in the world of tempered distributions, we have

$$\int_{-\infty}^{\infty}\mathrm{e}^{-\mathrm{i}kx}\,\mathrm{d}x = 2\pi\,\delta(k) \tag{8.42}$$

and the Fourier transform of 1 is indeed 2π times the Dirac δ.

The translation and rephasing properties of the Fourier transform provide us with the simple corollaries

$$\mathcal{F}[\delta(x-a)] = \mathrm{e}^{-\mathrm{i}ka} \qquad \text{and} \qquad \mathcal{F}[\mathrm{e}^{-\mathrm{i}\ell x}] = 2\pi\,\delta(k-\ell)\,, \tag{8.43}$$

whilst we also have

$$\begin{aligned}\mathcal{F}[\cos(\ell x)] &= \pi\,(\delta(k+\ell)+\delta(k-\ell))\\ \mathcal{F}[\sin(\ell x)] &= \mathrm{i}\pi\,(\delta(k+\ell)-\delta(k-\ell))\ .\end{aligned} \tag{8.44}$$

In particular, a highly localised signal in physical space (such as a δ function) has a very spread out representation in Fourier space. Conversely, a highly spread out (yet periodic) signal in physical space (such as a sine wave) is highly localised in Fourier space. This is further illustrated in problem sheet 3, where you compute the Fourier transform of a Gaussian. Going further, the fact that Fourier transforms turns multiplication by x into differentiation *wrt* k shows that the Fourier transform of a polynomial involves derivatives of δ-functions, and conversely the Fourier transform of derivatives of δ-functions is a polynomial.

For another example, consider the Heaviside step function

$$\Theta(x) = \begin{cases} 1 & x > 0 \\ 0 & \text{else.}\end{cases} \tag{8.45}$$

We first note that $\Theta(x) = \lim_{\epsilon\to 0^+} \Theta(x)\,\mathrm{e}^{-\epsilon x}$ and that for any $\epsilon > 0$

$$\int_{-\infty}^{\infty} \mathrm{e}^{-\mathrm{i}kx}\,\Theta(x)\,\mathrm{e}^{-\epsilon x}\,\mathrm{d}x = \int_0^{\infty} \mathrm{e}^{-(\epsilon+\mathrm{i}k)x}\,\mathrm{d}x = \frac{1}{\epsilon+\mathrm{i}k} \tag{8.46}$$

so that, naively taking $\epsilon \to 0$, we might think that the Fourier transform of $\Theta(x)$ is just $1/\mathrm{i}k$. However, the presence of ϵ was clearly important to ensure convergence of the integral as $x \to \infty$, so to really understand what this transform means we must treat $\mathcal{F}\Theta$ as a distribution and see how it acts on a test function ϕ. For finite ϵ and any small $\delta > 0$ we have

$$\begin{aligned}\mathcal{F}\Theta[\phi] &= \lim_{\epsilon\to 0^+} \int_{-\infty}^{\infty} \frac{1}{\epsilon+\mathrm{i}k}\,\phi(k)\,\mathrm{d}k \\ &= \int_{|k|>\delta} \frac{1}{\mathrm{i}k}\,\phi(k)\,\mathrm{d}k + \lim_{\epsilon\to 0^+} \int_{-\delta}^{\delta} \left[\frac{\phi(k)-\phi(0)}{\epsilon+\mathrm{i}k} + \frac{\phi(0)}{\epsilon\ +\mathrm{i}k}\right]\mathrm{d}k\end{aligned} \tag{8.47}$$

where it is clearly safe to take $\epsilon \to 0$ whenever $|k| > \delta > 0$. For the remaining terms, as $\delta \to 0$ we have

$$\int_{-\delta}^{\delta} \frac{\phi(k)-\phi(0)}{\epsilon+\mathrm{i}k}\,\mathrm{d}k = \frac{1}{i}\int_{-\delta}^{\delta} \frac{d\phi}{dk}\,\mathrm{d}k + \ \mathcal{O}(\epsilon) = \mathcal{O}(\epsilon) \tag{8.48}$$

since the test function ϕ is smooth, and finally

$$\begin{aligned}\lim_{\epsilon\to 0^+} \int_{-\delta}^{\delta} \frac{\phi(0)}{\epsilon+\mathrm{i}k}\,\mathrm{d}k &= -\mathrm{i}\phi(0) \lim_{\epsilon\to 0^+} \ln(\epsilon+\mathrm{i}k)\Big|_{-\delta}^{\delta} \\ &= \pi\phi(0)\,.\end{aligned} \tag{8.49}$$

Combining the pieces, altogether we have

$$\mathcal{F}\Theta[\phi] = \pi\phi(0) + \lim_{\delta\to 0} \int_{|k|>\delta} \frac{1}{\mathrm{i}k}\,\phi(k)\,\mathrm{d}k \tag{8.50}$$

showing that, as a distribution, the Fourier transform of $\Theta(x)$ is

$$\mathcal{F}[\Theta(x)] = \begin{cases} \dfrac{1}{\mathrm{i}k} & k \neq 0 \\ \pi\delta(k) & k = 0\,. \end{cases} \tag{8.51}$$

This is sometimes written as $\mathcal{F}[\Theta(x)] = \text{p.v.}\,(\mathrm{i}k)^{-1} + \pi\delta(k)$ where the letters p.v. stand for the (Cauchy) *principal value* and mean that we should exclude the point $k = 0$ from any integral containing this term. What happens at $k = 0$ is instead governed by the δ-function.

8.4 Linear systems and transfer functions

Fourier transform are often used in the systematic analysis of linear systems which arise in many applications. Suppose we have a linear operator $\mathcal{L}$ acting on input $I(t)$ to give output $O(t)$. For example, $\mathcal{L}$ may represent the workings of an amplifier that can modify both the amplitude and phase of individual frequency components of an input signal.

We first write the input signal in terms of its Fourier transform $\tilde{I}(\omega)$:

$$I(t) = \frac{1}{2\pi} \int_{\mathbb{R}} \mathrm{e}^{\mathrm{i}\omega t}\, \tilde{I}(\omega)\, \mathrm{d}\omega$$

via the Fourier inversion theorem. This expresses the input as a linear combination of components with various definite frequencies ω, with the amplitude and phase of each component given respectively by the modulus and argument of $\tilde{I}(\omega)$. In this context, it is sometimes called the *synthesis* of the input, while the Fourier transform $\tilde{I}(\omega) = \int_{\mathbb{R}} \mathrm{e}^{-\mathrm{i}\omega t}\, I(\omega)\, \mathrm{d}\omega$ itself is known as the *resolution* of the pulse (into its frequency components).

Now suppose that $\mathcal{L}$ modifies the amplitudes and phases via a complex function $\tilde{R}(\omega)$ to produce the output

$$O(t) = \frac{1}{2\pi} \int_{\mathbb{R}} \mathrm{e}^{\mathrm{i}\omega t}\, \tilde{R}(\omega)\, \tilde{I}(\omega) \mathrm{d}\omega\,. \tag{8.52}$$

$\tilde{R}(\omega)$ is called the *transfer function* of the system and its inverse Fourier transform $R(t)$ is called the *response function*[34]. Thus the transfer and response functions are related via

$$\tilde{R}(\omega) = \int_{\mathbb{R}} \mathrm{e}^{\mathrm{i}\omega t}\, R(t)\, \mathrm{d}t \qquad \text{and} \qquad R(t) = \frac{1}{2\pi} \int_{\mathbb{R}} \mathrm{e}^{\mathrm{i}\omega t}\, \tilde{R}(\omega)\, \mathrm{d}\omega\,.$$

Equation (8.52) shows that $R(t)$ is the output $O(t)$ of the system when the input has $\tilde{I}(\omega) = 1$ — in other words when the input signal is $I(t) = \delta(t)$. Hence the response function $R(t)$ is closely related to the Green's function when $\mathcal{L}$ is a differential operator.

According to (8.52) and the convolution theorem, the output is

$$O(t) = \mathcal{F}^{-1}[\tilde{R}(\omega)\tilde{I}(\omega)] = R * I(t) = \int_{\mathbb{R}} R(t-u)\, I(u)\, \mathrm{d}u \tag{8.53}$$

Causality (and the absence of a background hum!) implies that if the input signal vanishes for all $t < t_0$ then there can be no output signal before t_0 either. Since the response function $R(t)$ is the output when the input $I(t) = \delta(t)$, and this input certainly vanishes for all $t < 0$, we see that $R(t) = 0$ for all $t < 0$. If we now assume that the was no input signal before $t = 0$ then (8.53) becomes

$$O(t) = \int_{-\infty}^{\infty} R(t-u)\, I(u)\, \mathrm{d}u = \int_{0}^{t} R(t-u)\, I(u)\, \mathrm{d}u \tag{8.54}$$

so that the output signal is formally the same as we found in our previous expressions in section 7.5 with Green's functions for initial value problems.

8.4.1 General form of transfer functions for ode's

We now consider the case with the relation linear finite order o.d.e. $\mathcal{L}_m I(t) = \mathcal{L}_n O(t)$, where $\mathcal{L}_m$ and $\mathcal{L}_n$ are the differential operators

$$\mathcal{L}_m = \sum_{j=0}^{m} b_j \frac{d^j}{dt^j} \qquad \text{and} \qquad \mathcal{L}_n = \sum_{i=0}^{n} a_i \frac{d^i}{dt^i}$$

[34] Warning! In various texts both $R(t)$ and $\tilde{R}(\omega)$ are referred to as the response or transfer function, in different contexts.

with constant coefficients (a_i, b_j). For simplicity, we'll consider the case $m = 0$ so that the *input* acts directly as a forcing term, but the fully general case is not much more difficult. Taking Fourier transforms we obtain

$$\tilde{I}(\omega) = \left[\sum_{i=0}^{n} a_i (\mathrm{i}\omega)^n\right] \tilde{O}(\omega) \tag{8.55}$$

and therefore

$$\tilde{R}(\omega) = \frac{1}{[a_0 + a_1 \mathrm{i}\omega + \cdots + a_n (\mathrm{i}\omega)^n]}. \tag{8.56}$$

Thus the transfer function is a rational function with an n^{th} degree polynomial in $(\mathrm{i}\omega)$ as the denominator. By the fundamental theorem of algebra, this polynomial will have n complex roots, counted with multiplicity. Assuming these roots are at point $c_j \in \mathbb{C}$ and allowing for repeated roots, we write

$$\tilde{R}(\omega) = \frac{1}{a_n} \prod_{j=1}^{J} \frac{1}{(\mathrm{i}\omega - c_j)_j^k} \tag{8.57}$$

where k_j is the multiplicity of the root at c_j, and $\sum_{j=1}^{J} k_j = n$. Using partial fractions, this can be written as a sum of terms of the form

$$\frac{\Gamma_{mj}}{(\mathrm{i}\omega - c_j)^m} \qquad \text{where } 1 \le m \le k_j \tag{8.58}$$

where Γ_{mj} are constants so that

$$\tilde{R}(\omega) = \sum_{j=1}^{J} \sum_{m=1}^{k_j} \frac{\Gamma_{mj}}{(\mathrm{i}\omega - c_j)^m}\,. \tag{8.59}$$

To find the response function $R(t)$, we need to compute the inverse Fourier transform of this function.

Let's define $\tilde{h}_m(\omega) := 1/(\mathrm{i}\omega - \alpha)^{m+1}$ with $m \ge 0$; by linearity of the Fourier transform, our job is done once we compute $\mathcal{F}^{-1}[\tilde{h}_m]$. We'll cheat. I'll give you the answer and we'll check it's correct by computing its Fourier transform[35]. Consider the function

$$h_0(t) := \begin{cases} \mathrm{e}^{\alpha t} & t > 0 \\ 0 & \text{else.} \end{cases} \tag{8.60}$$

Provided $\mathrm{Re}(\alpha) < 0$ the Fourier transform is easily computed to be

$$\tilde{h}_0(\omega) = \int_{-\infty}^{\infty} \mathrm{e}^{-\mathrm{i}\omega t}\, h_0(t)\, \mathrm{d}t = \int_{0}^{\infty} \mathrm{e}^{-\mathrm{i}\omega t}\, \mathrm{e}^{\alpha t}\, \mathrm{d}t = \frac{1}{\mathrm{i}\omega - \alpha} \tag{8.61}$$

[Note that if $\mathrm{Re}(\alpha) > 0$ then the above integral is certainly divergent. Indeed recalling the theory of linear constant coefficient ode's, we see that the c_j's above are the roots of the

[35] Going in the 'forwards' direction is most simply done with some complex analysis you'll meet next term, but you can also do it by differentiating under the integral if you're careful.

auxiliary equation and the equation has solutions with terms $\mathrm{e}^{c_j t}$ which grow exponentially if $\mathrm{Re}(c_j) > 0$. Such exponentially growing functions are problematic for Fourier theory, so here we will consider only the case $\mathrm{Re}(c_j) < 0$ for all j, corresponding to 'stable' odes whose solutions do not grow unboundedly as $t \to \infty$. The whole subjects of stability and control grow from these remarks.]

Next consider the function

$$h_1(t) := \begin{cases} t\mathrm{e}^{\alpha t} & t > 0 \\ 0 & \text{else,} \end{cases} \tag{8.62}$$

so $h_1(t) = t h_0(1)$. Recalling that 'multiplication becomes differentiation' for Fourier transforms (so $\mathcal{F}[xf(x)] = \mathrm{i}d\mathcal{F}[f]/dk$), we obtain

$$\tilde{h}_1(\omega) = \mathrm{i}\frac{d}{d\omega}\frac{1}{\mathrm{i}\omega - \alpha} = \frac{1}{(\mathrm{i}\omega - \alpha)^2} \tag{8.63}$$

(which may also be derived directly by evaluating the $\int_0^\infty te^{\alpha t}e^{-iwt}\,dt$). Similarly (or using proof by induction), for $\mathrm{Re}(\alpha) < 0$ we have

$$h_m(t) = \begin{cases} \dfrac{t^m}{m!}\,\mathrm{e}^{\alpha t} & t > 0 \\ 0 & \text{else} \end{cases} \qquad \text{has Fourier transform} \qquad \tilde{h}_m(\omega) = \frac{1}{(\mathrm{i}\omega - \alpha)^{m+1}} \tag{8.64}$$

with $m \geq 0$. Thus, for such stable systems, we can use this in (8.54) to easily construct the output from the input. Notice that all the $h_m(t)$ decay as $t \to \infty$, but after $t = 0$ they can initially increase to some finite time maximum (at $t = t_m = m/|\alpha|$ if $\alpha < 0$ and real for example). We also see that the response function $R(u) = 0$ for $u < 0$ so that, as expected, the upper limit in (8.53) should be t and the output $O(t)$ depends only on the input at earlier times.

To see more clearly the relation of above formalism to Green's functions, let's consider the familiar equation

$$\frac{d^2y}{dt^2} + 2p\frac{dy}{dt} + (p^2 + q^2)y = f(t) \tag{8.65}$$

which, provided $p > 0$, describes the motion of a forced, damped oscillator. Since $p > 0$, the drag force $-2py'$ acts opposite to the direction of velocity so the motion is damped. We assume that the forcing term $f(t)$ is zero for $t < 0$. Also $y(t)$ and $y'(t)$ are also zero for $t < 0$ and we have initial conditions $y(0) = y'(0) = 0$. The Fourier transformed equation is $(\mathrm{i}\omega)^2\tilde{y} + 2\mathrm{i}p\omega\tilde{y} + (p^2 + q^2)\tilde{y} = \tilde{f}$ and so

$$\tilde{y} = \frac{\tilde{f}}{-\omega^2 + 2\mathrm{i}p\omega + (p^2 + q^2)} =: \tilde{R}(\omega)\,\tilde{f}(\omega) \tag{8.66}$$

which solves the equation algebraically in Fourier space. To find the solution in real space we take the inverse Fourier transform to find

$$y(t) = \int_0^t R(t-u)\,f(u)du = \int_0^t \left[\frac{1}{2\pi}\int_{-\infty}^{\infty} \frac{\mathrm{e}^{\mathrm{i}\omega(t-u)}}{p^2 + q^2 + 2\mathrm{i}p\omega - \omega^2}\,\mathrm{d}\omega\right] f(u)\,\mathrm{d}u\,. \tag{8.67}$$

where the quantity in square brackets is the response function $R(t-u)$. Now consider $\mathcal{L}R(t-u)$, using this integral formulation. Assuming that formal differentiation within the integral sign is valid we have

$$\begin{aligned}
&\frac{d^2}{dt^2}R(t-u) + 2p\frac{d}{dt}R(t-u) + (p^2+q^2)R(t-u) \\
&\quad = \frac{1}{2\pi}\int_{-\infty}^{\infty} \mathrm{e}^{\mathrm{i}\omega(t-u)} \left[\frac{(\mathrm{i}\omega)^2 + 2\mathrm{i}p\omega + (p^2+q^2)}{p^2+q^2+2\mathrm{i}p\omega-\omega^2}\right] \mathrm{d}\omega \\
&\quad = \frac{1}{2\pi}\int_{-\infty}^{\infty} \mathrm{e}^{\mathrm{i}\omega(t-u)}\,\mathrm{d}\omega = \delta(t-u),
\end{aligned} \tag{8.68}$$

where we used that 1 is the Fourier transform of the δ-function. Therefore, the Green's function $G(t,u)$ is simply the response function $R(t-u)$ by (mutual) definition. In the problem sheets you're asked to fill in the details of this example, computing both $R(t)$ and the Green's function explicitly.

Fourier transforms can also be used to solve ode's on the full line $\mathbb{R}$, so long as the functions involved have sufficiently good asymptotic properties for the Fourier integrals to exist. As an example consider suppose $y : \mathbb{R} \to \mathbb{R}$ solves the ode

$$\frac{d^2y}{dx^2} - A^2 y = -f(x) \tag{8.69}$$

and is such that $y \to 0$ and $y' \to 0$ as $|x| \to \infty$. We take A to be a positive real constant. Taking the Fourier transform, we can solve the equation in Fourier space trivially to find

$$\tilde{y}(k) = \frac{\tilde{f}(k)}{A^2+k^2} \tag{8.70}$$

and so to recover the solution $y(x)$ we need to take the inverse Fourier transform of the product $\tilde{f}(k) \times 1/(A^2+k^2)$. From the convolution theorem, this will be the convolution of $f(t)$ with a function whose Fourier transform is $1/(A^2+k^2)$. Consider the function

$$h(x) = \frac{\mathrm{e}^{-\mu|x|}}{2\mu} \qquad \text{where} \qquad \mu > 0\,. \tag{8.71}$$

Since $h(x)$ is even, its Fourier transform can be written as

$$\tilde{h}(k) = \mathrm{Re}\left(\frac{1}{\mu}\int_0^{\infty} \exp\left[-(\mu+\mathrm{i}k)x\right]\mathrm{d}x\right) = \frac{1}{\mu}\mathrm{Re}\left(\frac{1}{\mu+\mathrm{i}k}\right) = \frac{1}{\mu^2+k^2}\,, \tag{8.72}$$

which identifies $h(x)$ as the function we seek. The convolution theorem then gives

$$y(x) = \frac{1}{2A}\int_{-\infty}^{\infty} \mathrm{e}^{-A|x-u|}\, f(u)\,\mathrm{d}u\,. \tag{8.73}$$

This solution is clearly in the form of a Green's function expression. Indeed the same expression may be derived using the Green's function formalism of chapter 7, applied to the infinite domain $(-\infty,\infty)$ and imposing suitable asymptotic boundary conditions on the Green's function for $|x| \to \infty$.

8.5 The discrete Fourier Transform

In realistic, physical situations or in numerical applications, we cannot add expect to know the value of $f(x)$ for *every* $x \in \mathbb{R}$, but only within some finite interval $x \in [-R, S]$. However, provided $|f(x)|$ is small outside this range, we may reasonably expect to approximate the Fourier transform by

$$\tilde{f}(k) = \int_{-\infty}^{\infty} \mathrm{e}^{-\mathrm{i}kx}\, f(x)\, \mathrm{d}x \approx \int_{-R}^{S} \mathrm{e}^{-\mathrm{i}kx}\, f(x)\, \mathrm{d}x\,. \tag{8.74}$$

Even within this range we cannot numerically evaluate this integral by computing $\mathrm{e}^{-\mathrm{i}kx}\, f(x)$ at *every* value of x, but will rather have to sample it at some finite set of points. For simplicity, let's assume these points are equally spaced, at $x_j = -R + j(R+S)/N$ for $j = 0, \ldots, N-1$ where N is some large positive integer. Then we can set

$$\tilde{f}(k) \approx \frac{R+S}{N} \sum_{j=0}^{N-1} \mathrm{e}^{-\mathrm{i}kx_j}\, f(x_j)\,. \tag{8.75}$$

Similarly, although the Fourier transform was originally valid for all $k \in \mathbb{R}$, in practice our computer's memory can only store the values of $\tilde{f}(k)$ for some finite set values of k. It's convenient to choose these to be at $k = k_m := 2\pi m/(R+S)$ for some integer(s) m. Then we have

$$\tilde{f}(k_m) \;\approx\; \frac{(R+S)\,\mathrm{e}^{\mathrm{i}k_m R}}{N} \sum_{j=0}^{N-1} \mathrm{e}^{-2\pi\mathrm{i}jm/N}\, f(x_j) \;=\; \frac{(R+S)\,\mathrm{e}^{\mathrm{i}k_m R}}{N} \sum_{j=0}^{N-1} f(x_j)\, \omega^{-mj} \tag{8.76}$$

where $\omega = \mathrm{e}^{2\pi\mathrm{i}/N}$ in an N^{th} root of unity.

Thus, for numerical purposes, computing Fourier transforms amounts to computing expressions of the form $F(m) := \frac{1}{N}\sum_{j=0}^{N-1} f(x_j)\,\omega^{-mj}$. Of course, unlike the exact Fourier transform, these truncations have thrown away much of the information about our function: we obviously cannot see structures that vary on scales shorter than our sampling interval $(R+S)/N$. Furthermore, since it is built from N^{th} roots of unity, evidently our approximate function obeys $F(m+N) = F(m)$ whereas our original function $f(x)$ and its exact Fourier transform $\tilde{f}(k)$ were not assumed to obey any periodicity conditions[36]. Nevertheless, we shall see that knowing the values of the *sums* $F(m)$ for all $m = 0, 1, \ldots, N-1$ is sufficient to reproduce the exact values of $f(x)$ at all the points x_k.

To proceed, let G be the set $\{1, \omega, \omega^2, \ldots, \omega^{N-1}\}$ of N^{th} roots of unity, and let $f : G \to \mathbb{C}$ and $g : G \to \mathbb{C}$ be functions on G. The space of such functions is a complex vector space, and we can define an inner product on this space by

$$(f, g) = \frac{1}{N} \sum_{j=0}^{N-1} f(\omega^j)^*\, g(\omega^j) \tag{8.77}$$

[36] In fact, if $|f(x)| \to 0$ sufficiently rapidly as $|x| \to \infty$ that we are justified in ignoring $x \notin [-R, S]$ then $\tilde{f}(k)$ will also decay as $m \to \infty$.

in analogy to our earlier treatment of functions on $\mathbb{R}$. It is a straightforward exercise to check that this inner product obeys the usual sesquilinearity properties

$$(f, c_1 g_1 + c_2 g_2) = c_1 (f, g_2) + c_2 (f, g_2) \qquad \text{and} \qquad (g, f)^* = (f, g)$$

for constants $c_{1,2}$, and that $(f, f) \geq 0$ with equality iff $f(\omega) = 0$ identically. Next, we claim that the functions $e_m(\omega^j) := \omega^{mj}$ obey $(e_m, e_n) = \delta_{mn}$ and so form a set of basis functions on G that are orthonormal wrt $(\ ,\ )$. To see this, note that

$$(e_m, e_m) = \frac{1}{N} \sum_{j=0}^{N-1} \omega^{-mj}\, \omega^{mj} = \frac{1}{N} \sum_{j=0}^{N-1} 1 = 1 \tag{8.78}$$

whilst whenever $m \neq n$ we have

$$(e_n, e_m) = \frac{1}{N} \sum_{j=0}^{N-1} \omega^{(m-n)j} = \frac{1}{N}\, \frac{\omega^{(m-n)N} - 1}{\omega^{(m-n)} - 1} = 0 \tag{8.79}$$

since $\omega^{(m-n)N} = 1$ for $m \neq n$ and ω an N^{th} root of unity.

These results provide us with a Fourier expansion for functions on G. We can expand

$$f(\omega^m) = \sum_{j=0}^{N-1} \hat{f}_j\, e_m(\omega^j) \qquad \text{where} \qquad \hat{f}_k \equiv (e_k, f) = \frac{1}{N} \sum_{k=0}^{N-1} \omega^{-jk}\, f(\omega^k)\,. \tag{8.80}$$

In fact, since G here is just a finite set, there are no issues about convergence to worry about, and the validity of this expansion is easily proved using the orthonormality of the $\{e_m\}$. Likewise, Parseval's theorem is easily proved by writing

$$\begin{aligned} (f, f) &= \frac{1}{N} \sum_{j=0}^{N-1} f(\omega^j)^*\, f(\omega^j) = \frac{1}{N} \sum_{j=0}^{N-1} \left(\sum_{l,m=0}^{N-1} \hat{f}_m^*\, \hat{f}_l\; e_m(\omega^j)^*\, e_l(\omega^j) \right) \\ &= \sum_{l,m} \hat{f}_m^*\, \hat{f}_l \left(\sum_{j=0}^{N-1} e_m(\omega^j)^*\, e_l(\omega^j) \right) = \sum_{l,m} \hat{f}_m^*\, \hat{f}_l\, \delta_{ml} = \sum_{m=0}^{N-1} \hat{f}_m^*\, \hat{f}_m = N(\hat{f}, \hat{f})\,, \end{aligned} \tag{8.81}$$

with no complications about exchanging the order of the finite sums. Again the Fourier transform preserves the inner product.

Now we can understand why knowledge of the sums

$$F(m) = \frac{1}{N} \sum_{j=0}^{N-1} f(x_j)\, \omega^{-mj}$$

for all m is sufficient to reproduce the exact values of the sampled function $f(x)$ at the sampling points $x = \{x_0, x_1, \ldots, x_{N-1}\}$. Defining a function $g : G \to \mathbb{C}$ by $g(\omega^j) := f(x_j)$, we have $F(m) = (e_m, g)$ and therefore

$$f(x_j) = \sum_{m=0}^{N-1} \omega^{jm}\, F(m) \tag{8.82}$$

so that the $f(x_j)$ can be recovered exactly from the $F(m)$.

Since the discrete Fourier transform acts linearly on the space of functions from $G \to \mathbb{C}$, and G is a finite set, we can represent it by a matrix. Let $\mathbf{U}$ be the $N \times N$ symmetric matrix with entries $U_{mj} = e_m(\omega^j) = \omega^{mj} = e_j(\omega^m)$ with $m, j = 0, 1, 2, \ldots, N-1$. Then if we let $\mathbf{f}$ be the (column) vector $\mathbf{f} = (f(x_0), f(x_1), \ldots, f(x_{N-1}))^{\mathrm{T}}$ the discrete Fourier transform may be written as the matirx multiplication

$$\hat{\mathbf{f}} = \mathbf{U}\mathbf{f}\,. \tag{8.83}$$

The matrix $\mathbf{U}/\sqrt{N}$ is in fact *unitary*, so $\mathbf{U}^{-1} = \mathbf{U}^\dagger/N$. To see this, note that $\mathbf{U}^\dagger$ has entries $U^\dagger_{jk} = e_k(\omega^j)^* = \omega^{-jk}$ and so

$$(\mathbf{U}\mathbf{U}^\dagger)_{mk} = \sum_{j=0}^{N-1} e_m(\omega^j)\, e_k^*(\omega^j) = N(e_k, e_m) = N\delta_{mk} \tag{8.84}$$

from the orthonormality properties of the basis functions $\{e_m\}$. Thus we also have

$$\mathbf{f} = \mathbf{U}^{-1}\hat{\mathbf{f}} = \frac{1}{N}\mathbf{U}^\dagger\hat{\mathbf{f}} \tag{8.85}$$

for the inverse transform.

Hopefully, you've been awake enough throughout this course to notice that the Fourier series for functions[37] $f : T^n \to \mathbb{C}$, Fourier transforms for functions $f : \mathbb{R}^n \to \mathbb{C}$ and discrete Fourier transform for functions $f : G \to \mathbb{C}$ have all looked rather similar. In particular, in each case we have an Abelian group $\mathcal{G}$ (either T^n, $\mathbb{R}^n$ or G) and maps $e_{\mathrm{k}} : \mathcal{G} \to \mathbb{C}$, given on T^n and $\mathbb{R}^n$ by $\exp(\mathrm{i}\mathbf{k}\cdot\mathbf{x})$, with $\mathbf{k} \in \mathbb{Z}^n$ and $\mathbf{k} \in \mathbb{R}^n$ respectively, and by $e_k(\omega^j) = \omega^{jk}$ on G. These functions all obey

$$e_{\mathbf{k}}(\mathbf{x}+\mathbf{y}) = e_{\mathbf{k}}(\mathbf{x})\, e_{\mathbf{k}}(\mathbf{y}) \tag{8.86}$$

and $e_{\mathbf{k}}(I) = 1$ where I is the identity element of the group $\mathcal{G}$ ($\mathbf{0}$ in $\mathbb{R}^n$, $\mathbf{1}$ in T^n and 1 in G). In fact, it's not much more work to establish Fourier theory for any Abelian group, though we won't do it here. There's also a powerful generalization of Fourier theory to non–Abelian groups, at least for compact groups, which you can read about here.

8.5.1 Fast Fourier transforms

Non-examinable. All the best bits are.

In the months that followed the Cuban missile crisis, geopolitical tensions were running high. The realization of just how close the world had come to a nuclear apocalypse persuaded many that a curb on the development of nuclear weapons was required, and negotiations were underway to work towards a Nuclear Test Ban Treaty. A major problem was that neither side trusted the other to stick to the terms of the Treaty. In particular,

[37] Here $T^n = S^1 \times S^1 \times \cdots \times S^1$ is an n-dimensional torus. Equivalently, we have considered this case when Fourier analysing functions periodic in n variables.

the US wanted to be sure they could tell whether or not a nuclear test had taken place deep within the Soviet Union without having to undertake politically sensitive visits to the actual site. Overground tests were relatively easy to spot, not least because of the fallout effects, but detecting underground tests was another matter.

During a meeting of President Kennedy's Scientific Advisory Committee, John Tukey of Princeton got interested in a proposal to place many sensitive seismological devices at locations surrounding the Soviet Union. These devices could monitor vibrations, recording this information over time. But in order to tell whether a test had occurred, one would have to separate out the signal of the explosion from other noises and rumblings of the Earth's crust. This called for Fourier analysis, which would separate out the frequencies of vibration, but the large landmass of Soviet Russia and the long period of time for which monitoring would be required meant that a powerful computer would be needed to perform the analysis. The problem is that to actually compute $\hat{f}(m)$ at even a single value of m using the formula

$$\hat{f}(m) \approx \frac{1}{N} \sum_{j=0}^{N-1} \omega^{-mj} f(x_j) \tag{8.87}$$

obtained above is very computationally expensive. Even if our computer is provided with a library containing the values of ω^{-mj}, the $f(x_j)$ will depend on what the seismometers record, so we shall need at least $N-1$ additions and $N+1$ multiplications: a total of $2N$ operations to compute $\hat{f}(m)$ for a single value of m. Thus, even given all the values of ω^{-mj}, computing $\hat{f}(m)$ for all $m = 0, \ldots, N-1$ this way will thus take $2N^2$ operations.

Together with James Cooley at IBM, Tukey realised that a much more efficient algorithm could be obtained by breaking the task down into smaller chunks. Suppose that $N = 2M$ for some integer M. Then for a function on the $N = 2M^{\text{th}}$ roots of unity we can write

$$\begin{aligned} \frac{1}{N} \sum_{j=0}^{N-1} \omega^{-mj}\, g(\omega^j) &= \frac{1}{2M} \sum_{j=0}^{2M-1} \omega^{-mj}\, g(\omega^j) \\ &= \frac{1}{2} \left[\frac{1}{M} \sum_{k=0}^{M-1} \omega^{-2kj}\, g(\omega^{2k}) + \frac{1}{M} \sum_{k=0}^{M-1} \omega^{-(2k+1)m}\, g(\omega^{2k+1}) \right] \end{aligned} \tag{8.88}$$

where in going to the second line we've separated out the even ($j = 2k$) and odd ($j = 2k+1$) terms in the sum. Now let η denote an M^{th} root of unity and define $G(\eta^k) \equiv g(\omega^{2k})$ and $H(\eta^k) \equiv g(\omega^{2k+1})$. Then we can write the *rhs* of (8.88) as

$$\frac{1}{2} \left[\frac{1}{M} \sum_{k=0}^{M-1} \eta^{-mk}\, G(\eta^k) + \frac{\omega^{-m}}{M} \sum_{k=0}^{M-1} \eta^{-mk}\, H(\eta^k) \right] = \frac{1}{2} \left[\hat{G}(m) + \omega^{-m} \hat{H}(m) \right], \tag{8.89}$$

where the final equality identifies the sums as being the discrete Fourier transforms of G and H as functions on the M^{th} roots of unity.

Given the values of $\hat{G}(m)$, $\hat{H}(m)$ and ω^{-m} for some specific m, these expressions show that we can compute the value of $\hat{f}(m)$ using no more than one addition and two

multiplications. Consequently, given all these values, we can compute $\hat{f}(m)$ for *all* $m \in \{0, 1, \ldots, N-1\}$ using at most $3 \times 2M = 6M$ operations. Suppose it takes no more that P_M operations to compute the discrete Fourier transform of any function on the M^{th} roots of unity. Computing the value of ω^{-m} for every $0 \leq m < 2M$ will cost no more than $2M$ multiplications, and so we will be able to compute the value of $\hat{f}(m)$ at *every* $m \in \{0, 1, \ldots, N-1\}$ using no more than $P_{2M} = 8M + 2P_M$ operations.

Now to the point. Let's prove inductively that when $N = 2^n$, $P_N \leq 2^{n+2}n = 4N \log_2 N$ — note that for $N \gg 1$ this is a vast saving over the $\sim 2N^2$ operations required by a 'direct' approach. When $n = 1$ the Fourier transform is completely given by

$$\begin{aligned} \hat{F}(1) &= \frac{1}{2}\left(F(1) + F(-1)\right) \\ \hat{F}(-1) &= \frac{1}{2}\left(F(1) + (-1)F(-1)\right) , \end{aligned} \tag{8.90}$$

and these values clearly take no more than 5 operations on $\{F(1), F(-1)\}$ to obtain. Thus, certainly $P_2 = 5 \leq 8$. Assuming the result when $N = 2^m$ for some m, our recurrence then shows that $P_{2^{m+1}} \leq 8 \cdot 2^m + 2 \times 2^{m+2}m = 2^{m+3}(m+1)$ and the induction holds.

Overnight, Cooley and Tukey's algorithm revolutionized our ability to actually compute Fourier transforms numerically. Aside from Nuclear Test Ban Treaties, nowadays their results (and further refinements) lie behind essentially all the image processing computations that enable you see what your friends are up to via iPhone. But they weren't the first to get there. Back in 1805 Gauss had been trying to reconstruct the orbits of comets Pallas and Juno from their various intermittent observations. In the margins of his notebooks, he'd discovered Cooley & Tukey's algorithm for himself as a means to speed up his calculations.

9 Characteristics

When we studied Laplace's equation $\nabla^2\phi = 0$ within a compact domain $\Omega \subset \mathbb{R}^n$, we imposed that ϕ obeyed one of the boundary conditions

$$\begin{aligned} \phi|_{\partial\Omega} &= f(x) \qquad \text{(Dirichlet)} \\ \mathbf{n}\cdot\nabla\phi|_{\partial\Omega} &= g(x) \quad \text{(Neumann)} \end{aligned}$$

for some specified functions $f, g : \partial\Omega \to \mathbb{C}$. We showed that there was a unique solution obeying Dirichlet boundary conditions, whereas the solution obeying Neumann conditions was unique up to the addition of a constant. On the other hand, in the case of a function $\phi : \Omega \times [0,\infty) \to \mathbb{C}$ that obeys the heat equation $\partial_t\phi = K\nabla^2\phi$ we imposed both a condition

$$\phi|_{\partial\Omega} \times (0,\infty) = f(x,t)$$

that holds on $\partial\Omega$ for all times, and also a condition

$$\phi|_{\Omega\times\{0\}} = g(x)$$

on the initial value of ϕ throughout Ω. Finally, for $\phi : \Omega \times [0,\infty) \to \mathbb{C}$ obeying the wave equation $\partial_t^2\phi = c^2\nabla^2\phi$ we imposed the boundary condition

$$\phi_{\partial\Omega} \times (0,\infty) = f(x,t)$$

and initial conditions

$$\phi|_{\Omega\times\{0\}} = g(x) \qquad\qquad \partial_t\phi|_{\Omega\times\{0\}} = h(x)$$

on both the value and time derivative of ϕ at $t = 0$.

In all cases, we prescribe the value of ϕ or its derivatives on a co-dimension 1 surface of the domain of ϕ — that is, a surface where one of the coordinates (time or space) is held fixed. The choice of exactly what ϕ should look like on this surface (*e.g.* the functions f, g and h above) are known as the *Cauchy data* for the pde, and solving the pde subject to these conditions is said to be a *Cauchy problem*. According to Hadamard, the Cauchy problem is *well–posed* if

- A solution to the Cauchy problem exists
- The solution is unique
- The solution depends continuously on the auxiliary data.

The first two conditions are clear enough. We could violate the first condition if we try to impose too many conditions on our solution, overconstraining the problem, whilst the second can be violated by not restricting the solution enough. To understand the final condition properly would require us to introduce a topology on the space of functions (for example, we could use one induced by the inner product $(\ ,\ )$), but intuitively it means that a small change in the Cauchy data should lead to only a small change in the solution

itself. This requirement is reasonable from the point of view of studying equations that arise in mathematical physics — since we can neither set up our apparatus nor measure our results with infinite precision, equations that can usefully model the physics had better obey this condition. (Some systems' behaviour, especially non-linear systems such as the weather, are exquisitely sensitive to the precise initial conditions. This is the arena of chaos theory.)

To gain some intuition for this final condition, let's consider a couple of examples where it is violated. Recall that evolution of some initial function via heat flow tends to smooth it: all sharp features become spread out as time progresses, and even two heat profiles that initially look very different end up looking very similar. For example, radiators and underfloor heating are both good ways to heat your room. On the other hand, suppose we specify $\phi(x,t)$ at some *late* time $t = T$ and try to evolve ϕ backwards in time using the heat equation, to see where our late–time profile came from. This problem will violate the final condition above, since even small flucutations in $\phi(x,T)$ will grow exponentially as time runs backwards, so that our early–time solutions will look very different.

For a second example, let Ω be the upper half plane $\{(x,y) \in \mathbb{R}^2 : y \geq 0\}$ and suppose $\phi : \Omega \to \mathbb{C}$ solves Laplace's equation $\nabla^2\phi = 0$ with boundary conditions

$$\phi(x,0) = 0 \qquad \text{and} \qquad \partial_y\phi(x,0) = g(x) \tag{9.1}$$

for some prescribed $g(x)$. Let's first take the case $g(x) = 0$ identically. Then the unique solution is $\phi = 0$ throughout Ω. Now instead suppose $g(x) = \frac{\sin(Ax)}{A}$ for some constant $A \in \mathbb{R}$. Separation of variables shows that the solution in this case is

$$\phi(x,y) = \frac{\sin(Ax)\,\sinh(Ay)}{A^2} \tag{9.2}$$

and again this solution is unique. So far, all appears well, but consider taking the limit $A \to \infty$. In this limit our second choice of Cauchy data $\sin(Ax)/A \to 0$ everywhere along the x-axis and so becomes equal to the first. However, at $x = \pi/2A$ we have $\phi(\pi/2A, y) = \sinh(Ay)/A^2$ which for any finite y grows exponentially as $A \to \infty$. Thus at large A our second solution is very different from the first even for initial data that is very close. Hence the problem is ill–posed.

9.1 The Method of Characteristics

We'd like to understand how and where to specify our Cauchy data so as to ensure such ill–posed problems do not arise. One technique for thinking about this is known as the *method of characteristics*, which you met first in 1A Differential Equations. We'll look in some more detail at this here, beginning with the case of 1^{st} order p.d.e.s with two independent variables.

9.1.1 Vector fields and integral curves

To get started, let's think about a (smooth) parameterised curve $C \subset \mathbb{R}^2$. We can view this as a map $\mathbf{x} : \mathbb{R} \to \mathbb{R}^2$ given by $X : s \mapsto (x(s), y(s))$. In other words, $s \in \mathbb{R}$ is our

Figure 13. *A parametrised curve $C \subset \mathbb{R}^2$, with its tangent vector at a point $s \in \mathbb{C}$.*

parameter telling us where we are along C and $(x(s), y(s))$ tell us where this point of the curve sits inside $\mathbb{R}^2$ (see figure 13). The tangent vector to C at s is given by the vector

$$\mathbf{v} = \begin{pmatrix} \dfrac{dx(s)}{ds} \\ \dfrac{dy(s)}{ds} \end{pmatrix} \tag{9.3}$$

whose components are the derivatives w.r.t. s of the components of the image. If we're given a function $\phi : \mathbb{R}^2 \to \mathbb{C}$ then its *restriction to* C is a function $\phi|_C : C \to \mathbb{C}$ given by $\phi_C : s \mapsto \phi(x(s), y(s))$. The *directional derivative* of ϕ_C along C is

$$\frac{d\phi_C(x(s), y(s))}{ds} = \frac{dx(s)}{ds}\, \partial_x \phi|_C + \frac{dy(s)}{ds}\, \partial_y \phi|_C = \mathbf{v} \cdot \nabla \phi|_C \tag{9.4}$$

as follows from the chain rule. In particular, if $\mathbf{v} \cdot \nabla \phi = 0$ then ϕ is constant along C.

Now suppose we're given a (suitably regular) vector field

$$\mathbf{u} = \begin{pmatrix} \alpha(x, y) \\ \beta(x, y) \end{pmatrix} \tag{9.5}$$

defined on (part of) $\mathbb{R}^2$. For example, $\mathbf{u}$ might describe the velocity of water flowing on the surface of a stream. An *integral curve* of $\mathbf{u}$ is then a curve $C \subset \mathbb{R}^2$ whose tangent vector at a point $(x, y) \in \mathbb{R}^2$ is given by $\mathbf{u}$. That is, the integral curves obey the equations

$$\frac{dx(s)}{ds} = \alpha(x(s), y(s)) \qquad \text{and} \qquad \frac{dy(s)}{ds} = \beta(x(s), y(s))\,. \tag{9.6}$$

If $\mathbf{u}$ represents the velocity field of a stream, then we can think of these curves as the flow lines of a fluid, whilst if $\mathbf{u} = \mathbf{B}$ represents the magnetic field vector, then the integral curves are the field lines. Notice that the integral curves are determined by a system of

Figure 14. *The curve B is transverse to the family of curves.*

1st order o.d.e.s (in the variable s) and hence always exist, at least locally. To fix a unique solution to these o.d.e.s, we must specify an initial condition. To do so, pick another curve $B \subset \mathbb{R}^2$ that is *transverse* to all the integral curves, meaning that the tangent vector to B is nowhere parallel to the tangent vectors $\mathbf{u}$ at the same point. Thus, at least locally, B will intersect all the integral curves, as shown in figure 14, and we can fix our solution to (9.6) by saying the intersection occurs at $s = 0$. If B is parametrised by $t \in \mathbb{R}$, so that t labels how far we are along B, then we can also label each member of our family of integral curves by the value of t at which they intersect B. In particular, the t^{th} integral curve of $\mathbf{u}$ will be given by $C_t = \{(x = x(s,t), y = y(s,t)) \in \mathbb{R}^2\}$ where

$$\left.\frac{\partial x(s,t)}{\partial s}\right|_t = \alpha|_{C_t} \qquad \left.\frac{\partial y(s,t)}{\partial s}\right|_t = \beta|_{C_t} \tag{9.7}$$

subject to the condition that $(x(s,0), y(s,0))$ lies on the curve B. If the Jacobian

$$J := \frac{\partial x}{\partial s}\frac{\partial y}{\partial t} - \frac{\partial x}{\partial t}\frac{\partial x}{\partial t} \tag{9.8}$$

is non–zero then the transformation can be inverted, solving for (t, s) in terms of (x, y). Knowing $t(x, y)$ and $s(x, y)$ means that if we're given a point $(x, y) \in \mathbb{R}^2$ then we can say which curve we're on (t) and how far we are along that curve (s). Thus, if $J \neq 0$ then the family of integral curves of $\mathbf{u}$ are space–filling and non–intersecting, at least in some region of the plane.

9.1.2 Characteristics for first order p.d.e.s

To see how these ideas apply to partial differential equations, we'll start with the case of a 1st order homogeneous p.d.e.. suppose $\phi : \mathbb{R}^2 \to \mathbb{C}$ solves

$$\alpha(x,y)\,\partial_x\phi + \beta(x,y)\,\partial_y\phi = 0 \tag{9.9}$$

subject to the condition $\phi|_B = h(t)$ for some function $h(t)$ along a curve $B \subset \mathbb{R}^2$ parameterised by t. From equation (9.4) we see that this equation is equivalent to the statement that the directional derivative of ϕ vanishes, and thus ϕ is constant, along the integral curves of the vector $\mathbf{u} = \begin{pmatrix} \alpha \\ \beta \end{pmatrix}$. In the context of differential equations, these integral curves are called the *characteristic curves* of the p.d.e.. At the intersection point of any given characteristic curve with B, the Cauchy data fixes ϕ to be h, and since $\mathbf{u} \cdot \nabla\phi = 0$ along each integral curve, ϕ takes the same value $h(t)$ all along the t^{th} integral curve, and so knowing where the integral curves actually are tells us what $\phi(x, y)$ is throughout (some region of) the plane.

Let's illustrate this with some examples. We start with a trivial case. Let $\phi : \mathbb{R}^2 \to \mathbb{C}$ obey

$$\partial_x \phi = 0 \tag{9.10}$$

subject to $\phi(0, y) = f(y)$ for some function f. Of course, we don't need any fancy method to solve this; clearly (9.10) says that $\phi(x, y)$ is a function of y only and then the Cauchy data along the y–axis fixes $\phi(x, y) = f(y)$ throughout $\mathbb{R}^2$. It's instructive to see how the method of characteristics reproduces this result. In this case, the vector field $\mathbf{u}$ is $\mathbf{u} = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$ so the integral curves are given by

$$\frac{dx}{ds} = 1 \qquad \frac{dy}{ds} = 0 \tag{9.11}$$

which has general solution $x = s + c$ and $y = d$ for some constants c, d. In this case, the curve B along which our Cauchy data is specified is the y–axis itself. We can parameterize this as $x = 0$, $y = t$ and the condition that the integral curves of $\mathbf{u}$ intersect B at $s = 0$ fixes $c = 0$ and $d = t$ so that

$$x = s \qquad y = t \tag{9.12}$$

define our family of curves. In this case, all the integral curves are just horizontal lines, with the y co–ordinate specifying which integral curve we're on. Now, the differential equation (9.10) can be written as $\partial_x \phi = \mathbf{u} \cdot \nabla\phi = 0$, or $\frac{\partial \phi}{\partial s}|_t = 0$ so that ϕ is constant along each integral curve. The Cauchy data fixes $\phi(s, t) = f(t)$ on the t^{th} curve, or in other words $\phi(x, y) = f(y)$ since $t = y$ in this case. Thus we've recovered our earlier solution.

For a slightly more interesting example, suppose now we want a solution of

$$\mathrm{e}^x \partial_x \phi + \partial_y \phi = 0 \tag{9.13}$$

subject to $\phi(x, 0) = \cosh x$. Let's first find the characteristics. The integral curves of $\mathbf{u} = \begin{pmatrix} \mathrm{e}^x \\ 1 \end{pmatrix}$ obey $dx/ds = \mathrm{e}^x$ and $dy/ds = 1$ and so are given by

$$\mathrm{e}^{-x} = -s + c \qquad y = s + d \tag{9.14}$$

for some constants c, d. The Cauchy data here is specified along the x–axis, which we treat as a parametrised curve B by setting $x = t$, $y = 0$. The condition that the characteristic curves intesect B at $s = 0$ fixes the constants c, d so that

$$\mathrm{e}^{-x} = -s + \mathrm{e}^{-t} \qquad y = s\,. \tag{9.15}$$

The differential equation (9.13) says that ϕ is again constant along these characteristics, and the Cauchy data fixes ϕ to be $\cosh t$ on the t^{th} curve. Inverting the relations (9.15) to find (s,t) as functions of (x,y) shows that

$$s = y \qquad t = -\ln(y + \mathrm{e}^{-x}) \tag{9.16}$$

and therefore our solution is $\phi(x,y) = \cosh[\ln(y+\mathrm{e}^{-x})]$ throughout $\mathbb{R}^2$. You can check by direct substitution that this does indeed solve our p.d.e. with the given boundary condition.

We can also use the method of characteristics to attack inhomogeneous problems such as

$$\partial_x \phi + 2\partial_y \phi = y\,\mathrm{e}^x \tag{9.17}$$

with $\phi = \sin x$ along the diagonal $y = x$. The characteristic curves of $\mathbf{u} = \binom{1}{2}$ are given by

$$x = s + t \qquad y = 2s + t \tag{9.18}$$

where we've used the fact that the Cauchy data here is fixed along the curve B given by $x = t$, $y = t$ to fix the values of $x(s)$ and $y(s)$ at $s = 0$. Equivalently,

$$s = y - x \qquad \text{and} \qquad t = 2x - y \tag{9.19}$$

which shows that specifying a point $(x,y) \in \mathbb{R}^2$ determines which characteristic curve we're on (t) and where we are along this curve (s).

However, in this inhomogeneous example ϕ is no longer constant along the characteristic curves, but instead obeys

$$\mathbf{u}\cdot\nabla\phi = \left.\frac{\partial\phi}{\partial s}\right|_t = y\,\mathrm{e}^x = (2s+t)\,\mathrm{e}^{s+t} \tag{9.20}$$

with initial data that $\phi(0,t) = \sin t$ at the point $s = 0$ on the t^{th} curve. Solving this differential equation for ϕ is straightforward since t is just a fixed parameter: we have

$$\begin{aligned}\phi(x,y) &= (2-t)\,\mathrm{e}^t + \sin t + (t+2s-2)\,\mathrm{e}^{s+t} \\ &= (2-2x+y)\,\mathrm{e}^{2x-y} + \sin(2x-y) + (y-2)\,\mathrm{e}^x\,,\end{aligned} \tag{9.21}$$

where in the last line we used (9.19).

Note the following features of the above construction:

– If any characteristic curve intersects the initial curve B more than once then the problem is over–determined. In this case the value of $h(t)$ must be constrained at all such multiple intersection points or no solution will exist. For example, in the case of a homogeneous equation, we must have $h(t_1) = h(t_2)$ for any points $t_1, t_2 \in B$ that intersect the same characteristic curve.

– If the initial curve B is itself a characteristic curve then either the solution either does not exist or, if it does, it will not be unique. The solution will fail to exist if the Cauchy data $h(t)$ does not vary along B in the same way as the differential equation says our solution ϕ itself should vary as we move along this characteristic curve. If it does, then our solution is not unique because it is not determined on any other characteristic.

– If the initial curve is transverse to all characteristics and intersects them once only, then the problem is well–posed for any $h(t)$ and has a unique solution $\phi(x, y)$ (at least in a neighbourhood of B). Note that the initial data cannot be propagated from one characteristic to another. In particular, we see that if $h(t)$ is discontinuous, then these discontinuities will propagate along the corresponding characteristic curve.

In summary, to solve the quasi–linear[38] equation $\alpha\phi_x+\beta\phi_y = f(u, x, y)$ with $\phi|_B = h(t)$ on an initial curve B, we first write down the equations (9.6) which are o.d.e.s determining the characteristic curves. These are solved subject to the condition that they intersect B when $s = 0$. We then algebraically invert these relations to obtain $t = t(x, y)$ and $s = s(x, y)$. Along any given characteristic curve C_t the p.d.e. for ϕ becomes

$$\left.\frac{\partial\phi}{\partial s}\right|_t = f(\phi, x, y)|_{C_t} \tag{9.22}$$

which is just an o.d.e. in the variable s. We solve this o.d.e. subject to the initial condition $\phi(s = 0, t) = h(t)$, which gives ϕ as a function of s and t. Finally, substituting in the relations $t = t(x, y)$ and $s = s(x, y)$ we obtain $\phi(x, y)$ for any x, y in a neighbourhood of B.

9.2 Characteristics for second order p.d.e.s

New features emerge when we try to generalize the idea of characteristics to higher order p.d.e.s. The 'type' of equation we're dealing with determines what kind of Cauchy data should be imposed where in order to have a unique solution, and whether these solutions may develop singularities even starting from smooth Cauchy data.

9.2.1 Classification of p.d.e.s

In this section we'll give a rough classification of second order p.d.e.s in a way that helps identify equations with similar properties. To start, suppose $\phi : \mathbb{R}^n \to \mathbb{C}$ and consider the general second order linear differential operator

$$\mathcal{L} := a^{ij}(x)\frac{\partial^2\phi}{\partial x^i\,\partial x^j} + b^i(x)\frac{\partial\phi}{\partial x^i} + c(x)\phi = 0 \tag{9.23}$$

where $(x^1, x^2, \ldots, x^n)$ are coordinates on $\mathbb{R}^n$ and where the coefficient functions a^{ij}, b^i and c are real–valued. Note we may assume that $a^{ij} = a^{ji}$ without loss of generality. Introducting an auxiliary variable $k \in \mathbb{R}^n$, we define the *symbol* of $\mathcal{L}$ to be the polynomial

$$\sigma(x, k) := \sum_{i,j=1}^{n} a^{ij}(x)k_ik_j + \sum_{i=1}^{n} b^i(x)k_i + c(x) \tag{9.24}$$

in k. Likewise, the *principal part* of the symbol is the leading term

$$\sigma^{\mathrm{p}}(x, k) = \sum_{i,j} a^{ij}(x)k_ik_j\,. \tag{9.25}$$

[38] In a *quasi–linear* equation the coefficients of the leading

Thus, for any fixed $x \in \mathbb{R}^n$, $\sigma^{\mathrm{p}}(x,k)$ defines a quadratic form in the k_i variables. Note also that since $a^{ij} = a^{ji}$ this quadratic form is real and symmetric. For example, the symbol of the Laplacian ∇^2 is $\sum_{i=1}^n (k_i)^2$ while the symbol of the heat operator $\partial/\partial x^0 - \nabla^2$ is $k_0 - \sum_{i=1}^n (k_i)^2$ where we treat the coordinate x^0 as time. The principal part of the symbol of the Laplacian is the same as the symbol itself, whilst for the heat operator the principal part of the symbol is $-\sum_i (k_i)^2$, the k_0 term being dropped.

The idea behind this definition is that principal part of the symbol tells us how the differential operator behaves when acting on very rapidly varying functions: for such functions we expect the higher–order derivatives to dominate over lower–order ones, or over the value of the function itself. We can also see that, if the coefficient functions $a^{ij}(x)$, $b^i(x)$ and $c(x)$ are in fact constant then the symbol of $\mathcal{L}$ is essentially its Fourier transform. More precisely, if $\tilde{\phi}(k) = \int_{\mathbb{R}^n} \mathrm{e}^{-\mathrm{i}k\cdot x}\, \phi(x)\, \mathrm{d}^n x$ is the Fourier transform of $\phi(x)$ then $\sigma(\mathrm{i}k)\tilde{\phi}(k)$ is the Fourier transform of $\mathcal{L}\phi(x)$ if $\mathcal{L}$ has constant coefficients.

We now classify our second–order p.d.e.'s according to the principal part of their symbol. We treat $\sigma^{\mathrm{p}}(x,k)$ as a symmetric, real–valued quadratic form $\sigma^{\mathrm{p}}(x,k) = \mathbf{k}^{\mathrm{T}}\mathbf{A}\mathbf{k}$ where $\mathbf{A}$ is the matrix with entries $a^{ij}(x)$. Recalling that the eigenvalues of a real, symmetric matrix are always real, a second order differential operator of the form (9.23) is said to be

- *elliptic* if the eigenvalues of the principal part of the symbol all have the same sign,
- *hyperbolic* if all but one of the eigenvalues of the principal part of the symbol have the same sign,
- *ultrahyperbolic* if there is more than one eigenvalue with each sign, and
- *parabolic* if the quadratic form is degenerate (there are zero eigenvalues).

This classification will be significant for the behaviour of solutions, especially in relation to their Cauchy data, via characteristics. Note that in general, the coefficient functions $a^{ij}(x)$ depend on the location $x \in \mathbb{R}^n$, so a single differential operator can be hyperbolic, ultrahyperbolic, parabolic or elliptic in different regions inside $\mathbb{R}^n$.

As an example, consider the general second–order linear differential operator on $\mathbb{R}^2$

$$\mathcal{L} = a(x,y)\frac{\partial^2}{\partial x^2} + 2b(x,y)\frac{\partial^2}{\partial x\,\partial y} + c(x,y)\frac{\partial^2}{\partial y^2} + d(x,y)\frac{\partial}{\partial x} + e(x,y)\frac{\partial}{\partial y} + f(x,y) \qquad (9.26)$$

The principal part of the symbol of this differential operator is

$$\sigma^{\mathrm{p}}(x,k) = (k_x,\, k_y)\begin{pmatrix} a(x,y) & b(x,y) \\ b(x,y) & c(x,y) \end{pmatrix}\begin{pmatrix} k_x \\ k_y \end{pmatrix} \qquad (9.27)$$

and so the equation is elliptic if $b^2 - ac < 0$, hyperbolic if $b^2 - ac > 0$ and parabolic if $b^2 - ac = 0$. (Since we are in two dimensions, ultrahyperbolic operators cannot arise.) Thus the wave operator is hyperbolic (since $c = 1$, $b = 0$, $a = -(\text{wave speed})^2$), the heat operator is parabolic ($a = 0$, $b = 0$, $c = -(\text{diffusion constant})$) and the Laplace operator is elliptic ($a = c = 1$, $b = 0$).

9.2.2 Characteristic surfaces

We now introduce the notion of a characteristic curve (in two dimensions) or characteristic surface (in > 2 dimensions) for second–order p.d.e.s. The surface $C \in \mathbb{R}^n$ defined by $f(x^1, x^2, \ldots, x^n) = 0$ is a *characteristic surface* of the operator $\mathcal{L}$ in (9.23) *at a point* $x \in \mathbb{R}^n$ if

$$a^{ij}(x)\,\frac{\partial f}{\partial x^i}\,\frac{\partial f}{\partial x^j} = 0\,, \qquad \text{or equivalently} \qquad (\nabla f)^{\mathrm{T}}\,\mathbf{A}\,(\nabla f) = 0\,. \tag{9.28}$$

C is a *characteristic surface* for $\mathcal{L}$ if it is characteristic everywhere.

Now let's look for characteristics of our different types of differential operator. Firstly, if $\mathcal{L}$ is elliptic, the matrix $\mathbf{A}$ is definite and so there are no non–trivial solutions of (9.28). Thus an elliptic operator has no (real) characteristic surfaces. Consequently, the method of characteristics is not going to be applicable to elliptic p.d.e.'s such as Laplace's equation (at least if we insist on working over the reals).

Next, consider a parabolic operator. For simplicity, we consider the case where it has only one zero eigenvalue and let $\mathbf{n}$ be the corresponding normalised eigenvector. Thus $\mathbf{An} = \mathbf{n}^{\mathrm{T}}\mathbf{A} = 0$ and $\mathbf{n}\cdot\mathbf{n} = 1$. We decompose ∇f as

$$\begin{aligned} \nabla f &= \mathbf{n}\,(\mathbf{n}\cdot\nabla f) + (\nabla f - \mathbf{n}\,(\mathbf{n}\cdot\nabla f)) \\ &=: \mathbf{n}\,(\mathbf{n}\cdot\nabla f) + \nabla_\perp f \end{aligned} \tag{9.29}$$

into its parts along $\mathbf{n}$ and orthogonal to $\mathbf{n}$ wrt the quadratic form $\mathbf{A}$. Then

$$\begin{aligned} (\nabla f)^{\mathrm{T}}\,\mathbf{A}\,(\nabla f) &= \left[\mathbf{n}\,(\mathbf{n}\cdot\nabla f) + \nabla_\perp f\right]^{\mathrm{T}}\,\mathbf{A}\,\left[\mathbf{n}\,(\mathbf{n}\cdot\nabla f) + \nabla_\perp f\right] \\ &= (\nabla_\perp f)^{\mathrm{T}}\,\mathbf{A}\,(\nabla_\perp f)\,, \end{aligned} \tag{9.30}$$

using the fact that $\mathbf{n}$ is a left– and right–eigenvector of $\mathbf{A}$, with eigenvalue 0. Now, the *rhs* of this equation involves only $\nabla_\perp f$ which lives in the (positive or negative) definite eigenspace of $\mathbf{A}$. Thus, just as in the elliptic case, there are no non–trivial solutions to $(\nabla_\perp f)^{\mathrm{T}}\,\mathbf{A}\,(\nabla_\perp f) = 0$. Therefore, if f is to define a characteristic surface, it must be independent of all the coordinates in directions orthogonal to $\mathbf{n}$. However, the value of $\mathbf{n}\cdot\nabla f$ is unconstrained by the characteristic equation, so surfaces whose normal vector is given by $\mathbf{n}$ are characteristic surfaces. Thus there is a unique characteristic surface through any point $x \in \mathbb{R}^n$ at which $\mathcal{L}$ is parabolic (with a single zero eigenvalue).

Finally, we consider a hyperbolic operator. In this case all eigenvalues of $\mathbf{A}$ but one have the same sign. Suppose for definiteness that only one eigenvalue is negative and let $-\lambda$ be this negative eigenvalue, with $\mathbf{m}$ the corresponding unit eigenvector. Decomposing ∇f into its parts along and perpendicular to $\mathbf{m}$ as before, we now have

$$\begin{aligned} (\nabla f)^{\mathrm{T}}\,\mathbf{A}\,(\nabla f) &= \left[\mathbf{m}\,(\mathbf{m}\cdot\nabla f) + \nabla_\perp f\right]^{\mathrm{T}}\,\mathbf{A}\,\left[\mathbf{m}\,(\mathbf{m}\cdot\nabla f) + \nabla_\perp f\right] \\ &= (\mathbf{m}\cdot\nabla f)^2\left(\mathbf{m}^{\mathrm{T}}\mathbf{A}\mathbf{m}\right) \;+\; (\nabla_\perp f)^{\mathrm{T}}\,\mathbf{A}\,(\nabla_\perp f) \\ &= -\lambda(\mathbf{m}\cdot\nabla f)^2 + (\nabla_\perp f)^{\mathrm{T}}\,\mathbf{A}\,(\nabla_\perp f)\,, \end{aligned} \tag{9.31}$$

The characteristic condition $(\nabla f)^{\mathrm{T}}\,\mathbf{A}\,(\nabla f) = 0$ thus determines $(\mathbf{m}\cdot\nabla f)$ in terms of $\nabla_\perp f$ via

$$\mathbf{m}\cdot\nabla f = \pm\sqrt{\frac{(\nabla_\perp f)^{\mathrm{T}}\,\mathbf{A}\,(\nabla_\perp f)}{\lambda}}\,. \tag{9.32}$$

Given any function f, defining a candidate for a characteristic surface, the value of the *rhs* of (9.32) is fixed. Thus, for either choice of sign, we can regard (9.32) as an o.d.e. determining the dependence of f on the variable pointing along the direction of $\mathbf{n}$. Such first–order o.d.e.'s will always have solutions and since we have two possible choices of sign, we can find two possible characteristic surfaces through any point $x \in \mathbb{R}^n$. In summary, there are *two* separate characteristic surfaces through any point $x \in \mathbb{R}^n$ at which a differential operator $\mathcal{L}$ is hyperbolic.

Let's clarify how this machinery works with a couple of examples. Recalling the differential operator (9.26) in $\mathbb{R}^2$, the surface $f(x,y) = 0$ is a curve C which is characteristic if

$$(\partial_x f,\, \partial_y f) \begin{pmatrix} a(x,y) & b(x,y) \\ b(x,y) & c(x,y) \end{pmatrix} \begin{pmatrix} \partial_x f \\ \partial_y f \end{pmatrix} = 0\,. \tag{9.33}$$

We can write the curve $f(x,y) = 0$ as $y = y(x)$, and then the fact that f stays constant along this curve implies

$$0 = \frac{\partial f}{\partial x} + \frac{\partial f}{\partial y}\frac{dy}{dx} \qquad \text{so that} \qquad \frac{\partial_x f}{\partial_y f} = -\frac{dy}{dx}\,. \tag{9.34}$$

Consequently, equation (9.33) becomes a quadratric equation in dy/dx with solution

$$\frac{dy}{dx} = -\frac{-b \pm \sqrt{b^2 - ac}}{a}\,. \tag{9.35}$$

If $b^2 - ac \geq 0$ we can solve this nonlinear o.d.e. to find the characteristic curves $y(x)$. In particular, as we saw before, hyperbolic operators (where $b^2 - ac > 0$) have two characteristic curves through each point, while parabolic operators ($b^2 - ac = 0$) have only one. As expected, elliptic operators ($b^2 - ac < 0$) have no real characteristic curves.

To pick a specific case, consider the equation $\partial_y^2\phi - xy\,\partial_x^2\phi = 0$. The second–order differential operator here has $a = -xy$, $b = 0$ and $c = 1$ so $b^2 - ac = xy$. Thus the equation is hyperbolic in the first ($x, y > 0$) and third ($x, y < 0$) quadrants, elliptic in the second and fourth quadrants and parabolic along the axes $x = 0$ or $y = 0$. In the hyperbolic region we have

$$\frac{-b \pm \sqrt{b^2 - ac}}{a} = \pm\frac{1}{\sqrt{xy}}\,, \tag{9.36}$$

so the two families of characteristics are given by

$$\frac{dy}{dx} = \pm\frac{1}{\sqrt{xy}} \qquad \text{with solution} \qquad \frac{1}{3}y^{3/2} \pm x^{1/2} = c \tag{9.37}$$

for some constant c. The substitutions

$$u = \frac{1}{3}y^{3/2} + x^{1/2}$$
$$v = \frac{1}{3}y^{3/2} - x^{1/2}$$

reduce the equation to the canonical form

$$\frac{\partial^2\phi}{\partial u\,\partial v} + \text{lower–order terms} = 0 \tag{9.38}$$

in the hyperbolic region, though we omit the (straightforward but tedious) proof.

9.2.3 d'Alembert's general solution of the wave equation

An especially important example of a hyperbolic equation and its characteristics is the wave equation

$$\frac{\partial^2\phi}{\partial t^2} - c^2\frac{\partial^2\phi}{\partial x^2} = 0 \tag{9.39}$$

with $\phi(x,0) = f(x)$ and $\partial_t\phi(x,0) = g(x)$. This equation is hyperbolic in the whole (x,t) plane, and the characteristics are easily calculated to be $x \pm ct = \text{const}$. We thus introduce new variables

$$u = x - ct \qquad \text{and} \qquad v = x + ct \tag{9.40}$$

whereupon the equation takes the especially simple canonical form

$$\frac{\partial^2\phi}{\partial u\,\partial v} = 0\,. \tag{9.41}$$

The general solution is obtained by first integrating with respect to u, giving $\partial\phi/\partial v = F(v)$, and then

$$\phi(x,t) = G(u) + \int^v F(y)\,\mathrm{d}y = G(u) + H(v) \tag{9.42}$$

for some arbitrary functions G and H. (Here G is the arbitrary integration constant from the v integral.) The general solution is thus the sum of two terms that are each constant along one of the two families of characteristics.

Let us now impose our initial conditions on the general solution (9.42). Recalling that at $u, v = x \mp ct$ we obtain

$$\begin{aligned} \phi(x,0) = G(x) + H(x) &= f(x) \\ \partial_t\phi(x,0) = -cG'(x) + cH'(x) &= g(x) \end{aligned} \tag{9.43}$$

Differentiating the first equation and adding $1/c$ times the second gives $2H'(x) = f'(x) + \frac{1}{c}g(x)$ so that

$$\begin{aligned} H(x) &= \frac{f(x) - f(0)}{2} + \frac{1}{2c}\int_0^x g(y)\,\mathrm{d}y \\ G(x) &= \frac{f(x) + f(0)}{2} - \frac{1}{2c}\int_0^x g(y)\,\mathrm{d}y \end{aligned} \tag{9.44}$$

and so we obtain d'Alembert's very elegant general solution

$$\begin{aligned} \phi(x,t) &= G(x-ct) + H(x+ct) \\ &= \frac{f(x+ct) + f(x-ct)}{2} + \frac{1}{2c}\int_{x-ct}^{x+ct} g(y)\,\mathrm{d}y\,. \end{aligned} \tag{9.45}$$

We see that $\phi(x,t)$ is determined fully by the values of the initial functions f, g in the interval $[x-ct, x+ct]$ of the x-axis, whose endpoints are cut out by the characteristics through the point (x,t). This interval is called the *domain of dependence* for the solution at (x,t). Conversely, the initial data at the point $(x_0,0)$ of the x–axis at time $t=0$ itself *influences* $\phi(x,t)$ at points (x,t) in the wedge–shaped region bounded by the characteristics $x \pm ct = x_0$ through $(x_0,0)$ — that is, in the region $x_0 - ct < x < x_0 + ct$. Thus disturbances

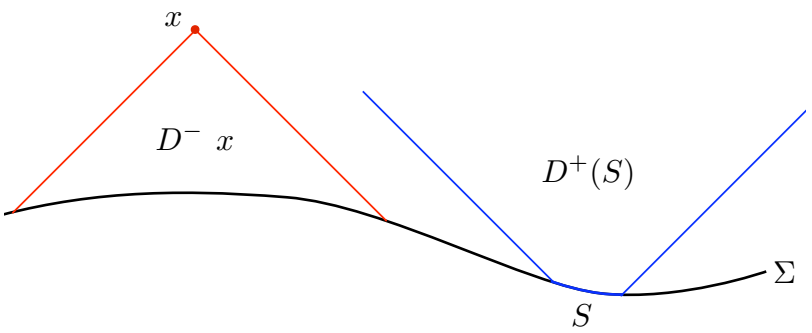


Figure 15. *Characteristics of the wave equation travel left and right with speed c. $D^-(p)$ is the (past) domain of dependence of a point p; the solution at x is governed by the Cauchy data on $D^-(x) \cap \Sigma$. The range of influence $D^+(S)$ of a set $S \subset \Sigma$ is the set of points the Cauchy data on S can influence.*

or signals travel only with speed c. (See figure 15.) In the final problem set, you'll show that the situation is very different for parabolic equations such as the heat equation, according to which signals can propagate arbitrarily rapidly.

Finally, notice that discontinuities in the initial data f propagate along characteristics. For example, suppose we have initial conditions $\phi(x,0) = \Theta(x)$ and $\partial_t \phi(x,0) = 0$, where as usual $\Theta(x)$ is the step function. Then the general solution is

$$\phi(x,t) = \frac{\Theta(x-ct) + \Theta(x+ct)}{2}\,. \tag{9.46}$$

This shows that the discontinuity (a unit step) which is initially located at $x = 0$ simply propagates out to the left and right with velocity $\pm c$, *i.e.* along the characteristic curves, each with half unit height.

9.2.4 Black holes

10 Green's functions for PDEs

In this final chapter we will apply the idea of Green's functions to PDEs, enabling us to solve the wave equation, diffusion equation and Laplace equation in unbounded domains. We will also see how to solve the inhomogeneous (*i.e.* forced) version of these equations, and uncover a relationship, known as Duhamel's principle, between these two classes of problem. In our construction of Green's functions for the heat and wave equation, Fourier transforms play a starring role via the 'differentiation becomes multiplication' rule. We derive Green's identities that enable us to construct Green's functions for Laplace's equation and its inhomogeneous cousin, Poisson's equation. We conclude with a look at the method of images — one of Lord Kelvin's favourite pieces of mathematical trickery.

10.1 Fourier transforms for the heat equation

Consider the Cauchy problem for the heat equation

$$\frac{\partial \phi}{\partial t} = D\nabla^2 \phi \tag{10.1}$$

on $\mathbb{R}^n \times [0, \infty)$, where D is the diffusion constant and where ϕ obeys the conditions

$$\phi|_{\mathbb{R}^n \times \{0\}} = f(\mathbf{x}) \qquad \text{and} \qquad \lim_{|\mathbf{x}| \to \infty} \phi(\mathbf{x}, t) = 0 \ \ \forall\, t\,. \tag{10.2}$$

Taking the Fourier transform w.r.t. the spatial variables we have

$$\frac{\partial}{\partial t}\tilde{\phi}(\mathbf{k}, t) = -D|\mathbf{k}|^2\, \tilde{\phi}(\mathbf{k}, t) \tag{10.3}$$

with initial condition $\tilde{\phi}(\mathbf{k}, 0) = \tilde{f}(\mathbf{k})$. This equation has a unique solution satisfying the initial conditions, given by

$$\tilde{\phi}(\mathbf{k}, t) = \tilde{f}(\mathbf{k})\, \mathrm{e}^{-D|\mathbf{k}|^2 t}\,. \tag{10.4}$$

Our solution $\phi(\mathbf{x}, t)$ itself is the inverse Fourier transform of the product of $\tilde{f}(\mathbf{k})$ with the Gaussian $\mathrm{e}^{-D|\mathbf{k}|^2 t}$, and the convolution theorem tells us that this will be the convolution of the initial data $f(\mathbf{x}) = \mathcal{F}^{-1}[\tilde{f}]$ with the inverse Fourier transform of the Gaussian. On the third problem sheet you've already shown that, for a Gaussian in one variable

$$\mathcal{F}[\mathrm{e}^{-a^2 x^2}] = \frac{\sqrt{\pi}}{a} \mathrm{e}^{-\frac{k^2}{4a^2}} \tag{10.5}$$

and therefore, setting $a^2 = 1/4Dt$ and treating t as a fixed parameter in performing the Fourier transforms, we find $\mathcal{F}^{-1}[\mathrm{e}^{-Dtk^2}] = \mathrm{e}^{-x^2/4Dt}/\sqrt{4\pi Dt}$ in one dimension, or

$$\mathcal{F}^{-1}[\mathrm{e}^{-D|\mathbf{k}|^2 t}] = \frac{1}{(4\pi Dt)^{n/2}} \exp\left(-\frac{|\mathbf{x}|^2}{4Dt}\right) =: S_n(\mathbf{x}, t) \tag{10.6}$$

in n dimensions, since the n–dimensional Gaussian is a product of n Gaussians in independent variables, each of which may be (inverse) Fourier transformed separately. The function $S_n(\mathbf{x}, t)$ is known as the *fundamental solution* of the diffusion equation.

Putting everything together, the general solution to our Cauchy problem is the convolution

$$\phi(\mathbf{x},t) = (f * S_n)(\mathbf{x},t) = \frac{1}{(4\pi Dt)^{n/2}} \int_{\mathbb{R}^n} f(\mathbf{y}) \, \exp\left(-\frac{|\mathbf{x}-\mathbf{y}|^2}{4Dt}\right) \mathrm{d}^n y \tag{10.7}$$

Notice that, provided f is integrable, this function indeed obeys $\phi \to 0$ as $|\mathbf{x}| \to \infty$. Also note the appearance of the dimensionless similarity variable $\eta^2 = \frac{|\mathbf{x}|^2}{4Dt}$ that we previously introduced.

For example, suppose instead we take the initial condition itself to be a Gaussian

$$f(\mathbf{x}) = \left(\frac{a}{\pi}\right)^{n/2} \phi_0 \, \mathrm{e}^{-a|\mathbf{x}|^2} \,, \tag{10.8}$$

normalised so that $\int_{\mathbb{R}^n} f(\mathbf{x}) \, \mathrm{d}^n x = \phi_0$. In this case, our general solution (10.7) gives

$$\begin{aligned}
\phi(\mathbf{x},t) &= \phi_0 \left(\frac{a}{4\pi^2 Dt}\right)^{n/2} \int_{\mathbb{R}^n} \exp\left(-a|\mathbf{y}|^2 - \frac{|\mathbf{x}-\mathbf{y}|^2}{4Dt}\right) \mathrm{d}^n y \\
&= \phi_0 \left(\frac{a}{4\pi^2 Dt}\right)^{n/2} \int_{\mathbb{R}^n} \exp\left(\frac{-(1+4aDt)|\mathbf{y}|^2 + 2\mathbf{x}\cdot\mathbf{y} - |\mathbf{x}|^2}{4Dt}\right) \mathrm{d}^n y \\
&= \phi_0 \left(\frac{a}{4\pi^2 Dt}\right)^{n/2} \exp\left(-\frac{a|\mathbf{x}|^2}{1+4aDt}\right) \int_{\mathbb{R}^n} \exp\left(\frac{-(1+4aDt)}{4Dt} \left|\mathbf{y} - \frac{\mathbf{x}}{1+4aDt}\right|^2\right) \mathrm{d}^n y \\
&= \phi_0 \left(\frac{a}{\pi^2} \, \frac{1}{1+4aDt}\right)^{n/2} \exp\left(-\frac{a|\mathbf{x}|^2}{1+4aDt}\right) \int_{\mathbb{R}^n} \mathrm{e}^{-|\mathbf{z}|^2} \, \mathrm{d}^n z \,,
\end{aligned} \tag{10.9}$$

where in going to the last line we've substituted

$$\mathbf{z} = \sqrt{\frac{1+4aDt}{4Dt}} \left(\mathbf{y} - \frac{\mathbf{x}}{1+4aDt}\right) \qquad \text{and thus} \qquad \mathrm{d}^n y = \left(\frac{4Dt}{1+4aDt}\right)^{n/2} \mathrm{d}^n z \,.$$

Thus finally

$$\phi(\mathbf{x},t) = \phi_0 \left(\frac{a/\pi}{1+4aDt}\right)^{n/2} \exp\left(-\frac{a|\mathbf{x}|^2}{1+4aDt}\right) . \tag{10.10}$$

Thus an initial Gaussian retains a Gaussian form, with its squared width $(1+4aDt)/a$ spreading linearly with t (recall linear growth of variance for diffusing probabilistic processes) while the total area remains constant (*c.f.* the conservation law we obtained for the heat equation in chapter 4) and the peak at $\mathbf{x} = 0$ drops as $t^{-1/2}$. This is as we saw in chapter 4, see in particular figure 8.

As a limiting case, suppose the initial profile Gaussian (10.8) becomes more and more sharply peaked around $\mathbf{x} = 0$, retaining the same total amount of heat ϕ_0. Then in the limit $f(\mathbf{x}) = \phi_0 \, \delta^n(\mathbf{x})$ and our solution (10.7) becomes simply

$$\begin{aligned}
\phi(\mathbf{x},t) &= \frac{\phi_0}{(4\pi Dt)^{n/2}} \int_{\mathbb{R}^n} \delta^{(n)}(\mathbf{y}) \, \exp\left(-\frac{|\mathbf{x}-\mathbf{y}|^2}{4Dt}\right) \mathrm{d}^n y \\
&= \phi_0 \, S_n(\mathbf{x},t) \,.
\end{aligned} \tag{10.11}$$

In other words, the fundamental solution *is* the solution (up to a constant factor) when the initial condition is a δ-function. For all $t > 0$, the δ-pulse spreads as a Gaussian. As $t \to 0^+$ we regain the δ function as a Gaussian in the limit of zero width while keeping the area constant (and hence unbounded height).

A striking property of this solution is that $|\phi| > 0$ everywhere throughout $\mathbb{R}^n$ for any finite $t > 0$, no matter how small. Thus, unlike for the wave equation, disturbances propagate via the heat equation arbitrarily rapidly — the presence of the spike of heat at the origin when $t = 0$ affects the solution at arbitrarily great distances (even if only by exponentially suppressed terms) immediately. Mathematically, this is a consequence of the fact that the heat equation is parabolic, and so has only one family of characteristic surfaces (in this case, they are the surfaces $t = \text{const.}$). Physically, we see that the heat equation is not compatible with Special Relativity; once again this is because it is really just a macroscopic approximation to the underlying statistical mechanics of microscopic particle motion.

10.1.1 The forced heat equation

In the previous section we solved the homogeneous equation with inhomogeneous boundary conditions. Here instead suppose ϕ solves the inhomgeneous (forced) heat equation

$$\frac{\partial \phi}{\partial t} - D\nabla^2 \phi = F(\mathbf{x}, t) \tag{10.12}$$

on $\mathbb{R}^n \times [0, \infty)$, but now with *homogeneous* boundary conditions:

$$\phi|_{\mathbb{R}^n \times \{0\}} = 0 \qquad \text{and} \qquad \lim_{|\mathbf{x}| \to \infty} \phi = 0 \ \ \forall\, t\,. \tag{10.13}$$

Note that the general case — the inhomogeneous equation with inhomogeneous boundary conditions — can be reduced to these two cases: We can write the solution as $\phi = \phi_{\mathrm{h}} + \phi_{\mathrm{f}}$ where ϕ_{h} satisfies the homogeneous equation with the given inhomogeneous boundary conditions while ϕ_{f} obeys the forced equation with homogeneous boundary conditions. (Such a decomposition will clearly apply to all the other equations we consider later.)

Turning to (10.12), we seek a Green's function $G(\mathbf{x}, t; \mathbf{y}, \tau)$ such that

$$\frac{\partial}{\partial t} G(\mathbf{x}, t; \mathbf{y}, \tau) - D\nabla^2 G(\mathbf{x}, t; \mathbf{y}, \tau) = \delta(t - \tau)\, \delta^{(n)}(\mathbf{x} - \mathbf{y}) \tag{10.14}$$

and where $G(\mathbf{x}, 0; \mathbf{y}, \tau) = 0$ in accordance with our homogeneous initial condition. Given such a Green's function, the function

$$\phi(\mathbf{x}, t) = \int_0^\infty \int_{\mathbb{R}^n} G(\mathbf{x}, t; \mathbf{y}, \tau)\, F(\mathbf{y}, \tau)\, \mathrm{d}^n y\, \mathrm{d}\tau\,, \tag{10.15}$$

solves (at least formally) the forced heat equation (10.12) using the defining equation (10.14) of the Green's function and the definition of the δ-functions.

To construct the Green's function, again take the Fourier transform of (10.14) w.r.t. the spatial variables $\mathbf{x}$, recalling that $\mathcal{F}[\delta^{(n)}(\mathbf{x} - \mathbf{y})] = \mathrm{e}^{-\mathrm{i}\mathbf{k}\cdot\mathbf{y}}$. After multiplying through by $\mathrm{e}^{Dk^2 t}$ we obtain

$$\frac{\partial}{\partial t}\left[\mathrm{e}^{D|\mathbf{k}|^2 t}\, \tilde{G}(\mathbf{k}, t; \mathbf{y}, \tau)\right] = \mathrm{e}^{-\mathrm{i}\mathbf{k}\cdot\mathbf{y} + D|\mathbf{k}|^2 t}\, \delta(t - \tau) \tag{10.16}$$

subject to the initial condition $\tilde{G}(\mathbf{k}, 0; \mathbf{y}, \tau) = 0$. This equation is easily solved, and we find that the Fourier transform of the Green's function is

$$\begin{aligned}\tilde{G}(\mathbf{k}, t; \mathbf{y}, \tau) &= \mathrm{e}^{-\mathrm{i}\mathbf{k}\cdot\mathbf{y} - D|\mathbf{k}|^2 t} \int_0^t \mathrm{e}^{D|\mathbf{k}|^2 u}\, \delta(u - \tau)\, \mathrm{d}u \\ &= \begin{cases} 0 & t < \tau \\ \mathrm{e}^{-\mathrm{i}\mathbf{k}\cdot\mathbf{y} - D|\mathbf{k}|^2(t-\tau)} & t > \tau \end{cases} \\ &= \Theta(t - \tau)\, \mathrm{e}^{-\mathrm{i}\mathbf{k}\cdot\mathbf{y} - D|\mathbf{k}|^2(t-\tau)}\,,\end{aligned} \tag{10.17}$$

where $\Theta(t - \tau)$ is the step function. Finally, taking the inverse Fourier transform in the $\mathbf{k}$ variables we recover the Green's function itself as

$$G(\mathbf{x}, t; \mathbf{y}, \tau) = \frac{\Theta(t - \tau)}{(2\pi)^n} \int_{\mathbb{R}^n} \mathrm{e}^{\mathrm{i}\mathbf{k}\cdot(\mathbf{x}-\mathbf{y})}\, \mathrm{e}^{-D|\mathbf{k}|^2(t-\tau)}\, \mathrm{d}^n k\,. \tag{10.18}$$

We recognise the integral here as the (inverse) Fourier transform of a Gaussian exactly as in (10.6), but where the resulting function has arguments $\mathbf{x}' = \mathbf{x} - \mathbf{y}$ and $t' = t - \tau$. Thus we immediately have

$$G(\mathbf{x}, t; \mathbf{y}, \tau) = \Theta(t - \tau)\, S_n(\mathbf{x} - \mathbf{y}, t - \tau) \tag{10.19}$$

where

$$S_n(\mathbf{x}', t') = \frac{1}{(4\pi D t')^{n/2}}\, \exp\left(-\frac{|\mathbf{x}'|^2}{4Dt'}\right)$$

is the *same* fundamental solution we encountered in studying the homogeneous equation with inhomogeneous boundary conditions.

10.1.2 Duhamel's principle

The fact that the *same* function $S_n(\mathbf{x}, t)$ appeared in both the solution to the homogeneous equation with inhomogeneous boundary conditions, and the solution to the inhomogeneous equation with homogeneous boundary conditions is not a coincidence. To see this, let's return to (10.7) but now suppose we impose

$$\phi|_{\mathbb{R}^n \times \{\tau\}} = f(\mathbf{x}) \tag{10.20}$$

at time $t = \tau$ (rather than at $t = 0$). A simple time translation of (10.7) shows that for times $t > \tau$, this problem is solved by

$$\phi_{\mathrm{h}}(\mathbf{x}, t) = \int_{\mathbb{R}^n} f(\mathbf{y})\, S_n(\mathbf{x} - \mathbf{y}, t - \tau)\, \mathrm{d}^n y\,. \tag{10.21}$$

Thus, the initial data $f(\mathbf{x})$ at $t = \tau$ has been propagated using the fundamental solution for a time $t - \tau$ up to time t. On the other hand, using the causality constraint from the step function, the solution (10.15) for the forced problem takes the form

$$\phi_{\mathrm{f}}(\mathbf{x}, t) = \int_0^t \left[\int_{\mathbb{R}^n} F(\mathbf{y}, \tau)\, S_n(\mathbf{x} - \mathbf{y}, t - \tau)\, \mathrm{d}^n y\right] \mathrm{d}\tau\,. \tag{10.22}$$

Now suppose that for each fixed time $t = \tau$, we view the forcing term $F(\mathbf{y}, t)$ as an *initial condition* (!) imposed at $t = \tau$. The integral in square brackets above represents the effect of this condition propagated to time t as in (10.21). Finally, the time integral in (10.22) expresses the solution ϕ_{f} to the forced problem as the accumulation (superposition) of the effects from all these conditions at times τ *earlier* than t, each propagated for time interval $t - \tau$ up to time t. The upper limit t of this integral arose from the step function $\Theta(t - \tau)$ in the Green's function (10.19) and expresses causality: the solution at time t depends only on the cumulative effects of 'initial' conditions applied at earlier times $\tau < t$. Conversely, an 'initial condition' applied at time τ cannot influence the past ($t < \tau$).

The relation between solutions to homogeneous equations with inhomogeneous boundary conditions and inhomogeneous equations with homogeneous boundary conditions is known as *Duhamel's principle*. Below, we'll see it in action in the wave equation, too.

10.2 Fourier transforms for the wave equation

In this section, we'll apply Fourier transforms to the wave equation. Suppose $F : \mathbb{R}^n \times [0, \infty)$ is a given forcing term and that ϕ solves the forced wave equation

$$\frac{\partial^2 \phi}{\partial t^2} - c^2 \nabla^2 \phi = F \tag{10.23}$$

on $\mathbb{R}^n \times (0, \infty)$, subject to the homogeneous initial conditions that

$$\phi|_{\mathbb{R}^n \times \{0\}} = 0\,, \qquad \partial_t \phi|_{\mathbb{R}^n \times \{0\}} = 0 \qquad \text{and} \qquad \lim_{|\mathbf{x}| \to \infty} \phi = 0\,, \tag{10.24}$$

and where c is the wave (phase) speed. As usual we seek a Green's function $G(\mathbf{x}, t; \mathbf{y}, \tau)$ that obeys the simpler problem

$$\left(\frac{\partial^2}{\partial t^2} - c^2 \nabla^2 \right) G(\mathbf{x}, t; \mathbf{y}, \tau) = \delta(t - \tau)\, \delta^{(n)}(\mathbf{x} - \mathbf{y}) \tag{10.25}$$

where the forcing term is replaced by δ-functions in all time and space variables, and where the Green's function obeys the same boundary conditions

$$G(\mathbf{x}, 0; \mathbf{y}, \tau) = 0\,, \qquad \partial_t G(\mathbf{x}, 0; \mathbf{y}, \tau) = 0 \qquad \text{and} \qquad \lim_{|\mathbf{x}| \to \infty} G(\mathbf{x}, t; \mathbf{y}, \tau) = 0 \tag{10.26}$$

as ϕ itself. Once again, if we can find such a Green's function then our problem (10.23) is solved by

$$\phi(\mathbf{x}, t) = \int_0^\infty \int_{\mathbb{R}^n} F(\mathbf{y}, \tau)\, G(\mathbf{x}, t; \mathbf{y}, \tau)\, \mathrm{d}^n y\; \mathrm{d}\tau\,, \tag{10.27}$$

at least formally.

Proceeding as before, we Fourier transform the defining equation for the Green's function wrt the spatial variables $\mathbf{x}$, obtaining

$$\frac{\partial^2}{\partial t^2} \tilde{G}(\mathbf{k}, t; \mathbf{y}, \tau) + |\mathbf{k}|^2 c^2\, \tilde{G}(\mathbf{k}, t; \mathbf{y}, \tau) = \mathrm{e}^{-\mathrm{i}\mathbf{k}\cdot\mathbf{y}}\, \delta(t - \tau)\,. \tag{10.28}$$

Again, this is subject to the conditions that both $\tilde{G}$ and $\partial_t \tilde{G}$ vanish at $t = 0$. Treating $\mathbf{k}$ as a parameter, we recognize this equation as an initial value problem in the variable t — essentially the same as the example given previously at the end of section 7.5. As we found there, The solution is

$$\tilde{G}(\mathbf{k}, t; \mathbf{y}, \tau) = \Theta(t - \tau)\, \mathrm{e}^{-\mathrm{i}\mathbf{k}\cdot\mathbf{y}}\, \frac{\sin\left(|\mathbf{k}|c(t-\tau)\right)}{c|\mathbf{k}|}\,, \tag{10.29}$$

as we found there.

To recover the Green's function itself we must compute the inverse Fourier transform

$$G(\mathbf{x}, t; \mathbf{y}, \tau) = \frac{\Theta(t-\tau)}{(2\pi)^n} \int_{\mathbb{R}^n} \mathrm{e}^{\mathrm{i}\mathbf{k}\cdot(\mathbf{x}-\mathbf{y})}\, \frac{\sin|\mathbf{k}|c(t-\tau)}{c|\mathbf{k}|}\, \mathrm{d}^n k \tag{10.30}$$

Unlike the case of the heat equation, here the form of the Green's function is sensitive to the number of spatial dimensions. To proceed, for definiteness we'll pick $n = 3$, which is physically the most important case. We introduce polar coordinates for $\mathbf{k}$ chosen so that

$$|\mathbf{k}| = k \qquad \text{and} \qquad \mathbf{k}\cdot(\mathbf{x}-\mathbf{y}) = k|\mathbf{x}-\mathbf{y}|\,\cos\theta$$

That is, we choose to align the z-axis in $\mathbf{k}$–space along whatever direction $\mathbf{x} - \mathbf{y}$ points. Thus, in three spatial dimensions the Green's function becomes

$$\begin{aligned} G(\mathbf{x}, t; \mathbf{y}, \tau) &= \frac{\Theta(t-\tau)}{(2\pi)^3} \int_{\mathbb{R}^3} \mathrm{e}^{\mathrm{i}k|\mathbf{x}-\mathbf{y}|\,\cos\theta}\, \frac{\sin kc(t-\tau)}{ck}\, \mathrm{d}^3 k \\ &= \frac{\Theta(t-\tau)}{(2\pi)^2 c} \int_0^\infty \left[\int_{-1}^1 \mathrm{e}^{\mathrm{i}k|\mathbf{x}-\mathbf{y}|\,\cos\theta}\, \mathrm{d}(\cos\theta)\right] \sin kc(t-\tau)\, k\, \mathrm{d}k \\ &= \frac{\Theta(t-\tau)}{2\pi\mathrm{i}c|\mathbf{x}-\mathbf{y}|} \left[\frac{1}{2\pi}\int_{-\infty}^\infty \mathrm{e}^{\mathrm{i}k|\mathbf{x}-\mathbf{y}|}\, \sin kc(t-\tau)\, \mathrm{d}k\right] \end{aligned} \tag{10.31}$$

where in going to the third line we used that fact that result of integrating over $\cos\theta$ leaves us with an even function of k. We recognise the remaining integral (the contents of the square bracket in the last line) as the inverse Fourier transform of $\sin kc(t-\tau)$, where the variable conjugate to k is $|\mathbf{x}-\mathbf{y}|$. From (8.43) we have that

$$\mathcal{F}^{-1}[\sin ka] = \frac{\mathrm{i}}{2}\left(\delta(x+a) - \delta(x-a)\right) \tag{10.32}$$

and therefore our Green's function is

$$\begin{aligned} G(\mathbf{x}, t; \mathbf{y}, \tau) &= \frac{\Theta(t-\tau)}{4\pi c|\mathbf{x}-\mathbf{y}|}\left[\delta(|\mathbf{x}-\mathbf{y}| + c(t-\tau)) - \delta(|\mathbf{x}-\mathbf{y}| - c(t-\tau))\right] \\ &= -\frac{1}{4\pi c|\mathbf{x}-\mathbf{y}|}\,\delta(|\mathbf{x}-\mathbf{y}| - c(t-\tau)) \end{aligned} \tag{10.33}$$

where we note that the first δ-function has no support in the region where the step function is non–zero, and that in the second line the argument of the δ–function already ensures $t - \tau > 0$ so the step function is superfluous. The fact that only this term contributes to our δ–function can be traced to the boundary conditions we imposed in (10.26). The Green's function here is often called the *retarded* Green's function.

Using this Green's function, our solution ϕ can finally be written as

$$\begin{aligned}\phi(\mathbf{x},t) &= -\int_0^\infty \frac{1}{4\pi c}\int_{\mathbb{R}^n}\frac{F(\mathbf{y},\tau)}{|\mathbf{x}-\mathbf{y}|}\,\delta(|\mathbf{x}-\mathbf{y}|-c(t-\tau))\,\mathrm{d}^n y\;\mathrm{d}\tau \\ &= -\frac{1}{4\pi c^2}\int_{\mathbb{R}^n}\frac{F(\mathbf{y},t_{\mathrm{ret}})}{|\mathbf{x}-\mathbf{y}|}\,\mathrm{d}^n y\end{aligned} \tag{10.34}$$

where the *retarded time* t_{ret} is defined by

$$ct_{\mathrm{ret}} := ct - |\mathbf{x}-\mathbf{y}|\,. \tag{10.35}$$

The retarded time illustrates the finite propagation speed for disturbances that obey the wave equation: the effect of the forcing term F at some point $\mathbf{y}$ is felt by the solution at a different location $\mathbf{x}$ only after time $t - t_{\mathrm{ret}} = |\mathbf{x}-\mathbf{y}|/c$ has elapsed. This is how long it took the disturbance to travel from $\mathbf{y}$ to $\mathbf{x}$, and is in perfect agreement with what we expect from our discussion of characterstics for the wave equation.

Above we solved the forced wave equation in $3+1$ dimensions. As an exercise, I recommend you show that the general solution to the forced wave equation with homogeneous boundary conditions in $1+1$ dimensions is

$$\begin{aligned}\phi(x,t) &= \int_0^t\int_{\mathbb{R}} F(y,\tau)\,\frac{\Theta(c(t-\tau)-|x-y|)}{2c}\,\mathrm{d}y\,\mathrm{d}\tau \\ &= \frac{1}{2c}\int_0^t\int_{x-c(t-\tau)}^{x+c(t-\tau)} F(y,\tau)\,\mathrm{d}y\,\mathrm{d}\tau\,.\end{aligned} \tag{10.36}$$

(Really — have a go! — it's not entirely trivial.) Thus, the retarded Green's function in $1{+}1$ dimensions is a step function, which in the second line we used to restrict the region over which we take the y–integral. Using the step function this way means that the order of the remaining integrations is important if we are to capture the correct, τ-dependent domain of influence (*i.e.* $y \in [x-c(t-\tau), x+c(t-\tau)]$) of the forcing term.

We can also see Duhamel's principle in operation for the wave equation here. Comparing to equation (9.45), we see that for $t > \tau$

$$\frac{1}{2c}\int_{x-c(t-\tau)}^{x+c(t-\tau)} F(y,\tau)\,\mathrm{d}y$$

is simply d'Alembert's solution to the homogeneous (unforced) wave equation in the case that the (inhomogeneous) initial data is given by

$$\phi(x,\tau) = 0 \qquad \text{and} \qquad \partial_t\phi(x,\tau) = F(x,\tau)\,, \tag{10.37}$$

with these conditions imposed when $t = \tau$. Hence the solution (10.36) of the forced equation with homogeneous initial data can again be viewed as a superposition of influences from the forcing term F used as an initial condition (here on the time–derivative of ϕ) for each $\tau < t$.

10.3 Poisson's equation

Poisson's equation for a function $\phi : \mathbb{R}^n \to \mathbb{C}$ is the forced Laplace equation

$$\nabla^2 \phi = -F(\mathbf{x}) \tag{10.38}$$

where as always the forcing term $F : \mathbb{R}^n \to \mathbb{C}$ is assumed to be given, and the minus sign on the *rhs* of (10.38) is conventional. We will again solve this equation by first constructing a Green's function for it, although the solution via Green's functions is less straightforward than for either the heat or wave equations — in particular, we will not obtain it via Fourier transforms (the Green's function itself will turn out not to be absolutely integrable). We also note that, since there is no time variable (the equation is elliptic), the solutions will have no notion of causality.

10.3.1 The fundamental solution

The *fundamental solution* G_n to Poisson's equation in n–dimensions is defined to be the solution to the problem

$$\nabla^2 G_n(\mathbf{x}; \mathbf{y}) = \delta^{(n)}(\mathbf{x} - \mathbf{y}) \,, \tag{10.39}$$

where the forcing term is chosen to be just an n–dimensional δ-function. Since the problem rotationally symmetric about the special point $\mathbf{y}$, the fundamental solution can only depend on the scalar distance from that point:

$$G_n(\mathbf{x}; \mathbf{y}) = G_n(|\mathbf{x} - \mathbf{y}|) \,. \tag{10.40}$$

Integrating both sides of (10.39) over a ball

$$B_r = \{\mathbf{x} \in \mathbb{R}^n \ : \ |\mathbf{x} - \mathbf{y}| \leq r.\}$$

of radius r centred on $\mathbf{y}$ we obtain

$$1 = \int_{B_r} \nabla^2 G_n \, \mathrm{d}V = \int_{\partial B_r} \mathbf{n} \cdot \nabla G_n \, \mathrm{d}S \tag{10.41}$$

where the integral of the δ-function gives 1, and we've used the divergence theorem to reduce the integral of $\nabla^2 G_n$ to an integral over the boundary sphere $\partial B_r = \{\mathbf{x} \in \mathbb{R}^n \ : |\mathbf{x} - \mathbf{y}| = r\}$. When $n = 3$, this is the surface of a 'standard' sphere, while it is a circle when $n = 2$ and a 'hypersphere' for $n > 3$. In each case, the outward pointing normal $\mathbf{n}$ points in the radial direction, so $\mathbf{n} \cdot \nabla G_n = dG_n/dr$. Thus we obtain

$$1 = \int_{\partial B_r} \frac{dG_n}{dr} \, r^{n-1} \, \mathrm{d}\Omega_n = r^{n-1} \frac{dG_n}{dr} \int_{S^{n-1}} \mathrm{d}\Omega_n \tag{10.42}$$

where we have used the fact that G is a function only of the radius, and where $\mathrm{d}\Omega_n$ is the measure on a unit S^{n-1}; for example

$$\mathrm{d}\Omega_n = \begin{cases} \sin\theta \, \mathrm{d}\theta \, \mathrm{d}\phi & \text{when n=3} \\ \mathrm{d}\theta & \text{when n=2} \end{cases} .$$

The remaining angular integral just gives the total 'surface area' A_n of our $(n-1)$–dimensional sphere. In particular, $A_2 = 2\pi$ is the circumference of a circle, whereas $A_3 = 4\pi$ is the total solid angle of a sphere in three dimensions[39]. Then

$$\frac{dG_n}{dr} = \frac{1}{Ar^{n-1}}\,. \tag{10.43}$$

This ode is easily solved to show that the fundamental solution is

$$G_n(\mathbf{x};\mathbf{y}) = \begin{cases} |\mathbf{x}-\mathbf{y}| + c_1 & n = 1 \\ \dfrac{1}{2\pi}\log|\mathbf{x}-\mathbf{y}| + c_2 & n = 2 \\ -\dfrac{1}{A_n(n-2)}\dfrac{1}{|\mathbf{x}-\mathbf{y}|^{n-2}} + c_n & n \geq 3 \end{cases} \tag{10.44}$$

When $n \geq 3$ we can fix the constant c_n to be zero by requiring $\lim_{r\to\infty} G(r) = 0$; however, this condition cannot be imposed in either one or two dimensions, and some other condition (usually suggested by the details of a specific problem) must instead be imposed.

Note that when $n > 1$ these fundamental solutions satisfy the Laplace equation for all $\mathbf{x} \in \mathbb{R}^n - \{\mathbf{y}\}$, but that they become singular at $\mathbf{x} = \mathbf{y}$. Thus we shall need to exercise special care when using them as Green's functions for the Poisson equation throughout $\mathbb{R}^n$.

10.3.2 Green's identities

Green's identities[40] establish a relationship between the fundamental solutions G_n and solutions of Poisson's equation.

First, suppose $\Omega \subset \mathbb{R}^n$ is a compact set with boundary $\partial\Omega$, and let $\phi, \psi : \Omega \to \mathbb{R}$ be a pair of functions on Ω that are regular throughout Ω. Then the product rule and divergence theorem give[41]

$$\begin{aligned} \int_\Omega \nabla\cdot(\phi\nabla\psi)\,\mathrm{d}V &= \int_\Omega \phi\,\nabla^2\psi + (\nabla\phi)\cdot(\nabla\psi)\,\mathrm{d}V \\ &= \int_{\partial\Omega} \phi\,(\mathbf{n}\cdot\nabla\psi)\,\mathrm{d}S \end{aligned} \tag{10.45}$$

where $\mathbf{n}$ is the outward pointing normal to $\partial\Omega$. This is *Green's first identity*. Simply interchanging ϕ and ψ we likewise find

$$\int_\Omega \nabla\cdot(\psi\nabla\phi)\,\mathrm{d}V = \int_\Omega \psi\,\nabla^2\phi + (\nabla\psi)\cdot(\nabla\phi)\,\mathrm{d}V = \int_{\partial\Omega} \psi\,(\mathbf{n}\cdot\nabla\phi)\,\mathrm{d}S\,, \tag{10.46}$$

and subtracting this equation from the previous one we arrive at

$$\int_\Omega \phi\,\nabla^2\psi - \psi\,\nabla^2\phi\;\,\mathrm{d}V = \int_{\partial\Omega} \phi\,(\mathbf{n}\cdot\nabla\psi) - \psi\,(\mathbf{n}\cdot\nabla\phi)\,\mathrm{d}S\,, \tag{10.47}$$

[39] You may enjoy showing that $A_n = 2\pi^{(n-1)/2}/\Gamma((n-1)/2)$ in general, where $\Gamma(t) = \int_0^\infty x^{t-1}\,\mathrm{e}^{-x}\,\mathrm{d}x$ is Euler's Gamma function. We won't need this result, though.

[40] Green's identities are sometimes called Green's theorems, but they're not to be confused with the two–dimensional version of the divergence theorem!

[41] I'm using the notation $\mathrm{d}V$ to denote the standard Cartesian measure $\mathrm{d}^n x$ on Ω, and $\mathrm{d}S$ to denote the measure on the $(n-1)$-dimensional boundary of Ω.

which is *Green's second identity.*

In order to make use of this result, we'd like to apply it to the case that $\psi = G_n$, our fundamental solution. However, $G_n(\mathbf{x}, \mathbf{y})$ is singular at $\mathbf{y}$ (at least when $n > 1$) so it's not clear that the derivation of (10.47) is valid, because the divergence theorem usually requires functions to be regular throughout Ω. Let's give a more careful derivation. Let B_ϵ be a ball of radius $\epsilon \ll 1$ centred on the dangerous point $\mathbf{y}$, and let Ω be the region

$$\Omega = B_r - B_\epsilon = \{\mathbf{x} \in \mathbb{R}^n : \epsilon \leq |\mathbf{x} - \mathbf{y}| \leq r\}\,. \tag{10.48}$$

Now G_n is perfectly regular everywhere within Ω, so we can apply Green's second identity with $\psi = G_n$ to find

$$\begin{aligned}
&\int_\Omega \phi\,\nabla^2 G_n - G_n \nabla^2 \phi \;\mathrm{d}V = -\int_\Omega G_n \nabla^2 \phi \;\mathrm{d}V \\
&= \int_{\partial\Omega} \phi\,(\mathbf{n}\cdot\nabla G_n) - G_n\,(\mathbf{n}\cdot\nabla\phi)\;\mathrm{d}S \\
&= \int_{S_r^{n-1}} \phi\,(\mathbf{n}\cdot\nabla G_n) - G_n\,(\mathbf{n}\cdot\nabla\phi)\;\mathrm{d}S + \int_{S_\epsilon^{n-1}} \phi\,(\mathbf{n}\cdot\nabla G_n) - G_n\,(\mathbf{n}\cdot\nabla\phi)\;\mathrm{d}S
\end{aligned} \tag{10.49}$$

where the first equality follows since $\nabla^2 G_n = 0$ in Ω, and we've included contributions from both boundary spheres (with radii r and ϵ) in the final line. On the inner boundary — a sphere of radius ϵ — the *outward*–pointing unit normal is $\mathbf{n} = -\hat{\mathbf{r}}$ and we have

$$\begin{aligned}
G_n|_{\text{inner bdry}} &= -\frac{1}{A_n(n-2)}\,\frac{1}{\epsilon^{n-2}} \\
\mathbf{n}\cdot\nabla G_n|_{\text{inner bdry}} &= -\frac{1}{A_n}\,\frac{1}{\epsilon^{n-1}}\,.
\end{aligned} \tag{10.50}$$

The measure on an $(n-1)$–dimensional sphere of radius ϵ is $\mathrm{d}S = \epsilon^{n-1}\,\mathrm{d}\Omega_n$ where again $\mathrm{d}\Omega_n$ is an integral over angles. Thus the final term in the last line of (10.49) is given by

$$-\int_{S_\epsilon^{n-1}} G_n\,(\mathbf{n}\cdot\nabla\phi)\;\mathrm{d}S = \epsilon\int(\mathbf{n}\cdot\nabla\phi)\;\mathrm{d}\Omega_n\,. \tag{10.51}$$

Since ϕ is regular at $\mathbf{y}$ by assumption, the value of the remaining integral is bounded, so this term vanishes as $\epsilon \to 0$. On the other hand, the penultimate term in the final line of (10.49) becomes

$$\int_{S_\epsilon^{n-1}} \phi\,(\mathbf{n}\cdot\nabla G_n)\,\mathrm{d}S = -\frac{1}{A_n}\int \phi\;\mathrm{d}\Omega_n = -\,\bar{\phi} \tag{10.52}$$

where $\bar{\phi}$ is the *average* value of ϕ on the small sphere surrounding $\mathbf{y}$. As the radius of this sphere shrinks to zero we have $\bar{\phi} \to \phi(\mathbf{y})$, the value of ϕ at the centre of the sphere. Putting all this together we find

$$\phi(\mathbf{y}) = \int_\Omega G_n \nabla^2\phi\;\mathrm{d}V + \int_{\partial\Omega} \phi\,(\mathbf{n}\cdot\nabla G_n) - G_n\,(\mathbf{n}\cdot\nabla\phi)\,\mathrm{d}S \tag{10.53}$$

as our new form of Green's second identity involving G_n, where now we take the boundary of Ω to be just the large sphere (the radius of the inner sphere having been shrunk to zero).

Finally, we take ϕ to be a solution to Poisson's equation $\nabla^2\phi = -F$, whereupon we obtain *Green's third identity*

$$\phi(\mathbf{y}) = -\int_\Omega G_n(\mathbf{x},\mathbf{y})\, F(\mathbf{x})\,\mathrm{d}V + \int_{\partial\Omega} \left[\phi(\mathbf{x})\,(\mathbf{n}\cdot\nabla G_n(\mathbf{x},\mathbf{y})) - G_n(\mathbf{x},\mathbf{y})\,(\mathbf{n}\cdot\nabla\phi(\mathbf{x}))\right]\,\mathrm{d}S \tag{10.54}$$

where the integrals are over the $\mathbf{x}$ variables. This is a remarkable formula. Recalling that $\mathbf{y}$ can be any point in $\mathbb{R}^n$, we see that (10.54) describes the solution throughout our domain in terms of the solution on the *boundary*, the known function G_n and the forcing term. Also notice that (unlike the previous cases we have considered in the course) the Green's function is here providing an expression for the solution with *in*homogeneous boundary conditions. Provided ϕ and $\mathbf{n}\cdot\nabla\phi$ tend to zero suitably fast at asymptotically large distances, the boundary terms in (10.54) can be neglected. In this case, Green's third identity also shows that G_n is the free–space Green's function for the Poisson equation; this also follows formally from the definition $\nabla^2 G_n = \delta^{(n)}(\mathbf{x}-\mathbf{y})$, since

$$\nabla^2\phi(\mathbf{y}) = -\int_{\mathbb{R}^n} (\nabla^2_{\mathbf{y}}\, G_n(\mathbf{x},\mathbf{y}))\, F(\mathbf{x})\,\mathrm{d}V = -\int_{\mathbb{R}^n} \delta^{(n)}(\mathbf{x}-\mathbf{y})\, F(\mathbf{x})\,\mathrm{d}V = -F(\mathbf{y}) \tag{10.55}$$

where the Laplacian is wrt $\mathbf{y}$.

There's something puzzling about equation (10.54) however. Setting $F = 0$, (10.54) provides an expression for the solution ϕ of the *Laplace* equation $\nabla^2\phi = 0$ in the interior of a domain Ω in terms of the values of both ϕ and $\mathbf{n}\cdot\nabla\phi$ on the boundary. But we already know that if Ω is a compact domain with boundary $\partial\Omega$, then $\phi|_{\partial\Omega}$ alone is enough to specify a *unique* solution to Laplace's equation (Dirichlet boundary condtions), while $\mathbf{n}\cdot\nabla\phi|_{\partial\Omega}$ alone gives a solution unique up to a constant (Neumann). How then should we interpret the Green's identity (10.54), involving *both* $\phi|_{\partial\Omega}$ and $\mathbf{n}\cdot\nabla\phi|_{\partial\Omega}$? The point is that whilst (10.54) (with $F = 0$) is a valid expression obeyed by any solution to Laplace's equation, it's not a constructive expression — we can't use it to *solve* for ϕ in terms of boundary data, because the boundary values of ϕ and $\mathbf{n}\cdot\nabla\phi$ cannot be specified independently.

10.3.3 Dirichlet Green's functions for the Laplace & Poisson equations

In view of this curious 'over–determined' property of equation (10.54), we now finally ask how *can* the Dirichlet[42] problem for the Laplace and Poisson equations be solved using Green's function techniques, in domains with boundaries? We do so by constructing a

[42]It's also interesting to ask about the Neumann problem (where $\mathbf{n}\cdot\nabla\phi$ is specified on the boundary), but in this course we'll discuss only the Dirichlet problem. The reason is that the Neumann problem is somewhat more complicated than the Dirichlet problem since (unlike the Dirichlet case) a consistency condition must be satisfied by the boundary data if a solution is to exist at all. Indeed, suppose we specify $\mathbf{n}\cdot\nabla\phi|_{\partial\Omega} = g$ for some choice of function $g : \partial\Omega \to \mathbb{R}$. It turns out that we cannot pick g freely, since

$$\int_{\partial\Omega} g\,\mathrm{d}^{n-1}S = \int_{\partial\Omega} \mathbf{n}\cdot\nabla\phi\,\mathrm{d}^{n-1}S = \int_\Omega \nabla^2\phi\,\mathrm{d}^{n-1}x = -\int_\Omega F\,\mathrm{d}^n x\,,$$

by the divergence theorem. Thus, in the Neumann case, the boundary data must be correlated with the integral of the forcing function F (the *rhs* of Poisson's equation), integrated over the whole domain. This consistency condition complicates the construction of a Green's function.

Dirichlet Green's function for the Laplacian operator on Ω (with $\mathbf{x}, \mathbf{y} \in \Omega$). This is defined to be the function $G(\mathbf{x};\mathbf{y}) := G_n(\mathbf{x};\mathbf{y}) + H(\mathbf{x},\mathbf{y})$ where H is finite for *all* $\mathbf{x} \in \Omega$ (including at $\mathbf{x} = \mathbf{y}$), and where H satisfies the Laplace equation throughout Ω. For G to be the Dirichlet Green's function, the boundary value of G should be chosen to cancel that of the fundamental solution G_n, so that $G|_{\partial\Omega} = 0$. Note that G also satisfies the Laplace equation whenever $\mathbf{x} \neq \mathbf{y}$.

We'll see a method for constructing such a Dirichlet Green's function in the following section (though in general it's a difficult problem — finding H requires solving Laplace's equation with non–trivial boundary conditions). For now, let's just suppose G exists. If so, then given G we can use it to solve Poisson's equation on Ω with Dirichlet boundary conditions for ϕ. To see this, suppose $\nabla^2\phi = -F$ inside Ω, with $\phi|_{\partial\Omega} = g$ for some given function $g : \partial\Omega \to \mathbb{R}$. Substituting $G_n = G - H$ into Green's third identity (10.54) gives

$$\phi(\mathbf{y}) = \int_{\partial\Omega} \left[\phi\,(\mathbf{n}\cdot\nabla[G-H]) \;-\; [G-H]\,(\mathbf{n}\cdot\nabla\phi)\right] \mathrm{d}S - \int_\Omega F(\mathbf{x})[G-H]\,\mathrm{d}V\,. \qquad (10.56)$$

Putting $\psi = H$ into Green's second identity (10.47) gives

$$\int_{\partial\Omega} \phi\,(\mathbf{n}\cdot\nabla H) - H\,(\mathbf{n}\cdot\nabla\phi)\,\mathrm{d}S = \int_\Omega F\,H\,\mathrm{d}V\,, \qquad (10.57)$$

where we've used the fact that $\nabla^2 H = 0$ throughout Ω, and that $\nabla^2\phi = -F$. Comparing this with (10.56) shows that all the H terms in (10.56) cancel. We thus obtain

$$\phi(\mathbf{y}) = \int_{\partial\Omega} \phi(\mathbf{x})\,(\mathbf{n}\cdot\nabla G(\mathbf{x},\mathbf{y})) \;-\; G(\mathbf{x},\mathbf{y})\,(\mathbf{n}\cdot\nabla\phi(\mathbf{x}))\,\mathrm{d}S - \int_\Omega F(\mathbf{x})\,G(\mathbf{x},\mathbf{y})\,\mathrm{d}V\,. \qquad (10.58)$$

Finally, having chosen H so as to ensure $G|_{\partial\Omega} = 0$ and using our boundary condition that $\phi|_{\partial\Omega} = g$, we get

$$\phi(\mathbf{y}) = \int_{\partial\Omega} g(\mathbf{x})\,\mathbf{n}\cdot\nabla G(\mathbf{x};\mathbf{y})\,\mathrm{d}S - \int_\Omega F(\mathbf{x})\,G(\mathbf{x};\mathbf{y})\,\mathrm{d}V\,. \qquad (10.59)$$

At last, this expression is constructive; the solution *throughout* Ω is given purely in terms of the known boundary conditions and the Green's function.

If instead we had a Neumann problem with $\mathbf{n}\cdot\nabla\phi|_{\partial\Omega} = g$ being specified, then instead of H we'd seek a harmonic function H' to make $\mathbf{n}\cdot\nabla G|_{\partial\Omega} = 0$. This condition defines H' only up to an additive constant. Then equation (10.58) gives us

$$\phi(\mathbf{y}) = -\int_{\partial\Omega} g(\mathbf{x})\,G(\mathbf{x};\mathbf{y})\,\mathrm{d}S - \int_\Omega F(\mathbf{x})\,G(\mathbf{x},\mathbf{y})\,\mathrm{d}V \qquad (10.60)$$

as the solution to the Neumann problem.

10.4 The method of images

For domains with sufficient symmetry we can sometimes use the elegant *method of images* (also called the reflection method) to construct the required Green's function. Indeed, this method can also be used for the Green's functions of the forced heat and wave equations

too, as well as for homogeneous equations. The key concept is to match the boundary conditions by placing a extending the domain beyond the region of interest, and placing a 'mirror' or 'image' source or forcing term in the unphysical region. We'll content ourselves with just illustrating how this works by looking at a few examples. (You can find more on the final problem sheet.)

10.4.1 Green's function for the Laplace's equation on the half–space

Let $\Omega = \{(x, y, z) \in \mathbb{R}^3 \,:\, z \geq 0\}$ and suppose $\phi : \Omega \to \mathbb{R}$ solves Laplace's equation $\nabla^2\phi = 0$ inside Ω, subject to

$$\phi(x, y, 0) = h(x, y) \qquad \text{and} \qquad \lim_{|\mathbf{x}|\to\infty} \phi = 0\,. \tag{10.61}$$

Before we can use the formula of equation (10.59), we must construct a Green's function which vanishes on $\partial\Omega$. As well as vanishing on the (x, y)–plane, we interpret the boundary condition on the asymptotic value of ϕ in the natural way by requiring G also vanishes as $|\mathbf{x}| \to \infty$. We'll set $\mathbf{x} = (x, y, z)$ and $\mathbf{y} := \mathbf{x}_0^+ = (x_0, y_0, z_0)$ in terms of Cartesian coordinates, with $z_0 > 0$.

We know that the free space Green's function

$$G_3(\mathbf{x}, \mathbf{x}_0^+) = -\frac{1}{4\pi}\frac{1}{|\mathbf{x} - \mathbf{x}_0^+|}$$

satisfies all the conditions *except* that

$$G_3(\mathbf{x}; \mathbf{x_0})|_{z=0} = -\frac{1}{4\pi}\frac{1}{[(x - x_0)^2 + (y - y_0)^2 + z_0^2]^{1/2}} \;\neq\; 0\,, \tag{10.62}$$

so that the homogeneous boundary condition $G|_{z=0} = 0$ does not hold for $G_3(\mathbf{x}; \mathbf{x}_0^+)$. We thus need to 'cancel' the nonzero boundary value of G_3 by adding on some function that solves Laplace's equation throughout our domain. Now let $\mathbf{x}_0^-$ be the point $(x_0, y_0, -z_0)$; in other words, $\mathbf{x}_0^-$ is the reflection of $\mathbf{x}_0^+$ in the boundary plane $z = 0$. The location $\mathbf{x}_0^- \notin \Omega$, so the Green's function $G_3(\mathbf{x}, \mathbf{x}_0^-)$ is regular everywhere within Ω, and so obeys Laplace's equation everywhere in the upper half–space. It's also clear from (10.62) that

$$G_3(\mathbf{x}; \mathbf{x}_0^-)|_{z=0} = G_3(\mathbf{x}; \mathbf{x}_0^+)|_{z=0}\,.$$

Thus the Dirichlet Green's function we seek is

$$\begin{aligned} G(\mathbf{x}; \mathbf{x}_0) &:= G_3(\mathbf{x}; \mathbf{x}_0^+) - G_3(\mathbf{x}; \mathbf{x}_0^-) \\ &= -\frac{1}{4\pi\,|\mathbf{x} - \mathbf{x}_0^+|} + \frac{1}{4\pi\,|\mathbf{x} - \mathbf{x}_0^-|}\,. \end{aligned} \tag{10.63}$$

Note that this expression obeys the asymptotic condition $\lim_{|\mathbf{x}|\to\infty} G(\mathbf{x}, \mathbf{x}_0) = 0$ as well as the boundary condtion $G(\mathbf{x}; \mathbf{x}_0)|_{z=0} = 0$.

The intuition behind this solution is as follows. Recall that the Green's function $G_3(\mathbf{x}; \mathbf{x}_0^+)$ obeyed $\nabla^2 G_3(\mathbf{x}; \mathbf{x}_0^+) = -\delta^{(3)}(\mathbf{x} - \mathbf{x}_0^+)$ and thus describes the contribution $\phi(\mathbf{x})$

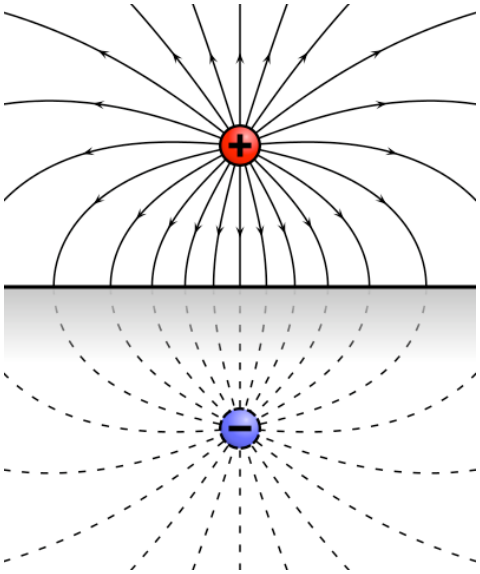


Figure 16. *The contribution to* (10.63) *from the image source in the unphysical region* $z < 0$ *cancels that of the source in the physical region along the plane* $z = 0$. *You can see more examples at this Wikipedia page, from where I took the picture.*

receives from a point source of unit strength placed at $\mathbf{x_0}^+$. On the other hand, if we were solving the problem on $\mathbb{R}^3$ rather than the upper half–space, then $G_3(\mathbf{x}; \mathbf{x}_0^-)$ would represent the contribution to $\phi(\mathbf{x})$ from a point source of *equal magnitude but opposite sign* placed at the mirror location $\mathbf{x}_0^-$. The combined effect of these two sources cancels out at any point $\mathbf{x}$ for which $|\mathbf{x} - \mathbf{x}_0^+| = \mathbf{x} - \mathbf{x}_0^-|$, in other words along the plane $z = 0$ (see figure 16). This is equivalent to the boundary condition we wanted.

To apply the formula (10.59), set $F = 0$ (we're considering Laplace's equation here) and note also that there is no contribution from the far field since $\phi \to 0$ asymptotically by our boundary condition. The *outward* normal from the domain at $z = 0$ points in the negative z-direction, so the only contribution to (10.59) comes from the lower boundary:

$$\begin{aligned}(\mathbf{n} \cdot \nabla G)|_{z=0} &= -\left.\frac{\partial G}{\partial z}\right|_{z=0} \\ &= \frac{1}{4\pi}\left(\frac{z + z_0}{|\mathbf{x} - \mathbf{x}_0^-|^3} - \frac{z - z_0}{|\mathbf{x} - \mathbf{x}_0^+|^3}\right)_{z=0} \\ &= \frac{z_0}{2\pi}\left[(x - x_0)^2 + (y - y_0)^2 + z_0^2\right]^{-3/2}.\end{aligned} \tag{10.64}$$

Therefore we get

$$\phi(x_0, y_0, z_0) = \frac{z_0}{2\pi}\int_{\mathbb{R}^2} \frac{h(x, y)}{\left[(x - x_0)^2 + (y - y_0)^2 + z_0^2\right]^{3/2}}\,\mathrm{d}x\,\mathrm{d}y \tag{10.65}$$

as the solution of the Dirichlet problem for the Laplace equation in the half space.

The method of images can also be applied to (some) more complicated domains. For example, suppose $\Omega = \{(x, y, z) \in \mathbb{R}^3 \ : \ a \leq z \leq b\}$ is the region between two planar boundaries. We can view each of the two boundaries as mirrors and then any special point $\mathbf{x}_0 \in \Omega$ gives rise to a *double infinity* of multiply reflected images — not only must $\mathbf{x}_0$ itself be reflected in each mirror plane, but each of the image points obtained in this way must then be reflected again in the *other* mirror. If the mirror charges are taken with alternating plus and minus signs, we can construct a Green's function that vanishes on both boundaries.

10.4.2 Method of images for the heat equation

We can also apply the method of images to the Green's functions that we developed for the forced wave and heat equations (with the initial conditions all being zero). For example, a chimney will provide a source of smoke $F(\mathbf{x}, t)$ from times $t > 0$ after the fire is lit. If this was a problem in $\mathbb{R}^3 \times [0, \infty)$ then from equation (10.15) the density of smoke at some point $\mathbf{x} \in \mathbb{R}^3$ at time t would be

$$\phi(\mathbf{x}, t) \stackrel{?}{=} \int_0^t \int_{\mathbb{R}^3} F(\mathbf{y}, \tau) \, \frac{1}{(4\pi D(t-\tau))^{3/2}} \, \exp\left(-\frac{|\mathbf{x}-\mathbf{y}|^2}{4D(t-\tau)}\right) \mathrm{d}^3 y \, \mathrm{d}\tau \tag{10.66}$$

using the Green's function $\Theta(t-\tau)\, S_3(\mathbf{x}-\mathbf{y}; t-\tau)$ for the heat (or diffusion) equation on $\mathbb{R}^3 \times [0, \infty)$. However, this is clearly incorrect in the present situation because the smoke does not diffuse into the ground ($z < 0$).

The condition that there be no flow of smoke across the plane $z = 0$ amounts to the Neumann condition that $\partial_z \phi|_{z=0} = 0$. We can ensure this is the case by modifying the Green's function to become

$$G(\mathbf{x}, t; \mathbf{x}_0, \tau) = \Theta(t-\tau) \, \left[S_3(\mathbf{x}-\mathbf{x}_0^+; t-\tau) + S_3(\mathbf{x}-\mathbf{x}_0^-; t-\tau)\right] \tag{10.67}$$

where $\mathbf{x}_0^\pm = (x_0, y_0, \pm z_0)$. Again, the second term here obeys the homogeneous diffusion equation $(\partial_t - D\nabla^2) S_3(\mathbf{x}-\mathbf{x}_0^-; t-\tau) = 0$ for all points $\mathbf{x}$ above ground. One can also easily check that the sum on the *rhs* of (10.67) indeed obeys the Neumann condition $\partial_z G|_{z=0} = 0$. Then the distribution of smoke at time $t > 0$ will be given by

$$\phi(\mathbf{x}, t) = \int_0^t \int_{\mathbb{R}^3} F(\mathbf{x}_0^+, \tau) \, \frac{\left[S_3(\mathbf{x}-\mathbf{x}_0^+; t-\tau) + S_3(\mathbf{x}-\mathbf{x}_0^-; t-\tau)\right]}{(4\pi D(t-\tau))^{3/2}} \, \mathrm{d}^3 x_0 \, \mathrm{d}\tau \tag{10.68}$$

in the region $z > 0$. We can imagine that the second term here describes the smoke emitted by a 'mirror chimney' — the reflection of the real chimney in the boundary plane. The unmodified Green's function (for $\mathbf{x} \in \mathbb{R}^3$) allows smoke to flow into the region $z < 0$, but this is exactly compensated by smoke flowing up into $z > 0$ from the mirror chimney. Note that we take the same source term $F(\mathbf{x}_0^+, \tau) = F(\mathbf{x}_0^-, \tau)$ in order for the smoke distributions to mirror eachother.

I want to emphasize that the second source of smoke in the $z < 0$ region is (of course) entirely fictitious. It's just a device we've introduced in order to help solve our problem

on the upper half space with the condition that no smoke flows across $z = 0$ in either direction. We wanted to find the smoke distribution at points $\mathbf{x}$ in the upper half space. Our solution (10.68) is indeed valid in the region $z > 0$, and obeys the boundary condition $\phi|_{z=0} = 0$ for all times. The uniqueness theorem for solutions of the heat equation on a domain Ω with Dirichlet boundary conditions on $\partial\Omega$ then assures us that we've found the solution we wanted. We could also evaluate (10.68) at points with $z < 0$ and in fact, were this region to be filled with air rather than ground and were the mirror chimney to actually exist, our solution would be correct there. But this is clearly irrelevant to the physical situation.

10.4.3 Method of images for inhomogeneous problems

For homogeneous diffusion or wave problems the method of images can be applied to the *initial data itself*, adapting our previous solutions to be applicable in the presence of extra boundaries.

For example consider the wave equation for $\phi(x,t)$ on the half-line $x \geq 0$, subject to the Neumann boundary condition that $\partial_x\phi(0,t) = 0$, and with initial conditions

$$\phi(x,0) = b(x) \qquad \text{and} \qquad \partial_t\phi(x,0) = 0 \qquad \text{where } x \geq 0\,, \tag{10.69}$$

and where

$$b(x) = \begin{cases} 1 & x_0 - a \leq x \leq x_0 + a \\ 0 & \text{else} \end{cases} \tag{10.70}$$

is the 'top-hat' function. (Physically, the Neumann condition at $x = 0$ physically models small amplitude waves in the vicinity of a frictionless wall.)

d'Alembert's general solution (9.45) shows that the solution on *whole* line $x \in \mathbb{R}$ would be a pair of boxes, each of height half and width $2a$, one traveling to the left and one to the right with speed c. This solution clearly does not satisfy the Neumann boundary condition at $x = 0$ (when the left moving box passes over the origin). To overcome this, we consider an initial 'image box' on the negative x axis, obtained by reflecting the given initial conditions in $x = 0$. Taking this image box to have the *same* sign as the original box, d'Alembert gives us the solution

$$\phi(x,t) = \frac{b(x-ct) + b(x+ct)}{2} + \frac{b(-x-ct) + b(-x+ct)}{2} \tag{10.71}$$

on the whole line. This describes *two* pairs of moving boxes, each member of each pair having height $1/2$. The solution satisfies the initial condition $\phi(x,0) = b(x)$ in the region $x \geq 0$ and satisfies the Neumann boundary condition at $x = 0$ for all time. Thus, $\phi(x,t)$ *restricted* to the region $x \geq 0$ is the solution to our original problem.

It's instructive to picture how this solution evolves in time (especially in the region $x \geq 0$). Let B_R and B_L denote the right and left moving boxes corresponding to the original initial box, and I_R and I_L the boxes from the initial 'image box'. I_L just moves off to the left and never appears as part of the solution for $x \geq 0$. B_R just moves off to the right and is always present in the $x \geq 0$ region. At time $t = (x_0 - a)/c$ the leading

edges of both B_L and I_R reach $x = 0$. As they pass through each other (for a time $2a/c$) the solution piles up to double height where they overlap and then B_L goes off into $x < 0$ while I_R emerges fully into $x \geq 0$. Thereafter, the solution in $x \geq 0$ is just two boxes of heights half, with centres separated by constant distance $2x_0$ (the initial separation of I_L and B_R) moving off to the right at speed c. If we view the solution near $x = 0$ just on the positive side, we see B_L "hit the wall", piling up to double height (and enclosing the same total area at all times) as it appears to be reflected back to the right into $x > 0$ with final shape unchanged, giving the trailing second right-moving box.
