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Introduction to Differential Equations 1

Differential equations are equations where variables are linked together by differentiation, for example

$$\frac{dy}{dx} = x^2,$$

or, more complicated

$$\frac{d^2y}{dx^2} + \sin x \left(\frac{dy}{dx}\right)^2 + y = e^x.$$

Differential equations are very important in physics. In many areas the processes we are interested in are best described by differential equations.

For example, in mechanics

$$m\frac{d^2x}{dt^2} = F(x,t)$$

describes the motion of a particle of mass m under the influence of a force F(x,t).

In quantum mechanics, the central equation is the Schrödinger equation for the wavefunction of a particle, $\psi(x,t)$,

$$-\frac{\hbar^2}{2m}\frac{\partial^2 \psi}{\partial x^2} + V(x)\psi = i\hbar \frac{\partial \psi}{\partial t}.$$

In electromagentism, Maxwell's equations, which determine the electric and magnetic fields, are differential equations, for example

$$\nabla \cdot \mathbf{E} = \frac{\partial E_x}{\partial x} + \frac{\partial E_y}{\partial y} + \frac{\partial E_z}{\partial z} = \rho(\mathbf{r})$$

where $E = (E_x, E_y, E_z)$ is the electric field and ρ the charge density.

Classification of Differential Equations 1.1

There are many different ways to classify differential equations and it is important that you are able to identify the different types of equations you will see.

Independent and Dependent Variables

The first thing you need to be able to determine is which variable(s) are *independent* and which are *depen*dent. For example, in

$$\frac{dy}{dx} = x^2$$

y depends on x, so x is independent and y is dependent.

Ordinary or Partial?

In an ordinary differential equation, or *ODE*, there is only one independent variable. For example, in

$$\frac{dy}{dx} = x^2,$$

y depends only on x.

In a partial differential equation, or PDE, there are more than one independent variables. For example, in the wave equation

$$\frac{\partial^2 y}{\partial x^2} = \frac{1}{c^2} \frac{\partial^2 y}{\partial t^2},$$

y depends on x and t.

PDEs are written in terms of partial derivatives. Generally, they are harder to solve than ODEs.

Linear or Non-linear?

An equation is *linear* if the highest power of the dependent variable or any of its derivatives is one. For example,

$$\frac{dy}{dx} = x^2$$

contains only the first power of dy/dx. Note that the higher power of the independent variable does not matter for this definition.

A *nonlinear* equation contains higher powers. For example

$$\frac{dy}{dx} = y^2$$

contains the second power of the dependent variable *y*.

Note that

$$\frac{dy}{dx} = \sin y$$

is also nonlinear; you can think of expanding sin y as a power series containing higher powers of y. We shall see a more formal definition oflinearity later.

Generally, non-linear equations are harder to solve than linear ones, though some methods work for both. Often, nonlinear equations can only be solved numerically.

Order of an Equation

The order of an equation is given by the highest derivative it contains. For example

$$\frac{dy}{dx} = x^2$$

is a first order equation, because it contains the first derivative of y. However

$$\frac{d^2y}{dx^2} + \frac{dy}{dx} + y = 0,$$

is second order, because of the second derivative.

Generally, lower order differential equations are easier to solve than higher order ones.

Homogeneous or Inhomogeneous?

A linear differential equation is said to be homogeneous if all the terms contain the dependent variable. Thus

$$\frac{d^2y}{dx^2} + \frac{dy}{dx} + y = 0$$

is homogeneous, while

$$\frac{dy}{dx} = x^2$$

is inhomogeneous because the x^2 term on the right hand side is independent of y.

Another way to see this is to realise that a homogeneous linear equation will always have a solution with the dependent variable equal to zero.

These are just a few of the many ways we can classify differential equations, but they are the important ones for this course.

First Order Differential Equations 2

Solving a First Order Differential Equation by Direct Integration 2.1

In this section, we shall look at how to solve a very simple differential equation of the form

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

Note that this is a first order, linear, inhomogeneous, ordinary differential equation. The important property is that there is no term proportional to y, only dy/dx.

Equations of this sort are easily solved by direct integration. We can see that

$$y = \int dx f(x),$$

where this is an indefinite integral. We can only really solve the eqution if the integral can be evaluated. However, we tend to say the equation is solved if we can write a solution in this form, even when there is no exact expression for the integral.

Example: Let us look at a particular example

$$\frac{dy}{dx} = x^2.$$

Then,

$$y = \int dx x^2 = \frac{x^3}{3} + A,$$

where *A* is the arbitrary integration constant.

There will always be one arbitrary constant in the general solution of a first order ODE.

Note that this method works for higher order equations if the dependent variable only appears in one order.

Example:

$$\frac{d^2y}{dx^2} = x^2,$$

integrating once gives

$$\frac{dy}{dx} = \frac{x^3}{3} + A \ .$$

Integrating again,

$$y = \int dx \left(\frac{x^3}{3} + A\right) = \frac{x^4}{12} + Ax + B$$
.

The general solution of a second order linear ODE will always contain exactly two arbitrary constants. In order to determine these constants we need some additional constraints, known as boundary conditions. We shall see more about this later.

2.2 Solving a First Order Differential Equation by Separation of Variables

In this section, we shall look at solving a first order ODE of the form

$$\frac{dy}{dx} = f(x)g(y).$$

The right hand side is a function of x and y, but it is *separable*, that is, it can be written as a *product* of a function of x and another function of y. Note that equations of this type are not generally linear, unless $g(y) \propto y$.

Equations of this sort can be solved by integration. We write

$$\frac{1}{g(y)}\frac{dy}{dx} = f(x),$$

then integrate to get

$$\int \frac{dy}{g(y)} = \int dx f(x).$$

These are two indefinite integrals; if we can do them both, we obtain an implicit equation for the dependent variable y.

Example: Looking at an example

$$\frac{dy}{dx} = e^{-x}y^2.$$

We get

$$\int \frac{dy}{y^2} = \int dx \, e^{-x}.$$

Integrating,

$$-\frac{1}{\nu}+A=-e^{-x}+B.$$

There are two arbitrary integration constants, A and B, but we can combine them, writing C = A - B, to get

$$\frac{1}{y} = e^{-x} + C,$$

or, explicitly,

$$y = \frac{1}{e^{-x} + C}.$$

Note that sometimes it will be obvious that your equation is of this form, but sometimes you may have to do some work to get it there.

Example: Take, for example, the equation

$$\frac{1}{y}\frac{dy}{dx} = \frac{1+x/y}{xy+y^2}e^x.$$

Multiplying through by y,

$$\frac{dy}{dx} = \frac{y+x}{y(x+y)}e^x = \frac{e^x}{y}.$$

Then

$$\int dy y = \int dx e^x,$$

so

$$\frac{1}{2}y^2 = e^x + A ,$$

and

$$y = \sqrt{2(e^x + A)}.$$

Note that the arbitrary constant does not always appear as y = something + C.

Second Order Differential Equations I: Homogeneous Equations

Linearity and the Superposition Principle

In this section, I shall look at the significance of an equation being linear. For a homogeneous equation, the formal definition that the equation is linear is that its solutions satisfy the *superposition pronciple*, that is, if f(x) and g(x) are solutions to the equation, then so is the linear combination

$$y = A f(x) + B g(x)$$

where A and B are arbitrary constants. This is most clear for second order ODEs, where there are, in general, two independent solutions, so I shall use this as an example.

Example: Consider the equation

$$\frac{d^2y}{dx^2} = y.$$

It is easy to see that this has solutions $y = e^x$ and $y = e^{-x}$, so let us look at the function

$$y = Ae^x + Be^{-x}$$
.

Then

$$\frac{dy}{dx} = Ae^x - Be^{-x}$$

and

$$\frac{d^2y}{dx^2} = Ae^x + Be^{-x} = y,$$

so the equation is satisfied.

An important consequence of the superposition principle is that, if we can find any two independent solutions to a second order linear homogeneous ODE, then we can write down the general solution as an arbitrary linear combination of the two.

For an inhomogeneous equation, we can still use the superposition principle – the general solution is a linear combination of a solution which satisfies the full ODE and one which satisfies just the inhomogeneous part. We shall see more of this later.

For a first order, linear, homogeneous, ODE, there is only one independent solution, so the superposition principle is less useful. What it tells us is that if we can find any solution to the equation, the general solution is obtained just by multiplying by an arbitrary constant.

3.2 Second order Homogeneous Equation with Constant Coefficients

In this section I shall show how to solve a second order linear homogeneous equation with constant coefficients. To start off, let us consider the example

$$\frac{d^2x}{dt^2} - \frac{dx}{dt} - 6x = 0,$$

Note that this is second order, linear and homogeneous - there are no terms independent of x - and the coefficients in front of all the terms are constants, not functions of t.

We look for a solution of the form $x = e^{mt}$. Then

$$\frac{dx}{dt} = me^{mt} = mx$$
$$\frac{d^2x}{dx^t} = m^2e^{mt} = m^2x.$$

Substituting in the equation, we get

$$m^2x - mx - 6x = 0.$$

Then, cancelling the xs, gives the auxiliary equation for m:

$$m^2 - m - 6 = 0$$
.

This has roots m = -2 and m = 3, so $x = e^{-2t}$ and $x = e^{3t}$ are solutions. Then the superposition principle tells us that the general solution is

$$x = Ae^{-2t} + Be^{3t},$$

where *A* and *B* are arbitrary constants.

There are various possibilities we need to consider for the roots of the auxiliary equation:

- 1. They could be real and different,
- 2. They could be real and identical.
- 3. They could be complex, in a complex conjugate pair (if the equation is real).

The previous example shows us what to do in the first case; we get exponential functions in the general solution.

In the second case, when the auxiliary equation has two equal roots, we need to do something a little different. We shall look at an example, using the equation

$$\frac{d^2x}{dt^2} - 2\frac{dx}{dt} + x = 0.$$

The auxiliary equation for this case is

$$m^2 - 2m - 1 = 0$$
,

which has repeated root m = 1. The obvious thing to do would be to write down the general solution as

$$x = Ae^t + Be^t$$
,

but this is **wrong**, because the two terms are identical, so we effectively have just one arbitrary constant, while the general solution requires two. To get the second solution, we multiply the first by t, so, in this case $x = te^t$. We can show that this is indeed a solution by substituting:

$$\frac{dx}{dt} = e^t + te^t$$
$$\frac{d^x}{dt^2} = e^t + e^t + te^t.$$

Substituting in the differential equation, we get

$$\frac{d^2}{dt^2} - 2\frac{dx}{dt} + x = (e^t + e^t + te^t) - 2(e^t + te^t) + (te^t) = 0,$$

as required. Hence the general solution of the equation is

$$x = Ae^t + Bte^t$$
.

In the third case, where the solutions to the auxiliary equation form a complex conjugate pair, say $m = \alpha \pm i\beta$, we can proceed as in the first example and write

$$x(t) = Ae^{\alpha t}e^{i\beta t} + Be^{\alpha t}e^{-i\beta t}.$$

This looks a bit odd, because it involves complex numbers, but in fact it does work as we shall see in the next section. However, we can express the complex exponentials in terms of sines and cosines using de Moivre's theorem, so an alternative way to write this is

$$x(t) = A'e^{\alpha t}\sin\beta t + B'e^{\alpha t}\cos\beta t,$$

where A' and B' are different arbitrary constants, which can be written in terms of the original A and B.

Remember that the specific solution for an actual problem will involve applying initial or boundary conditions to determine the arbitrary constants in the general solution. Take our first example, where we found

$$x = Ae^{-2t} + Be^{3t}.$$

Since we have two arbitrary constants, we require two conditions to determine them. Suppose we are given initial conditions x = 0 and dx/dt = v when t = 0. This requires

$$y(0) = A + B = 0$$

 $y'(0) = -2A + 3B = v$.

The first condition gives A = -B, so from the second we get -5A = v. Hence A = v/5 and B = -v/5, which means the specific solution is

$$x(t) = \frac{v}{5}(e^{3t} - e^{2t}).$$

3.3 Complex Exponentials

In this section, I shall discuss the use of complex exponentials, $y = e^{i\alpha x}$, in the solution of differential equations, particularly those for oscillating systems.

It may at first seem a strange thing to introduce complex numbers to describe physical quantities which are real, given by real equations. The reason we do it is because it is easier to work with complex exponentials than with sines and cosines. This is particularly true when we have a damped oscillator: it is much easier to differentiate

$$x = e^{(\alpha + i\beta)t}$$

than

$$x = e^{\alpha t} \cos \beta t$$
.

So, what do these complex solutions mean? In fact, they have no physical significance. They appear only in the general solution to the equation. Once we put in (real) boundary conditions, the specific solution always ends up real.

Example: Let us take a simple example of an undamped harmonic oscillator

$$\frac{d^2x}{dt^2} + \omega^2 x = 0,$$

with initial conditions x(0) = 0 and x'(0) = v.

Following our usual method, we get the auxiliary equation

$$m^2 + \omega^2 = 0,$$

so $m = \pm i\omega$. The general solution can therefore be written as

$$x(t) = Ae^{i\omega t} + Be^{-i\omega t}$$

which involves complex numbers.

Now we apply the initial conditions to get

$$x(0) = A + B = 0$$

$$x'(0) = i\omega A - i\omega B = v.$$

From the first equation, B = -A, and then from the second $A = v/2i\omega$. So we can write the specific solution as

$$x(t) = \frac{v}{\omega} \frac{1}{2i} (e^{i\omega t} - e^{-i\omega t}) = \frac{v}{\omega} \sin \omega t,$$

which is real. The complex numbers have disappeared now we have a specific solution corresponding to the real initial conditions.

We do not have to work with complex numbers if we prefer not to. The general solution can also be written as

$$x(t) = A' \cos \omega t + B' \sin \omega t.$$

You can verify this by substituting in the differential equation, but can you see how to use De Moivre's theorem to show directly how to get from one form to the other, expressing the arbitrary constants A' and B' in terms of A and B?

Note that there are cases where the dependent variable real is a complex quantity and the differential equation involves imaginary terms. An example of this is the Schrödinger equation. Although the wavefunction is not someting which is physically measurable, its complex nature is an intrinsic part of the theory of quantum mechanics. In cases such as this, the comments made in this section do not apply – the wavefunction will in general be complex, even if we use real initial conditions.

4 Second Order Differential Equations II: Boundary Conditions and Inhomogeneous Equations

4.1 Initial and Boundary Value Problems

When we have a second order ODE, there are two arbitrary constants in the general solution. This means that we need two additional conditions to find these constants and turn the general solution into a specific solution.

These conditions can given for the same value of the independent variable or at different values. The problem is said to be an *initial value problem*, or *IVP*, if the value is the same, for example x(0) = 0 and x'(0) = 0. If the values are different, for example x(0) = x(a) = 0, it is a *boundary value problem*, or *BVP*.

A typical initial value problem would occur in mechanics, where we are given the initial position and velocity of a particle.

A typical boundary value problem would be finding the solutions to the Schrödinger equation, where the wavefunction goes to zero as $x \to \pm \infty$.

Let us look at an example of each type of problem. Assume that we have found the same solution to the differential equation in each case:

$$x(t) = A \sin \omega t + B \cos \omega t$$

SO

$$x'(t) = A\omega\cos\omega t - B\omega\sin\omega t$$

For the IVP, I shall use the condition x(0) = 0, x'(0) = 1. Putting these in, we get

$$x(0) = B = 0$$

$$x'(0) = A\omega = 1$$
,

so clearly $A = 1/\omega$ and B = 0. This gives the specific solution

$$x(t) = \frac{1}{\omega} \sin \omega t.$$

For the BVP, I shall make x(0) = 0 and $x(\tau) = 0$. This gives

$$x(0) = B = 0$$

$$x(1) = A \sin \omega \tau + B \cos \omega \tau = 0.$$

So B=0 and A=0 unless $\sin \omega \tau = 0$, which requires $\omega \tau$ to be an integer multiple of π . If that is the case, A can have any value.

This example highlights an important point: IVPs will generally have a solution (unless the conditions given are contradictory) while for BVPs this may not be the case.

Example: Consider a damped oscillator governed by the differential equation

$$\frac{d^2x}{dt^2} + 4\frac{dx}{dt} + 5x = 0,$$

which initially is at rest but has displacement x = 1.

The auxiliary equation is

$$m^2 + 4m + 5 = 0$$
,

which has solutions $m = -2 \pm i$. Thus the general solution can be written as

$$x(t) = Ae^{-2t}\cos t + Be^{-2t}\sin t.$$

Differentiating this, we get the velocity

$$x'(t) = -2Ae^{-2t}\cos t - Ae^{-2t}\sin t - 2Be^{-2t}\sin t + Be^{-2t}\cos t.$$

Putting in the initial conditions, x(0) = 1 gives

$$A=1$$
,

while x'(0) = 0 gives

$$-2A + B = 0,$$

so B = 2. Thus the specific solution is

$$x(t) = e^{-2t} \cos t + 2e^{-2t} \sin t$$
.

Example: Consider the differential equation

$$\frac{d^2y}{dx^2} - \frac{dy}{dx} - 2y = 0$$

with boundary conditions y(0) = 0 and y(ln2) = 1.

The auxiliary equation is

$$m^2 - 2m - 2 = 0$$
.

which has solutions m = -1 and m = 2. Hence the general solution is

$$v(x) = Ae^{-x} + Be^{2x}.$$

Putting in the boundary conditions, at x = 0,

$$A+B=0$$
,

and at $x = \ln 2$,

$$Ae^{-\ln 2} + Be^{2\ln 2} = \frac{1}{2}A + 4B = 1.$$

Solving these equations gives A = -2/7 and B = 2/7, so

$$y = -\frac{2}{7}(e^{-x} - e^{2x}).$$

4.2 Complementary Functions and Particular Integrals

In this section I shall look at solving a second order, linear, inhomogeneous equation with constant coefficients. The example I shall look at later is

$$\frac{d^2x}{dt^2} + 4x = \sin t.$$

This could represent an undamped harmonic oscillator with an applied force which oscillates in time, given by the inhomogeneous term $\sin t$.

The method we shall use divides the solution in two parts, called the *complementary function* and *particular integral*. Let us start by expressing the general inhomogeneous equation in a more abstract form

$$\hat{D}x = f$$

where \hat{D} is the *differential operator* on the left hand side, in this case $\hat{D} = d^2/dt^2 + 4$ and f, the inhomogeneous term on the right hand side, here $f = \sin t$. We first solve the homogeneous equation

$$\hat{D}x_c=0$$
,

to find the *complementary function* x_c . For equations with constant coefficients, you can do this using the method described in section 3.2. Note that the complementary function, for a second order equation, will contain two arbitrary constants. Next we find a solution, called the *particular integral*, x_p , to the full inhomogeneous problem

$$\hat{D}x_p = f$$
.

 x_p can be any function which satisfies the equation - we do not have to worry about it satisfying any initial or boundary conditions here. The general solution to the inhomogeneous problem is then the sum of the complementary function and the particular integral:

$$x = x_c + x_p$$
.

We can see that it satisfies the differential equation because

$$\hat{D}x = \hat{D}(x_c + x_p) = \hat{D}x_c + \hat{D}x_p = 0 + f.$$

It also has two arbitrary constants, in x_c , which is required for the general solution of a second order, ordinary differential equation. That is why we have to include the complementary function. Note that we have assumed the equation is linear, as only then is $\hat{D}(x_c + x_p) = \hat{D}x_c + \hat{D}x_p$. The method does not work for non-linear problems.

Example: Let us now apply this method to the example we started with,

$$\frac{d^2x}{dt^2} + 4x = \sin t.$$

The complementary function satisfies the homogeneous equation

$$\hat{D}x_c = \frac{d^2x_c}{dt^2} + 4x_c = 0.$$

Following our usual procedure, the auxilliary equation is

$$m^2 + 4 = 0$$
,

so $m = \pm 2i$ and we can write the complementary function as

$$x_c(t) = Ae^{2it} + Be^{-2it}$$
 or $x_c(t) = A\sin 2t + B\cos 2t$.

When the function on the right hand side is a sine or cosine, the particular integral we chose takes the form

$$x_p = a\cos t + b\sin t.$$

Note that here, a and b are not arbitrary constants, as in the complementary function. They are constants which we are going to determine by substituting this solution into the differential equation.

Differentiating,

$$\frac{dx_p}{dt} = -a\sin t + b\cos t$$

and

$$\frac{d^2x_p}{dt^2} = -a\cos t - b\sin t,$$

so, substituting this into the differential equation, we get

$$(-a\cos t - b\sin t) + 4(a\cos t + b\sin t) = \sin t.$$

Equating coefficients of the sine and cosine terms gives

$$-a + 4a = 0$$

$$-b + 4b = 1$$
.

Hence, a = 0 and b = 1/3, so the particular integral is

$$x_p = \frac{1}{3}\sin t.$$

The full solution is then

$$x(t) = x_c(t) + x_p(t) = A \sin 2t + B \cos 2t + \frac{1}{3} \sin t.$$

There are many ways to find particular integrals corresponding to different functions on the right hand side of the inhomogenous equation. You can look these up in a text book when you need them. Here, we will just consider the case of a harmonic function, $\sin(\omega t)$ or $\cos(\omega t)$, as above. This is a common form in physics, as we often like to consider driving systems in this way. Usually, the function we need to try is then

$$x_p(t) = a\sin(\omega t) + b\cos(\omega t), \tag{4.1}$$

with a and b constants to be determined.

Example: As a second, slightly more complicated, example, consider the equation

$$\frac{d^2x}{dt^2} + 2\frac{dx}{dt} + 10x = \cos 2t.$$

This could represent a damped oscillator with harmonic driving term.

In this case, the complemetary function satisfies

$$\hat{D}x_c = \frac{d^2x_c}{dt^2} + 2\frac{dx_c}{dt} + 10x_c = 0.$$

We solve this in the usual way, obtaining the auxiliary equation

$$m^2 + 2m + 10 = 0.$$

This is has solutions $m = -1 \pm 3i$. I will use sines and cosines rather than complex numbers to write the complementary function as

$$x_c = Ae^{-t}\cos 3t + Be^{-t}\sin 3t,$$

with A and B arbitrary constants.

The particular integral is a solution to the inhomogeneous equation:

$$\frac{d^2x_p}{dt^2} + 2\frac{dx_p}{dt} + 10x_p = \cos 2t.$$

We use the trial solution:

$$x_p = a\cos 2t + b\sin 2t.$$

Then

$$\frac{dx_p}{dt} = -2a\sin t + 2b\cos t$$

and

$$\frac{d^2x_p}{dt^2} = -4a\cos t - 4b\sin t,$$

Substituting into the equation, we get

$$(-4a\cos t - 4b\sin t) + 2(-2a\sin t + 2b\cos t) + 10(a\cos 2t + b\sin 2t) = \cos 2t$$
.

Equating coefficients of the sines and cosines gives

$$6b - 4a = 0$$

$$6a + 4b = 1.$$

Solving these simultaneous equations gives a = 3/26 and b = 2/26, so the particular integral is

$$x_p(t) = \frac{1}{26}(3\cos 2t + 2\sin 2t).$$

The general solution is then

$$x(t) = Ae^{-t}\cos 3t + Be^{-t}\sin 3t + \frac{1}{26}(3\cos 2t + 2\sin 2t).$$

The constants *A* and *B* depend on the initial conditions, but after a long time, the terms they multiply go to zero and we are left with a displacement which goes at the frequency of the driving term. This is what we would expect for a damped oscillator.

The form for the particular integral given above usually works for harmonic driving terms. However, it can fail if the inhomogeneous term is identical to one of the parts of the complementary function. If we are dealing with a driven oscillator, this corresponds to the case with no damping and the driving term being at the resonant frequency. Then we would find $\hat{D}x_p = 0$, so it would not be possible to solve the resulting simultaneous equations. What we then do is multiply the trial function by t:

$$x_p(t) = at\sin(\omega t) + bt\cos(\omega t), \tag{4.2}$$

Example: Suppose now instead we are asked to find the particular integral for

$$\frac{d^2x}{dt^2} + 4x = \sin 2t.$$

The difference here is that the function $\sin 2t$ is part of the complementary function. Hence we have to try

$$x_p = at\sin 2t + bt\cos 2t.$$

Now we have

$$\begin{aligned} \frac{dx_p}{dt} &= (a\sin 2t + b\cos 2t) + 2t(a\cos 2t - b\sin 2t) \\ \frac{d^2x_p}{dt^2} &= 2(a\cos 2t - b\sin 2t) + 2(a\cos 2t - b\sin 2t) - 4t(a\sin 2t + b\cos 2t) \\ &= 4(a\cos 2t - b\sin 2t) - 4t(a\sin 2t + b\cos 2t) \end{aligned}$$

Now substituting in the differential equation gives

$$4(a\cos 2t - b\sin 2t) - 4t(a\sin 2t + b\cos 2t) + 4t(a\sin 2t + b\cos 2t) = sin 2t.$$

The terms containing t cancel, leaving

$$4a\cos 2t - 4b\sin 2t = \sin 2t$$
.

This is easily solved by taking a = 0 and b = -1/4, so the particular integral is

$$x_p = -\frac{t}{4}\cos 2t.$$

Note that if we had not realised that $\sin 2t$ was part of the complementary function, and tried the same function as in the previous example, we would not have been able to find a solution. The method thus 'fails safe' in that we get a warning something is wrong. However, it is relatively easy to find complementary functions, so it is usually best to do this first so that we can chose the correct trial function for the particular integral.

4.3 Complex Numbers Again

We found that calculating the particular integral is a bit messy, because of the need to include both sine and cosine terms. Here, we look at how to simplify the treatment, for harmonic driving terms, using complex numbers.

Example:

$$\frac{d^2x}{dt^2} + 2\frac{dx}{dt} + 10x = e^{2it}.$$

We have already found the complementary function. It is

$$x_c(t) = Ae^{-t}\cos 3t + Be^{-t}\sin 3t,$$

with *A* and *B* arbitrary constants.

Now let's solve for the particular integral, trying the solution

$$x_p(t) = ae^{2it},$$

where a is a complex number which we need to find. The differentiation is now much simpler:

$$\frac{dx_p}{dt} = 2iae^{2it} \qquad \frac{d^2x_p}{dt^2} = -4ae^{2it}.$$

Substituting in the differential equation,

$$-4ae^{2it} + 4iae^{2it} + 10ae^{2it} = e^{2it}$$
.

This requires

$$a = \frac{1}{6+4i} = \frac{1}{52}(6-4i) = \frac{1}{26}(3-2i)$$

so

$$x_p(t) = \frac{1}{26}(3-2i)e^{2it} = \frac{1}{26}(3-2i)(\cos 2t + i\sin 2t)$$
$$= \frac{1}{26}(3\cos 2t + 2\sin 2t) + i\frac{1}{26}(-2\cos 2t + 3\sin 2t).$$

So, what is the physical meaning of a complex driving term $f(t) = f^{(r)}(t) + if^{(i)}(t)$? We can't apply a complex force to an oscillator.

We have found that the complex driving term leads to a complex particular integral, $x_p(t) = x_p^{(r)}(t) + ix_p^{(i)}(t)$. Using the \hat{D} notation, we have

$$\hat{D}(x_p^{(r)}(t) + ix_p^{(i)}(t)) = f^{(r)}(t) + if^{(i)}(t). \tag{4.3}$$

Provided \hat{D} is real (the coefficients are all real), we can equate real and imaginary parts, to get

$$\hat{D}x_p^{(r)}(t) = f^{(r)}(t)$$
 and $\hat{D}x_p^{(i)}(t) = f^{(i)}(t)$. (4.4)

So $x_p^{(r)}(t)$ is the particular integral for the real, physical, driving term $f^{(r)}(t)$ and $x_p^{(i)}(t)$ is the particular integral for the real, physical, driving term $f^{(i)}(t)$

More concretely, for the example we have just looked at, we get

$$\left(\frac{d^2 x_p^{(r)}}{dt^2} + 2 \frac{d x_p^{(r)}}{dt} + 10 x_p^{(r)}\right) + i \left(\frac{d^2 x_p^{(i)}}{dt^2} + 2 \frac{d x_p^{(i)}}{dt} + 10 x_p^{(i)}\right) = \cos 2t + i \sin 2t .$$
(4.5)

Equating real and imaginary parts gives

$$\frac{d^2x_p^{(r)}}{dt^2} + 2\frac{dx_p^{(r)}}{dt} + 10x_p^{(r)} = \cos 2t \tag{4.6}$$

$$\frac{d^2x_p^{(i)}}{dt^2} + 2\frac{dx_p^{(i)}}{dt} + 10x_p^{(i)} = \sin 2t.$$
 (4.7)

We have solved two separate problems: one is for the driving term $\cos 2t$ (note the solution is the same as we found previously), the other for $\sin 2t$.

Using complex numbers like this simplifies finding the particular integral, though we have to take the real (or imaginary) part at the end of the calculation to get the actual solution. However, in physics we often don't bother doing this, and talk about the complex oscillation (or, more generally, wave) as the actual solution. We then need to have formulae to calculate the physical quantities which we may be interested in, for example, the time averaged intensity of the wave, from the complex form. If we have two oscillating terms represented by complex functions $a = a_0 e^{i\omega t}$ and $b = b_0 e^{i\omega t}$ (a_0 , b_0 complex numbers), the time average of the product of the real parts (or the imaginary parts, the expression is the same) is

$$\langle ab \rangle = \frac{1}{2} \operatorname{Re} \left\{ ab^* \right\} \,. \tag{4.8}$$

The intensity of our oscillator is thus

$$\langle I \rangle = \frac{1}{2} \operatorname{Re} \left\{ x_p x_p^* \right\} = \frac{1}{2} |x_p|^2. \tag{4.9}$$

In the example above, we get

$$\langle I \rangle = \frac{1}{2} (ae^{2it} \times a^* e^{-2it}) = \frac{1}{2} |a|^2 = \frac{1}{2} \left| \frac{1}{6+4i} \right|^2 = \frac{1}{104}.$$
 (4.10)

5 Introduction to Partial Differential Equations

Partial differential equations are one of the most important mathematical tools we use to understand physical systems. They tend to occur whenever something depends on more than one variable: for example, when we look at waves on a string, the displacement depends on both the position, x, and the time, t.

5.1 Examples of PDEs

We are going to meet primarily the following partial differential equations:

1. The Wave Equation

$$\nabla^2 u = \frac{1}{c^2} \frac{\partial^2 u}{\partial t^2} \,. \tag{5.1}$$

u is the displacement of the wave. ∇^2 is the *Laplacian operator*, which becomes simply $\partial^2 u/\partial x^2$ in one dimension (such as a wave on a string). c is the speed of the wave.

2. The Laplace Equation

$$\nabla^2 u = 0. ag{5.2}$$

Applies to many systems: often u is a potential, such as in electrostatics (without any charges), gravitation, hydrodynamics.

3. Diffusion Equation

$$\nabla^2 u = \frac{1}{h^2} \frac{\partial u}{\partial t} \,. \tag{5.3}$$

Describes diffusion of gases, chemicals, heat. u is the density or temperature. h^2 is a diffusion constant.

4. The Schrödinger Equation

$$-\frac{\hbar^2}{2m}\nabla^2\psi + V\psi = i\hbar\frac{\partial\psi}{\partial t}.$$
 (5.4)

Here, ψ is the wavefunction, $V(\mathbf{r})$ is the potential, m is the particle mass and \hbar is Planck's constant divided by 2π .

5.2 Notation and Terminology

Partial differential equations obviously involve partial differentiation. Remember that if we have a function u(x,t), then $\partial u/\partial x$ is the differential of u with respect to x, treating t as a constant. For example, if $u = \sin x e^{-t}$,

$$\frac{\partial u}{\partial x} = \cos x e^{-t} , \quad \frac{\partial u}{\partial t} = -\sin x e^{-t} , \quad \frac{\partial^2 u}{\partial x^2} = -\sin x e^{-t} , \quad \frac{\partial^2 u}{\partial x \partial t} = \frac{\partial^2 u}{\partial t \partial x} = -\cos x e^{-t} .$$

Partial differentiation can get more complicated than this, but we shall not need that here.

The Laplacian operator, ∇^2 is a shorthand for the derivative

$$\nabla^2 u = \frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} + \frac{\partial^2 u}{\partial z^2} \,. \tag{5.5}$$

In two dimensions, we drop one of the derivatives, usually z.

All the equations given above are second order PDEs (because the highest derivative is the second). There is a single dependent variable (u or ψ), and at least two independent variables. They are also all linear equations: the dependent variable only occurs as the first power (there are, for example, no u^2 terms). This is important for the method we are going to use to solve them, which involves the superposition principle: if we have two solutions to the equation, the sum, or any linear combination, of these is also a solution.

The method we are going to use to solve these equations is known as the *separation of variables*. I will say a little bit about some other methods, but we do not expect you to learn how to use them here.

6 The Wave Equation in One Dimension

In one dimension, such as when we are considering waves on a string, the wave equation is

$$\frac{\partial^2 u}{\partial x^2} = \frac{1}{c^2} \frac{\partial^2 u}{\partial t^2} \,, \tag{6.1}$$

where u(x,t) is the displacement of the string for position x at time t. c is the speed of the wave, which can be written $c = \sqrt{T/\mu}$, where T is the tension and μ the mass per unit length. We will not be looking at the physical origin of the equations here, just how to solve them.

We shall first consider the case of a string of length L fixed to rigid supports at either end, where x = 0 and x = L. This gives us some *boundary conditions*: u(0,t) = 0 = u(L,t). We always need to know the boundary conditions in order to solve a PDE.

We are now going to go through solving the equation by the method of separation of variables. this is our standard recipe, which you need to learn and practice.

6.1 Separate the Variables

Our boundary conditions must be satisfied at special values of x but for all values of time. We can achieve this by writing a solution which is factorised in the form u(x,t) = X(x)T(t), where X is a function just of x, and T a function of only t. If X satisfies the boundary conditions, that is X(0) = 0 = X(L), then u will satisfy them whatever the behaviour of T(t). If we can make this factorisation, then we have separated the variables.

We now substitute our u into the differential equation. We have

$$\frac{\partial^2 u}{\partial x^2} = \frac{\partial^2}{\partial x^2} [X(x)T(t)] = T \frac{d^2 X}{dx^2} \quad \text{and} \quad \frac{1}{c^2} \frac{\partial^2 u}{\partial t^2} = \frac{1}{c^2} X \frac{d^2 T}{dt^2}. \tag{6.2}$$

Substituting in Eq.(6.1) gives

$$T\frac{d^2X}{dx^2} = \frac{1}{c^2} X \frac{d^2T}{dt^2} \,. \tag{6.3}$$

If we now divide through by XT, we get

$$\frac{1}{X(x)}\frac{d^2X(x)}{dx^2} = \frac{1}{c^2}\frac{1}{T(t)}\frac{d^2T(t)}{dt^2}.$$
 (6.4)

Since the left hand side is a function just of x, and the right hand side just of t, the only way this equation can be satisfied is if both sides are equal to a constant. Let's call this constant N. It is sometimes known as the *separation constant*. We now have two separate, *ordinary differential equations*, one for X and the other for T:

$$\frac{d^2X}{dx^2} = NX\tag{6.5}$$

and

$$\frac{d^2T}{dt^2} = Nc^2T. ag{6.6}$$

Note that we have not specified the sign of N. If N < 0, these equations look like the description of an harmonic oscillator, so they have oscillatory solutions. If N > 0 they have exponentially growing and decaying solutions. We can guess which is appropriate, either by thinking about the physics, or, more mathematically, by looking at how we can satisfy the boundary conditions.

6.2 Satisfy the Boundary Conditions

In the present case, the boundary conditions are y(0,t) = 0 = y(L,t), which means that X(0) = 0 = X(L). The function X is thus equal to zero at two distinct points. This allows us to determine the sign of N, because oscillatory functions can have two such zeros, but exponential functions cannot.

We can rule out N = 0, because the solutions would then take the form X(x) = Ax + B, where A and B are arbitrary integration constants. The boundary conditions then require A = 0 = B, which just gives us the trivial solution X(x) = 0 for all x.

If N > 0, say $N = k^2$, with k real, the general solution would be $X(x) = Ae^{kx} + Be^{-kx}$. Again, this can only be satisfied if A = 0 = B, giving X(x) = 0.

So *N* must be negative. If we take $N = -k^2$, Eq.(6.5) becomes

$$\frac{d^2X}{dx^2} = -k^2X\,, (6.7)$$

which has general solution

$$X(x) = A\cos kx + B\sin kx. \tag{6.8}$$

We now apply the boundary conditions. X(0) = A, so as we require X(0) = 0, A = 0. Then, $X(L) = B \sin kL$. We cannot take B = 0, as that gives the trivial solution, X(x) = 0 everywhere, so $\sin kL = 0$, giving $k = k_n = n\pi/L$, where n is any integer (we can exclude n = 0, because, again, this gives X(x) = 0). So, we have

$$X_n(x) = B_n \sin\left(\frac{n\pi x}{L}\right), \quad \text{for } n = 1, 2, 3, \dots,$$
 (6.9)

where we add the subscript n to remind us that there are different solutions corresponding to different values of n.

Now we know the values of k, and hence N, we can solve Eq.(6.6) to find T(t):

$$\frac{d^2T}{dt^2} = Nc^2T = -k_n^2c^2T = -\frac{n^2\pi^2c^2}{L^2}T = -\omega_n^2T,$$
(6.10)

Where the frequency, $\omega_n = k_n c = n\pi c/L$. This equation again has the form of a harmonic oscillator, so the solution is

$$T_n(t) = C_n \sin \omega_n t + D_n \cos \omega_n t$$
 or $T_n(t) = C_n \cos (\omega_n t + \phi_n)$, (6.11)

where C_n , D_n and ϕ_n are arbitrary constants. We cannot proceed further to find these without more constraints. In this case, we need to know some *initial conditions* – what the string is doing at some initial time, t = 0.

At this point, we now have a set of solutions to the wave equation, satisying the boundary conditions, of the form

$$u_n(x,t) = X_n(x)T_n(t) = B_n \sin(k_n x)\cos(\omega_n t + \phi_n) = B_n \sin\left(\frac{n\pi x}{L}\right)\cos\left(\frac{n\pi ct}{L} + \phi_n\right). \tag{6.12}$$

These solutions describe the fundamental (n = 1) and harmonics, of the standing waves on the string.

6.3 Construct the General Solution

We now have a set of particular solutions, the standing waves, which satisfy the wave equation and our boundary conditions at x = 0 and x = L. We are now going to use the superposition principle to construct the most general solution which satisfies the boundary conditions.

The superposition applies to any differential equation which is linear (and homogeneous), meaning that the dependent variable (u in the wave equation) and its derivatives appear only as the first power. It state that if u_1 and u_2 are solutions to the equation, then $u = c_1u_1 + c_2u_2$, with c_1 and c_2 arbitrary constants, is also a solution. We have often used this property of waves – when talking about constructive and destructive interference of two waves, we think of the resultant amplitude as being the sum of the amplitudes of the two waves considered separately.

Applying the superposition principle, we can say that any linear combination of our standing wave solutions will also be a solution to the wave equation, satisfying the same boundary conditions. Thus, the most general solution we can write down will be

$$u(x,t) = \sum_{n=1}^{\infty} B_n \sin\left(\frac{n\pi x}{L}\right) \cos\left(\frac{n\pi ct}{L} + \phi_n\right). \tag{6.13}$$

Notice that this solution is no longer separable, in the form u(x,t) = X(x)T(t).

6.4 Satisfy the Initial Conditions

In order to determine the arbitrary constants B_n and ϕ_n in Eq(6.13), we need to know what the string is doing at some initial time, which we can take as t = 0. We may be told, for example, that it is held stationary but in some fixed shape, or that it has zero displacement and some position dependent velocity.

Let us take a particular example, where the string is initially at rest $(\partial u/\partial t = 0$ for all x at t = 0), but is held in a triangular shape, displaced by a distance d at its midpoint:

$$u(x,0) = f(x) = \begin{cases} 2dx/L & 0 \le x \le L/2\\ 2d(1-x/L) & L/2 \le x \le L \end{cases}$$
 (6.14)

before being released.

Calculating the velocity,

$$\frac{\partial u}{\partial t} = \sum_{n=1}^{\infty} -B_n \frac{n\pi c}{L} \sin\left(\frac{n\pi x}{L}\right) \sin\left(\frac{n\pi ct}{L} + \phi_n\right). \tag{6.15}$$

For this to be zero everywhere, we simply require all the $\phi_n = 0$. Then our solution simplifies to

$$u(x,t) = \sum_{n=1}^{\infty} B_n \sin\left(\frac{n\pi x}{L}\right) \cos\left(\frac{n\pi ct}{L}\right),\tag{6.16}$$

which gives

$$u(x,0) = \sum_{n=1}^{\infty} B_n \sin\left(\frac{n\pi x}{L}\right). \tag{6.17}$$

You should recognise this as something like a Fourier series. In fact, it is a half-range sine series, because there are only sines in the expansion, and the fundamental mode correponds to only half a wavelength. Hence we can find the coefficients B_n by using Fourier theory to expand our initial displacement, Eq.(6.14) as a half range sine series. They are given by

$$B_n = \frac{2}{L} \int_0^L dx f(x) \sin\left(\frac{n\pi x}{L}\right). \tag{6.18}$$

In our particular case (you should make sure that you can show this)

$$B_n = \begin{cases} -\frac{8d}{\pi^2} \frac{1}{n^2} (-1)^{(n+1)/2} & \text{for odd } n \\ 0 & \text{for even } n \end{cases}$$
 (6.19)

Hence we have a solution which satisfys both initial and boundary conditions

$$u(x,t) = \frac{8d}{\pi^2} \left[\sin\left(\frac{\pi x}{L}\right) \cos\left(\frac{\pi ct}{L}\right) - \frac{1}{9} \sin\left(\frac{3\pi x}{L}\right) \cos\left(\frac{3\pi ct}{L}\right) + \frac{1}{25} \sin\left(\frac{5\pi x}{L}\right) \cos\left(\frac{5\pi ct}{L}\right) - \frac{1}{49} \sin\left(\frac{7\pi x}{L}\right) \cos\left(\frac{7\pi ct}{L}\right) + \dots \right] .$$
(6.20)

On blackboard there is a python script which generates an animation of this solution as it changes with time.

6.5 Summary

We have solved the wave equation

$$\frac{\partial^2 u}{\partial x^2} = \frac{1}{c^2} \frac{\partial^2 u}{\partial t^2} \,,$$

with boundary conditions u(0,t) = 0 = u(L,t), and initial conditions on the displacement of the string. The procedure involved the following steps:

1. We looked for a separable solution u(x,t) = X(x)T(t) and used it to write the wave equation in the form

$$\frac{1}{X(x)}\frac{d^2X(x)}{dx^2} = \frac{1}{c^2}\frac{1}{T(t)}\frac{d^2T(t)}{dt^2} = N.$$

- 2. By considering the boundary conditions, we decided that N must be negative: $N = -k^2$. We then applied the boundary conditions to solve for X(x), finding the allowed values of k, which we called k_n .
- 3. We used these k to find the form of T(t).
- 4. We applied the superposition to express the general solution as a linear combination of the separarble solutions. This gives the most general solution to the equation for our boundary conditions.
- 5. We used a Fourier expansion to determine the arbitrary constants in the general solution from the initial conditions.

We will be using this recipe repeatedly in this course, for all the PDEs we study, so you need to be very familiar with it and be able to apply it yourself to new problems. For example, in the case of waves on a string, you should be able to figure out how to deal with different boundary conditions (for example, $\partial u/\partial x = 0$ at one or both ends of the string), different initial displacements, and initial conditions on the velocity of the string rather than its displacement.

6.6 D'Alembert's Solution to the Wave Equation

Though the method of separation of variables is a very useful technique, you should not get the impression that it is the only approach we can use. for example, D'Alembert showed that, for the wave equation

$$\frac{\partial^2 u}{\partial x^2} = \frac{1}{c^2} \frac{\partial^2 u}{\partial t^2} ,$$

the most general solution is

$$u(x,t) = f(x-ct) + g(x+ct), (6.21)$$

where the functions f and g are completely arbitrary – any (differentiable) functions will satisfy the equation. This solution consists of two shapes, given by the functions f and g, one which, f is moving in the

direction of increasing x, while the other, g moves to decreasing x. If you look at the animation of the Fourier expansion for the wave, you can see these two shapes: starting from the triangular form, we get one triangle moving to the left, another to the right. There is another python script showing how we construct the same result using D'Alembert's solution.

We are not asking you to be able to use this method to solve the wave equation.

7 Similar Wave Problems

In the previous section we saw, in detail, the solution of the wave equation with boundary conditions where we fix both ends of the string, and with the initial condition that the string is at rest. In this section we will look at how this solution changes when we use different initial and boundary conditions, and also what happens when we add a damping term to the motion of the string.

7.1 Changing the Initial Conditions

In the previous example, I chose initial conditions where the string was at rest, v(x,0) = 0, but with some given displacement u(x,0) = f(x). Another possibilty would be to have zero displacement, u(x,0) = 0 but some initial velocity profile v(x,0) = f(x). For example, we could hit the string with a hammer, as in a piano. We start from the general solution, Eq.(6.13)

$$u(x,t) = \sum_{n=1}^{\infty} B_n \sin\left(\frac{n\pi x}{L}\right) \cos\left(\frac{n\pi ct}{L} + \phi_n\right). \tag{7.1}$$

Putting t = 0,

$$u(x,0) = \sum_{n=1}^{\infty} B_n \sin\left(\frac{n\pi x}{L}\right) \cos\left(\phi_n\right),\tag{7.2}$$

so we can make u(x,0) = 0 by making all $\phi_n = -\pi/2$. Remembering that $\cos(\theta - \pi/2) = \sin\theta$, this gives

$$u(x,t) = \sum_{n=1}^{\infty} B_n \sin\left(\frac{n\pi x}{L}\right) \sin\left(\frac{n\pi ct}{L}\right). \tag{7.3}$$

Of course, we could have just written our general solution for T(t) as $\sin(\omega_n t + \phi_n)$ and chosen $\phi_n = 0$.

Now we differentiate with respect to t and get

$$v(x,t) = \sum_{n=1}^{\infty} B_n \left(\frac{n\pi c}{L} \right) \sin\left(\frac{n\pi x}{L} \right) \cos\left(\frac{n\pi ct}{L} \right). \tag{7.4}$$

Letting t = 0, and putting v(x,0) = f(x)

$$v(x,0) = \sum_{n=1}^{\infty} B_n \left(\frac{n\pi c}{L} \right) \sin\left(\frac{n\pi x}{L} \right) = f(x) = \sum_{n=1}^{\infty} b_n \sin\left(\frac{n\pi x}{L} \right), \tag{7.5}$$

where the b_n are the coefficients in the half-range sine series for f(x). Equating the coefficients, we see that the B_n we require to complete the solution in Eq.(7.3) are

$$B_n = \left(\frac{L}{n\pi c}\right)b_n. \tag{7.6}$$

7.2 Changing the Boundary Conditions

In the initial treatment of the wave equation, I chose boundary conditions where both ends of the string are fixed. That's the natural boundary condition for a string, but other boundary conditions can occur for different sorts of wave. If we look at one dimensionsl waves on a rod, we can have one or both ends unconstrained. Then the boundary condition is for the gradient, $\partial u/\partial x$, to be zero. We can get this for a wave on a string, but it is necessary to have tension in the string, so we need to do something like attaching the end to a massless ring moving on a frictionless rod, which is not very realistic. The $\partial u/\partial x = 0$ boundary condition applies for sound waves at the open end of a pipe, such as an organ pipe.

Let's next look at how the solution changes when we have $\partial u/\partial x = 0$ at both ends, x = 0 and x = L. The separation of variables process is exactly the same, so we can start from Eq(6.8):

$$X(x) = A\cos kx + B\sin kx. \tag{7.7}$$

We require dX/dx = 0 for x = 0 and x = L, so we differentiate:

$$\frac{dX}{dx} = -Ak\sin kx + Bk\cos kx. \tag{7.8}$$

Putting x=0 gives Bk, so we must have B=0 to satisfy the boundary condition. Then, for x=L, we require $-Ak\sin kL=0$. So, for a non trivial solution, we must have $\sin kL=0$, which means $kL=n\pi$. The solutions for X(x) are thus

$$X(x) = A\cos\left(\frac{n\pi x}{L}\right),\tag{7.9}$$

with n = 0, 1, 2... In this case, we do not omit the value n = 0, because that gives a non-trivial solution, X(x) = A, representing a constant displacement. This makes sense for these boundary conditions: if we only fix the gradient, we can displace the whole rod or string and still satisfy the conditions.

Actually, I have not done the case of n = 0, and thus k = 0, completely correctly. Returning to the differential equation for X(x), Eq.(6.5), we get, for k = 0,

$$\frac{d^2X}{dx^2} = 0\,, (7.10)$$

which has general solution X(x) = A + Bx. For the boundary conditions we are looking at, we must have B = 0, so X(x) = A is, in fact, correct. However, there may be cases where both terms are needed.

Having found the values of k, we can go on to solve Eq.(6.6) for T(t). For n > 0, the solutions are identical to those we found previously, Eq.(6.11). For n = 0 we again need to be careful, as the general solution will be

$$T_0(t) = A_0 + B_0 t . (7.11)$$

In this case, it may be necessary to have both terms, as the initial conditions may make the whole string move with some velocity, requiring $B_0 \neq 0$.

With these considerations, we can now assemble the general solution from the separable solutions, using the superposition principle. We separate out the n = 0 term, because it looks different:

$$u(x,t) = A_0 + B_0 t + \sum_{n=1}^{\infty} A_n \cos\left(\frac{n\pi x}{L}\right) \cos\left(\frac{n\pi ct}{L} + \phi_n\right). \tag{7.12}$$

Going further requires some initial conditions. I will not do this here. The main point to note is that we now have cosines rather than sines for X(x), so the Fourier series we get will be a half-range cosine series.

Another possible combination of boundary conditions is to have one need fixed, and the other end unconstrained. Then, for example, we may have u=0 at x=0 and $\partial u/\partial x=0$ at x=L. We will look at this problem in the next tutorial. The main complication is that the fundamental mode in this case is a quarter of a wavelength, so we need to deal with a quarter-range Fourier series, rather than the half-range series of the other cases we have seen.

The final boundary conditions I will introduce here are *periodic boundary conditions*. We get these when we connect the two ends together, for example, if we consider waves on a circular hoop. Of course, there is no boundary here, but we do require the condition that the displacement is continuous as we go round the loop. This is probably clearer if we use an angular coordinate, writing $x = a\theta$, where a is the radius of the hoop and θ the angle. Then, the wave equation becomes

$$\frac{1}{a^2}\frac{\partial^2 u}{\partial \theta^2} = \frac{1}{c^2}\frac{\partial^2 u}{\partial t^2} \,. \tag{7.13}$$

The separation of variables looks very similar: we write $u(\theta,t) = H(\theta)T(t)$ and get equations for H and T:

$$\frac{d^2H}{d\theta^2} = -k^2H \quad \text{and} \quad \frac{d^2T}{dt^2} = -k^2\frac{c^2}{a^2}T. \tag{7.14}$$

The general solution for H is

$$H(\theta) = A\cos(k\theta + \phi), \tag{7.15}$$

where A and ϕ are our arbitrary constants. For the boundary condition we need the solution when $\theta = 2\pi$ to join up correctly with the one at $\theta = 0$. We require $H(0) = H(2\pi)$, so the hoop is not broken. Thus

$$H(0) = A\cos\phi = H(2\pi) = A\cos(2\pi k + \phi)$$
 (7.16)

This requires k to be an integer, $n = 0, 1, 2 \dots$ Again n = 0 is fine here. With this constraint, the boundary conditions are satisfied for any values of A and ϕ , so

$$H_n(\theta) = A_n \cos(n\theta + \phi_n) = A'_n \cos n\theta + B'_n \sin n\theta, \qquad (7.17)$$

where the second form may be more useful for Fourier series. Solving for the corresponding $T_n(t)$, we get the same solution as for the original problem, Eq.(6.11), but with $\omega_n = nc/a$. Then, the general solution obtained by superposition is

$$u(\theta, t) = A_0' + \sum_{n=1}^{\infty} (A_n' \cos n\theta + B_n' \sin n\theta) \cos \left(\frac{nct}{a} + \phi_n\right). \tag{7.18}$$

In this case, we will require a full-range Fourier series to fit the initial conditions.

7.3 Damped Waves

One of the obviously unphysical properties of the solutions we have found is that the string carries on oscillating indefinitely. In reality, for any mechanical system, there will be damping effects which mean that the wave decays with time, and the string eventually returns to equilibrium. We can modify our wave equation to account for this dissipation by adding a damping term. Recalling the damped oscillations we found in the ODE section, we write

$$\frac{\partial^2 u}{\partial x^2} = \frac{1}{c^2} \left(\frac{\partial^2 u}{\partial t^2} + 2\kappa \frac{\partial u}{\partial t} \right),\tag{7.19}$$

where κ is a constant which determines the strength of the damping. We will solve this with the 'fixed' boundary conditions u(0,t) = 0 = u(L,t). Note that equation is not the only way to add damping, but it is a simple model which will give us decaying waves.

Let us now look at finding separable solutions, of the form u(x,t) = X(x)T(t). Substituting this, we get

$$T\frac{d^{2}X}{dt^{2}} = \frac{1}{c^{2}} \left(X\frac{d^{2}T}{dt^{2}} + 2\kappa X\frac{dT}{dt} \right). \tag{7.20}$$

Now dividing through by XT gives

$$\frac{1}{X}\frac{d^2X}{dt^2} = \frac{1}{T}\frac{1}{c^2} \left(\frac{d^2T}{dt^2} + 2\kappa \frac{dT}{dt} \right). \tag{7.21}$$

We make the same argument that both sides of this must be equal to a constant, and that this constant must be negative, so we write it as $-k^2$. This gives us the equations for X and T:

$$\frac{d^2X}{dt^2} = -k^2X \qquad \frac{d^2T}{dt^2} + 2\kappa \frac{dT}{dt} + c^2k^2T = 0.$$
 (7.22)

The *X* equation is the same as for the undamped string, so we can just write down the solution:

$$X_n(x) = B_n \sin\left(\frac{n\pi x}{L}\right) = B_n \sin(k_n x),$$

with n = 1, 2, ... Then for T we solve using our standard method for homogeneous equations with constant coefficients. We write $T(t) = e^{mt}$ and substitute, which leads to the auxiliary equation

$$m^2 + 2\kappa m + c^2 k_n^2 = 0. (7.23)$$

This has solution

$$m = -\kappa \pm \sqrt{\kappa^2 - c^2 k_n^2} \,. \tag{7.24}$$

There are various possibilities here. Let us just consider the case where $\kappa < ck_n$ for all n. Then all the modes of the system are underdamped: the argument of the square root is negative, so we can write $m = -\kappa \pm i\omega_n$, where $\omega_n^2 = c^2k_n^2 - \kappa^2$. We then have the general solution

$$T_n(t) = C_n e^{-\kappa t} \cos(\omega_n t + \phi_n). \tag{7.25}$$

Combining this with X, and using superposition, we can now write down the general solution for u(x,t),

$$u(x,t) = e^{-\kappa t} \sum_{n=1}^{\infty} B_n \sin\left(\frac{n\pi x}{L}\right) \cos(\omega_n t + \phi_n).$$
 (7.26)

There are two differences compared to the undamped case: the damping causes the amplitude of the motion to decay, and the frequencies ω_n are modified. Note that we can also have the case where some of the modes are overdamped – the time dependence is a simple exponential decay.

The solution is completed by using some initial conditions to find the Fourier amplitudes B_n and the phases π_n . Note that u(x,0) is the same as for the undamped case, but when differentiating to obtain the initial velocity, it is necessary to take account of the $e^{-\kappa t}$ factor, which gives a more complicated expression.

8 The Laplace Equation in Two Dimensions

We are next going to look at using the separation of variables method to solve the Laplace and diffusion equations. These equations turn up in a wide range of physical problems, including electrostatics, gravitation, hydrodynamics and chemical reactions. However, to avoid thinking about too many different systems, we will just use the example of the temperature distribution in a solid body, where conduction is the main heat transport mechanism. The temperature, $T(\mathbf{r},t)$ is then given by the diffusion equation,

$$\nabla^2 T = \frac{1}{h^2} \frac{\partial T}{\partial t} \,, \tag{8.1}$$

where $h^2 = \kappa/\rho C$ is the diffusion constant, also know as the *thermal diffusivity*. Here κ is the thermal conductivity, ρ the density and C the heat capacity of the material. In the case when the system is in a steady state, $\partial T/\partial t = 0$, so the temperature is determined by the Laplace equation, $\nabla^2 T = 0$. We will consider the case of a two dimensional sheet, so we have a temperature distribution T(x,y) and the Laplace equation becomes

$$\frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2} = 0. {(8.2)}$$

Notice that this looks something like the wave equation (if c = 1), with two second derivatives. The difference is that they must have opposite sign, while in the wave equation they have the same sign. This difference leads to some modification of the mathematical solutions, as we shall see.

In thermal problems, there tend to be two sorts of boundary conditions. One is when some point or edge is kept at constant temperature, say T=0, by contact with a heat bath. The other occurs when there is nothing in contact with the edge, so no heat can flow into or out of the system. We know that heat flow is proportional to the temperature gradient, $\partial T/\partial x$, so this leads to a boundary condition like $\partial T/\partial x=0$.

8.1 Solving the Laplace Equation by Separation of Variables

We are going to consider an example of a two-dimensional rectangular metal plate. The plate has width L and is very (infinitely) long in the other direction. One of the short sides is kept at a temperature $T=T_0$, while the other three sides are maintained at T=0. We will find the steady state temperature distribution in the sheet.

We will now go through the steps in our separation of variables recipe. Starting from the Laplace equation, Eq.(8.2), we look for the separable solution T(x, y) = X(x)Y(y). Substituting this solution and dividing by XY, we get

$$\frac{1}{X(x)}\frac{d^2X(x)}{dx^2} + \frac{1}{Y(y)}\frac{d^2Y(y)}{dy^2} = 0.$$
 (8.3)

From this, we can deduce, as before, that

$$\frac{1}{X(x)}\frac{d^2X(x)}{dx^2} = -\frac{1}{Y(y)}\frac{d^2Y(y)}{dy^2} = N,$$
(8.4)

where N is our separation constant.

Next, we have to decide on the sign of N. Note that we are going to get different types of equations for X and Y: one will have trigometric solutions, the other exponentials. We can decide the sign for N, and thus which is which, by looking at the boundary conditions. We know that X has to go to zero at x=0 and x=L, so we are going to need trigonometric functions for this. Exponentials are fine for Y, as we would expect it to decrease steadily from T_0 to zero as we move from y=0 to $y\to\infty$. So we chose N to be negative, say $N=-k^2$ again. This gives us two ordinary differential equations for X and Y:

$$\frac{d^2X}{dx^2} = -k^2X$$
 and $\frac{d^2Y}{dy^2} = k^2Y$. (8.5)

We can write the general solution of these equations as

$$X(x) = A\cos kx + B\sin kx$$
 and $(y) = Ce^{ky} + De^{-ky}$. (8.6)

It is not essential to get the choice of the sign of N right. If we chose $N = +k^2$, we would find exponential instead of trigonometic solutions for X(x). Then, applying the boundary conditions, we would eventually decide that k must be imaginary, making N negative as required. However, it is a lot less painful to make the right choice at the start.

Now we apply the boundary conditions to find the constants A,B,C and D. We know that X(0) = 0 = X(L), so, as in the wave equation calculation, we can deduce that A = 0 and $k = n\pi/L$, with n any integer. In the y direction, $Y(y) \to 0$ as $y \to \infty$, so we can only have the decaying exponetial and thus C = 0 and $Y(y) = De^{-ky}$. Hence the solution for T(x,y) = X(x)Y(y) looks like

$$T(x,y) = De^{-n\pi y/L}B\sin\left(\frac{n\pi x}{L}\right) = Pe^{-n\pi y/L}\sin\left(\frac{n\pi x}{L}\right),\tag{8.7}$$

where the constant P = DB.

This solution satisfies the Laplace equation and our boundary conditions (except on y = 0) for n any integer. Hence we can write down the general solution

$$T(x,y) = \sum_{n=1}^{\infty} P_n e^{-n\pi y/L} \sin\left(\frac{n\pi x}{L}\right). \tag{8.8}$$

We now have to make our solution satisfy the boundary condition $T(x,0) = T_0$ for all x. Putting y = 0 in our general solution gives the condition

$$T(x,y) = \sum_{n=1}^{\infty} P_n \sin\left(\frac{n\pi x}{L}\right) = T_0.$$
 (8.9)

We again have a half-range Fourier sine series, so we can use

$$P_{n} = \frac{2}{L} \int_{0}^{L} dx f(x) \sin\left(\frac{n\pi x}{L}\right) = \frac{2T_{0}}{L} \int_{0}^{L} dx \sin\left(\frac{n\pi x}{L}\right)$$
$$= -\frac{2T_{0}}{L} \frac{L}{n\pi} \left[\cos\left(\frac{n\pi x}{L}\right)\right]_{0}^{L} = -\frac{2T_{0}}{n\pi} (\cos n\pi - 1) .. \tag{8.10}$$

This is equal to zero for even n and $4T_0/n\pi$ for odd n. We substitute these P_n back in our general solution to get

$$T(x,y) = \sum_{\text{odd } n} \frac{4T_0}{n\pi} e^{-n\pi y/L} \sin\left(\frac{n\pi x}{L}\right). \tag{8.11}$$

This gives the full solution to our problem; it satisfies the Laplace Equation, and the boundary conditions on all four edges of the plate.

9 The Diffusion Equation

We are next going to look at the diffusion equation, which in one dimension takes the form

$$\frac{\partial^2 F}{\partial x^2} = \frac{1}{D} \frac{\partial F}{\partial t} \,, \tag{9.1}$$

where F(x,t) is the quantity which diffuses, and D is the *diffusion constant*. D has dimensions of [length]²/[time], and in the S.I. system its units are m^2s^{-1} . There are many phenomena which are governed by the diffusion equation. Obviously, we talk about the diffusion of gases and chemicals, in which case F will be the concentration. Other concentrations, such as defects in solids and spin densities can diffuse in similar ways. Although the maths does not care which physical system we are dealing with, we shall talk primarily about the flow of heat by thermal conduction, in which case, F is the temperature, so we shall re-write it as T. Then we call D the *thermal diffusivity*: $D = K/\rho C$, where K is the thermal conductivity, ρ the density and C the heat capacity of the material. For metals, $D \sim 10^{-4} \text{m}^2 \text{s}^{-1}$. It is convenient to define $h = \sqrt{D}$. In these terms, the one dimensional diffusion equation becomes

$$\frac{\partial^2 T}{\partial x^2} = \frac{1}{h^2} \frac{\partial T}{\partial t} \,, \tag{9.2}$$

where T(x,t) is the temperature of the point x at time t.

9.1 Thermal Relaxation in a Rod with both ends held at T=0

For our first example, we will consider a rod of length L, with both ends held at a temperature T=0 at all times. We assume the surface of the rod is perfectly insulated along its length, so there is no heat flow out of the sides, only through the ends. The temperature in this rod will be well described by the one-dimensional diffusion equation. The rod is not in thermal equilibrium: at time t=0, the temperature distribution is given by function f(x). We shall use the same triangular distribution as we did for the plucked string:

$$f(x) = \begin{cases} 2T_0 x/L & 0 \le x \le L/2 \\ 2T_0 (1 - x/L) & L/2 \le x \le L \end{cases}$$
 (9.3)

This provides our initial condition: T(x,0) = f(x). The boundary conditions are that T(0,t) = 0 = T(L,t).

We now go through the separation of variables process again, but this time for the diffusion equation. We separate $T(x,t) = X(x)\theta(t)$ (T is temperature now, so we cannot use it for the time function), then substitute to get

$$\frac{1}{X(x)} \frac{d^2 X(x)}{dx^2} = \frac{1}{h^2} \frac{1}{\theta(t)} \frac{d\theta(t)}{dt} \,. \tag{9.4}$$

We then make the usual argument that one side is a function just of x, the other just of t, so if they are to be satisfied for all x and t, they must be equal to a constant. We know that the boundary conditions require X=0 both at x=0 and x=L, so we must get oscillatory solutions for X, which requires a negative constant, $-k^2$.

We get two ordinary differential equations

$$\frac{d^2X}{dx^2} = -k^2X \quad \Rightarrow \quad X(x) = A\cos kx + B\sin kx \tag{9.5}$$

and

$$\frac{d\theta}{dt} = -h^2 k^2 \theta \quad \Rightarrow \quad \theta(t) = C e^{-h^2 k^2 t} \,. \tag{9.6}$$

As before, the boundary conditions T(0,t)=0=T(L,t) equate to X(0)=0=X(L), and thus A=0 and $k=n\pi/L$. So we have solutions

$$T_n(x,t) = X(x)\theta(t) = B_n \sin\left(\frac{n\pi x}{L}\right) e^{-t/\tau_n} \quad \text{where} \quad \tau_n = \frac{1}{h^2 k^2} = \left(\frac{L}{n\pi h}\right)^2. \tag{9.7}$$

Now we use the superposition principle to get the general solution

$$T(x,t) = \sum_{n} T_n(x,t) = \sum_{n} B_n \sin\left(\frac{n\pi x}{L}\right) e^{-t/\tau_n}.$$
 (9.8)

This solution satisfies the diffusion equation and the boundary conditions at either end of the bar.

The final step is to satisfy the initial condition T(x,0) = f(x). Putting t = 0 in the general solution gives

$$T(x,0) = \sum_{n} B_n \sin\left(\frac{n\pi x}{L}\right) = f(x), \qquad (9.9)$$

so, once again, we need to find the half-range Fourier sine series for f(x).

We have

$$B_{n} = \frac{2}{L} \int_{0}^{L} dx f(x) \sin\left(\frac{n\pi x}{L}\right)$$

$$= \frac{2}{L} \frac{2T_{0}}{L} \left(\int_{0}^{L/2} dx x \sin\left(\frac{n\pi x}{L}\right) + \int_{L/2}^{L} dx (L-x) \sin\left(\frac{n\pi x}{L}\right)\right). \tag{9.10}$$

Doing the two integrals in the bracket separately, using integration by parts

$$\int_{0}^{L/2} dx \, x \sin\left(\frac{n\pi x}{L}\right) = \frac{L}{n\pi} \left\{ -\left[x\cos\left(\frac{n\pi x}{L}\right)\right]_{0}^{L/2} + \int_{0}^{L/2} dx \cos\left(\frac{n\pi x}{L}\right) \right\}$$

$$= \frac{L}{n\pi} \left\{ -\frac{L}{2}\cos\left(\frac{n\pi}{2}\right) + \frac{L}{n\pi} \left[\sin\left(\frac{n\pi x}{L}\right)\right]_{0}^{L/2} \right\}$$

$$= \frac{L}{n\pi} \left\{ -\frac{L}{2}\cos\left(\frac{n\pi}{2}\right) + \frac{L}{n\pi}\sin\left(\frac{n\pi}{2}\right) \right\}$$
(9.11)

and

$$\int_{L/2}^{L} dx (L - x) \sin\left(\frac{n\pi x}{L}\right) = \frac{L}{n\pi} \left\{ -L \left[\cos\left(\frac{n\pi x}{L}\right)\right]_{L/2}^{L} + \left[x\cos\left(\frac{n\pi x}{L}\right)\right]_{L/2}^{L} - \int_{L/2}^{L} dx \cos\left(\frac{n\pi x}{L}\right) \right\}
= \frac{L}{n\pi} \left\{ -L \left(\cos(n\pi) - \cos\left(\frac{n\pi}{2}\right)\right) + L\cos(n\pi) - \frac{L}{2}\cos\left(\frac{n\pi}{2}\right) - \frac{L}{n\pi} \left[\sin\left(\frac{n\pi x}{L}\right)\right]_{L/2}^{L} \right\}
= \frac{L}{n\pi} \left\{ \frac{L}{2}\cos\left(\frac{n\pi}{2}\right) + \frac{L}{n\pi}\sin\left(\frac{n\pi}{2}\right) \right\}.$$
(9.12)

Combining these, we get

$$B_n = \frac{2}{L} \frac{2T_0}{L} 2 \frac{L^2}{n^2 \pi^2} \sin\left(\frac{n\pi}{2}\right) = \frac{8T_0}{n^2 \pi^2} \sin\left(\frac{n\pi}{2}\right). \tag{9.13}$$

The final factor, $\sin(n\pi/2)$ is zero for even n. For odd n, it alternates in sign, +1 for n=1,5,9... and -1 for n=3,7,11..., which can be expressed as $(-1)^{(n-1)/2}$. We now have the complete solution

$$T(x,t) = \sum_{n} B_{n} \sin\left(\frac{n\pi x}{L}\right) e^{-t/\tau_{n}} = \frac{8T_{0}}{\pi^{2}} \sum_{n \text{ odd}} \frac{1}{n^{2}} (-1)^{(n-1)/2} \sin\left(\frac{n\pi x}{L}\right) e^{-t/\tau_{n}}.$$

$$= \frac{8T_{0}}{\pi^{2}} \left[\sin\left(\frac{\pi x}{L}\right) e^{-\pi^{2}h^{2}t/L^{2}} - \frac{1}{9} \sin\left(\frac{3\pi x}{L}\right) e^{-9\pi^{2}h^{2}t/L^{2}} + \frac{1}{25} \sin\left(\frac{5\pi x}{L}\right) e^{-25\pi^{2}h^{2}t/L^{2}}... \right]. \tag{9.14}$$

We see that the temparature distribution consists of a series of spatial harmonics, like the waves on a string. However, these harmonics decay, due to the exponential term, with the higher harmonics decaying more quickly. In the limit $t \to \infty$, $T(x,t) \to 0$ everywhere, as we would expect: the bar reaches thermal equilibrium with the reservoir holding the ends at T=0. There is a python script producing an animation of T(x,t) on Blackboard.

9.2 Thermal Relaxation of an Isolated Body

In the previous example, the ends of the rod were held at T=0, so heat was able to flow into or out of the reservoir which maintained that temperature. Next we are going to consider a rod where the ends are insulated, just like the sides. At time t=0, we will start with the same triangular distribution as before, Eq.(9.3). We expect that, with time, the temperature distribution will flatten out, as the heat becomes distributed uniformly along the rod.

We know that the rate of heat flow is proportional to the temperature gradient, $\partial T/\partial x$, so, as no heat flows out of the ends of the rod, the boundary conditions are that $\partial T/\partial x = 0$ at x = 0 and x = L for all t. This is the difference from the previous example, where we had T = 0 at these points. Clearly the separation starts in the same way, so we know we have $T(x,t) = X(x)\theta(t)$, with

$$X(x) = A\cos kx + B\sin kx \tag{9.15}$$

We now apply the new boundary conditions, which become dX/dx = 0 at x = 0 and x = L. We have

$$\frac{dX}{dx} = -Ak\sin kx + Bk\cos kx. \tag{9.16}$$

This must be zero at x=0, which implies B=0. The boundary condition at x=L then requires $\sin kL=0$, so again $k=n\pi/L$, with n integer. However, in this case, n=0 is allowed, because a constant, non-zero temperature along the bar, for which dT/dx=0 everywhere, is a valid solution. Indeed, the final equilibrium state of the system will be exactly this. Thus $X(x)=A_n\cos(n\pi x/L)$, for n>0, and $X(x)=A_0$ for n=0. The equation for $\theta(t)$ is

$$\frac{d\theta}{dt} = -h^2 k^2 \theta = -\frac{h^2 n^2 \pi^2}{L^2} \theta \,. \tag{9.17}$$

For n > 0, we have $\theta(t) = Ce^{-t/\tau_n}$, with $\tau_n = (L/n\pi h)^2$ as before. For n = 0, the solution is simply $\theta(t) = C_0$, a constant. Thus our general solution becomes

$$T(x,t) = A_0 + \sum_{n=1}^{\infty} A_n \cos\left(\frac{n\pi x}{L}\right) e^{-t/\tau_n} .$$
 (9.18)

The final step, using the Fourier series for f(x) to determine the coefficients A_n , is now different, because we require a half-range *cosine* series instead of the previous sine series. We have

$$T(x,0) = A_0 + \sum_{n=1}^{\infty} A_n \cos\left(\frac{n\pi x}{L}\right) = f(x) = \frac{1}{2}a_0 + \sum_{n=1}^{\infty} a_n \cos\left(\frac{n\pi x}{L}\right), \tag{9.19}$$

where the a_n are the Fourier coefficients

$$a_n = \frac{2}{L} \int_0^L dx \, f(x) \cos\left(\frac{n\pi x}{L}\right). \tag{9.20}$$

We see that, in general, $A_n = a_n$, except for n = 0, when $A_0 = a_0/2$.

You should make sure that you can do the integrals to find the A_n . The result is

$$A_0 = \frac{T_0}{2}$$
 and $A_n = \frac{4T_0}{n^2\pi^2} \left(2\cos\left(\frac{n\pi}{2}\right) - \cos(n\pi) - 1\right)$. (9.21)

Calculating these coefficients, we find that A_n is only non-zero when n = 2, 6, 10, 14... The full solution is

$$T(x,t) = \frac{T_0}{2} - \frac{16L}{\pi^2} \left[\frac{1}{2^2} \cos\left(\frac{2\pi x}{L}\right) e^{-2^2 \pi^2 h^2 t/L^2} + \frac{1}{6^2} \cos\left(\frac{6\pi x}{L}\right) e^{-6^2 \pi^2 h^2 t/L^2} \dots \right]. \tag{9.22}$$

We again see harmonics which decay away for large t. In the limit $T \to \infty$, $T(x,t) \to T_0/2$. The bar has a constant, uniform temperature, as we predicted.

9.3 The Physics of Diffusion

Although we are mainly talking about the mathematics of partial differential equations, the previous examples have taught us some of the physics of diffusion and thermal relaxation, which you may not have met before. to summarise, we have found

- 1. Sinusoidal harmonics are important part of the solutions to the diffusion equation.
- 2. These harmonics decay away exponentially with time.
- 3. The time constant of the decay, the *relaxation time*, is proportional to the square of the wavevector, k^2 , and hence λ^{-2} , and also to L^2 . Hence the longest wavelength harmonic (the fundamental) decays away the most slowly.
- 4. It follows that if we write the initial distribution as a Fourier series, normally the first term is the most important in determining the behaviour at long times.

Looking more closely at the dependence of the relaxation time on the wavelength of the harmonic, λ , (or equivalently, the harmonic number n), we see that the n^2 dependence suppresses higher harmonics very quickly. We can make the n dependence explicit by writing

the exponential decay as e^{-n^2t/τ_1} , where $\tau_1 = (L/h\pi)^2$ is the relaxation time for the fundamental, n=1. Hence at time $t=\tau_1$, the amplitude of the $n^{\rm th}$ harmonic has decayed by e^{-n^2} . This becomes very small quite rapidly with increasing n: $e^{-1} \approx 0.37$, $e^{-4} \approx 0.02$, $e^{-9} \approx 1.2 \times 10^{-4}$, $e^{-16} \approx 1.1 \times 10^{-7}$. So by this time, any contribution beyond the fundamental and the first harmonic is going to be very hard to detect (bear in mind that the higher harmonics tend to start off smaller too).

The other interesting dependence is that on the length of the bar, L. The relaxation times are all proportional to L^2 , so they get longer very rapidly as L increases. In the world of our experience this sort of dependence is unusual: if we double the distance we walk, it takes twice as long, but in a diffusion problem, doubling the length slows the relaxation by a factor of 4. This is why the Christmas turkey takes so long to cook

Values of the thermal diffusivity, h^2 , vary between about $10^{-4} \mathrm{m}^2 \mathrm{s}^{-1}$ for metals to $\sim 10^{-7} \mathrm{m}^2 \mathrm{s}^{-1}$ for good insulators like cork. We can use this to get a very rough idea about how far heat travels into an object in one second. taking n=1 and $\tau_1=1$ s, the distance is $L\sim \pi h$, which is ~ 3 cm for a metal, and ~ 1 mm for cork. These feel like reasonable estimates.

On a much smaller scale, our bodies can function because ions diffuse into and out of our cells. Chemical diffusion constants for ions are of order $D \sim 10^{-9} \mathrm{m}^2 \mathrm{s}^{-1}$, and our cells have diameters $L \sim 10^{-6} \mathrm{m}$. So the diffusion times are $\tau \sim L^2/\pi^2 D \sim 10^{-4} \mathrm{s}$, which is reasonable quick on our timescales. What would happen if we could scale up a person so our cells were 1 cm across? The timescale would increase to $10^4 \mathrm{s}$, which is definitely too slow!

10 Inhomogeneous Boundary Conditions

You may have noticed that in all the examples we have considered, the boundary conditions have taken the form of the function, or, in the some cases, its derivative, being equal to zero at the boundary points. Such boundary conditions are said to be *homogeneous*.

The fact that our boundary conditions are homogeneous was important in the procedure we use, because it is a requirement for the superposition principle to work. Suppose we have the boundary condition, at x = 0, that u(0,t) = 0. If we find two solutions satisfying this condition, so $u_1(0,t) = 0 = u_2(0,t)$, then any linear combination of these will also satisfy it:

$$u(0,t) = c_1 u_1(0,t) + c_2 u_2(0,t) = 0.$$
(10.1)

Next, suppose instead our boundary condition is u(0,t) = 1, so $u_1(0,t) = 1 = u_2(0,t)$. These are known as *inhomogeneous* boundary conditions. Now, for our superposition

$$u(0,t) = c_1 u_1(0,t) + c_2 u_2(0,t) = c_1 + c_2 \neq 1.$$
(10.2)

Though our superposition may satisfy the differential equation, assuming it is linear, it will not satisfy the boundary conditions (unless we add an additional constraint on the coefficients). We can also think about this physically. We will look at a thermal diffusion problem with a bar, where one end is held at $T = T_0$, the other at T = 0. We know that, in the steady state, the bar will have a linear heat gradient from T_0 to 0. However, the solutions we found in Eq.(9.14) all decay to zero as $t \to \infty$, so they cannot represent such a steady state. In fact, in this case, the problem is fairly easy to fix, as we shall see next.

10.1 Thermal Relaxation in a Rod with Ends Held at Different Temperatures

We are interested in the behaviour for t > 0. Then the boundary conditions are T(0,t) = 0 and $T(L,t) = T_0$. The initial condition is that T(x,0) = 0 for all x. The way will solve this problem is to divide the solution into two parts: one which satisfies the boundary conditions and provides the final steady state form, the other which satisfies the initial conditions and provides the time dependence. This is something like what we do with ordinary differential equations, where we use a complementary function and a particular integral. In order to describe the steady state final form, we need a solution with no time dependence, $T(x,t) = T_{\infty}(x)$, so the differential equation becomes simply

$$\frac{d^2 T_{\infty}}{dx^2} = 0. {(10.3)}$$

This has general solution $T_{\infty}(x) = Ax + B$. We find the constants A and B by fitting the inhomogeneous boundary conditions: $T_{\infty}(0) = B = 0$ and $T_{\infty}(L) = T_0 = AL$. Hence $A = T_0/L$ and B = 0.

We next use the superposition principle and write the full solution as

$$T(x,t) = T_{\infty}(x) + \tilde{T}(x,t) = T_0 x/L + \tilde{T}(x,t),$$
 (10.4)

where $\tilde{T}(x,t)$ satisfies the partial differential equation, including the time dependence. However, the boundary condition, at x=L, on \tilde{T} is not the same as for T: $T(L,t)=T_0=T_0+\tilde{T}(L,t)$, so $\tilde{T}(L,t)=0$ and we have restored the homogeneous boundary conditions. We also need to re-think the initial condition: $T(x,0)=0=T_0x/L+\tilde{T}(x,0)$, so $\tilde{T}(x,0)=-T_0x/L$.

The calculation of $\tilde{T}(x,t)$ proceeds in exactly the same way as Sec 9.1, except our initial f(x) is now $-T_0x/L$. Thus the Fourier coefficients become

$$B_{n} = \frac{2}{L} \int_{0}^{L} dx \, f(x) \sin\left(\frac{n\pi x}{L}\right) = -\frac{2}{L} \frac{T_{0}}{L} \int_{0}^{L} dx \, x \sin\left(\frac{n\pi x}{L}\right)$$

$$= -\frac{2T_{0}}{L^{2}} \frac{L}{n\pi} \left\{ -\left[x\cos\left(\frac{n\pi x}{L}\right)\right]_{0}^{L} + \int_{0}^{L} dx \cos\left(\frac{n\pi x}{L}\right) \right\}$$

$$= -\frac{2T_{0}}{L^{2}} \frac{L}{n\pi} \left\{ -L\cos n\pi + \left[\sin\left(\frac{n\pi x}{L}\right)\right]_{0}^{L} \right\} = \frac{2T_{0}}{n\pi} \cos n\pi = \frac{2T_{0}}{n\pi} (-1)^{n} . \tag{10.5}$$

We can now put together our full solution:

$$T(x,t) = T_{\infty}(x) + \tilde{T}(x,t) = T_{0}x/L + \sum_{n=1}^{\infty} B_{n} \sin\left(\frac{n\pi x}{L}\right) e^{-t/\tau_{n}}$$

$$= T_{0}x/L + \frac{2T_{0}}{\pi} \sum_{n=1}^{\infty} \frac{(-1)^{n}}{n} \sin\left(\frac{n\pi x}{L}\right) e^{-n^{2}\pi^{2}h^{2}t/L^{2}}.$$
(10.6)

There is an animation of this on Blackboard.

10.2 Waves on a String Driven by Oscillating one End

A natural way to excite waves on a string is to hold onto one end and make it oscillate. The boundary condition is then $u(0,t) = u_0 \cos \omega_0 t$, which is clearly inhomogeneous. Here, we will look at solving the wave equation

$$\frac{\partial^2 u}{\partial x^2} = \frac{1}{c^2} \frac{\partial^2 u}{\partial t^2} \tag{10.7}$$

with this boundary condition at x = 0 and u(L, t) = 0.

As in the last section, we will express the solution as a sum of two terms

$$u(x,t) = u_{\infty}(x,t) + \tilde{u}(x,t), \qquad (10.8)$$

where u_{∞} satisfies the inhomogeneous boundary condition but not the initial conditions, while \tilde{u} satisfies the initial conditions and homogeneous boundary conditions with $\tilde{u}=0$ at both ends of the string. If there were any damping of the string, this latter term would be transient, disappearing as $t \to \infty$, leaving the 'steady state' solution $u_{\infty}(x,t)$.

We will use the trick of replacing the inhomogeneous driving term by a complex function $u_0e^{-i\omega t}$, so the actual solution will be the real part of the complex function which we find. Clearly, the driving term means that the string will oscillate at the same frequency, ω_0 . Hence we look for separable solutions of the form

$$u_{\infty}(x,t) = X(x)e^{-i\omega_0 t}. \tag{10.9}$$

Substituting in the wave equation, we get

$$e^{-i\omega_0 t} \frac{d^2 X}{dx^2} = -\frac{\omega_0^2}{c^2} X e^{-i\omega_0 t} \,. \tag{10.10}$$

Thus

$$\frac{d^2X}{dx^2} = -\frac{\omega_0^2}{c^2}X\,, (10.11)$$

Then, as usual,

$$X(x) = A\cos\left(\frac{\omega_0 x}{c}\right) + B\sin\left(\frac{\omega_0 x}{c}\right). \tag{10.12}$$

and

$$u_{\infty}(x,t) = \left(A\cos\left(\frac{\omega_0 x}{c}\right) + B\sin\left(\frac{\omega_0 x}{c}\right)\right)e^{-i\omega_0 t}.$$
 (10.13)

We now need to satisfy the boundary conditions. At x = 0 we have

$$u_{\infty}(0,t) = Ae^{-i\omega_0 t} = u_0 e^{-i\omega_0 t}, \qquad (10.14)$$

so $A = u_0$. We also require $u_{\infty}(L, t) = 0$, so

$$u_{\infty}(L,t) = u_0 \cos\left(\frac{\omega_0 L}{c}\right) + B \sin\left(\frac{\omega_0 L}{c}\right) = 0.$$
 (10.15)

This requires

$$B = -u_0 \cot\left(\frac{\omega_0 L}{c}\right). \tag{10.16}$$

Then, taking the real part to get the actual solution,

$$u_{\infty}(x,t) = u_0 \left(\cos\left(\frac{\omega_0 x}{c}\right) - \cot\left(\frac{\omega_0 L}{c}\right) \sin\left(\frac{\omega_0 x}{c}\right) \right) \cos\omega_0 t . \tag{10.17}$$

The full solution would require us to construct $\tilde{u}(x,t)$, which is just the homogeneous problem we solved earlier. If the string was at rest and undisplaced at t=0, the initial condition on \tilde{u} would be $\tilde{u}(x,0)=-u_{\infty}(x,0)$, which would give us the Fourier series solution. We will not find this here.

10.3 Waves on an Infinite String with Damping

We can make the previous problem more realistic by adding damping so that the transient part $\tilde{u}(x,t)$ would decay away in time, leaving just the 'steady state' part $u_{\infty}(x,t)$. However, the fixed boundary problem is tricky to solve with damping. Instead, here we will find the steady state solution for a damped semi-infinite string, driven so that $u(0,t) = u_0 \cos \omega_0 t$. The wave equation for the damped string is

$$\frac{\partial^2 u}{\partial x^2} = \frac{1}{c^2} \left(\frac{\partial^2 u}{\partial t^2} + 2\kappa \frac{\partial u}{\partial t} \right). \tag{10.18}$$

We will proceed like the previous example, using a complex driving term $u_0e^{-i\omega_0t}$ and look for solutions of the form

$$u_{\infty}(x,t) = X(x)e^{-i\omega_0 t}$$
. (10.19)

Substituting into the wave equation gives

$$\frac{d^2X}{dx^2} = -\frac{1}{c^2}(\omega_0^2 + 2i\kappa\omega_0)X.$$
 (10.20)

The solutions have complex wavevector: $X(x) = Ae^{i(k+i\alpha)x}$, with

$$-(k+i\alpha)^2 = (-k^2 + \alpha^2 - 2ik\alpha) = -\frac{1}{c^2}(\omega_0^2 + 2i\kappa\omega_0).$$
 (10.21)

Equating real and imaginary parts:

$$k^2 - \alpha^2 = \frac{\omega_0}{c}$$
 and $k\alpha = \frac{\kappa\omega_0}{c^2}$. (10.22)

This is easy enough to solve exactly, but, to avoid messy expressions, we will assume $\alpha \ll k$, so the α^2 term in the second equation can be neglected. Then $k = \omega_0/c$ and $\alpha = \kappa/c$. We keep only the positive solution, because we want a wave which propagates forward and gets smaller as x increases. Putting the bits together,

$$u_{\infty}(x,t) = Ae^{i\left(\frac{\omega_0}{c} + i\frac{\kappa}{c}\right)x}e^{-i\omega_0 t}.$$
 (10.23)

The boundary condition $u_{\infty}(0,t) = u_0 \cos \omega_0 t$ then gives $A = u_0$. Taking the real part to get the physical solution

$$u_{\infty}(x,t) = u_0 e^{-\frac{\kappa}{c}x} \cos\left(\frac{\omega_0}{c}x - \omega_0 t\right). \tag{10.24}$$

This is a travelling wave, with frequency ω_0 , which decays in amplitude as it propagates along the string. Note that in this, the damping term causes a decay with position, rather than time.

As previously, we will not find the full solution, which requires adding a transient term satisfying the homogeneous boundary condition, then using Fourier methods (in this case, a Fourier transform would be required, because the string is infinite, so any wavevector k is allowed in the general solution).

10.4 Thermal Waves

In this section, we will put together the techniques we have just learned to go through the maths underlying the Ångström bar experiment which some of you will be working on in the laboratory sessions. In this experiment, one end of a bar is driven so that its temparture oscillates in time, while the other end is held isolated.

The temperature in the bar satisfies the diffusion

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

where $D = h^2$ in our previous notation. I am going to use the variable, T, in these equations to mean the difference between the temperature of the bar and the environment temperature, so negtaive values simply mean that the temperature is below that of the environment. We can always add a constant to any solution of the diffusion equation, which means we can choose any origin for our temperature scale. One end of the bar, x = 0, is in contact with a reservoir whose temperature oscillates, so that

$$T(0,t) = T_0 \cos \omega t \,, \tag{10.25}$$

with T_0 a constant. The other end, x = L, is isolated, so $\partial T/\partial x = 0$. However, to simplify the maths, I shall assume that the bar has infinite length. This is a fairly good approximation, because we will find that the temperature oscillations decay exponentially as they travel down the bar. Thus, the other boundary condition is simply that $T(x,t) \to 0$ as $x \to \infty$.

We look for a solution with two parts,

$$T(x,t) = T_{\infty}(x,t) + \tilde{T}(x,t),$$
 (10.26)

were $T_{\infty}(x,t)$ satisfies the inhomogeneous boundary condition, but not the initial conditions, while $\tilde{T}(x,t)$ satisfies homogeneous boundary conditions and ensures that the full solution T(x,t) satisfies the initial conditions. We know that $\tilde{T}(x,t)$ is transient: it will decay exponentially with time, so that, at long times $T(x,t) = T_{\infty}(x,t)$. We will not bother calculating the transient. In the experiment, it is better to wait for it to decay away before taking data, rather than try to include it in the analysis.

As before, We will change the driving term to $T(0,t) = T_0 e^{-i\omega t}$, so at the end we will need to take the real part to get the physical solution. We look for an oscillating solution of the form

$$T_{\infty}(x,t) = X(x)e^{-i\omega t} . \tag{10.27}$$

Substituting this in the diffusion equation gives

$$De^{-i\omega t}\frac{d^2X}{dt^2} = -i\omega e^{-i\omega t}X, \qquad (10.28)$$

so

$$\frac{d^2X}{dx^2} = -i\frac{\omega}{D}X. ag{10.29}$$

If we look for a solution of the form $X(x) = e^{(-\alpha + ik)x}$, we find

$$(-\alpha + ik)^2 = \alpha^2 - k^2 - 2i\alpha k = -i\frac{\omega}{D}.$$
 (10.30)

This requires $\alpha = k$ and $\omega = 2\alpha kD$. The general solution is then

$$X(x) = Ae^{(-\alpha + ik)x} + Be^{-(-\alpha + ik)x}.$$
 (10.31)

For the temperature difference to go to zero as $x \to \infty$, we must have B = 0. Thus the separable solution we get is of the form

$$T_{\infty}(x,t) = Ae^{-\alpha x}e^{i(kx-wt)}$$
.

This represents a decaying wave travelling along the bar. We find A by applying the boundary condition $T_{\infty}(0,t) = T_0 exp - i\omega t$. This gives $A = T_0$. Finally, taking the real part, we get the physical solution

$$T_{\infty}(x,t) = T_0 e^{-\alpha x} \cos(kx - \omega t). \tag{10.32}$$

Remember there is also a transitent part to the solution, which decays with time. We can estimate how long you will have to wait by looking at the decay time for the lowest frequency component, which is, Eq.(9.7),

$$\tau_1 = \left(\frac{L}{\pi h}\right)^2 = \frac{1}{D} \left(\frac{L}{\pi}\right)^2 \tag{10.33}$$

For the experiment, we want to know how long it will take for the transient to decay out as far as the furthest measurement point, which is approximately 20 cm along the bar, so we take L=0.2 m. Then, using $D\sim 10^{-4}\,\mathrm{m}^2\mathrm{s}^{-1}$, we get $\tau_1\sim 1$ minute. You will probably have to wait a few minutes for the transient to decay sufficiently.

The superposition principle makes it easy to solve for the case when the oscillating temperature at the end of the bar is not a simple cosine wave. If we express this function as a Fourier series, we need to make a superposition of solutions with all the frequencies which appear, chosing their amplitudes to match the Fourier coefficients. Thus, for a wave which is symmetric about t = 0, with Fourier series representation

$$T(0,t) = \frac{1}{2}a_0 + \sum_{n=1}^{\infty} a_n \cos(\omega_n t), \qquad (10.34)$$

we get

$$T(x,t) = \frac{1}{2}a_0 + \sum_{n=1}^{\infty} a_n e^{-\alpha_n x} \cos(k_n x - \omega_n t)$$
 (10.35)

where

$$\alpha_n = k_n = \sqrt{\frac{\omega_n}{2D}} \,. \tag{10.36}$$

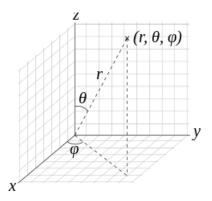
All the frequency components decay as we move along the bar, due to the $e^{-\alpha_n x}$ term. But $\alpha_n \propto \sqrt{\omega_n}$, so the higher frequency components decay most rapidly. As the wave propagates along the bar, it becomes more and more like a cosine wave.

Thermal waves provide an explanation for permafrost: in places where the average annual temperature is lower than freezing, the ground below a depth of a couple of meters remains frozen, even in the summer when the surface temperatures can get quite high. We have an oscillating temperature with a period of 1 year (along with much rapider daily oscillations and variations due to the weather). So how deep do we have to go before thermal waves at that frequency decay away? We have seen that the decay constant, $\alpha = \sqrt{(\omega/2D)}$. Dry soil is a pretty good insulator, and D values $\sim 10^{-7} \mathrm{m}^2 \mathrm{s}^{-1}$ are typical. A period of 1 year corresponds to angular frequency $\omega \sim 2 \times 10^{-7} \mathrm{s}^{-1}$. This gives $\alpha \sim 1 \mathrm{m}^{-1}$, so below a few meters, the soil temperature will be pretty much constant and equal to the annual average temperature.

11 Spherical Polar Coordinates

In physics, we frequently deal with objects which have spherical symmetry, from stars to atoms. In such systems, it is nearly always best to work with spherical polar coordinates.

In physics (but not in astronomy), we define (r, θ, ϕ) as in the figure below.



Spherical polars are related to cartesian coordinates by

$$x = r \sin \theta \cos \phi$$

$$y = r \sin \theta \sin \phi$$

$$z = r \cos \theta$$
. (11.1)

The element of volume is $dV = r^2 \sin \theta \, dr \, d\theta \, d\phi$. To cover all space, we require $0 \le r \le \infty$, $0 \le \theta < \pi$ and $0 \le \phi < 2\pi$.

The Laplacian operator in spherical polars is

$$\nabla^2 = \frac{1}{r^2} \frac{\partial}{\partial r} \left(r^2 \frac{\partial}{\partial r} \right) + \frac{1}{r^2 \sin \theta} \frac{\partial}{\partial \theta} \left(\sin \theta \frac{\partial}{\partial \theta} \right) + \frac{1}{r^2 \sin^2 \theta} \frac{\partial^2}{\partial \phi^2} \,. \tag{11.2}$$

We will first look at problems where the solutions are spherically symmetric, that is, they depend only on r, not on θ and ϕ . Then the Laplacian simplifies, as the θ and ϕ derivative sare zero. If we have a function F(r),

$$\nabla^2 F(r) = \frac{1}{r^2} \frac{d}{dr} \left(r^2 \frac{dF(r)}{dr} \right). \tag{11.3}$$

11.1 The Laplace Equation

We will solve $\nabla^2 V = 0$ when V(r) depends only on r. We thus have

$$\frac{1}{r^2}\frac{d}{dr}\left(r^2\frac{dV}{dr}\right) = 0. ag{11.4}$$

Multiplying both sides by r^2 and integrating gives

$$r^2 \frac{dV}{dr} = A \,, \tag{11.5}$$

where A is the integration constant. Dividing by r^2 and integrating again gives the general solution

$$V(r) = -\frac{A}{r} + B, \qquad (11.6)$$

where B is another constant.

We now need boundary conditions to determine these constants. If, for example, V was an electrosatic potential, we would want $V \to 0$ as $r \to \infty$, so B = 0 and V(r) = -A/r. this is the Coulomb potential for a point charge, Q, at the origin, $V(r) = Q/4\pi\varepsilon_0 r$. Note that we cannot show that $A = -Q/4\pi\varepsilon_0$ just by solving the Laplace equation, because the potential satisfies the Poisson equation, not the Laplace equation, in the presence of a charge.

11.2 The Wave Equation

In three dimensions, the wave equation is

$$\nabla^2 u = \frac{1}{c^2} \frac{\partial^2 u}{\partial t^2} \,. \tag{11.7}$$

We will look for spherically symmetric solutions, so $u(\mathbf{r},t) = u(r,t)$, and the wave equation can be written

$$\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial u}{\partial r}\right) = \frac{1}{c^2}\frac{\partial^2 u}{\partial t^2} \,. \tag{11.8}$$

As previously, we look for separable solutions u(r,t) = R(r)T(t), and substitute in the wave equation to get

$$\frac{1}{R(r)} \frac{1}{r^2} \frac{d}{dr} \left(r^2 \frac{dR(r)}{dr} \right) = \frac{1}{T(t)} \frac{1}{c^2} \frac{d^2 T(t)}{dt^2} \,. \tag{11.9}$$

Each side is a function of just one of the variables, so we know it must be equal to a constant. We want wave-like solutions which oscillate in time (and space), so we make this constant negative. To make the units nice, we put it equal to $-(\omega/c)^2$. Then we find

$$\frac{d^2T(t)}{dt^2} = -\omega^2 T(t), \qquad (11.10)$$

which has oscillatory solutions of the form $T(t) \sim e^{\pm i\omega t}$ (or we can express this in terms of sines and cosines).

The equation for R(r) is a little more difficult to solve. It is

$$\frac{1}{r^2}\frac{d}{dr}\left(r^2\frac{dR(r)}{dr}\right) = -\left(\frac{\omega}{c}\right)^2R(r) = -k^2R(r),\tag{11.11}$$

where $k = \omega/c$. The trick to solving this is to define a new variable $\chi(r)$ by $R(r) = \chi(r)/r$. Then

$$\frac{dR}{dr} = -\frac{1}{r^2}\chi + \frac{1}{r}\frac{d\chi}{dr} \tag{11.12}$$

and

$$r^2 \frac{dR}{dr} = -\chi + r \frac{d\chi}{dr} \,. \tag{11.13}$$

Differentiating again

$$\frac{d}{dr}\left(r^2\frac{dR}{dr}\right) = -\frac{d\chi}{dr} + \frac{d\chi}{dr} + r\frac{d^2\chi}{dr^2} = r\frac{d^2\chi}{dr^2}.$$
 (11.14)

Then Eq.(11.11) becomes

$$\frac{1}{r}\frac{d^2\chi}{dr^2} = -\frac{k^2}{r}\chi \,. \tag{11.15}$$

We can cancel the 1/r then solve to get $\chi(r) \sim e^{\pm ikr}$, so

$$R(r) \sim \frac{e^{\pm ikr}}{r} \,. \tag{11.16}$$

We can combine this with the solution for T(t) to get the full solution

$$u(r,t) = \frac{A}{r}e^{i(kr - \omega t)} + \frac{B}{r}e^{-i(kr + \omega t)},$$
(11.17)

where A and B are arbitrary constants. I have written this so that the first term represents a spherical wave going out from the origin, while the second term represents one going towards the origin. Depending on the boundary conditions, we may require one or the other, or both, to solve a particular problem.

Note that there are number of conventions about the signs of the ω and k terms in the exponentials. I prefer to fix the sign of ω to be negative. Then the sign of k gives the direction of the waves. We can see the direction by looking at how points of constant phase move with time. In the first term, constant phase corresponds to $kr - \omega t = \text{const.}$ Differentiating with repect to t, we get $kdr/dt = \omega$. So if k > 0, dr/dt > 0 and the points of constant phase move to increasing r with time – we have an outgoing wave. Other conventions also exist: for example $e^{-i(kr-\omega t)}$ also represents an outgoing wave.

12 Spherical Harmonics

In the previous section, we looked for solutions to the Laplace equation and the wave equation which had no angular dependence, just depending on the distance from the origin, r in spherical polar coordinates. The underlying assumption was that we have a system with spherical symmetry, so that any boundary conditions etc also depend only on r. However, even with spherical symmetry, we can find solutions which do have an angular dependence. For example, the ground state of the hydrogen atom is spherically symmetric, but many of the excited states do have some angular dependence – these are the $p,d\ldots$ orbitals which you may have met in chemistry. For any such problem, we always find the same angular functions, which are known as *spherical harmonics*.

We will derive the spherical harmonics by looking at the separation of variables, in spherical polar coordinates, for the three dimensional Laplace equation. However, we would get the same angular functions if we solved the wave equation or the diffusion equation, or the Schrödinger equation with a spherically symmetric potential V(r), like in the hydrogen atom.

We will solve

$$\nabla^{2}V = \frac{1}{r^{2}}\frac{\partial}{\partial r}\left(r^{2}\frac{\partial V}{\partial r}\right) + \frac{1}{r^{2}\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial V}{\partial\theta}\right) + \frac{1}{r^{2}\sin^{2}\theta}\frac{\partial^{2}V}{\partial\phi^{2}} = 0,$$
 (12.1)

by separating the variables so $V(r,\theta,\phi) = R(r)P(\theta)F(\phi)$. Then

$$\frac{1}{r^2} \frac{\partial}{\partial r} \left(r^2 \frac{\partial V}{\partial r} \right) = P(\theta) F(\phi) \frac{1}{r^2} \frac{d}{dr} \left(r^2 \frac{dR(r)}{dr} \right)
\frac{1}{r^2 \sin \theta} \frac{\partial}{\partial \theta} \left(\sin \theta \frac{\partial V}{\partial \theta} \right) = \frac{R(r) F(\phi)}{r^2 \sin \theta} \frac{d}{d\theta} \left(\sin \theta \frac{dP(\theta)}{d\theta} \right)
\frac{1}{r^2 \sin^2 \theta} \frac{\partial^2 V}{\partial \phi^2} = \frac{R(r) P(\theta)}{r^2 \sin^2 \theta} \frac{d^2 F(\phi)}{d\phi^2}.$$
(12.2)

Dividing by V = RPF and substituting, we get

$$\frac{1}{R(r)} \frac{1}{r^2} \frac{d}{dr} \left(r^2 \frac{dR(r)}{dr} \right) + \frac{1}{P(\theta)} \frac{1}{r^2 \sin \theta} \frac{d}{d\theta} \left(\sin \theta \frac{dP(\theta)}{d\theta} \right) + \frac{1}{F(\phi)} \frac{1}{r^2 \sin^2 \theta} \frac{d^2 F(\phi)}{d\phi^2} = 0. \tag{12.3}$$

We cannot quite separate yet, because the variables are still mixed together in some terms. So next, multiply by $r^2 \sin^2 \theta$:

$$\frac{\sin^2 \theta}{R(r)} \frac{d}{dr} \left(r^2 \frac{dR(r)}{dr} \right) + \frac{\sin \theta}{P(\theta)} \frac{d}{d\theta} \left(\sin \theta \frac{dP(\theta)}{d\theta} \right) + \frac{1}{F(\phi)} \frac{d^2 F(\phi)}{d\phi^2} = 0. \tag{12.4}$$

We now see that the first two terms depend only on r and θ , and the final term depends only on ϕ . We can therefore argue that the final term, and the sum of the first two terms, must be equal to constants. We thus have

$$\frac{1}{F(\phi)} \frac{d^2 F(\phi)}{d\phi^2} = \text{constant}. \tag{12.5}$$

Now the variable ϕ is defined in the range $0 \to 2\pi$. To make $F(\phi)$ single valued, it must repeat so that $F(\phi) = F(\phi + 2\pi)$ This means the solutions we require are periodic, so the separation constant must be negative. We write

$$\frac{1}{F(\phi)} \frac{d^2 F(\phi)}{d\phi^2} = -m^2 \,, \tag{12.6}$$

which has solutions

$$F(\phi) \sim \left\{ \begin{array}{c} \sin m\phi \\ \cos m\phi \end{array} \right\} \sim \left\{ \begin{array}{c} e^{im\phi} \\ e^{-im\phi} \end{array} \right\}. \tag{12.7}$$

Imposing our periodicity requirement, $\sin m(\phi + 2\pi) = \sin(m\phi + 2m\phi)$, and for this to be equal to $\sin(m\phi)$, m must be an integer.

We next substitute back into Eq.(12.4). The final term is equal to $-m^2$, so

$$\frac{\sin^2 \theta}{R(r)} \frac{d}{dr} \left(r^2 \frac{dR(r)}{dr} \right) + \frac{\sin \theta}{P(\theta)} \frac{d}{d\theta} \left(\sin \theta \frac{dP(\theta)}{d\theta} \right) - m^2 = 0.$$
 (12.8)

Dividing through by $\sin^2 \theta$.

$$\frac{1}{R(r)}\frac{d}{dr}\left(r^2\frac{dR(r)}{dr}\right) + \frac{1}{\sin\theta P(\theta)}\frac{d}{d\theta}\left(\sin\theta\frac{dP(\theta)}{d\theta}\right) - \frac{m^2}{\sin^2\theta} = 0.$$
 (12.9)

We have now managed to separate the r dependence, in the first term, from the rest, which depend only on θ . For the $P(\theta)$ terms, we have

$$\frac{1}{\sin\theta P(\theta)} \frac{d}{d\theta} \left(\sin\theta \frac{dP(\theta)}{d\theta} \right) - \frac{m^2}{\sin^2\theta} = \text{constant}.$$
 (12.10)

We are not going to go into the details of solving for $P(\theta)$. It is known that Eq.(12.10) has well behaved solutions only if the constant is equal to -l(l+1), where l is an integer. Thus $P(\theta)$ satisfies

$$\frac{1}{\sin\theta} \frac{d}{d\theta} \left(\sin\theta \frac{dP(\theta)}{d\theta} \right) - \frac{m^2}{\sin^2\theta} P(\theta) + l(l+1)P(\theta) = 0. \tag{12.11}$$

The solutions are known as associated Legendre functions, or sometimes, associated Legendre polynomials. They are written

$$P(\theta) = P_I^m(\cos\theta), \qquad (12.12)$$

where the l and m labels refer to the integers l and m in Eq.(12.11). There is an additional requirement that $l \ge |m|$. So for l = 0 we can only have m = 0, but for l = 1, m can take the values -1, 0 and +1, while for l = 3, m = -2, -1, 0, +1, +2 are allowed.

To complete the solution, we still have to solve for R(r). Substituting in Eq.(12.9), we get

$$\frac{d}{dr} \left(r^2 \frac{dR(r)}{dr} \right) - l(l+1)R(r) = 0.$$
 (12.13)

We look for solutions of the form $R(r) = r^{\nu}$. Then $r^2 dR/dr = \nu r^{\nu+1}$, and the first term is $\nu(\nu+1)r^{\nu}$. The equation is thus satisfied if $\nu(\nu+1) = l(l+1)$. There are two possibilities: $\nu = l$ and $\nu = -(l+1)$. We thus have the general solution

$$R(r) = Ar^{l} + Br^{-(l+1)}, (12.14)$$

where the constants A and B are determined by the boundary conditions on the problem.

The important thing to notice here is that all the angular dependence here comes from the terms in the Laplacian operator. So we can add other terms to the equation, and as long as they have no angular dependence, we will be able to separate variables in the same way and get the same factors for the angular variables. For example, the same angular factors occur when we solve the Schrödinger equation in atomic physics, because the Coulomb potential due to the nucleus is spherically symmetric. Because of this we give the angular dependent part of the solution a special name: we call them *spherical harmonics*. For all these spherically symmetric equations, the separable solutions take the form

$$f(r,\theta,\phi) = R(r)Y_I^m(\theta,\phi), \qquad (12.15)$$

where the spherical harmonics are

$$Y_l^m(\theta,\phi) = P_l^m(\cos\theta)e^{im\phi}. \tag{12.16}$$

You will find when you study quantum mechanics further that the spherical harmonics are eigenstates of the angular momentum operator, with the l and m labels telling us about the angular momentum of a state.

12.1 Properties of Spherical Harmonics

The following table shows full expressions for the lowest few spherical harmonics. There is no need to learn any of these expressions; you will be given them when you need them.

l = 0

$$Y_0^0(\theta,\phi) = \sqrt{\frac{1}{4\pi}}$$

l = 1

$$Y_1^{-1}(\theta,\phi) = \sqrt{\frac{3}{8\pi}} \sin\theta \, e^{-i\phi}$$

$$Y_1^0(\theta,\phi) = \sqrt{\frac{3}{4\pi}} \cos\theta$$

$$Y_1^1(\theta,\phi) = -\sqrt{\frac{3}{8\pi}} \sin\theta \, e^{i\phi}$$

l = 2

$$\begin{split} Y_2^{-2}(\theta,\phi) &= \sqrt{\frac{15}{32\pi}} \sin^2 \theta \, e^{-2i\phi} \\ Y_2^{-1}(\theta,\phi) &= \sqrt{\frac{15}{8\pi}} \sin \theta \cos \theta \, e^{-i\phi} \\ Y_2^{0}(\theta,\phi) &= \sqrt{\frac{5}{16\pi}} (3\cos^2 \theta - 1) \\ Y_2^{1}(\theta,\phi) &= -\sqrt{\frac{15}{8\pi}} \sin \theta \cos \theta \, e^{i\phi} \\ Y_2^{2}(\theta,\phi) &= \sqrt{\frac{15}{32\pi}} \sin^2 \theta \, e^{2i\phi} \end{split}$$

There are some obvious patterns in this table. Firstly, the functions get more complicated with increasing values of l. There are also more of them, because of the restriction $|m| \le l$. So, for l = 0, we have only m = 0, and this is just a constant. For l = 1, we have m = -1,0 and -1. The corresponding associated Legendre functions just contain the first power of $\cos \theta$ and $\sin \theta$. Moving on to l = 2, we get five functions, and these are up to second order in sines and cosines. More generally, for higher values of l, we get functions up to the l^{th} order in the sines and cosines; for even l we get only even powers, and for odd l they are odd powers.

To show that these functions are indeed solutions to Eq.(12.11), we can substitute in these equations. For l = 0, m must also be zero, so the associated Legendre equation becomes

$$\frac{1}{\sin\theta} \frac{d}{d\theta} \left(\sin\theta \frac{dP(\theta)}{d\theta} \right) = 0. \tag{12.17}$$

From our table, $P(\theta)$ is a constant, so $dP/d\theta = 0$ and the equation is clearly satisfied.

For l = 1 and m = 0, we have

$$\frac{1}{\sin\theta} \frac{d}{d\theta} \left(\sin\theta \frac{dP(\theta)}{d\theta} \right) + 2P(\theta) = 0.$$
 (12.18)

For this case, we use $P(\theta) \sim \cos \theta$, so $dP/d\theta = -\sin \theta$. Then

$$\frac{d}{d\theta} \left(\sin \theta \frac{dP(\theta)}{d\theta} \right) = \frac{d}{d\theta} (-\sin^2 \theta) = -2\sin \theta \cos \theta . \tag{12.19}$$

Substituting, the left hand side is

$$\frac{1}{\sin\theta} \frac{d}{d\theta} \left(\sin\theta \frac{dP(\theta)}{d\theta} \right) + 2P(\theta) = -2\cos\theta + 2\cos\theta = 0, \qquad (12.20)$$

so the equation is satisfied.

The constants in the expressions for the spherical harmonics are chosen to normalise the functions such that

$$\int_0^{2\pi} d\phi \int_0^{\pi} \sin\theta \, d\theta \, |Y_l^m(\theta,\phi)|^2 = 1.$$
 (12.21)

As an example, we consider the $l=1,\,m=0$ harmonic. This is

$$Y_1^0(\theta,\phi) = \sqrt{\frac{3}{4\pi}}\cos\theta$$
 (12.22)

The integral is thus

$$\int_{0}^{2\pi} d\phi \int_{0}^{\pi} \sin\theta \, d\theta \, \frac{3}{4\pi} \cos^{2}\theta = \frac{3}{2} \int_{0}^{\pi} \sin\theta \, d\theta \, \cos^{2}\theta \,. \tag{12.23}$$

Writing $u = \cos \theta$, $du = -\sin \theta d\theta$, so

$$\frac{3}{2} \int_0^{\pi} \sin \theta \, d\theta \, \cos^2 \theta = -\frac{3}{2} \int_1^{-1} du \, u^2 = -\frac{3}{2} \left[\frac{u^3}{3} \right]_1^{-1} = 1,$$
 (12.24)

as expected.