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1B METHODS
LECTURE NOTES

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PART II:

PDEs on bounded domains: Separation of variables

Introduction

Here we begin our study of some of the most important partial differential equations of physics and applied mathematics viz. the wave equation, the diffusion equation and the Laplace equation. We will introduce the method of **separation of variables** which provides a simple but extremely useful means of solution in a wide variety of practical situations. The method involves reducing the PDEs to a set of Sturm-Liouville ODEs. Later in Part IV we will develop a further method of solution (developing associated Green's functions) that can be applied in further contexts, such as in the presence of inhomogeneous (forcing) terms.

3 THE WAVE EQUATION

3.1 Physical significance

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 $\phi(\underline{x}, t)$ characterising the disturbance will satisfy the **wave equation**:

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

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.

To illustrate the physical origin of the wave equation consider small transverse (1 dimensional) vibrations of an elastic string with ends fixed at $x = 0$ and $x = L$. We make the following (physically sensible) assumptions:
– the string is uniform (mass per unit length μ is constant);
– the string is perfectly elastic and offers no resistance to bending;
– the string performs small transverse motions so the deflection and slope remain small in absolute value (we will retain terms only to first order in these quantities);
– we will include gravity (taking the x-axis to be horizontal).
Let $y(x, t)$ denote the vertical deflection of the point at x. 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 vertical, the total horizontal force is zero. Also by Newton's law, $\mu\delta x\partial^2 y/\partial t^2$ is the total vertical force. Thus we get respectively:

$$T_A\cos\theta_A = T_B\cos\theta_B = T = \text{constant} \tag{1}$$

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

Dividing through by the quantities in eq. (1) we get

$$\frac{\mu\delta x}{T}\frac{\partial^2 y}{\partial t^2} = \frac{T_B\sin\theta_B}{T_B\cos\theta_B} - \frac{T_A\sin\theta_A}{T_A\cos\theta_A} - \frac{\mu g\delta x}{T}. \tag{3}$$

Now

$$\frac{T_B\sin\theta_B}{T_B\cos\theta_B} - \frac{T_A\sin\theta_A}{T_A\cos\theta_A} = \tan\theta_B - \tan\theta_A = \left(\frac{\partial y}{\partial x}\right)_B - \left(\frac{\partial y}{\partial x}\right)_A \approx \frac{\partial^2 y}{\partial x^2}\delta x$$

and eq. (3) becomes (after dividing through by $\mu\delta x/T$):

$$\frac{\partial^2 y}{\partial t^2} = c^2\frac{\partial^2 y}{\partial x^2} - g \qquad \text{where} \qquad c^2 = T/\mu$$

i.e. a *forced* wave equation. Neglecting gravity (setting $g=0$) gives the standard wave equation. c (having units of a velocity) 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 $y(0,t)=y(L,t)=0$ for all t) we would expect to have to provide the initial position $y(x,0)$ and the initial velocity $\partial y/\partial t(x,0)$ for $0<x<L$ of all points along the string.

3.2 The method of separation of variables – illustrated by waves on a finite string

Consider the following problem:

$$\frac{\partial^2 y}{\partial t^2} = c^2\frac{\partial^2 y}{\partial x^2}$$

$$\begin{aligned} \text{BCs}: &\quad y(0,t)=y(L,t)=0 \quad \text{for all } t; \\ \text{ICs}: &\quad y(x,0)=\phi(x) \quad \partial y/\partial t(x,0)=\psi(x) \quad \text{for } 0<x<L. \end{aligned}$$

where ϕ and ψ are specified functions on $(0,L)$. It may be shown that this problem, with the given initial and boundary conditions, is well-posed i.e. has a unique solution, as expected from our physical considerations above.

To find this solution, the **method of separation of variables** begins by considering a solution of the following form

$$y(x,t) = X(x)T(t)$$

in which the variables have been "separated", as a product of two single-variable functions. Substituting into the wave equation (and denoting x–derivatives with a prime, and t–derivatives with a dot) gives

$$c^2 X''T = X\ddot{T} \quad \text{i.e.} \quad \frac{1}{c^2}\frac{\ddot{T}}{T} = \frac{X''}{X}$$

Now the key observation is that the LHS (resp. RHS) is a function only of t (resp. only of x) so the only way that they can be equal is for both sides to be equal to the same *constant* which we call $-\lambda$:

$$\frac{1}{c^2}\frac{\ddot{T}}{T} = \frac{X''}{X} = -\lambda$$

so

$$X'' + \lambda X = 0 \tag{4}$$
$$\ddot{T} + \lambda c^2 T = 0 \tag{5}$$

and we get two SL eigenvalue equations with related eigenvalues.

Solving eq. (4), if $\lambda = -\mu^2$ is non-positive we get

$$X = \alpha \cosh \mu x + \beta \sinh \mu x$$

and the BCs $X(0) = X(L) = 0$ give $\alpha = \beta = 0$. Hence λ must be positive and writing $\lambda = \mu^2$ (with $\mu > 0$), we get

$$X = \alpha \cos \mu x + \beta \sin \mu x.$$

Using the BCs we get $\alpha = 0$ (from $X(0) = 0$) and then $X(L) = 0$ gives $\beta \sin \mu L = 0$ i.e. $\mu = n\pi/L$ so

$$\lambda_n = \frac{n^2\pi^2}{L^2} \qquad n = 1, 2, 3, \ldots$$

Note that these are the eigenvalues of the SL system

$$(X')' = -\lambda X$$

having $p(x) = 1$, $q(x) = 0$ and weight function $w(x) = 1$. The associated eigenfunctions

$$X_n(x) = \sin \frac{n\pi x}{L}$$

are called the **normal modes**, corresponding to n half-wavelengths fitting spatially into the domain. The lowest mode $n = 1$ is called the **fundamental mode** and for $n > 1$ they are called harmonics or overtones.

Knowing X_n and λ_n we can return to the time equation eq. (5) and derive the associated time functions $T_n(t)$:

$$\ddot{T}_n + \frac{n^2\pi^2c^2}{L^2}T_n = 0$$

so

$$T_n(t) = \gamma_n \cos\left[\frac{n\pi ct}{L}\right] + \delta_n \sin\left[\frac{n\pi ct}{L}\right],$$

and our specific solution so far is

$$y_n = X_n(x)T_n(t) = \sin\left[\frac{n\pi x}{L}\right]\left(A_n \cos\left[\frac{n\pi ct}{L}\right] + B_n \sin\left[\frac{n\pi ct}{L}\right]\right).$$

The next insight is to note that the wave equation is *linear* (and the BCs are *homogeneous*) so we can superpose solutions to obtain more general solutions of the form

$$y(x,t) = \sum_{n=1}^{\infty} \sin\left[\frac{n\pi x}{L}\right]\left(A_n \cos\left[\frac{n\pi ct}{L}\right] + B_n \sin\left[\frac{n\pi ct}{L}\right]\right) \tag{6}$$

Finally now, the initial conditions require

$$y(x,0) = \phi(x) = \sum_{n=1}^{\infty} A_n \sin\left[\frac{n\pi x}{L}\right]$$

and

$$\frac{\partial y}{\partial t}(x,0) = \psi(x) = \sum_{n=1}^{\infty} \frac{n\pi c}{L} B_n \sin\left[\frac{n\pi x}{L}\right]$$

i.e. the coefficients A_n, B_n are determined from the initial conditions as the Fourier sine series coefficients of ϕ, ψ:

$$\begin{aligned} A_n &= \frac{2}{L}\int_0^L \phi(x)\sin\left[\frac{n\pi x}{L}\right]dx, \\ B_n &= \frac{2}{n\pi c}\int_0^L \psi(x)\sin\left[\frac{n\pi x}{L}\right]dx \end{aligned}$$

completing our solution eq. (6).

Summary of the method:
(1) Separate the variables by writing y as a product of single-variable functions;
(2) Determine the allowed form for the eigenvalues (constants of separation) from the BCs;
(3) Determine the form of all corresponding single-variable eigenfunctions;
(4) Sum over possible separated-variable solutions to form a general series solution;
(5) Determine the coefficients in the general series solution from the initial conditions (using SL orthogonality of the eigenfunctions, to form SL eigenfunction expansions of the initial-value functions). □

Exercise: the plucked string. Determine the full solution for a string initially plucked at its centre i.e. in the above notation $\psi(x) = 0$ and

$$\phi(x) = \begin{cases} 2kx/L & 0 \le x \le L/2 \\ 2k(L-x)/L & L/2 \le x \le L \end{cases}$$

You'll need to check that the Fourier sine series of $\phi(x)$ is

$$\phi(x) = \frac{8k}{\pi^2}\left[\frac{1}{1^2}\sin\frac{\pi x}{L} - \frac{1}{3^2}\sin\frac{3\pi x}{L} + \frac{1}{5^2}\sin\frac{5\pi x}{L} - \cdots\right]$$

3.3 Separation of variables for 2D polar co-ordinates: Bessel's equation, waves on a drum

The previous example lead to very simple SL problems (constant coefficients and weight function $w(x) = 1$) typical of separation of variables in cartesian (rectangular) co-ordinates. For problems with circular or cylindrical symmetry, separation of variables leads to a more interesting equation, known as Bessel's equation, having non-constant weight function and coefficient function $p(x)$.

Consider the wave equation with two spatial dimensions and time, on the unit disc:

$$\frac{\partial^2 u}{\partial t^2} = c^2 \nabla^2 u \quad x^2 + y^2 \leq 1$$

Later we'll specify BCs and ICs. But first, separating the time from the space variables $u(x, y, t) = V(x, y)T(t)$ we get

$$\ddot{T} = -\lambda c^2 T \qquad \nabla^2 V = -\lambda V$$

where we take λ to be non-negative, since (as before) this will be required by our BCs (cf later). Now let us use polar co-ordinates for the space dimensions, and separate these variables too, writing:

$$V = R(r)\Theta(\theta).$$

Then for $\nabla^2 V = -\lambda V$ the Laplacian in polar co-ordinates

$$\nabla^2 V = \frac{\partial^2}{\partial r^2} V + \frac{1}{r^2}\frac{\partial^2}{\partial \theta^2} V + \frac{1}{r}\frac{\partial}{\partial r} V$$

gives (introducing a second constant μ of separation):

$$\begin{aligned} \Theta'' + \mu\Theta &= 0, \\ r^2 R'' + rR' + (\lambda r^2 - \mu)R &= 0. \end{aligned}$$

The Θ equation gives $\Theta = a\cos\sqrt{\mu}\theta + b\sin\sqrt{\mu}\theta$. Due to the circular geometry, Θ must be periodic with period 2π (as θ and $\theta + 2\pi$ are the same physical point), which implies that $\mu = m^2$ (m an integer) and the radial eigenvalue problem becomes

$$r^2 R'' + rR' + (\lambda r^2 - m^2)R = 0. \tag{7}$$

After dividing by r, we get the standard Sturm-Liouville form

$$\frac{d}{dr}\left[r\frac{d}{dr}R\right] - \frac{m^2}{r}R = -\lambda r R \quad r \leq 1, \tag{8}$$

having $p(r) = r$, $q(r) = -m^2/r$ and weight function $w(r) = r$.
(Jumping ahead slightly, note that $p(0) = 0$ and we will later impose BCs $R(1) = 0$ and $R(0)$ bounded, so the LHS of the above equation will be self adjoint.)

Now, substituting $z = \sqrt{\lambda}r$, we get

$$z^2\frac{d^2}{dz^2}R + z\frac{d}{dz}R + (z^2 - m^2)R = 0, \tag{9}$$

which is **Bessel's equation of order** m.

When m is an integer eq. (9) has two linearly independent solutions conventionally called:
• $J_m(z)$, the Bessel function of the first kind of order m, which is *regular at the origin* (and zero there for all $m > 0$);
• $Y_m(z)$, the Bessel function of the second kind of order m, which is *singular at the origin*. (It is sometimes also called the Weber function or Neumann function). Don't confuse the (quite standard) notation Y_m here with our previous use of this for normalised eigenfunctions!

Since Y_m is singular at the origin it will not generally appear in our solutions for problems on a full disc $r \leq a$ (although it generally does appear in problems on an annulus $0 < b \leq r \leq a$ having the origin excluded). We will mostly be concerned with J_m for $m = 0, 1, 2, \ldots$

There is a huge literature on properties of Bessel functions J_α and Y_α, of all (not necessarily integer) orders $\alpha \in \mathbb{R}$ (defined by eq. (9) with α replacing m). We will state here (without proof) some properties relevant to our purposes (but see exercise sheet 1 No. 8 and sheet 2 No. 10 for some derivations). For a more complete account and further properties see for example, chapter 12 of M. Boas "Mathematical Methods in the Physical Sciences".

- Using the Frobenius method of power series in eq. (9) we can derive the formula

$$J_p(z) = \left(\frac{z}{2}\right)^p \sum_{k=0}^{\infty} \frac{(-1)^k}{k!(p+k)!} \left(\frac{z}{2}\right)^{2k} \qquad p = 0, 1, 2, \ldots$$

  (Remark: this formula actually holds for all $p \in \mathbb{R}$ if we replace factorials by the Gamma function $(p+k)! \rightsquigarrow \Gamma(p+k+1)$.)
  We will not give an expression here for Y_p; but see for example Boas' book.

- Small z behaviour. As $z \to 0$:

$$J_p(z) = \frac{1}{p!}\left(\frac{z}{2}\right)^p + O(z^{p+2}) \qquad p = 0, 1, 2, \ldots$$

$$Y_0(z) = O(\ln z) \qquad Y_p(z) = O(\frac{1}{z^p}) \quad p = 1, 2, \ldots$$

- Large z (asymptotic) behaviour. As $z \to \infty$:

$$\begin{aligned} J_p(z) &= \left(\frac{2}{\pi z}\right)^{1/2} \cos\left[z - \frac{p\pi}{2} - \frac{\pi}{4}\right] + O(z^{-3/2}) \\ Y_p(z) &= \left(\frac{2}{\pi z}\right)^{1/2} \sin\left[z - \frac{p\pi}{2} - \frac{\pi}{4}\right] + O(z^{-3/2}). \end{aligned}$$

  Hence we see that J_p and Y_p each have an infinite number of zeroes and turning points (characteristic of our eigenvalue problems). The figure shows graphs of the first few Bessel funtions of integer order.

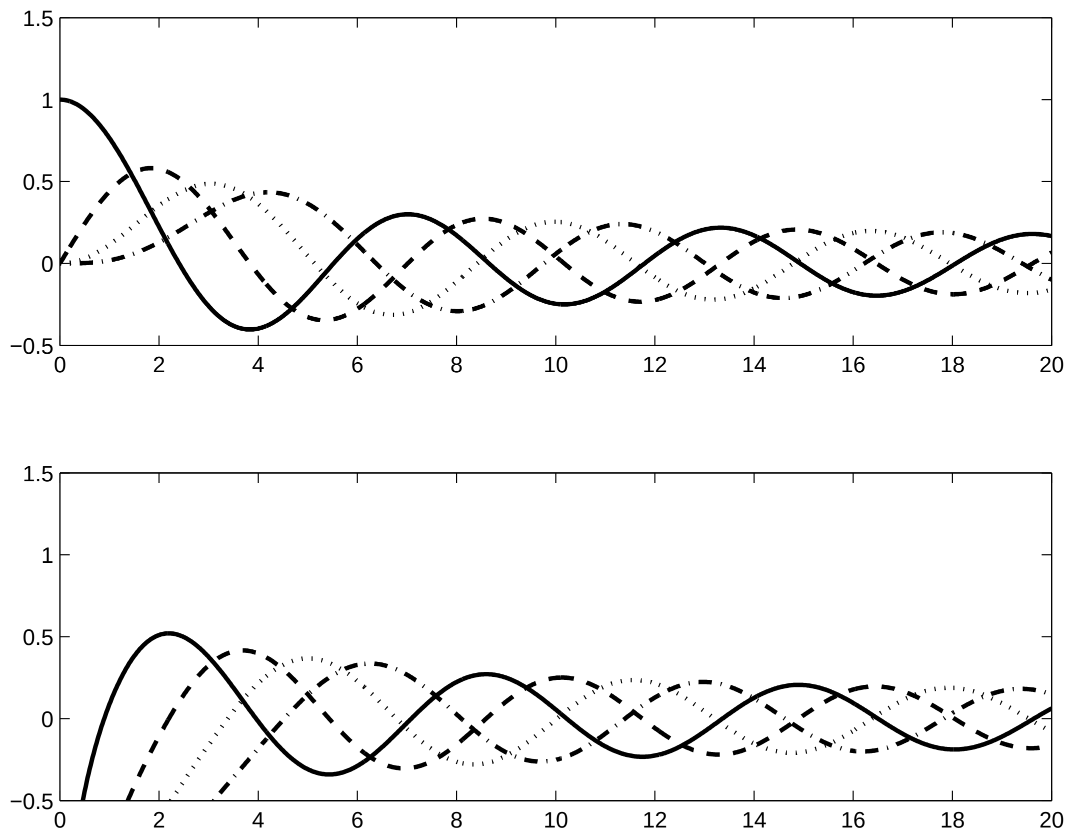

Figure 1: Upper panel: Plots of the Bessel functions of the first kind $J_0(x)$ (solid); $J_1(x)$ (dashed); $J_2(x)$ (dotted); and $J_3(x)$ (dot-dashed). Lower panel: Plots of the Bessel functions of the second kind $Y_0(x)$ (solid); $Y_1(x)$ (dashed); $Y_2(x)$ (dotted); and $Y_3(x)$ (dot-dashed).

Example: the vibrating drum

Returning to our radial equation eq. (9) we see that a priori, the dilated Bessel functions $J_m(\sqrt{\lambda_{mn}}r)$ and $Y_m(\sqrt{\lambda_{mn}}r)$ are appropriate eigenfunctions with eigenvalues λ_{mn} to be determined from the BCs. (Here for each order m of Bessel function we have introduced a second subscript n as we expect a discrete series of eigenvalues). As a concrete example, consider a vibrating drum: we will demand (i) that u is finite when $r = 0$ and (ii) that $u = 0$ when $r = 1$ corresponding to the edge of the drum being clamped. Then (i) excludes Bessel functions Y_m of the second kind and (ii) requires the eigenvalues to be square roots of the zeroes of the Bessel functions of the first kind

$$J_m(\sqrt{\lambda_{mn}}) = 0.$$

For each order m, consider them in increasing order $0 < \lambda_{m1} < \lambda_{m2} < \ldots$ and write $j_{mn} = \sqrt{\lambda_{mn}}$. Then for the spatial component of our solution we have

$$V_{mn}(r, \theta) = J_m(j_{mn}r)\left[\alpha_{mn}\cos m\theta + \beta_{mn}\sin m\theta\right].$$

Note that for $m = 0$ we have simply $V_{0n}(r, \theta) = \alpha_{0n}J_0(j_{0n}r)$. From the time equation $\ddot{T} = -\lambda c^2 T$, we see that for each m, n the associated time function is

$$T(t) = \gamma_{mn}\cos j_{mn}ct + \kappa_{mn}\sin j_{mn}ct.$$

Putting all this together (and relabelling products of arbitrary constants) our general solution incorporating the (homogeneous) BCs takes the form:

$$\begin{aligned} u(r,\theta,t) \;\; = \;\; & \sum_{n=1}^{\infty} J_0(j_{0n}r)\left(A_{0n}\cos j_{0n}ct + C_{0n}\sin j_{0n}ct\right) \\ & + \sum_{m=1}^{\infty}\sum_{n=1}^{\infty} J_m(j_{mn}r)\left(A_{mn}\cos m\theta + B_{mn}\sin m\theta\right)\cos j_{mn}ct \\ & + \sum_{m=1}^{\infty}\sum_{n=1}^{\infty} J_m(j_{mn}r)\left(C_{mn}\cos m\theta + D_{mn}\sin m\theta\right)\sin j_{mn}ct. \end{aligned}$$

To complete the formulation of the problem we need to specify the initial displacement and initial velocity of the drum surface:

$$\begin{aligned} u(r,\theta,0) &= \phi(r,\theta) \\ \frac{\partial u}{\partial t}(r,\theta,0) &= \psi(r,\theta). \end{aligned}$$

The constants in the general solution above are then fixed by expanding ϕ and ψ as Fourier series in θ, and in terms of a series of Bessel functions $J_k(j_{kn}r)$ for the radial co-ordinate. For the latter we use the fact that these (SL eigen-)functions (*for each fixed k, and varying n*) are orthogonal with respect to the weight function $w(r) = r$. Explicitly we have (cf example sheet 1 No. 8 and sheet 2 No. 10 for derivations):

$$\int_0^1 J_k(j_{kn}r)\,J_k(j_{km}r)\,r\,dr = \frac{1}{2}[J_k'(j_{kn})]^2\delta_{mn} = \frac{1}{2}[J_{k+1}(j_{kn})]^2\delta_{mn}. \qquad (10)$$

Indeed from our SL theory we know that the LHS above must be proportional to δ_{mn}, and the particular form of the proportionality factors above can be derived from the power series formulas for the Bessel functions.

Example. To illustrate the above orthogonality formula in action, consider the simple case where the drum is initially at rest so $\phi(r,\theta) = 0$ and is hit by a drumstick at the centre so that

$$\frac{\partial u}{\partial t}(r,\theta,0) = \Psi(r)$$

is a function of r only. The solution is then also independent of θ and all constants are zero except for C_{0n}. (The A_{0n}'s are all zero since $\phi(r,\theta) = 0$ at $t = 0$). Using eq. (10) we get (as you can check):

$$\begin{aligned} u(r,\theta,t) &= \sum_{n=1}^{\infty} J_0(j_{0n}r)C_{0n}\sin[j_{0n}ct], \\ C_{0m} &= \frac{2}{cj_{0m}}\frac{\int_0^1 \Psi(r)rJ_0(j_{0m}r)dr}{[J_0'(j_{0m})]^2}. \end{aligned}$$

Interestingly, the fundamental frequency for a drum of general diameter d is $2j_{01}c/d \sim 4.8c/d$ (where we have rescaled our expression above to make $r_{\max} = d/2$), which is higher than that of a string of length d (which is $\pi c/d$). Also, the fundamental response of the drum is just a Bessel function, showing that we actually experience these functions rather frequently.

Exercise in orthogonality. Going back to the case of general initial conditions, use the orthogonality relations eq. (10) and the Fourier orthogonality relations for sine and cosine functions to write down integral expressions for A_{mn}, B_{mn} in terms of ϕ and C_{mn}, D_{mn} in terms of ψ. Note that the Fourier orthogonality relations ensure that the Bessel function orthogonality integrals that arise along the way, involve two Bessel functions always of the *same* order.

3.4 Energetics for the wave equation

Consider again small transverse vibrations of an elastic string with endpoints fixed at $x = 0, L$, with mass density μ per unit length and tension T (both constant). Write $c^2 = T/\mu$. We have:

$$\begin{aligned} \frac{\partial^2 y}{\partial t^2} &= c^2\frac{\partial^2 y}{\partial x^2},\ y(0,t) = y(L,t) = 0,\ y(x,0) = \phi(x),\ \frac{\partial y}{\partial t}(x,0) = \psi(x), \\ y(x,t) &= \sum_{n=1}^{\infty}\left[a_n\cos\left(\frac{n\pi ct}{L}\right) + b_n\sin\left(\frac{n\pi ct}{L}\right)\right]\sin\left(\frac{n\pi x}{L}\right), \qquad (11) \\ a_n &= \frac{2}{L}\int_0^L \phi(x)\sin\left(\frac{n\pi x}{L}\right)dx, \\ b_n &= \frac{2}{n\pi c}\int_0^L \psi(x)\sin\left(\frac{n\pi x}{L}\right)dx. \end{aligned}$$

Now, we can consider the total kinetic energy K of the string, defined as

$$K = \int_0^L \frac{1}{2}\mu \left(\frac{\partial y}{\partial t}\right)^2 dx, \tag{12}$$

To get an expression for potential energy consider a small element δs of the string:

$$\begin{aligned} PE &= T \times \text{extension} = T(\delta s - \delta x), \\ &= T\left[\sqrt{1 + \left(\frac{\partial y}{\partial x}\right)^2} - 1\right]\delta x. \end{aligned}$$

Integrating along the whole string, the potential energy is

$$\begin{aligned} V &= T\int_0^L \left[\left(1 + \left[\frac{\partial y}{\partial x}\right]^2\right)^{1/2} - 1\right] dx, \\ &\simeq \frac{T}{2}\int_0^L \left(\frac{\partial y}{\partial x}\right)^2 dx, \end{aligned} \tag{13}$$

using a Taylor series expansion, since $\partial y/\partial x$ is small.

Therefore, the total energy is

$$E = K + V = \frac{\mu}{2}\int_0^L \left[\left(\frac{\partial y}{\partial t}\right)^2 + c^2\left(\frac{\partial y}{\partial x}\right)^2\right] dx.$$

Substituting the form of the solution (11) into the expression for K yields (using Fourier trig function orthogonality):

$$\begin{aligned} K &= \frac{\mu}{2}\int_0^L \sum_{n=1}^{\infty}\sum_{m=1}^{\infty} \sin\left(\frac{n\pi x}{L}\right)\sin\left(\frac{m\pi x}{L}\right) \\ &\quad \times \left(\frac{n\pi c}{L}\left[b_n\cos\left(\frac{n\pi ct}{L}\right) - a_n\sin\left(\frac{n\pi ct}{L}\right)\right]\right) \\ &\quad \times \left(\frac{m\pi c}{L}\left[b_m\cos\left(\frac{m\pi ct}{L}\right) - a_m\sin\left(\frac{m\pi ct}{L}\right)\right]\right) dx, \\ &= \frac{\mu L}{4}\sum_{n=1}^{\infty}\frac{n^2\pi^2c^2}{L^2}\left[a_n^2\sin^2\left(\frac{n\pi ct}{L}\right) + b_n^2\cos^2\left(\frac{n\pi ct}{L}\right)\right. \\ &\quad \left. - 2a_nb_n\cos\left(\frac{n\pi ct}{L}\right)\sin\left(\frac{n\pi ct}{L}\right)\right]. \end{aligned}$$

A similar calculation can be done for the potential energy and combining the two, all trig terms drop out (e.g. using $\sin^2 + \cos^2 = 1$), and we get the simple total energy expression

$$E = \frac{\mu c^2\pi^2}{4L}\sum_{n=1}^{\infty} n^2(a_n^2 + b_n^2),$$

which is independent of time i.e. just like an oscillating mass attached to an elastic spring, PE and KE are continuously inter-converted during the motion while conserving the total energy. Finally, recall that the period of oscillation (i.e. period of the fundamental mode) is

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

and we can average over a period to get

$$\overline{K} = \frac{c}{2L}\int_0^{\frac{2L}{c}} K dt = \overline{V} = \frac{c}{2L}\int_0^{\frac{2L}{c}} V dt = \frac{E}{2},$$

i.e. there is an equipartition of energy between average potential and kinetic energies.

3.5 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, for example with 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 $c_\pm = \sqrt{\tau/\mu_\pm}$ differs either side of $x = 0$. Consider an incident wave propagating to the right from $x = -\infty$. The most general form is (using subscript I to denote "incident"):

$$W_I = A_I \cos[w(t - x/c_-) + \phi_I] \tag{14}$$

with amplitude A_I and phase ϕ_I. It is convenient to represent such waves in terms of a complex exponential

$$W_I = \Re\left(I \exp\left[i\omega\left(t - x/c_-\right)\right]\right) \tag{15}$$

where $I = I_r + iI_i$ is a complex number and $\Re$ denotes the real part.
Remark on notation: in $I = I_r + iI_i$ the capital I stands for "incident" and subscripts r and i denote real and imaginary parts. In a moment we'll also have complex numbers R and T for "reflected" and "transmitted" with similar subscripts r and i denoting real and imaginary parts.

To see the equivalence of eq. (14) and eq. (15) it is convenient to consider I in polar form $I = |I|e^{i\xi}$. Then

$$\Re\left(I \exp\left[i\omega\left(t - \frac{x}{c_-}\right)\right]\right) = |I|\Re\left(\exp\left[i\omega\left(t - \frac{x}{c_-}\right) + \xi\right]\right)$$

so $A_I = |I|$ and $\phi_I = \xi$ i.e. the amplitude and phase of the wave are just the modulus and argument of the complex number I.

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. Using subscripts T for "transmitted" and R for "reflected" we write

$$\begin{aligned} W_T &= \Re\left(T\exp\left[i\omega\left(t-\frac{x}{c_+}\right)\right]\right) \\ W_R &= \Re\left(R\exp\left[i\omega\left(t+\frac{x}{c_-}\right)\right]\right) \\ \text{with} \quad T &= T_r + iT_i \quad R = R_r + iR_i. \end{aligned}$$

The latter quantities define the new amplitudes and phases via their moduli and arguments. These coefficients T and R are determined by physical matching conditions at $x = 0$.

(a) we assume the string does not break so the displacement at $x = 0$ must be continuous *for all time* i.e.

$$W_I|_{x=0^-} + W_R|_{x=0^-} = W_T|_{x=0^+}$$

so (using the fact that if $\Re Ae^{iwt} = \Re Be^{iwt}$ for all t then $A = B$ as complex numbers) we get

$$I + R = T. \tag{16}$$

(b) the point $x = 0$ has no inertia (but see a different situation on example sheet 2!...) and thus the total vertical force at $x = 0$ must vanish:

$$\tau \left.\frac{\partial y}{\partial x}\right|_{x=0^-} = \tau \left.\frac{\partial y}{\partial x}\right|_{x=0^+}$$

i.e.

$$\frac{R}{c_-} - \frac{I}{c_-} = -\frac{T}{c_+}. \tag{17}$$

The two equations eqs. (16,17) then suffice to fix the two complex numbers R and T in terms of I and solving we get

$$\begin{aligned} R &= \left(\frac{c_+ - c_-}{c_+ + c_-}\right) I, \\ T &= \left(\frac{2c_+}{c_+ + c_-}\right) I. \end{aligned}$$

This has several interesting properties: (i) 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; (ii) if $\mu_+ = \mu_-$ then $c_+ = c_-$ and so $R = 0$ and $T = I$ as expected. If the string to the right is very much heavier $\mu_+ \gg \mu_-$, then $c_+ \ll c_-$so $T \sim 0$ and almost all the wave is reflected with the reflected wave having phase shift π ($R \approx -I$). On the other hand if the string to the right $x > 0$ is very much lighter $\mu_+ \ll \mu_-$, then $c_+ \gg c_-$ so $T \sim 2I$ and $R \sim I$. Thus 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.

4 The diffusion equation

4.1 Physical significance

The **diffusion equation** (also known as the **heat equation**) is (like the wave equation) one of the most important equations of physics and applied mathematics. It describes the transport of quantities that "diffuse" as a consequence of spatial gradients in their concentration. A classic example is heat (characterised in terms of temperature) which diffuses from hot regions to cooler regions and the diffusion is driven by temperature gradients. Other examples include chemical species in solution that diffuse in the presence of concentration gradients.

Let $c(\underline{x}, t)$ denote the concentration of a 'species' A. Our basic assumption (also known as Fick's law, or Fourier's law of thermal conduction in the case of heat) is that the flux of A is proportional to the negative concentration gradient

$$\underline{J} = -D\,\nabla c \tag{18}$$

D is called the diffusion coefficient which we assume to be constant. The meaning of the term 'flux' is the following: if $\underline{n}$ is a unit vector then locally at $(\underline{x}, t)$ the amount of A crossing a small area at $(\underline{x}, t)$ with normal $\underline{n}$ is $\underline{J} \cdot \underline{n}$ per unit area per second. Thus diffusion occurs from high to low concentration, as $\underline{J}$ points opposite to the concentration gradient.

Consider now a volume V with surface S and suppose that species A is *conserved* as it sloshes around by diffusion. The total content in V is $\int_V c\, dV$. By eq. (18) the amount crossing the surface is $\int_S -D\,\nabla c \cdot \underline{n}\, dS$ where $\underline{n}$ is the outward pointing normal to the surface. Then the requirement of conservation can be expressed as follows "rate of decrease of total c in V equals the rate at which c is transported out across the boundary. Thus we can write

$$-\frac{\partial}{\partial t}\int_V c\, dV = \int_S -D\,\nabla c \cdot \underline{n}\, dS.$$

Applying the divergence theorem to RHS gives

$$-\frac{\partial}{\partial t}\int_V c\, dV = \int_V \nabla \cdot (-D\nabla c)\, dV$$

i.e. $\int_V (\partial c/\partial t - D\nabla^2 c)\, dV = 0$. Since this holds for all volumes we get

$$\frac{\partial c}{\partial t} = D\nabla^2 c$$

which is the diffusion equation for c.

Heat diffusion. In the case of temperature and heat flow we have the following facts from thermodynamics: if $\theta(\underline{x}, t)$ is the temperature distribution then the heat flux is given by (Fourier's law of conduction)

$$\underline{q} = -k\nabla\theta$$

where k is the thermal conductivity. Also the heat content of a region V is $\int_V \sigma\rho\,\theta\, dV$ where σ is the specific heat and ρ is the density, both assumed constant here. Then conservation of energy via the above argument gives

$$\frac{\partial\theta}{\partial t} = D\,\nabla^2\theta \quad \text{where} \quad D = \frac{k}{\sigma\rho}.$$

Random walks and diffusion. The diffusion equation also arises in the study of probabilistic processes, especially in the theory of random walks and Brownian motion. Consider a particle moving in one dimension x viewed at discrete time intervals Δt. Let $P_N(x)$ be its probability density function (PDF) after N steps. We assume the following probabilistic behaviour: in each step (regardless of the time or position of the particle) it has PDF $p(\xi)$ to move distance ξ in one step. Thus the process is homogeneous (independent of position) and memoryless ($p(\xi)$ does not depend on the previous history of the particle). We will also assume that $p(\xi)$ has mean zero i.e. there is no drift in the mean position of the particle. By considering all possible ways that the particle can get to a position x at stage $N+1$ from stage N we easily see that

$$P_{N+1}(x) = \int_{-\infty}^{\infty} p(\xi)P_N(x-\xi)\, d\xi.$$

Now suppose the motion in each step is small i.e. $p(\xi)$ is concentrated near $\xi = 0$, and expand $P_N(x-\xi)$ as a Taylor series:

$$\begin{aligned} P_{N+1}(x) &\approx \int_{-\infty}^{\infty} p(\xi)P_N(x) + p(\xi)P_N'(x)(-\xi) + p(\xi)P_N''(x)\tfrac{\xi^2}{2}\, d\xi \\ &= P_N(x) - P_N'(x)\langle\xi\rangle + P_N''(x)\tfrac{\langle\xi^2\rangle}{2}. \end{aligned}$$

Here by assumption the mean $\langle\xi\rangle = 0$, and $\langle\xi^2\rangle$ is the variance of PDF p. Writing $P_N(x)$ as $P(x, N\Delta t)$ we get

$$P(x,(N+1)\Delta t) - P(x, N\Delta T) = \frac{\partial^2}{\partial x^2}P(x, N\Delta t)\frac{\langle\xi^2\rangle}{2}. \tag{19}$$

Next *assume that the variance* $\langle\xi^2\rangle$ *is proportional to* Δt:

$$\frac{\langle\xi^2\rangle}{2} = D\Delta t. \tag{20}$$

Then in the limit of small Δt eq. (19) becomes the diffusion equation in one space dimension

$$\frac{\partial P}{\partial t} = D\frac{\partial^2 P}{\partial x^2}.$$

The assumed behaviour of the variance eq. (20) occurs commonly in actual physical processes. For example suppose the particle is a foreign body in a (1-dimensional) background gas of particles that randomly collide with it, having very many independent random hits per unit time (even for very small time intervals). The number of hits M in time Δt will then be proportional to Δt. Thus the 'microscopic origin' of $p(\xi)$ is the sum of many independent identical random variables $X_1 + X_2 + \ldots + X_M$ with $X_i = X$ for all i (characterising a single hit), and by elementary probability theory, the variance is then proportional to M and so to Δt. This kind of analysis provides an explanation of Brownian motion – the random jiggling (as seen under a microscope) of tiny pollen grains that have fallen into a liquid. It was used by Einstein in 1905 to provide compelling evidence for the existence of atoms, which was still much doubted at that time!

4.2 Similarity solutions and the error function erf(z)

Let's consider the one dimensional diffusion equation

$$\frac{\partial \theta}{\partial t} = D\frac{\partial^2 \theta}{\partial x^2} \qquad \theta = \theta(x,t). \tag{21}$$

The dimensionless combination x^2/Dt (reflecting the characteristic linear-time spread of variance in diffusion processes noted above) plays a special role for the equation and we introduce the so-called *similarity variable*

$$\eta = \frac{x}{2\sqrt{Dt}}.$$

We now seek solutions of eq. (21) that depend on x, t only through the combination η i.e. $\theta(x,t) = \theta(\eta(x,t))$ (without imposing any BCs or ICs). Straightforward chain rule differentiation gives

$$\frac{\partial \theta}{\partial t} = \frac{\partial \eta}{\partial t}\frac{\partial \theta}{\partial \eta} = -\frac{\eta}{2t}\frac{\partial \theta}{\partial \eta}$$

$$\frac{\partial \theta}{\partial x} = \frac{\partial \eta}{\partial x}\frac{\partial \theta}{\partial \eta} = \frac{1}{2\sqrt{Dt}}\frac{\partial \theta}{\partial \eta}$$

$$\frac{\partial^2 \theta}{\partial x^2} = \frac{\partial}{\partial x}\left(\frac{1}{2\sqrt{Dt}}\frac{\partial \theta}{\partial \eta}\right) = \frac{1}{2\sqrt{Dt}}\frac{\partial}{\partial x}\frac{\partial \theta}{\partial \eta} = \frac{1}{4Dt}\frac{\partial^2 \theta}{\partial \eta^2}$$

and the diffusion equation becomes the ODE

$$\frac{d^2\theta}{d\eta^2} = -2\eta\frac{d\theta}{d\eta}.$$

Setting $X = d\theta/d\eta$ we get $dX/d\eta = -2\eta X$ so $X = C\exp -\eta^2$ and

$$\theta = c\,\frac{2}{\sqrt{\pi}}\int_0^\eta e^{-u^2}\,du = c\,\mathrm{erf}\left(\frac{x}{2\sqrt{Dt}}\right)$$

where we have introduced the error function

$$\mathrm{erf}(z) = \frac{2}{\sqrt{\pi}}\int_0^z e^{-u^2}\,du$$

which is scaled so that $\mathrm{erf}(0) = 0$ and $\mathrm{erf}(z) \to \pm 1$ as $z \to \pm\infty$. The function $\theta(x,t) = \mathrm{erf}(x/2\sqrt{Dt})$ is plotted in the figure (with $D = 1$) for times $t = 10^{-3}, 10^{-2}, 10^{-1}, 10^{0}$. Note that as $t \to 0$ θ approaches the step function with jump discontinuity from -1 to 1 as x crosses 0.

Although we have not incorporated any BCs this function can be used as an early-time approximation to diffusion problems in a finite domain, near to interior points where the initial concentration $\theta(x,0)$ has a jump discontinuity. Intuitively, it takes some time for the interior solution to "feel" the influence of boundaries and BCs there. We will see an illustration of this in the next example.

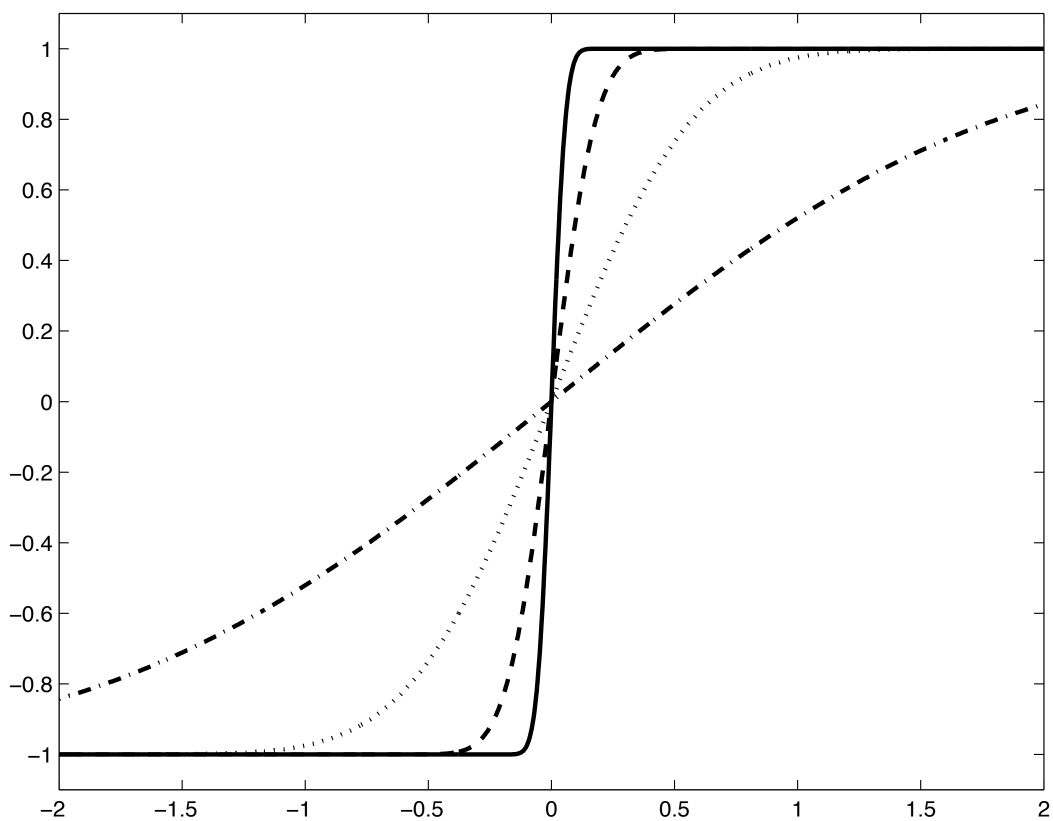

Figure 2: Plots (with $D = 1$) of the error function $\mathrm{erf}(x/2\sqrt{Dt})$ for times $t = 10^{-3}$ (solid); $t = 10^{-2}$ (dashed); $t = 10^{-1}$ (dotted); and $t = 10^{0}$ (dot-dashed).

Example. (Heat conduction in a finite bar)

Consider a finite bar $-L \leq x \leq L$ of length $2L$ with initial temperature

$$\theta(x,0) = H(x) = \begin{cases} 1 & 0 < x \leq L \\ 0 & -L \leq x < 0 \end{cases}$$

and boundary conditions for all $t \geq 0$:

$$\theta(L,t) = 1 \qquad \theta(-L,t) = 0. \tag{22}$$

Subject to these conditions we aim to use the method of separation of variables to solve the heat equation eq. (21). But there is a hiccup at the start: recall that we proceed by (a) finding separated (eigenfunction) solutions $f_n(x,t) = X_n(x)T_n(t)$ *that satisfy the BCs* and then (b) *superposing* them to form $\sum_n c_n X_n(x) T_n(t)$, (c) then choosing coefficients c_n to match the initial conditions (expanded as infinite series in the eigenfunctions). The problem is with (b) – in this example *our BCs are not homogeneous so we cannot superpose solutions that individually satisfy the BCs, to obtain a combination that still satisfies the BCs!* One way to deal with this is to identify any *particular* solution θ_s of the diffusion equation which satisfies the given BCs, and then consider solving the problem for $\hat{\theta} = \theta - \theta_s$ which will then have *homogeneous* BCs (and we'll correspondingly modified θ's ICs to apply to $\hat{\theta}$).

For θ_s we will seek a *steady state solution* $\theta_s(x)$ that will then physically correspond to the late-time behaviour of θ, when all transients have decayed. Thus we seek θ_s with

$$\frac{\partial \theta_s}{\partial t} = 0 = D\frac{\partial^2 \theta_s}{\partial x^2}$$

so $\theta_s = Ax + B$ and imposing the BCs we get

$$\theta_s(x) = \frac{(x+L)}{2L}.$$

Thus our problem for $\hat{\theta}(x,t) = \theta(x,t) - \theta_s(x)$ becomes

$$\frac{\partial \hat{\theta}}{\partial t} = D\,\frac{\partial^2 \hat{\theta}}{\partial x^2}$$

$$\begin{array}{ll} \text{BCs:} & \hat{\theta}(\pm L,t) = 0 \quad \text{for all } t > 0 \text{ (homogeneous now!)} \\ \text{ICs:} & \hat{\theta}(x,0) = H(x) - \frac{(x+L)}{2L} \qquad \text{for } -L \leq x \leq L \end{array}$$

and we can now straightforwardly apply our standard separation of variables method: setting $\hat{\theta}(x,t) = X(x)T(t)$ gives as usual

$$\dot{T} = -D\lambda T \qquad X'' = -\lambda X$$

for some constant λ. If $\lambda < 0$ then the BCs allow only $X(x) = 0$. Thus λ is positive and

$$X(x) = A\cos\sqrt{\lambda}x + B\sin\sqrt{\lambda}x.$$

The BCs $X(\pm L) = 0$ impose

$$A\cos\sqrt{\lambda}L = 0 \quad \text{and} \quad \mathrm{B}\sin\sqrt{\lambda}\mathrm{L} = 0.$$

If $A \neq 0$ then $\cos\sqrt{\lambda}L = 0$ so we get

$$\sqrt{\lambda_m} = \frac{m\pi}{2L} \qquad m = 1, 3, 5, \ldots$$

and so then $B = 0$ and the corresponding eigenfunctions are

$$X_m(x) = A_m \cos\frac{m\pi x}{2L} \qquad \lambda_m = \frac{m^2\pi^2}{4L^2}. \tag{23}$$

On the other hand, if $B \neq 0$ then $\sin\sqrt{\lambda}L = 0$ so we get

$$\sqrt{\lambda_n} = \frac{n\pi}{L} \qquad n = 1, 2, 3, \ldots$$

so then $A = 0$ and the eigenfunctions are

$$X_n(x) = B_n \sin\frac{n\pi x}{L} \qquad \lambda_n = \frac{n^2\pi^2}{L^2}. \tag{24}$$

Note that the first set eq. (23) of eigenfunctions are all even and the second set eq. (24) are all odd functions. Our initial condition $\hat{\theta}(x, 0)$ for $\hat{\theta}$ is an *odd* function so we retain only the second set i.e. we take $A_m = 0$ for all m. With λ_n from eq. (24) the time equation gives

$$T_n(t) = C_n \exp(-\frac{-Dn^2\pi^2}{L^2}t).$$

The general solution for $\hat{\theta}$ (with odd initial condition $\hat{\theta}(x, 0)$) is thus

$$\hat{\theta}(x, t) = \sum_{n=1}^{\infty} b_n \sin\frac{n\pi x}{L} \exp(-\frac{-Dn^2\pi^2}{L^2}t).$$

Imposing the initial condition fixes the b_n's:

$$\sum_{n=1}^{\infty} b_n \sin\frac{n\pi x}{L} = H(x) - \frac{(x + L)}{2L}$$

so

$$Lb_m = \int_{-L}^{L} \hat{\theta}(x, 0) \sin\frac{n\pi x}{L}\, dx = \int_0^L \sin\frac{n\pi x}{L}\, dx - \frac{1}{2}\int_{-L}^{L} \sin\frac{n\pi x}{L}\, dx - \frac{1}{2L}\int_{-L}^{L} x \sin\frac{n\pi x}{L}\, dx.$$

After some integration by parts (for the last integral) we get simply

$$b_m = \frac{1}{m\pi}$$

and the transient and full solutions are

$$\begin{aligned}
\hat{\theta} &= \sum_{n=1}^{\infty} \frac{1}{n\pi} \sin\left(\frac{n\pi x}{L}\right) \exp\left(-\frac{n^2\pi^2 Dt}{L^2}\right), \\
\theta &= \frac{(x+L)}{2L} + \sum_{n=1}^{\infty} \frac{1}{n\pi} \sin\left(\frac{n\pi x}{L}\right) \exp\left(-\frac{n^2\pi^2 Dt}{L^2}\right).
\end{aligned} \tag{25}$$

In the figure we plot the solution $\theta(x, t_0)$ for times $t_0 = 0, 10^{-3}, 10^{-2}, 10^{-1}, 10^{0}$. For these t_0's we also plot the function

$$\theta_i(x, t_0) = \frac{1}{2}\left(1 + \operatorname{erf}\left[\frac{x}{2\sqrt{Dt}}\right]\right). \tag{26}$$

which represents the error function suitably translated and rescaled to fit the initial step function data for θ). We see that θ_i is graphically indistinguishable from θ for all the plotted times except the latest time $t_0 = 10^0$ confirming the validity of the similarity solution as an excellent approximation for early times.

5 The Laplace equation

Our third fundamentally important equation of study is the **Laplace equation**

$$\nabla^2 \psi = 0 \tag{27}$$

in some domain $\mathcal{D}$. We have no initial conditions (as there is no time co-ordinate) and we will consider two kinds of boundary conditions on the boundary $\delta\mathcal{D}$ of $\mathcal{D}$:
(i) **Dirichlet conditions:** if ψ is given on the boundary, then there is a unique solution throughout $\mathcal{D}$;
(ii) **Neumann conditions:** if the normal derivative $\underline{n} \cdot \nabla\psi$ is given on the boundary then ψ is uniquely defined throughout $\mathcal{D}$ up to an additive constant (here $\underline{n}$ is the outward pointing unit normal to the boundary).

5.1 Physical and mathematical significance

The Laplace equation is very important in physics and applied mathematics but even more, it also plays a fundamental role in some other areas of *pure* mathematics. The study of its solutions (in more general contexts of differentiable manifolds and locally compact groups) is an area of study in its own right called **harmonic analysis** – solutions of Laplace's equation are sometimes called **harmonic functions**.

Applications of Laplace's equation include the following:

(a) **Steady state** heat conduction (or diffusion) – in the heat equation we seek solutions that are independent of time, and then the heat equation becomes the Laplace equation.

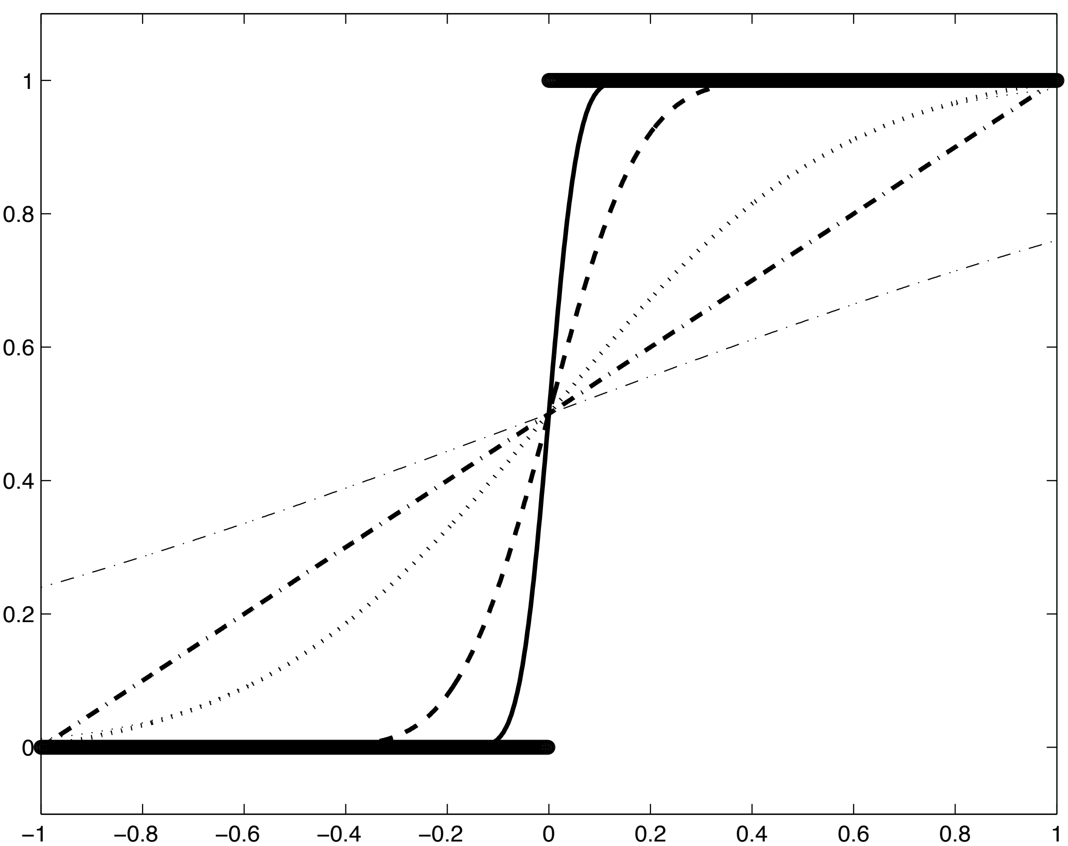

Figure 3: Plots (with $L = 1$ and $D = 1$) of θ as defined in eq. (25) for: $t = 0$ (very thick line); $t = 10^{-3}$ (thick solid line); $t = 10^{-2}$ (thick dashed); $t = 10^{-1}$ (thick dotted); $t = 10^{0}$ (thick dot-dashed). Also plotted is the error function approximation, as defined in (26) for: $t = 10^{-3}$ (thin solid line); $t = 10^{-2}$ (thin dashed); $t = 10^{-1}$ (thin dotted); $t = 10^{0}$ (thin dot-dashed). Only the last line is visible.

(b) For **incompressible fluid flow** (with velocity field $\underline{v}(x,t)$) in a region with no sources or sinks. If the flow is **irrotational** i.e. curl $\underline{v} = 0$ (i.e. zero vorticity) then $\underline{v}$ can be expressed in terms of a so-called **velocity potential** ϕ: $\underline{v} = \nabla\phi$. Then the incompressibility condition $\nabla \cdot \underline{v} = 0$ gives $\nabla^2\phi = 0$.

(c) **Potential theory:** in a variety of physical scenarios of particle dynamics involving motion in space under the action of forces, we have a force field (i.e. a force defined at each point in space) that can be expressed as the gradient of a potential: $\underline{F} = -\nabla\psi$. Such forces are called **conservative forces** since (as a consequence of Newton's laws) there is a corresponding conservation of total (kinetic plus potential) energy. Examples include the gravitational force and the electric field force. In these cases it is physical law that the integral of the normal component of force, integrated over a closed surface, is proportional to the total amount of source inside (viz. mass and electric charge in our examples). Thus using the divergence theorem we see that the potential must satisfy the Laplace equation in any region free of sources e.g. the gravitational potential due to any mass distribution in the region outside the masses.

(d) **Complex analysis:** any function of a complex variable $f : \mathbb{C} \to \mathbb{C}$ may be written via real and imaginary parts as $f(z) = u(x,y) + iv(x,y)$ where $z = x + iy$. For a well defined notion of derivative with respect to z to exist i.e. we want $\lim_{\delta z\to 0}(f(z+\delta z) - f(z))/\delta z$ to be independent of how δz tends to zero in the 2-dimensional complex plane, it can be shown that it is necessary and sufficient that $u_x = v_y$ and $u_y = -v_x$ hold (these are the so-called Cauchy-Riemann equations, subscripts denoting partial derivatives). Thus (by taking a further derivative of these equations) we see that both u and v must satisfy the 2-dimensional Laplace equation. Such functions f are called **complex analytic** or **holomorphic** functions and they have a very rich and beautiful theory (cf Complex Analysis and Complex Methods courses) with many applications.

We now consider the solution of Laplace's equation by separation of variables in different co-ordinate systems: cartesian, plane polar, cylindrical and spherical polar co-ordinates.

5.2 3D cartesian co-ordinates

We have $\psi_{xx} + \psi_{yy} + \psi_{zz} = 0$ and substituting $\psi(x,y,z) = X(x)Y(y)Z(z)$ we get

$$\frac{X''}{X} + \frac{Y''}{Y} + \frac{Z''}{Z} = 0.$$

Each ratio (being a function of a different single variable) must thus be constant so we can write

$$X'' = -\lambda X \quad Y'' = -\mu Y \quad Z'' = (\lambda + \mu)Z.$$

Note that the constant in the Z equation is not a third independent constant, as the three ratios must sum to zero.

Our (by now rather familiar!...) procedure is:
(i) find eigenvalues λ_l, μ_m and associated eigenfunctions $X_l(x), Y_m(y)$ by applying the

x, y-BCs (yet to be specified). Note: here we assume that these BCs are *homogeneous.*
(ii) then solve for $Z_{lm}(z)$ and write the product solution

$$P_{lm}(x, y, z) = X_l(x)Y_m(y)Z_{lm}(z)$$

i.e. we treat z like we did the time co-ordinate in the wave and heat equations. The z-BCs (assumed generally not homogeneous) are not applied yet here – see (iv) below.
(iii) next define a general solution by summing over l, m:

$$\psi(x, y, z) = \sum_{l,m} a_{lm} X_l(x)Y_m(y)Z_{lm}(z)$$

which still satisfies the x, y-BCs (because they were homogeneous).
(iv) determine the coefficients a_{lm} using the z-BCs.

In the above the roles of x, y, z can be interchanged to match the BC homogeneities and geometry of the given problem. Note that as before, we get rather simple SL problems from cartesian co-ordinate separations.

Example: steady heat conduction

Consider the problem of steady heat conduction in a semi-infinite rod of rectangular cross-section, heated at one end and having fixed temperature zero on its other surfaces. We assume the rod lies along the z-axis for $z \geq 0$ with rectangular cross-section $0 \leq x \leq a, 0 \leq y \leq b$. If $\psi(x, y, z)$ denotes the steady temperature field we then have:

$$\nabla^2 \psi = 0$$

$$\begin{aligned} z\text{-BCs:} \quad & \psi(x, y, 0) = \Theta(x, y) \quad \psi \to 0 \text{ as } z \to \infty \\ x, y\text{-BCs:} \quad & \psi(0, y, z) = \psi(a, y, z) = \psi(x, 0, z) = \psi(x, b, z) = 0. \end{aligned}$$

Separating variables as above gives $\psi = X_l Y_m Z_{lm}$ and solving the X equation with $X(0) = X(a) = 0$ gives

$$\lambda_l = \frac{l^2 \pi^2}{a^2} \qquad X_l = \sqrt{\frac{2}{a}} \sin\left(\frac{l\pi x}{a}\right) \qquad l = 1, 2, 3, \ldots$$

where for convenience we have normalised the eigenfunctions i.e. $\int_0^a X_l^2 \, dx = 1$.

Similarly solving the Y equation with $Y(0) = Y(b) = 0$ gives

$$\mu_m = \frac{m^2 \pi^2}{b^2} \qquad Y_m = \sqrt{\frac{2}{b}} \sin\left(\frac{l\pi x}{b}\right) \qquad m = 1, 2, 3, \ldots$$

Using the above (positive) λ, μ values, the general solution of the Z equation is

$$Z = \alpha \exp\left[\left(\frac{l^2}{a^2} + \frac{m^2}{b^2}\right)^{1/2} \pi z\right] + \beta \exp\left[-\left(\frac{l^2}{a^2} + \frac{m^2}{b^2}\right)^{1/2} \pi z\right].$$

Since ψ remains bounded as $z \to \infty$, we have $\alpha = 0$. Thus our general solution is

$$\psi(x, y, z) = \qquad (28)$$
$$\frac{2}{\sqrt{ab}} \sum_{l=1}^{\infty} \sum_{m=1}^{\infty} a_{lm} \sin\left(\frac{l\pi}{a}x\right) \sin\left(\frac{m\pi}{b}y\right) \exp\left[-\left(\frac{l^2}{a^2} + \frac{m^2}{b^2}\right)^{1/2} \pi z\right].$$

The coefficients a_{lm} are determined by the boundary condition at $z = 0$:

$$\psi(x, y, 0) = \Theta(x, y) = \frac{2}{\sqrt{ab}} \sum_{l=1}^{\infty} \sum_{m=1}^{\infty} a_{lm} \sin\left(\frac{l\pi}{a}x\right) \sin\left(\frac{m\pi}{b}y\right).$$

Using the orthogonality of the sine functions we easily get

$$a_{pq} = \frac{2}{\sqrt{ab}} \int_0^b \int_0^a \Theta(x, y) \sin\left(\frac{p\pi}{a}x\right) \sin\left(\frac{q\pi}{b}y\right) \, dxdy \qquad (29)$$

completing the solution.

Note that the sine functions arise because of the homogeneous Dirichlet BCs on x and y. If instead we had homogeneous Neumann conditions $\partial\psi/\partial x = 0$ and $\partial\psi/\partial y = 0$ on the y and x boundaries respectively (which physically corresponds to *insulated* boundaries i.e. no heat flow across the boundary) then we would get cosine eigenfunctions. Furthermore if the bar were *finite* of length L, with an extra BC $\psi(x, y, L) = f(x, y)$ then we would expect both positive and negative exponentials in the Z part of the solution (i.e. both α and β now generally non-zero there).

As a specific concrete case consider $\Theta = 1$ i.e. the end of the rod is kept at constant temperature 1. Then from eq, (29) we get (as you can check)

$$a_{pq} = \begin{cases} \frac{8}{\pi^2}\frac{\sqrt{ab}}{pq} & \text{if } p, q \text{ both odd} \\ 0 & \text{otherwise} \end{cases}$$

so

$$\begin{aligned} \psi(x, y, z) &= 16 \sum_{l=1}^{\infty} \sum_{m=1}^{\infty} \frac{\sin\left[\frac{(2m-1)\pi y}{b}\right] \sin\left[\frac{(2l-1)\pi x}{a}\right]}{\pi^2(2l-1)(2m-1)} \exp[-k_{l,m}\pi z], \\ k_{l,m}^2 &= \frac{(2l-1)^2}{a^2} + \frac{(2m-1)^2}{b^2}. \end{aligned}$$

Thus we see that the rod is hotter in the middle, and for large z the solution is dominated by lower harmonics i.e. with k_{lm} small so l, m small.

5.3 Plane polar co-ordinates

In plane polar coordinates with $\psi = \psi(r, \theta)$, Laplace's equation becomes

$$\nabla^2\psi = 0 = \frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial}{\partial r}\psi\right) + \frac{1}{r^2}\frac{\partial^2}{\partial\theta^2}\psi.$$

We write $\psi = R(r)\Theta(\theta)$ and separate variables giving

$$\Theta'' = -\lambda\Theta \tag{30}$$

$$\frac{r}{R}\,(rR')' = \lambda \tag{31}$$

with separation constant λ.

For the angular equation: since θ is an angular co-ordinate we have (by single-valuedness) $\Theta(\theta + 2\pi) = \Theta(\theta)$ i.e. Θ must have period 2π and for $\lambda \neq 0$ eq. (30) gives the discrete series of eigenvalues and eigenfunctions:

$$\lambda_n = n^2 \qquad \Theta_n(\theta) = a_n \cos n\theta + b_n \sin n\theta \qquad n = 1, 2, 3, \ldots \tag{32}$$

For $\lambda = 0$ eq. (30) gives $\Theta_0 = a + b\theta$ and periodicity requires that $b = 0$ so $\Theta_0(\theta)$ is constant (just like in Fourier series) and the formula eq. (32) above actually holds for $n = 0$ too.

For the radial equation: we again treat the cases $\lambda = n^2 > 0$ and $\lambda = 0$ separately. For $n \neq 0$ we have

$$r(rR_n')' - n^2 R_n = 0.$$

Let us search for power law solutions, i.e. assume that $R_n \propto r^\beta$. Substituting this into the radial equation, we get $\beta^2 - n^2 = 0$ i.e. $\beta = \pm n$ and so

$$R_n(r) = c_n r^n + d_n r^{-n}, \;\; n = 1, 2, 3 \ldots$$

and our n^{th} separated solution is

$$\psi_n(r, \theta) = (a_n \cos n\theta + b_n \sin n\theta)(c_n r^n + d_n r^{-n}) \qquad n = 1, 2, 3, \ldots,$$

For $n = 0$ we have $(rR_0')' = 0$ so

$$R_0 = d_0 \log r + c_0 = \psi_0(r, \theta)$$

and $\psi_0(r, \theta) = c_0 + d_0 \log r$ (as Θ_0 was constant).

Thus our general solution for Laplace's equation in polar coordinates is

$$\psi(r, \theta) = c_0 + d_0 \log r + \sum_{n=1}^{\infty} (a_n \cos n\theta + b_n \sin n\theta)(c_n r^n + d_n r^{-n}). \tag{33}$$

This general solution contains a rather large number of different constants but this number can often be immediately reduced by the geometry of the region being considered:
- If the problem is defined on the interior of a disc $r \leq a$ then for regularity at $r = 0$ we immediately have $d_0 = d_n = 0$ and we can absorb the c_n's, introducing $\alpha_n = a_n c_n$ and $\beta_n = b_n c_n$.
- Similarly if the problem is defined on an infinite domain with $r \to \infty$ and excludes the origin e.g. the outside of a finite disc, then a condition that ψ remain bounded asymptotically requires $d_n = c_n = 0$ for $n > 0$ and $c_0 = \lim_{r\to\infty} \psi$ (which must be independent

of θ.
• Things are more complicated in an annular region $a \le r \le b$ where all constants potentially survive.
• In all cases the constants are finally determined in the usual way by expanding the boundary conditions (functions of θ) for the $r =$ constant boundaries as Fourier series in θ.

Example: Laplace's equation in the unit disc

Consider Laplace's equation in the unit disc $r \le 1$with BC $\psi(1,\theta) = f(\theta)$ being a given function on the boundary. With regularity at the origin, our general solution becomes

$$\psi(r,\theta) = \frac{a_0}{2} + \sum_{n=1}^{\infty}(a_n \cos n\theta + b_n \sin n\theta) r^n.$$

and then setting $r = 1$ we have

$$f(\theta) = \psi(1,\theta) = \frac{a_0}{2} + \sum_{n=1}^{\infty}(a_n \cos n\theta + b_n \sin n\theta),$$

so

$$a_n = \frac{1}{\pi}\int_0^{2\pi} f(\theta)\cos n\theta d\theta \qquad \text{and} \qquad b_n = \frac{1}{\pi}\int_0^{2\pi} f(\theta)\sin n\theta d\theta$$

are just the Fourier coefficients of $f(\theta)$. Note that the influence of the higher harmonics (i.e. larger n) becomes localized near the edge $r = 1$ due to the r^n factor.

5.4 Cylindrical polar coordinates

In this case, Laplace's equation is

$$\nabla^2\psi = 0 = \frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial}{\partial r}\psi\right) + \frac{1}{r^2}\frac{\partial^2}{\partial\theta^2}\psi + \frac{\partial^2}{\partial z^2}\psi.$$

We separate variables by writing $\psi = R(r)\Theta(\theta)Z(z)$ and the Laplace equation separates as follows (where we have chosen to write the separation constants as $-\lambda$ and μ):

$$\Theta'' = -\lambda\Theta$$

$$Z'' = \mu Z$$

$$r\frac{d}{dr}\left(r\frac{d}{dr}R\right) + (\mu r^2 - \lambda)R = 0.$$

(To see this, first separate z from (r,θ) and then separate the resulting (r,θ) equation after suitably multiplying it through by r^2).
For the θ equation: exactly as for plane polar co-ordinates above, we will require that λ be non-negative and we get again (cf eq. (32)):

$$\lambda_n = n^2 \qquad \Theta_n(\theta) = a_n \cos n\theta + b_n \sin n\theta \qquad n = 0, 1, 2, 3, \ldots$$

For the z equation: here (for simplicity) we will treat only the case of non-negative μ. (Note that if μ is negative the corresponding Z functions are sines and cosines that do not decay for large $|z|$. Hence negative μ values will not be relevant for problems in a semi-infinite domain with the solution ψ required to tend to zero asymptotically). Writing $\mu = k^2$ we get

$$\mu = k^2 \qquad Z_k = c_k e^{-kz} + d_k e^{kz}$$

For the r equation: with the above $\lambda = n^2$ and $\mu = k^2$, if we substitute $z = kr$ into the radial equation we get Bessel's equation of order n (as you should check) and so

$$R_{nk} = \alpha_n J_n(kr) + \beta_n Y_n(kr).$$

All these can then be combined to form a general solution. Assuming (indeed expecting) that the eigenvalue k for each n will be quantized by the boundary conditions into an infinite discrete set k_{n_j} with $j = 1, 2, \ldots$, we finally write our general solution in cylindrical polar coordinates as

$$\begin{aligned} \psi(r,\theta,z) &= \sum_{n=0}^{\infty}\sum_{j=1}^{\infty}[\alpha_{jn}J_n(k_{n_j}r) + \beta_{jn}Y_n(k_{n_j}r)] \\ &\quad \times[a_n\cos n\theta + b_n \sin n\theta][c_j e^{-k_{n_j}z} + d_j e^{k_{n_j}z}]. \end{aligned} \tag{34}$$

Example: Heat conduction in an infinite wire

Consider the problem of **steady** heat conduction in a semi-infinite rod with **circular** cross-section of radius a, kept heated at one end at a uniform constant temperature T_0, and maintained with fixed temperature zero on its other (curved) surface. In terms of equations we want to find the steady temperature field $\psi(r,\theta,z)$ with:

$$\frac{\partial}{\partial t}\psi = \kappa\nabla^2\psi = 0$$

$$\psi(r,\theta,0) = T_0 \quad \text{and} \quad \psi \to 0 \text{ as } z \to \infty$$

$$\psi(a,\theta,z) = 0.$$

Because of the rotational symmetry of the boundary conditions, the (unique) solution will not depend on θ, so $b_n = 0 = a_n$ for all $n > 0$ in eq. (34) (but a_0 remains nonzero). Similarly, all the d_j must be zero because of the far field condition, and all the β_{jn} must be zero because of the regularity of the solution at $r = 0$, and so

$$\begin{aligned} \psi(r,\theta,z) &= \sum_{j=1}^{\infty} A_j J_0\left(k_j\frac{r}{a}\right)e^{-k_j z/a}, \\ T_0 &= \sum_{j=1}^{\infty} A_j J_0\left(k_j\frac{r}{a}\right), \end{aligned}$$

where the k_j can now be identified as the zeroes of J_0. The coefficients can be calculated by using the orthogonality relations (with suitable weight function) satisfied by the Bessel functions.

Exercise (calculation of A_j's) By using the Bessel function orthogonality relations, and the recursion relation between J_0' and J_1 (see exercise sheet 2 No. 10), show that the solution to this problem is

$$\psi(r,\theta,z) = \sum_{j=1}^{\infty} \frac{2T_0}{k_j J_1(k_j)} J_0\left(k_j \frac{r}{a}\right) e^{-k_j z/a}.$$

5.5 Laplace's equation in spherical polar co-ordinates; Legendre polynomials

Recall the definition of spherical polar co-ordinates (r,θ,ϕ) of a point P with position vector $\underline{P}$ in 3D space:
• r is the distance of P from the origin, so $r \geq 0$;
• θ is the angle that $\underline{P}$ makes with the positive z axis. We have $0 \leq \theta \leq \pi$;
• for ϕ, if we project $\underline{P}$ into the xy-plane then ϕ is the angle of the projection measured counterclockwise from the positive x axis, so $0 \leq \phi < 2\pi$.

Thus $r = 1$ is the equation of a unit sphere centred at the origin with N and S poles on the z axis at $z = 1, -1$ respectively. θ is the latitude on the sphere (N pole having $\theta = 0$, equator having $\theta = \pi/2$ and S pole having $\theta = \pi$) and ϕ is the longitude with $\phi = 0$ in the xz-plane and $\phi = \pi/2$ in the yz-plane. Note that the co-ordinate system is singular at the origin: if $r = 0$ then $(0,\theta,\phi)$ is the same point for all θ, ϕ but away from the origin there is a one-to-one correspondence between (x,y,z) and (r,θ,ϕ).

From the above we get:

$$\begin{aligned} x &= r\sin\theta\cos\phi; \\ y &= r\sin\theta\sin\phi; \\ z &= r\cos\theta; \\ dV &= r^2\sin\theta\, dr\, d\theta\, d\phi, \end{aligned}$$

where dV is a volume element. The Laplace equation $\nabla^2\psi = 0$ becomes:

$$\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\psi\right) + \frac{1}{r^2\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\psi\right) + \frac{1}{r^2\sin^2\theta}\frac{\partial^2}{\partial\phi^2}\psi = 0.$$

In this course we will restrict attention to axisymmetric solutions i.e. $\psi = \psi(r,\theta)$ ***being independent of angle*** ϕ ***around the*** z ***axis.***
Thus we can omit the third term in the above form of Laplace's equation.

Separating variables we write $\psi(r,\theta) = R(r)\Theta(\theta)$ and substitution into Laplace's equation (followed by multiplying through by $\frac{r^2}{R\Theta}$) gives

$$\frac{1}{R}\frac{d}{dr}\left(r^2\frac{d}{dr}R\right) + \frac{1}{\Theta\sin\theta}\frac{d}{d\theta}\left(\sin\theta\frac{d}{d\theta}\Theta\right) = 0$$

i.e.

$$\begin{aligned} \left([\sin\theta]\Theta'\right)' + \lambda[\sin\theta]\Theta &= 0, && (35) \\ \left(r^2R'\right)' - \lambda R &= 0, && (36) \end{aligned}$$

where λ is the separation constant.

For the θ equation, eq. (35):
this is an especially interesting equation and will lead to the so-called **Legendre polynomials**.

To solve eq. (35) we make the substitution $x = \cos\theta$. Since $0 \leq \theta \leq \pi$ we have $-1 \leq x \leq 1$ and

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

So eq. (35) becomes

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

i.e.

$$-\frac{d}{dx}\left[(1-x^2)\frac{d}{dx}\Theta\right] = \lambda\Theta. \tag{37}$$

This equation is in standard Sturm-Liouville form, with $p(x) = 1 - x^2$, $q(x) = 0$, and weight function $w(x) = 1$. It is known as **Legendre's equation**.

Legendre polynomials

We require a bounded solution of eq. (37) on $[-1, 1]$. Note that the endpoints $x = \pm 1$ are included here, corresponding to $\theta = 0, \pi$ i.e. points on the z axis in space. Let us seek a series solution

$$\Theta \quad = \quad \sum_{n=0}^{\infty} a_n x^n.$$

Substituting this form into (37), we obtain

$$\begin{aligned}
(1-x^2)\frac{d^2}{dx^2}\Theta - 2x\frac{d}{dx}\Theta + \lambda\Theta \quad &= \quad 0, \\
(1-x^2)\sum_{n=2}^{\infty} a_n n(n-1)x^{n-2} - 2\sum_{n=1}^{\infty} a_n n x^n + \lambda\sum_{n=0}^{\infty} a_n x^n \quad &= \quad 0.
\end{aligned}$$

Considering the coefficient of x^n,

$$\begin{aligned}
0 \quad &= \quad a_{n+2}(n+2)(n+1) - n(n-1)a_n - 2na_n + \lambda a_n, \\
a_{n+2} \quad &= \quad \left[\frac{n(n+1) - \lambda}{(n+1)(n+2)}\right] a_n. \qquad (38)
\end{aligned}$$

Since this recurrence relation relates a_{n+2} to a_n, we can generate two linearly independent solutions Θ_0 and Θ_1 starting from a_0 and a_1 respectively:

$$\Theta = a_0\Theta_0(x) + \Theta_1(x_)$$

with

$$\Theta_0 = a_0\left[1+\frac{(-\lambda)x^2}{2!}+\frac{(-\lambda)(6-\lambda)x^4}{4!}+\frac{(-\lambda)(6-\lambda)(20-\lambda)x^6}{6!}+\ldots\right],$$
$$\Theta_1 = a_1\left[x+\frac{(2-\lambda)x^3}{3!}+\frac{(12-\lambda)(2-\lambda)x^5}{5!}+\ldots\right].$$

Now the recurrence relation eq. (38) implies

$$\frac{a_{n+2}}{a_n}\to 1 \quad \text{as} \quad \mathrm{n}\to\infty$$

so by the ratio test the two infinite series will converge for $|x|<1$.

But here comes a subtle and crucially important point: the infinite series for Θ_0 and Θ_1 can be shown to generally *diverge* at $x=\pm1$! As an illustrative example consider $\lambda=0$ so the recurrence relation is $a_{n+2}=\frac{n}{n+2}a_n$. If $x=\pm1$ then the Θ_0 series reduces to just a constant, but the Θ_1 series becomes $\pm(1+\frac{1}{3}+\frac{1}{5}+\frac{1}{7}+\cdots)$, a so-called *harmonic series*, which is known to be divergent. For other generic λ values the series (generally both) will diverge in a similar harmonic manner for $x=\pm1$. This follows from *Gauss' test* for convergent series which is applicable to our recurrence relation eq. (38). We will not elaborate on this test here, but if you're interested you can find a full exposition in the book by Arfken and Weber p295-6.

Recall that $x=\pm1$ correspond to physically significant points (i.e. points on the z axis) so it appears that our method of solution of the Laplace equation has failed! Actually no – we have been a little too hasty: looking again at the recurrence relaton eq.(38) we see that if λ takes the form

$$\lambda_m = m(m+1) \qquad m=0,1,2,3,\ldots$$

then the numerator will be zero when n reaches m and all subsequent a_n's will be zero i.e. the series terminates at m terms so it becomes *convergent* and the corresponding Θ function is a *polynomial* of degree m. Thus we get a sequence of polynomials $P_m(x)$ of increasing degree m for $m=0,1,2,\ldots$ coming alternately from the Θ_0 and Θ_1 series for even and odd m. The overall scaling of the polynomials (corresponding to choice of a_0, a_1 values) is conventionally chosen so that $P_m(1)=1$. With this scaling, these polynomials are called the **Legendre polynomials**.

The first five Legendre polynomials are:

$$\begin{array}{llr} m=0 & \lambda=0 & P_0(x)=1; \\ m=1 & \lambda=2 & P_1(x)=x; \\ m=2 & \lambda=6 & P_2(x)=\frac{3x^2-1}{2}; \\ m=3 & \lambda=12 & P_3(x)=\frac{5x^3-3x}{2}; \\ m=4 & \lambda=20 & P_4(x)=\frac{35x^4-30x^2+3}{8}. \end{array} \tag{39}$$

and they are plotted in the figure.

Legendre polynomials have many tantalising special properties:
• When m is an odd (resp. even) integer then P_m is an odd (resp. even) function;

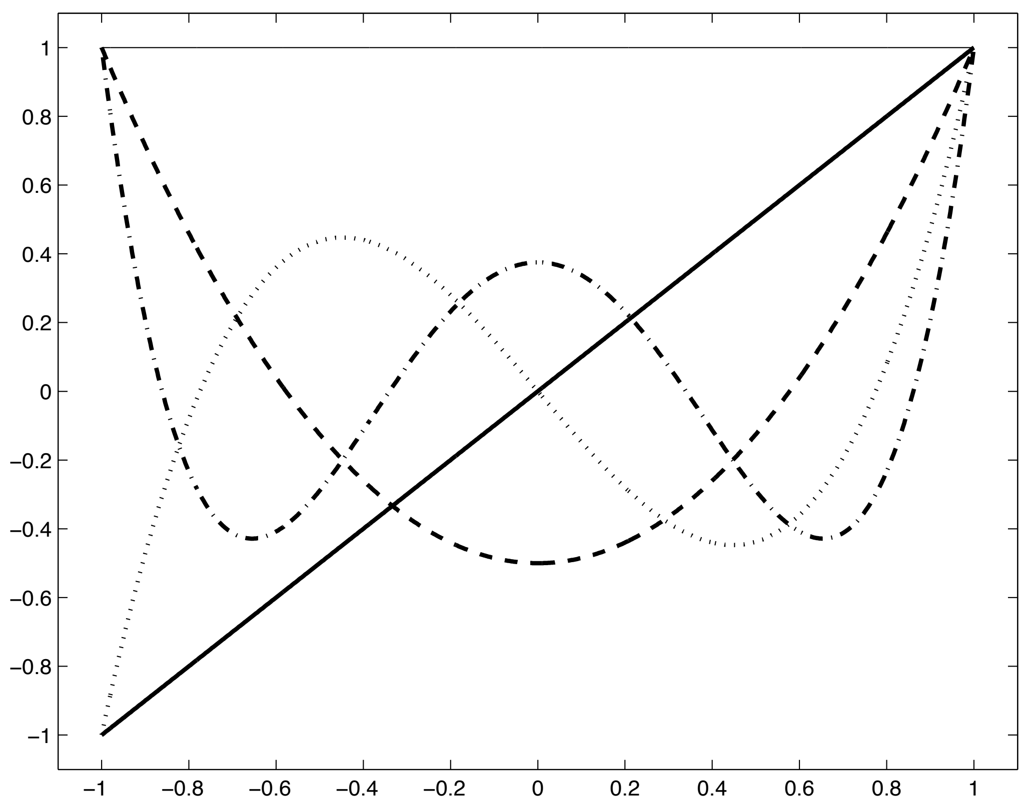

Figure 4: Legendre polynomials $P_0(x)$ (thin solid line); $P_1(x)$ (thick solid); $P_2(x)$ (dashed); $P_3(x)$ (dotted); $P_4(x)$ (dot-dashed).

• It can be shown that P_m has m zeroes in $[-1,1]$;
• The Legendre polynomials are SL eigenfunctions with weight function $w(x)=1$ so

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

(Note that we have not imposed any boundary conditions and for SL theory, the self-adjointness of the SL differential equation here come from $p(x) = 1-x^2$ being zero at the endpoints);
• Due to the condition that $P(1)=1$ the Legendre polynomials are not normalised, but in fact

$$\int_{-1}^{1} P_m^2(x)\,dx = \frac{2}{2m+1}$$

as we'll derive below (and by a different method on exercise sheet 2);
• From general SL theory, bounded functions on $[-1,1]$ can be represented as series of Legendre polynomials:

$$\begin{aligned} f(x) &= \sum_{n=0}^{\infty} a_n P_n(x), \\ a_n &= \frac{(2n+1)}{2}\int_{-1}^{1} f(x)P_n(x)\,dx; \end{aligned}$$

• *Optional remark:* we have been lead to the Legendre polynomials via a rather tortuous route of taming a potentially divergent infinite series. But they arise in more direct ways. Recall the Gram-Schmidt process of linear algebra: given a set of vectors $v_1, v_2, \ldots v_n$ we turn them sequentially into an orthonormal set $\hat{w}_1, \hat{w}_2, \ldots$ with the same span (and here 'hat' denotes 'normalised vector') viz. $w_1 = v_1, w_2 = v_2 - (v_2\cdot\hat{w}_1)\hat{w}_1, w_3 = v_3 - (v_3\cdot\hat{w}_1)\hat{w}_1 - (v_3\cdot\hat{w}_2)\hat{w}_2$ etc i.e. we successively take the v's and subtract off components parallel to all already obtained w's (and normalise the result), giving the next vector orthogonal to all previous w's. Now we can play the same game with vectors v being *polynomials* f, g on $[-1,1]$ and inner product (f,g) being $\int_{-1}^{1} f(x)g(x)\,dx$. If we start with the sequence of simple powers $1, x, x^2, x^3, \ldots$ for the v's and apply the Gram-Schmidt process we get precisely (up to scale) the Legendre orthogonal polynomials $P_n(x)$! (as you can readily check for the first few by direct calculation – you'll need to suitably un-normalise the resulting polynomials w to have $w(1)=1$, to get the exact Legendre polynomials.)
• *Optional remark:* the Legendre polynomials are just the simplest example of a class of orthogonal polynomials that can be defined by taking a specific weight function in the inner product formula i.e. $(f,g) = \int_a^b w(x)f(x)g(x)\,dx$. For example we have Hermite polynomials, Laguerre polynomials and Chebyshev polynomials with $w(x)$ being e^{-x^2}, e^{-x} and $(1-x^2)^{-1/2}$ respectively and on intervals $(-\infty,\infty)$, $(0,\infty)$ and $[-1,1]$ respectively. Hermite and Laguerre polynomials arise as eigenfunctions of SL systems occurring in quantum mechanics, in the solution of the time independent Schrödinger equation for the harmonic oscillator and hydrogen atom wavefunctions respectively.

Now back to our:

General axisymmetric solution of the Laplace equation

So far we have $\psi(r,\theta) = R(r)\Theta(\theta)$ and

$$\Theta_n(\theta) = P_n(x) = P_n(\cos\theta) \quad \text{with} \quad \lambda = n(n+1).$$

The radial equation then becomes

$$(r^2 R_n')' - n(n+1)R_n \;=\; 0.$$

Trying a solution of the form $R_n \propto r^\beta$, we get

$$\beta(\beta+1) \;=\; n(n+1)$$

so $\beta = n$ or $-(n+1)$ and our basic separated solution is

$$\psi_n(r,\theta) = \left(a_n r^n + b_n r^{-(n+1)}\right) P_n(\cos\theta).$$

and finally the general axisymmetric solution is

$$\psi(r,\theta) = \sum_{n=0}^{\infty} \left(a_n r^n + b_n r^{-(n+1)}\right) P_n(\cos\theta). \tag{40}$$

The constants a_n and b_n are determined by expanding boundary conditions in terms of the Legendre polynomials. It is important to remember the $2/(2n+1)$ normalisation factor, and also to be careful with the actual argument of the functions viz. $\cos\theta$ vs. θ.

If the problem is defined on the interior of a sphere then $b_n = 0$ for the solution to be regular at the origin. Similarly, if the problem is defined on an infinite domain that excludes the origin (for example *outside* a sphere) then the typical requirement that ψ remain bounded as $r \to \infty$ implies that $a_n = 0$, for $n > 0$ and a_0 is the asymptotic ψ value. For problems between shells $r_1 < r < r_2$, both a_n and b_n are in general non-zero, and the coefficients need to be determined by applying the boundary conditions on both the inner and outer shells.

Example: Laplace's equation inside the unit sphere

Let's find the solution to Laplace's equation inside the unit sphere, subject to an axisymmetric boundary condition on $r = 1$, i.e. $\psi(1,\theta) = f(\theta)$. In the general solution (40) we immediately have that $b_n = 0$ (for regularity at the origin). Then at $r = 1$ we have

$$\begin{aligned}
f(\theta) &= \sum_{n=0}^{\infty} a_n P_n(\cos\theta),\; 0 \le \theta \le \pi, \\
F(x) &= \sum_{n=0}^{\infty} a_n P_n(x),\; x = \cos\theta,\; -1 \le x \le 1, \\
a_n &= \frac{(2n+1)}{2}\int_{-1}^{1} F(x) P_n(x)\,dx,
\end{aligned}$$

where F is a function such that $F(\cos\theta) = f(\theta)$ i.e. we wish to see the given $f(\theta)$ as a function of $\cos\theta$ rather than θ.

Generating function for Legendre polynomials

If $f_n(x)$ for $n = 0, 1, 2, \ldots$ is any sequence of functions then a **generating function** for the sequence is a function $G(x, r)$ with an extra variable r such that the f_n's arise as coefficients in the power series expansion of G w.r.t. r:

$$G(x,r) = \sum_{n=0}^{\infty} f_n(x) r^n.$$

Thus G neatly encapsulates the whole family of f's, which can be reconstructed (by the usual Taylor series formula, viewing x as a parameter) as

$$f_n(x) = \frac{1}{n!} \frac{d^n G(x,r)}{dr^n}\bigg|_{r=0}.$$

We now derive a generating function for the Legendre polynomials $P_n(x)$ (scaled so that $P_n(1) = 1$). We will motivate its construction from physics considerations (but this is not essential). Consider a unit point charge on the z axis at $z = 1$. Its potential is axisymmetric (i.e. independent of ϕ) and at any point P with position vector $\underline{P}$ the potential is $1/d$ where d is the distance from P to the charge. If $\underline{k}$ denotes the unit vector in the z direction then we have

$$d^2 = |\underline{P} - \underline{k}|^2 = \underline{P} \cdot \underline{P} - 2\underline{P} \cdot \underline{k} + \underline{k} \cdot \underline{k} = r^2 - 2r\cos\theta + 1$$

and the potential is

$$\psi(r,\theta) = \frac{1}{\sqrt{1 - 2r\cos\theta + r^2}}.$$

This function satisfies Laplace's equation (from electrostatic theory, or just check it directly!) and it is regular near the origin. Hence using our general form of such axisymmetric solutions (with $b_n = 0$) we must be able to write

$$\begin{aligned} \frac{1}{\sqrt{1 - 2r\cos\theta + r^2}} &= \sum_{n=0} a_n P_n(\cos\theta) r^n, \\ \frac{1}{\sqrt{1 - 2rx + r^2}} &= \sum_{n=0} a_n P_n(x) r^n. \end{aligned} \tag{41}$$

Here by definition of the P_n's, $P_n(1) = 1$ but they may be rescaled by the a_n's. However putting $x = 1$ in eq. (41) we get

$$\frac{1}{1-r} = \sum_{n=0}^{\infty} a_n r^n$$

so $a_n = 1$ for all n and we have our **generating function for Legendre polynomials**:

$$\begin{aligned} \sum_{n=0}^{\infty} P_n(x) r^n &= \frac{1}{\sqrt{1 - 2rx + r^2}}, \\ \frac{1}{n!} \frac{d^n}{dr^n} \left[\frac{1}{\sqrt{1 - 2rx + r^2}} \right]_{r=0} &= P_n(x). \end{aligned} \tag{42}$$

Eq. (42) can be used to derive the normalisations of the P_n's (recalling that we have already imposed to condition $P_n(1) = 1$) – squaring both sides and integrating from -1 to 1 gives

$$\int_{-1}^{1} \frac{dx}{1 - 2rx + r^2} = \sum_{m=0}^{\infty} r^m \sum_{n=0}^{\infty} r^n \int_{-1}^{1} P_n(x) P_m(x)\, dx = \sum_{n=0}^{\infty} r^{2n} \int_{-1}^{1} P_n^2(x)\, dx$$

where we have used the orthogonality of the P_n's. On the other hand we can evaluate the LHS integral (exercise! - start by substituting $y = 2rx$) to get

$$\int_{-1}^{1} \frac{dx}{1 - 2rx + r^2} = \frac{1}{r} \log\left(\frac{1+r}{1-r}\right)$$

and forming the difference of the standard powers series for $\log(1 \pm r)$ for $|r| < 1$, we get

$$\frac{1}{r} \log\left(\frac{1+r}{1-r}\right) = \sum_{n=0}^{\infty} \frac{2}{2n+1} r^{2n} = \sum_{n=0}^{\infty} r^{2n} \int_{-1}^{1} P_n^2(x)\, dx$$

giving

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