PH20107: LINEAR EQUATIONS OF SCIENCE

1. PDEs AND LINEARITY

"Partial differential equations are the basis of all physical theorems. In the theory of sound in gases, liquids and solids, in the investigations of elasticity, in optics, everywhere partial differential equations formulate basic laws of nature which can be checked against experiments".

Bernhard Riemann, German mathematician (1826-1866) (http://commons.wikimedia.org/wiki/File:Bernhard_Riemann_3.jpg)

Partial Differential Equations (PDEs) are the 'language' in which the mathematical laws which describe an enormous range of fundamental physical phenomena and processes are expressed.

Some examples of the types of scientific (physical, chemical and biological) and engineering problems that use PDEs:

- using aerodynamics to design a faster Formula One car;
- predicting the weather;
- modelling blood flow in human veins;
- designing the static and dynamic properties of buildings and bridges;
- modelling and predicting population growth.

PDEs first emerged around the beginning of the 18th century[1], and have remained an active area of research for mathematicians, scientists and engineers ever since. Some of the most important PDEs that have been developed are:

- Euler's equations for the dynamics of rigid bodies and the motion of an ideal fluid;
- Newton's law of cooling;
- Lagrange's equations of motion;
- Hamilton's equations of motion;
- Laplace's and Poisson's equations for potential theory and electrostatics;
- Fourier's equation for the diffusion of heat;
- d'Alembert's wave equation;
- the Navier-Stokes equations for the motion of viscous fluids;
- Maxwell's equations for electromagnetic fields;
- the Schrödinger and Dirac equations in quantum mechanics.

1.1. Partial Differential Equations

- Any equation containing partial differential coefficients is known as a partial differential equation (PDE).
- The **order** of a PDE is equal to the order of the highest partial differential coefficient occurring in it.

Check your understanding:

What is the order of the following PDEs?

$$5xy^2\frac{\partial u}{\partial x}+3y\frac{\partial u}{\partial y}=10u$$ 1st order PDE

$$f_1(x,y)\frac{\partial^2 u}{\partial x^2}+f_2(x,y)\frac{\partial u}{\partial y}=0$$ 2nd order PDE

[1] Florian Cajori, 1928. "The Early History of Partial Differential Equations and of Partial Differentiation and Integration" *The American Mathematical Monthly* 35(9): 459-467. (http://www.jstor.org/stable/2298771)

- It is generally much more difficult to solve PDEs compared to ODEs (ordinary differential equations). There are no general methods for solving any arbitrary PDE – only for certain special types of linear PDEs.
- The general solution of an ODE of order *n* contains *n* arbitrary constants.
- The general solution of a PDE usually contains arbitrary **functions**, rather than arbitrary constants, as shown by the following examples:

Example 1:

If

$$u = y\, f(x), \tag{1.1}$$

where $f(x)$ is an arbitrary function of *x*, then

$$\frac{\partial u}{\partial y} = f(x), \tag{1.2}$$

and we can then substitute (1.2) into (1.1) to give:

$$y\frac{\partial u}{\partial y} = u\,. \tag{1.3}$$

The function *u* given in equation (1.1) (which contains an arbitrary function of *x*) is therefore a solution of the 1st order PDE given in equation (1.3).

Example 2:

If

$$u = f(x+y) + g(x-y), \tag{1.4}$$

where $f(x+y)$ and $g(x-y)$ are arbitrary functions of $x+y$ and $x-y$ respectively, then

$$\frac{\partial u}{\partial x} = f'(x+y) + g'(x-y), \tag{1.5}$$

$$\frac{\partial^2 u}{\partial x^2} = f''(x+y) + g''(x-y), \tag{1.6}$$

$$\frac{\partial u}{\partial y} = f'(x+y) - g'(x-y), \tag{1.7}$$

$$\frac{\partial^2 u}{\partial y^2} = f''(x+y) + g''(x-y), \tag{1.8}$$

where the 'dash' notation (f' etc.) means differentiation with respect to the appropriate argument (i.e. $(x+y)$ or $(x-y)$).

By comparing equations (1.6) and (1.8), we therefore find that:

$$\frac{\partial^2 u}{\partial x^2} = \frac{\partial^2 u}{\partial y^2}\,. \tag{1.9}$$

So the function *u* given in equation (1.4) (which contains two arbitrary functions) is therefore a solution to the 2nd order PDE given in equation (1.9).

1.2. Homogeneity

A PDE is homogeneous if all its terms involve the dependent variable and/or one of its derivatives.

Check your understanding:

Are the following PDEs homogeneous or inhomogeneous?

$\frac{\partial^2 T}{\partial x^2} - \frac{1}{\kappa}\frac{\partial T}{\partial t} = 0$ Homogeneous

$R\frac{\partial Q}{\partial t} + \frac{Q}{C} = V$ Inhomogeneous

$\frac{\partial^2 y}{\partial x^2} + \frac{\partial y}{\partial t} - \sin x = 0$ Inhomogeneous

1.3. Operators

Reminder: An operator is a mathematical rule which, when applied to a function, produces another function.

For example, the operator to multiply a function *u* by 2 can be written as:

$$L(u) = 2u \qquad (1.10)$$

We can also have differential operators, such as:

$$L(u) = \frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2}$$

and

$$M(u) = \frac{\partial^2 u}{\partial x^2} - x\frac{\partial u}{\partial y} + 2u\,.$$

Here, the differential operators are:

$$L = \left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2}\right) \text{ and } M = \left(\frac{\partial^2}{\partial x^2} - x\frac{\partial}{\partial y} + 2\right).$$

1.4. Linear Operators

An operator *L* is linear if it satisfies the following:

$$L(a\psi) = aL(\psi) \qquad (1.11)$$

$$L(\psi + \Phi) = L(\psi) + L(\Phi) \qquad (1.12)$$

Therefore, by combining equations (1.11) and (1.12), the general definition of a linear operator *L* is that it meets the following condition:

$$L(a\psi + b\Phi) = aL(\psi) + bL(\Phi) \qquad (1.13)$$

where Ψ and Φ are functions, and *a* and *b* are non-zero constants.

In general, equation (1.13) can be extended to any number of functions:

$$L\left(\sum_{j=1}^{k} a_j\psi_j + b_j\Phi_j\right) = \sum_{j=1}^{k} a_j L(\psi_j) + \sum_{j=1}^{k} b_j L(\Phi_j) \qquad (1.14)$$

where $u_1, u_2, u_3 \ldots\ldots u_k$ are *k* functions and $c_1, c_2, c_3 \ldots\ldots c_k$ are *k* constants. This is known as the principle of linear superposition.

Example 3:

If $L(\psi) = \frac{\partial \psi}{\partial x}$, then *L* represents the operator *differentiation with respect to x.*

Is *L* a linear operator? Check by substituting into equation (1.13):

$$L(a\psi + b\Phi) = \frac{\partial}{\partial x}(a\psi + b\Phi)$$
$$= a\frac{\partial \psi}{\partial x} + b\frac{\partial \Phi}{\partial x}$$
$$= a\,L(\psi) + b\,L(\Phi)$$

In other words, in this example L is a linear operator.

Example 4:

If $L(\psi) = \sqrt{\psi}$, then L is the *square root* operator.

Is L a linear operator? Again, check by substituting into equation (1.13)

$$L(a\psi + b\Phi) = \sqrt{a\psi + b\Phi}$$

$$a\,L(\psi) + b\,L(\Phi) = a\sqrt{\psi} + b\sqrt{\Phi}$$

So:

$$L(a\psi + b\Phi) \neq a\,L(\psi) + b\,L(\Phi)$$

In other words, in this example L is not a linear operator.

1.5. Combining Linear Operators

Sum:

If L and M are two linear operators, then the sum of L and M is defined as:

$$(L+M)(\psi) = L(\psi) + M(\psi) \qquad (1.15)$$

$L+M$ is also a linear operator ***(Homework**: show this!)*

Product:

The result of multiplying two linear operators L and M is the same as applying the individual operators L and M in turn.

In other words:

$$LM(\psi) = L\left(M(\psi)\right) \qquad (1.16)$$

Again, LM is also a linear operator ***(More homework**: show this!)*

Other properties of linear operators:

- ***Commutative (for addition):***

$$L + M = M + L \qquad (1.17)$$

- ***Associative:***

$$(L+M) + N = L + (M + N) \qquad (1.18)$$

$$(LM)\,N = L(M\;N) \qquad (1.19)$$

- ***Distributive:***

$$L(c_1 M + c_2 N) = c_1 LM + c_2 LN \qquad (1.20)$$

Linear operators **with constant coefficients** also have the following property:

- ***Commutative (for products):***

$$LM = ML \qquad (1.21)$$

1.6. Linear Differential Operators

We've already seen that the d/dx operator is linear. It must also be the case that any higher order differential operators (d^2/dx^2 , d^3/dx^3 etc.) must also be linear.

The following is therefore a general expression for a linear differential operator:

$$L(y) = a_n(x)\frac{d^n y}{dx^n} + a_{n-1}(x)\frac{d^{n-1}y}{dx^{n-1}} + a_{n-2}(x)\frac{d^{n-2}y}{dx^{n-2}} \ldots\ldots \\ \ldots\ldots + a_2(x)\frac{d^2 y}{dx^2} + a_1(x)\frac{dy}{dx} + a_0(x)\, y \qquad (1.22)$$

1.7. Linear Differential Equations

If $L(y)$ is a linear differential operator, then the equation $L(y) = f(x)$ is a linear differential equation. If $f(x) = 0$, it is a homogeneous linear differential equation. If $f(x) \neq 0$, it is inhomogeneous.

1.8. Linear Partial Differential Equations

A PDE is linear iff it fulfils both of the following conditions:

i. Both the dependent variable (i.e. *u* in most of the examples below) and its derivatives occur only to the first power[2];

ii. The PDE does not contain any products of the dependent variable and its derivatives.

If both of these conditions are not fulfilled, the PDE is nonlinear.

Check your understanding:

Are the following PDEs linear or nonlinear?

$$\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} = 0$$ Linear

$$\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial Z}{\partial r}\right) = \frac{1}{c^2}\frac{\partial^2 Z}{\partial t^2}$$ Linear

$$u\frac{\partial^2 u}{\partial x^2} + \left(\frac{\partial u}{\partial y}\right)^2 = u^2$$ Nonlinear

$$i\frac{\partial \psi}{\partial t} = -\frac{1}{2}\frac{\partial^2 \psi}{\partial x^2} + \kappa|\psi^2|\psi$$ Nonlinear

$$\frac{1}{c^2}\frac{\partial^2 \psi}{\partial t^2} - \nabla^2\psi + \frac{m^2c^2}{\hbar^2}\psi = 0$$ Linear

The most general 1st order PDE for two independent variables *x* and *y*, and dependent variable *u* is therefore:

$$A(x,y)\frac{\partial u}{\partial x} + B(x,y)\frac{\partial u}{\partial y} + C(x,y)\,u = D(x,y) \qquad (1.23)$$

and the most general 2nd order PDE for $u(x,y)$ is:

[2] i.e. no terms containing u^2., u^3, $\left(\frac{\partial u}{\partial x}\right)^2$, $\left(\frac{\partial u}{\partial y}\right)^3$ etc.

$$A(x,y)\frac{\partial^2 u}{\partial x^2}+B(x,y)\frac{\partial^2 u}{\partial x\partial y}+C(x,y)\frac{\partial^2 u}{\partial y^2}+D(x,y)\frac{\partial u}{\partial x}+E(x,y)\frac{\partial u}{\partial y}+F(x,y)u=G(x,y) \quad (1.24)$$

Or, using shorthand notation:

$$A(x,y)u_x+B(x,y)u_y+C(x,y)u=D(x,y)$$

$$A(x,y)u_{xx}+B(x,y)u_{xy}+C(x,y)u_{yy}+D(x,y)u_x+E(x,y)u_y+F(x,y)u=G(x,y) \quad (1.25)$$

Equation (1.24) can be rewritten in the form

$$L(u)=G(x,y), \quad (1.26)$$

where

$$L=A\frac{\partial^2}{\partial x^2}+B\frac{\partial^2}{\partial x\partial y}+C\frac{\partial^2}{\partial y^2}+D\frac{\partial}{\partial x}+E\frac{\partial}{\partial y}+F \quad (1.27)$$

Equations (1.24) and (1.26) are said to be ***homogeneous*** if $G(x,y)=0$, and ***inhomogeneous*** if $G(x,y)\neq 0$.

[3] This naming is by analogy with the classification of conic sections, which are described by the general second-order algebraic equation $Ax^2+Bxy+Cy^2+Dx+Ey+F=0$.

1.9. Types of 2nd Order Linear PDEs

All 2nd order linear PDEs of the form shown in equation (1.24) can be classified as parabolic, hyperbolic, or elliptic[3]. The type of equation is determined by the particular values taken by the coefficients of the equation:

i. ***Elliptic equations:***

$$B^2-4AC<0 \quad (1.28)$$

ii. ***Hyperbolic equations:***

$$B^2-4AC>0 \quad (1.29)$$

iii. ***Parabolic equations:***

$$B^2-4AC=0 \quad (1.30)$$

Check your understanding:

Are the following PDEs parabolic, hyperbolic or elliptic?

$$3\frac{\partial^2 u}{\partial x^2}+4\frac{\partial^2 u}{\partial x\partial y}-\frac{\partial^2 u}{\partial y^2}+6\frac{\partial u}{\partial x}=0$$ Hyperbolic

$$\frac{\partial^2 Z}{\partial r^2}-2\frac{\partial^2 Z}{\partial r\partial t}+\frac{\partial^2 Z}{\partial t^2}=1$$ Parabolic

$$4\frac{\partial^2 u}{\partial x^2}+\frac{\partial^2 u}{\partial y^2}+2\frac{\partial u}{\partial x}=\sin x$$ Elliptic

1.10. What do these classifications mean physically?

- ***Elliptic equations:***

  Elliptic PDEs describe steady-state phenomena, and are characterised by the minimum of a certain quantity (often energy). They generally arise from a physical problem that involves a diffusion process that has reached equilibrium, e.g. a steady-state temperature distribution.

- ***Hyperbolic equations:***

  Hyperbolic PDEs describe vibrating systems and wave motion. They usually describe physical phenomena for which there is transport or propagation of a physical entity or information. Hyperbolic equations can support solutions with discontinuities, such as a shock wave.

- ***Parabolic equations:***

  Parabolic PDEs represent the transition between hyperbolic and elliptic PDEs. Physically, they tend to arise in time-dependent diffusion and transient heat flow problems. They usually describe the evolutionary process that leads to a steady state described by an elliptic equation.

1.11. Examples of linear PDEs within the physical sciences

- **Poisson Equation**

$$\nabla^2 \Phi = -S(\mathbf{r}) \tag{1.31}$$

This equation can be applied in a number of ways, including electrostatics, gravitational fields, steady-state diffusion and heat conduction, image and shape processing.

- **Laplace Equation**

$$\nabla^2 \Phi = 0 \tag{1.32}$$

The homogeneous equivalent to Poisson's Equation.

- **Diffusion Equation**

$$\nabla^2 \Phi - \frac{1}{\kappa}\frac{\partial \Phi}{\partial t} = -S(\mathbf{r}, t) \tag{1.33}$$

This is based on Fick's Laws of diffusion.

- **Wave Equation**

$$\nabla^2 \Phi - \frac{1}{c^2}\frac{\partial^2 \Phi}{\partial t^2} = -S(\mathbf{r}, t) \tag{1.34}$$

D'Alembert developed a method for solving the wave equation, and applied it to problems such as vibrating strings in musical instruments.

- **Helmholtz Equation**

$$\nabla^2 \Phi + \lambda \Phi = 0 \tag{1.35}$$

This equation often arises as a result of applying the separation of variables method to a time-dependent PDE, and represents the time-independent form of this original equation.

- **Schrödinger Equation (time-dependent and time-independent forms):**

$$-\frac{\hbar^2}{2m}\nabla^2 \Phi + V(\mathbf{r})\,\Phi = i\hbar\frac{\partial \Phi}{\partial t} \tag{1.36}$$

$$-\frac{\hbar^2}{2m}\nabla^2 \Phi + V(\mathbf{r})\,\Phi = E\,\Phi \tag{1.37}$$

These equations describe the quantum mechanical wavefunction of a physical system, either as it evolves in time, or in the steady state.

2. FORMULATING A PDE FROM A PHYSICAL PROBLEM

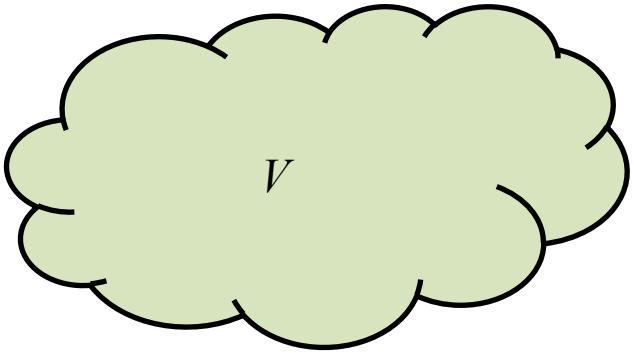
Where do the equations in Section 1.11 come from?

Let's look at the ***diffusion equation*** as an example. It arises in the description of many physical processes, such as:

- diffusion of a chemical species;
- temperature distribution and heat flow in a body;
- distribution of neutrons in a nuclear reactor.

2.1. Diffusion of a chemical species

Let $\rho(\mathbf{r}, t)$ be the concentration of a chemical (say in air or water), and consider the species diffusing into or out of some arbitrary volume V, as shown in the diagram below:



Let the total amount of the species in the volume V be M. So

$$M = \int_V \rho(\mathbf{r}, t)\, dV \tag{2.1}$$

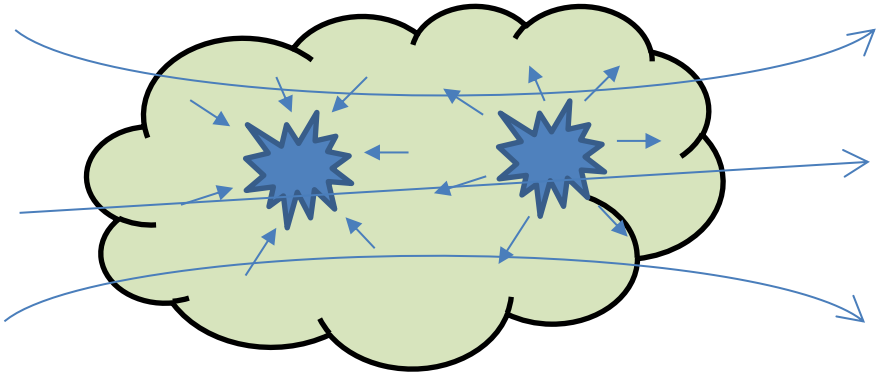
The change in the total amount of the species in the volume V during a time δt is therefore:

$$\begin{aligned} \Delta M &= \int_V \rho(\mathbf{r}, t+\delta t)\, dV - \int_V \rho(\mathbf{r}, t)\, dV \\ &= \delta t \int_V \frac{\partial \rho}{\partial t}\, dV \end{aligned} \tag{2.2}$$

There are two ways in which this change can arise:

i. Creation/destruction of the species (for example, due to a chemical reaction):

ii. Diffusion in or out of the surface of V:



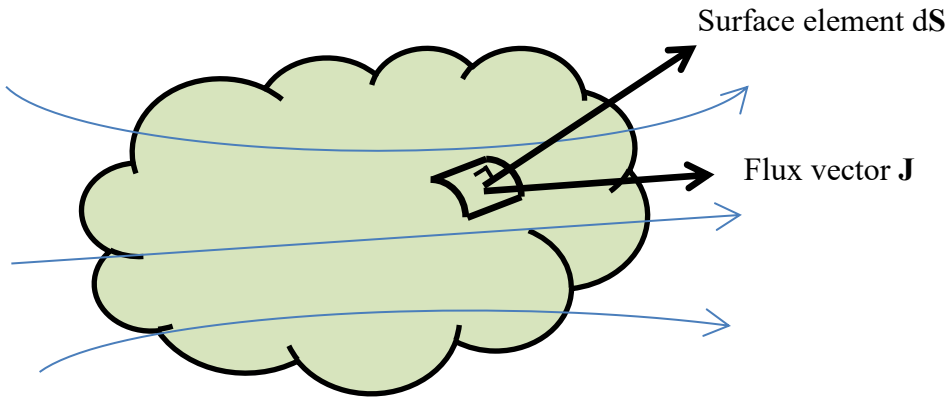
2.2. Creation/destruction of the species

The change in the total amount of the species in the volume V during a time δt due to creation or destruction of the species is:

$$\Delta M_1 = \delta t \int_V Q(\mathbf{r}, t)\, dV\,, \tag{2.3}$$

where $Q(\mathbf{r}, t)$ is the rate of production of the species per unit volume per unit time.

2.3. Diffusion in or out of the surface of V



The flux vector **J** represents the net flow of the species through the surface element.

Fick's Law states that the flux **J** is in the direction of the most rapid decrease in concentration, i.e. in the direction of $-\nabla\rho$. So $\mathbf{J} = -D\nabla\rho$, where D is the diffusion constant.

The change in the total amount of the species in the volume V during a time δt due to diffusion in/out of the surface of V is:

$$\Delta M_2 = \delta t \int_S -\mathbf{J}\cdot d\mathbf{S}$$

$$\Delta M_2 = D\,\delta t \int_S \nabla\rho \cdot d\mathbf{S} \qquad (2.4)$$

We can now put (2.2), (2.3) and (2.4) together, as follows:

$$\Delta M = \Delta M_1 + \Delta M_2 \qquad (2.5)$$

$$= \delta t \int_V Q(\mathbf{r},t)\,dV + D\,\delta t \int_S \nabla\rho \cdot d\mathbf{S} \qquad (2.6)$$

But we already know that $\Delta M = \delta t \int_V \frac{\partial \rho}{\partial t}\,dV$.

So $$\int_V \frac{\partial \rho}{\partial t}\,dV = \int_V Q(\mathbf{r},\mathrm{t})\,dV + D\int_S \nabla\rho\cdot d\mathbf{S} \qquad (2.7)$$

But the Divergence Theorem states that

$$\int_S \mathbf{A}\cdot d\mathbf{S} = \int_V \nabla\cdot\mathbf{A}\,d\mathbf{V} \qquad (2.8)$$

So

$$\int_S \nabla\rho\cdot d\mathbf{S} = \int_V \nabla\cdot\nabla\rho\,dV = \int_V \nabla^2\rho\,dV$$

Substituting this back into equation (2.7) gives:

$$\int_V \frac{\partial \rho}{\partial t}\,dV = \int_V Q(\mathbf{r},\mathrm{t})\,dV + D\int_V \nabla^2\rho\,dV \qquad (2.9)$$

But this equation holds for any volume V, so we can shrink V to a point to give:

$$\frac{\partial \rho}{\partial t} = Q(\mathbf{r},\mathrm{t}) + D\nabla^2\rho \qquad (2.10)$$

Or:

$$\nabla^2\rho - \frac{1}{D}\frac{\partial \rho}{\partial t} = -\frac{Q(\mathbf{r},\mathrm{t})}{D} \qquad (2.11)$$

Source term

In other words, the Diffusion Equation (cf.equation (1.33)).

2.4. The temperature distribution of a body

In a similar way we can derive the diffusion equation which describes the temperature distribution $T(\mathbf{r},t)$ in a body:

$$\nabla^2 T - \frac{\rho c}{\kappa}\frac{\partial T}{\partial t} = -\frac{P(\mathbf{r})}{\kappa}, \qquad (2.12)$$

where ρ is the density of the body, c is the heat capacity per unit mass, κ is the thermal conductivity, and $P(\mathbf{r})$ is the rate of heat generation per unit volume.

The derivation of this equation is based on the following principles:

- The rate of heat flow across a surface is proportional to the temperature gradient across the surface;
- Conservation of energy.

Suppose we are interested in the steady state concentration or temperature distribution. In this case:

$$\frac{\partial \rho}{\partial t} = 0 \qquad (2.13)$$

and

$$\frac{\partial T}{\partial t} = 0. \qquad (2.14)$$

So equations (2.11) and (2.12) reduce to:

$$\nabla^2 \rho = -\frac{Q(\mathbf{r})}{D} \qquad (2.15)$$

$$\nabla^2 T = -\frac{P(\mathbf{r})}{\kappa} \qquad (2.16)$$

These are examples of the Poisson Equation (cf. equation (1.31)).

Equation (2.16) could, for example, be used to describe the temperature distribution in a heated body, e.g. a nuclear reactor.

If there are no source terms, equations (2.15) and (2.16) reduce to:

$$\nabla^2 \rho = 0 \qquad (2.17)$$

and

$$\nabla^2 T = 0, \qquad (2.18)$$

which are examples of Laplace's Equation (cf. equation (1.32)).

3. SOLVING PDES BY SEPARATION OF VARIABLES

3.1. Introduction

Many PDEs (especially linear homogeneous PDEs) can be solved using the *separation of variables* method. This method works by magically (well, maybe not!) converting the PDE to a set of ODEs that we can then solve. It doesn't always work, though – whether or not a PDE is separable isn't always an easy question to determine. Moreover, even when we can separate the variables, it's often hard to move past this step. Still, it's generally a good idea to give it a go.

Before diving into applying the method, we first need to cover some preliminaries, however: a reminder of linear superposition and boundary conditions.

3.2. Linear Superposition

Recall the general 2nd order linear PDE for two independent variables x and y, and dependent variable u:

$$A(x,y)\frac{\partial^2 u}{\partial x^2}+B(x,y)\frac{\partial^2 u}{\partial x\partial y}+C(x,y)\frac{\partial^2 u}{\partial y^2}+D(x,y)\frac{\partial u}{\partial x}+E(x,y)\frac{\partial u}{\partial y}+F(x,y)u=G(x,y) \quad (3.1)$$

This can be rewritten in the form

$$L(u)=G(x,y), \quad (3.2)$$

where

$$L=A\frac{\partial^2}{\partial x^2}+B\frac{\partial^2}{\partial x\partial y}+C\frac{\partial^2}{\partial y^2}+D\frac{\partial}{\partial x}+E\frac{\partial}{\partial y}+F\ . \quad (3.3)$$

Suppose that v is a particular solution of the inhomogeneous linear equation (3.2) (i.e. when $G\neq 0$), and that w is a particular solution of the associated homogeneous equation (i.e. when $G=0$).

Then

$$L(v)=G(x,y) \quad (3.4)$$

and

$$L(w)=0 \quad (3.5)$$

Therefore, if $u=v+w$, and adding equations (3.4) and (3.5):

$$L(u)=L(v+w)=L(v)+L(w)=G(x,y)+0=G(x,y) \quad (3.6)$$

In other words, if v is a particular solution of a linear equation, and w is a particular solution of the associated homogeneous linear equation, then $u=v+w$ is also a solution of the equation.

More generally, equation (3.5) can have many solutions (often infinitely many solutions), which we can write as w_k. So we can write the solution to equation (3.1) as

$$u=v+\sum_k c_k\, w_k \quad (3.7)$$

where c_1, c_2, c_3.... are constant coefficients.

To obtain a complete solution, we then have to apply the relevant boundary conditions to fix the values of the coefficients c_k.

3.3. Example of applying boundary conditions

Consider the wave equation in 1D:

$$\frac{\partial^2\phi}{\partial x^2}-\frac{1}{c^2}\frac{\partial^2\phi}{\partial t^2}=0 \quad (3.8)$$

This can be rewritten in the form

$$L(\phi) = 0 \tag{3.9}$$

where

$$L = \frac{\partial^2}{\partial x^2} - \frac{1}{c^2}\frac{\partial^2}{\partial t^2} \tag{3.10}$$

Comparing with equation (1.34), there is no source term $S(\mathbf{r}, t)$.

Solutions to (3.8) are of the form $\phi(x, t) = e^{i(kx-kct)}, e^{i(kx+kct)}$, for any value of *k*.

The general solution is then:

$$\phi(x,t) = \sum_k \left[A_k e^{i(kx-kct)} + B_k e^{i(kx+kct)} \right] \tag{3.11}$$

coefficients for each value of *k*

sum over all possible values of *k*

The values of *k*, A_k and B_k are fixed by the boundary conditions.

Suppose the boundary conditions are:

$$\phi(x,0) = \sin 3x \tag{3.12}$$

and

$$\dot{\phi}(x,0) = 0\,, \tag{3.13}$$

where $\dot{\phi}$ means $\frac{\partial \phi}{\partial t}$.

Start with boundary condition (3.13), and substitute into (3.11):

$$\begin{aligned} \dot{\phi}(x,0) &= \sum_k \left[-ikc\, A_k e^{ikx} + ikc\, B_k e^{ikx} \right] \\ &= \sum_k -ikc\left(A_k - B_k\right) e^{ikx} \end{aligned} \tag{3.14}$$

But the boundary condition is that $\dot{\phi}(x,0) = 0$ for **all** values of *x*.

Looking at (3.14), this can only be the case if $A_k = B_k$.

Substituting this into (3.11) gives:

$$\phi(x,t) = \sum_k A_k e^{ikx}\left(e^{-ikct} + e^{ikct}\right) = \sum_k 2A_k e^{ikx}\cos(kct) \tag{3.15}$$

Now substitute boundary condition (3.12) into(3.15):

$$\phi(x,0) = \sum_k 2A_k e^{ikx} = \sin 3x \tag{3.16}$$

But

$$\sin 3x = \frac{e^{i3x}}{2i} - \frac{e^{-i3x}}{2i} \tag{3.17}$$

So

$$\sum_k 2A_k e^{ikx} = \frac{e^{i3x}}{2i} - \frac{e^{-i3x}}{2i}\,. \tag{3.18}$$

Equation (3.18) can only be true for all values of *x* (as it must be) if:

$$2A_3 = \frac{1}{2i}, \tag{3.19}$$

$$2A_{-3} = -\frac{1}{2i}, \tag{3.20}$$

and all other coefficients $A_k = 0$.

Substituting these coefficients into (3.15) gives:

$$\begin{aligned}\phi(x,t) &= \sum_k 2A_k e^{ikx}\cos(kct) \\ &= \frac{1}{2i}\, e^{i3x}\cos(3ct) - \frac{1}{2i}\, e^{-i3x}\cos(-3ct) \\ &= \sin(3x)\cos(3ct)\end{aligned} \qquad (3.21)$$

So applying the boundary conditions has transformed the infinite number of unknowns in (3.11) into a unique solution.

3.4. Separation of Variables Method

How to apply the method? The starting point is to take the unknown function (say $u(x,t)$), and to "separate its variables", i.e. to make the ansatz that:

$$u(x,t) = X(x)T(t), \qquad (3.22)$$

where $X(x)$ is a function of *x* only, and $T(t)$ is a function of *t* only.

For example, consider the 1D wave equation again, with no sources:

$$\frac{\partial^2\phi}{\partial x^2} - \frac{1}{c^2}\frac{\partial^2\phi}{\partial t^2} = 0 \qquad (3.23)$$

Look for a separable solution of the form

$$\phi(x,t) = X(x)\,T(t), \qquad (3.24)$$

where $X(x)$ is a function of *x* only, and $T(t)$ is a function of *t* only. Differentiating (3.24) gives:

$$\frac{\partial^2\phi}{\partial x^2} = \frac{d^2X}{dx^2}\,T \qquad (3.25)$$

$$\frac{\partial^2\phi}{\partial t^2} = X\,\frac{d^2T}{dt^2} \qquad (3.26)$$

Substitute into (3.23) to give:

$$\frac{d^2X}{dx^2}\,T - \frac{1}{c^2}\,X\,\frac{d^2T}{dt^2} = 0 \qquad (3.27)$$

Divide by XT, and rearrange such that the LHS is a function of *x* only, and the RHS is a function of *t* only:

$$\frac{1}{X}\frac{d^2X}{dx^2} = \frac{1}{c^2T}\frac{d^2T}{dt^2} \qquad (3.28)$$

Notice the important facts that:

- the LHS of equation (3.28) is a function of *x* only, while the RHS is a function of *t* only;
- the LHS of equation (3.28) has to be equal to the RHS for ***any*** values of *x* and *t*.

The only way in which this can be possible is if both sides of equation (3.28) are independently equal to the same constant.

This constant is called a separation constant, and we have some freedom in choosing what it should be. (At least we have some freedom mathematically – the physics will often constrain our choice more, as we will see in the following examples).

In this example, we will see later that our separation constant will need to be a negative number. We will therefore call it $-k^2$.

So

$$\frac{1}{X}\frac{d^2X}{dx^2} = \frac{1}{c^2T}\frac{d^2T}{dt^2} = -k^2 \qquad (3.29)$$

Or:

$$\frac{d^2X}{dx^2} = -k^2X \tag{3.30}$$

$$\frac{d^2T}{dt^2} = -k^2c^2T \tag{3.31}$$

In other words, separation of variables has enabled us to transform the original PDE containing two independent variables into two ODEs. Note that these two ODEs are linked together, though, as they both contain *k*. So they aren't independent of each other – changing the value of *k* will change both ODEs.

Solving equations (3.30) and (3.31) gives:

$$X(x) = a_k e^{ikx} + b_k e^{-ikx} \tag{3.32}$$

$$T(t) = c_k e^{ickt} + d_k e^{-ickt} \tag{3.33}$$

So

$$\phi(x,t) = X(x)\,T(t) = \left(a_k e^{ikx} + b_k e^{-ikx}\right)\left(c_k e^{ickt} + d_k e^{-ickt}\right) \tag{3.34}$$

The values of a_k, b_k, c_k and d_k are fixed by boundary conditions. One possible solution is:

$$\phi(x,t) = e^{i(kx-\omega t)}, \tag{3.35}$$

which is a forward-travelling wave, with wavevector $k = 2\pi/\lambda$ and angular frequency $\omega = ck$.

Notes:

- For now (i.e. without any boundary conditions), any value of *k* is allowed, as ϕ satisfies the original PDE (3.23) for any value of *k*.
- If we had used a positive separation constant (say $+k^2$), our solutions would have been $X(x) = a_k e^{kx} + b_k e^{-kx}$ and $T(t) = c_k e^{ckt} + d_k e^{-ckt}$, i.e. the wave would exponentially increase or decrease in space and time – this would not represent a physically meaningful solution, unless the wave is constrained to a finite region of space.
- *X* and *T* should be labelled to indicate the particular value of *k* chosen, i.e.

$$X_k(x) = a_k e^{ikx} + b_k e^{-ikx} \tag{3.36}$$

$$T_k(t) = c_k e^{ickt} + d_k e^{-ickt} \tag{3.37}$$

- Because of linearity, the general solution is the sum over all possible solutions:

$$\phi(x,t) = \sum_k X_k(x)\,T_k(t) \tag{3.38}$$

- *k* is really a continuous variable here, so $\sum_k$ really means $\int dk$
- Similar considerations apply to the solution of other PDEs by separation of variables.
- Separation of variables can be applied when there are more than two independent variables, e.g.

$$\phi(x,t) = X(x)\,Y(y)\,Z(z)\,T(t)$$

or, in other co-ordinate systems, e.g.

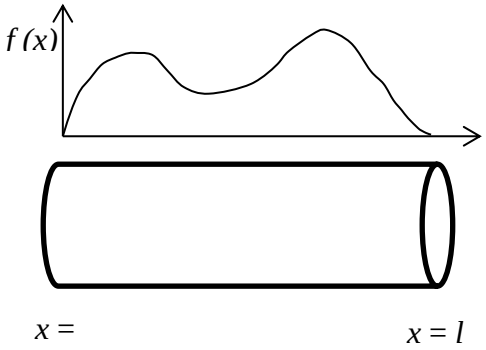
$$\phi(\mathbf{r},t) = R(\mathbf{r})\,\Theta(\theta)\,\Phi(\phi)\,T(t)$$

- An equation may be separable in one co-ordinate system, but not in another. It's important to choose the co-ordinate system most appropriate to the geometry of the problem.

4. SOLVING SOME REAL PDEs BY SEPARATION OF VARIABLES

4.1. Solving the Diffusion Equation in 1D Cartesian co-ordinates

Suppose a tube of length l is filled with a chemical solution, and at time $t=0$ the concentration profile of this solution is $f(x)$. The ends of the tube are open to reservoirs of pure solvent, which will wash away any of the chemical that diffuses to the ends of the tube. So the concentration is $\rho = 0$ at $x=0$ and $x=l$.



Question: What is the concentration profile at later times?

The 1D diffusion equation with no source is

$$\frac{\partial^2 \rho}{\partial x^2} = \frac{1}{c}\frac{\partial \rho}{\partial t}\,, \tag{4.1}$$

where $\rho(x,t)$ is the concentration, and c the diffusion constant. Look for a separable solution:

$$\rho(x,t) = X(x)\,T(t) \tag{4.2}$$

So:

$$T\,\frac{d^2X}{dx^2} = \frac{1}{c}X\,\frac{dT}{dt} \tag{4.3}$$

Divide by $\rho = X\,T$:

$$\frac{1}{X}\frac{d^2X}{dx^2} = \frac{1}{cT}\frac{dT}{dt} = -\alpha^2\,, \tag{4.4}$$

where we've introduced $-\alpha^2$ (again for physical meaningfulness defined as being negative) as the separation constant.

So:

$$\frac{dT}{dt} = -\alpha^2 cT \qquad \Rightarrow T(t) = e^{-\alpha^2 ct} \tag{4.5}$$

and

$$\frac{d^2X}{dx^2} = -\alpha^2 X \qquad \Rightarrow X(x) = A\sin\alpha x + B\cos\alpha x \tag{4.6}$$

So the general solution becomes:

$$\rho(x,t) = X(x)\,T(t) = \sum_{\alpha}\left(A_\alpha \sin\alpha x + B_\alpha \cos\alpha x\right)e^{-\alpha^2 ct} \tag{4.7}$$

Having found the general solution, we now apply the boundary conditions to find the required solution.

Boundary conditions 1 and 2 are that $\rho = 0$ at $x=0$ and $x=l$.

Boundary condition 1:

$$\rho(0,t) = \sum_{\alpha} B_\alpha\, e^{-\alpha^2 ct} = 0 \tag{4.8}$$

To satisfy (4.8) for **all** t, we therefore need $B_\alpha = 0$ for all values of α.

Boundary condition 2:

$$\rho(l,t) = \sum_{\alpha} A_{\alpha} \sin \alpha l \, e^{-\alpha^2 c t} = 0 \qquad (4.9)$$

To satisfy (4.9) for **all** t, we need the following to be true for all α:

$$A_{\alpha} \sin \alpha l = 0 \qquad (4.10)$$

Given that we already know that $B_{\alpha} = 0$, it would not be physically meaningful to also have $A_{\alpha} = 0$, as this would then just reduce to $\rho(x,t) = 0$.

Therefore:

$$\sin \alpha l = 0 \qquad (4.11)$$

In other words,

$$\alpha l = n\pi \quad \Rightarrow \quad \alpha = \frac{n\pi}{l}, \qquad (4.12)$$

where n is any integer.

So we can now switch the label on our summation to n instead of α:

$$\rho(x,t) = \sum_{n} A_n \sin\left(\frac{n\pi x}{l}\right) e^{-\frac{n^2\pi^2 c}{l^2}t} \qquad (4.13)$$

Look at the form of equation (4.13). The spatial variation in concentration, which is described by the factor $\sin\left(\frac{n\pi x}{l}\right)$, is damped out in time by the $e^{-\frac{n^2\pi^2 c}{l^2}t}$ factor. (As expected, the higher the value of the diffusion constant c, the quicker the damping).

Now consider boundary condition 3 (i.e. that at time $t = 0$ the concentration profile is $f(x)$:

Boundary condition 3:

$$\rho(x,0) = f(x) \qquad (4.14)$$

$$\Rightarrow \quad f(x) = \sum_{n} A_n \sin\left(\frac{n\pi x}{l}\right). \qquad (4.15)$$

At this point, refer to the Appendix to these notes (as well as Appendix C from the Fourier half of PH20107), which shows that the Fourier series for an **odd** function $f(x)$ in the range $-L < x < L$ contains only **sine** terms, and is given by:

$$f(x) = \sum_{n} b_n \sin\left(\frac{n\pi x}{L}\right), \qquad (4.16)$$

where

$$b_n = \frac{2}{L}\int_0^L f(x) \sin\left(\frac{n\pi x}{L}\right) dx. \qquad (4.17)$$

So, by comparing equation (4.15) with equation (4.16), we can therefore write:

$$A_n = \frac{2}{l}\int_0^l f(x) \sin\left(\frac{n\pi x}{l}\right) dx \qquad (4.18)$$

Equations (4.13) and (4.18) therefore provide the complete solution for $\rho(x,t)$ for any starting profile $f(x)$.

In other words, the general solution to equation (4.1), given the boundary conditions that $\rho = 0$ at $x = 0$ and $x = l$, and that the concentration profile at time $t = 0$ is $f(x)$, is given by:

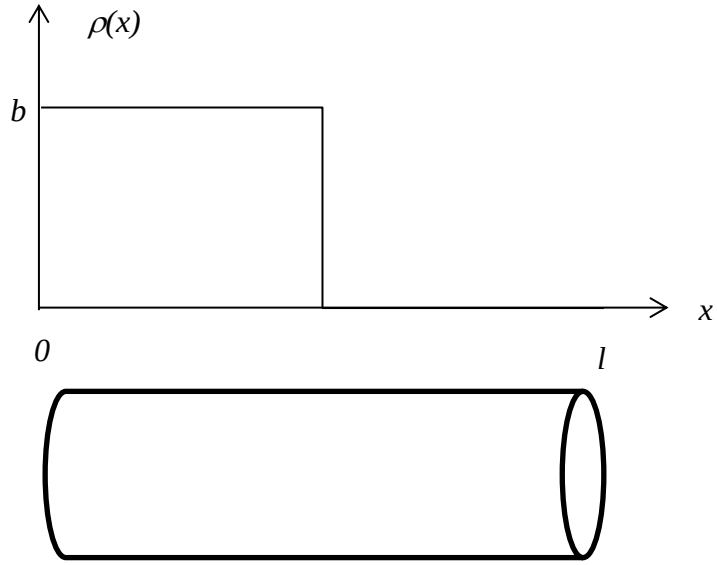
$$\rho(x,t) = \sum_{n} A_n \sin\left(\frac{n\pi x}{l}\right) e^{-\frac{n^2\pi^2 c}{l^2}t}, \qquad (4.19)$$

where

$$A_n = \frac{2}{l}\int_0^l f(x) \sin\left(\frac{n\pi x}{l}\right) dx \qquad (4.20)$$

Now try an example of a specific initial concentration profile $f(x)$:

$$f(x)=\begin{cases} b & 0<x<l/2 \\ 0 & l/2<x<l \end{cases} \tag{4.21}$$



Substituting (4.21) into (4.18) gives:

$$A_n=\frac{2}{l}\int_0^{l/2} b\sin\left(\frac{n\pi x}{l}\right)dx \tag{4.22}$$

$$=\frac{2b}{l}\left(\frac{-l}{n\pi}\right)\left[\cos\left(\frac{n\pi x}{l}\right)\right]_0^{l/2} \tag{4.23}$$

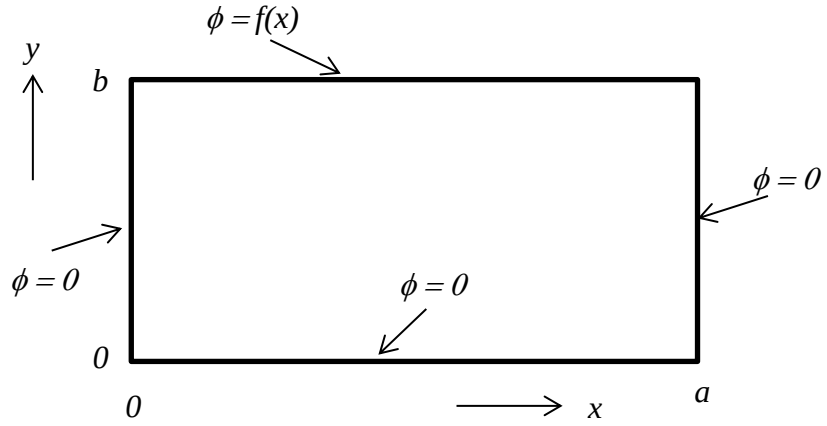
$$=\frac{2b}{n\pi}\left(1-\cos\left(\frac{n\pi}{2}\right)\right) \tag{4.24}$$

So:

$$\rho(x,t)=\frac{2b}{\pi}\sum_{n=1}^{\infty}\frac{\left(1-\cos\left(\frac{n\pi}{2}\right)\right)}{n}\sin\left(\frac{n\pi x}{l}\right)e^{-\frac{n^2\pi^2 c}{l^2}t} \tag{4.25}$$

4.2. Solving Laplace's Equation in 2D Cartesian co-ordinates

Find the function $\phi(\mathbf{r})$ which satisfies Laplace's Equation in the region shown below:



This diagram could, for example, represent the temperature distribution of a plate, with the temperature of the edges fixed as shown.

Laplace's Equation is:

$$\nabla^2\phi=0 \tag{4.26}$$

Given the rectangular geometry of the region, the Cartesian co-ordinate system looks the best to use.

So we write Laplace's Equation as

$$\frac{\partial^2\phi}{\partial x^2}+\frac{\partial^2\phi}{\partial y^2}=0 \qquad (4.27)$$

Let's try separation of variables, with

$$\phi(x,y)=X(x)\,Y(y) \qquad (4.28)$$

Substitute (4.28) into (4.27) to give:

$$\frac{d^2X}{dx^2}Y+X\frac{d^2Y}{dy^2}=0 \qquad (4.29)$$

$$\Rightarrow \quad \frac{1}{X}\frac{d^2X}{dx^2}=-\frac{1}{Y}\frac{d^2Y}{dy^2}=-k^2 \qquad (4.30)$$

Again note the sign of the separation constant.

If you are solving the Laplace equation in Cartesian coordinates, the hint of what sign you should use for the separation constant comes from the boundary conditions. If (say) the conditions at the boundaries of the domain in the *x* variable are the same (as they are in this example), but those at the boundaries of the domain in the *y* variable are different (again, as they are in this example), choose the sign of the constant such that it will lead to oscillatory/periodic solutions in the *x* variable.

So this means that we should use $\frac{1}{X}\frac{d^2X}{dx^2}=-k^2$, not $\frac{1}{X}\frac{d^2X}{dx^2}=+k^2$.

Separating the two ODEs in equation (4.30) gives:

$$\frac{d^2X}{dx^2}=-k^2X \quad \Rightarrow X=A\sin(kx)+B\cos(kx) \qquad (4.31)$$

$$\frac{d^2Y}{dy^2}=+k^2Y \quad \Rightarrow \begin{cases} Y=Ce^{ky}+De^{-ky} \\ OR \\ Y=C\sinh(ky)+D\cosh(ky) \end{cases} \qquad (4.32)$$

(Remember that $\sinh x=\frac{e^x-e^{-x}}{2}$ and $\cosh x=\frac{e^x+e^{-x}}{2}$).

Substituting back into (4.28) gives:

$$\phi(x,y)=\sum_k\left(A_k\sin(kx)+B_k\cos(kx)\right)\left(C_k\sinh(ky)+D_k\cosh(ky)\right) \qquad (4.33)$$

Now we apply the boundary conditions (provided by the labelling in the diagram above), in order to determine the values of A_k, B_k, C_k, D_k,and k.

Boundary condition 1 (left-hand edge):

$$\phi(0,y)=\sum_k B_k\left(C_k\sinh(ky)+D_k\cosh(ky)\right)=0 \qquad (4.34)$$

Since equation (4.34) must be true for **all** values of *y*, it must be the case that:

$$B_k=0 \qquad (4.35)$$

Boundary condition 2 (bottom edge):

$$\phi(x,0)=\sum_k A_kD_k\sin(kx)=0 \qquad (4.36)$$

Since equation (4.36) must be true for **all** values of *x*, it must be the case that:

$$D_k=0 \qquad (4.37)$$

(It wouldn't be physically meaningful to have $A_k = 0$ as well as $B_k = 0$, as this would then just reduce to $\phi(x, y) = 0$).

So we can now rewrite equation (4.33) as:

$$\phi(x, y) = \sum_k A_k C_k \sin(kx)\sinh(ky) = \sum_k E_k \sin(kx)\sinh(ky) \quad (4.38)$$

Boundary condition 3 (right-hand edge):

$$\phi(a, y) = \sum_k E_k \sin(ka)\sinh(ky) = 0 \quad (4.39)$$

Since equation (4.39) must be true for **all** values of *y*, it must be the case that:

$$\sin(ka) = 0 \quad \Rightarrow k = \frac{n\pi}{a} \ , \quad (4.40)$$

where *n* is an integer.

So we can now rewrite equation (4.38) as:

$$\phi(x, y) = \sum_n E_n \sin\left(\frac{n\pi x}{a}\right)\sinh\left(\frac{n\pi y}{a}\right) \quad (4.41)$$

(Note the relabelling from *k* to *n* in equation (4.41)).

Boundary condition 4 (top edge):

Finally:

$$\phi(x, b) = \sum_n E_n \sin\left(\frac{n\pi x}{a}\right)\sinh\left(\frac{n\pi b}{a}\right) = f(x), \quad (4.42)$$

which can be rewritten as:

$$f(x) = \sum_n \left(E_n \sinh\left(\frac{n\pi b}{a}\right)\right)\sin\left(\frac{n\pi x}{a}\right) \quad (4.43)$$

Again, we already know that the Fourier series for an **odd** function $f(x)$ in the range $-L < x < L$ is given by:

$$f(x) = \sum_n b_n \sin\left(\frac{n\pi x}{L}\right), \quad (4.44)$$

where

$$b_n = \frac{2}{L}\int_0^L f(x)\sin\left(\frac{n\pi x}{L}\right) dx. \quad (4.45)$$

So, by comparing equation (4.43) with equation (4.44), we can therefore write:

$$E_n \sinh\left(\frac{n\pi b}{a}\right) = \frac{2}{a}\int_0^a f(x)\sin\left(\frac{n\pi x}{a}\right) dx \quad (4.46)$$

$$\Rightarrow \quad E_n = \frac{2}{a\sinh(n\pi b/a)}\int_0^a f(x)\sin\left(\frac{n\pi x}{a}\right) dx \quad (4.47)$$

Equations (4.41) and (4.47) therefore provide the complete solution for $\rho(x, t)$ for any starting profile $f(x)$.

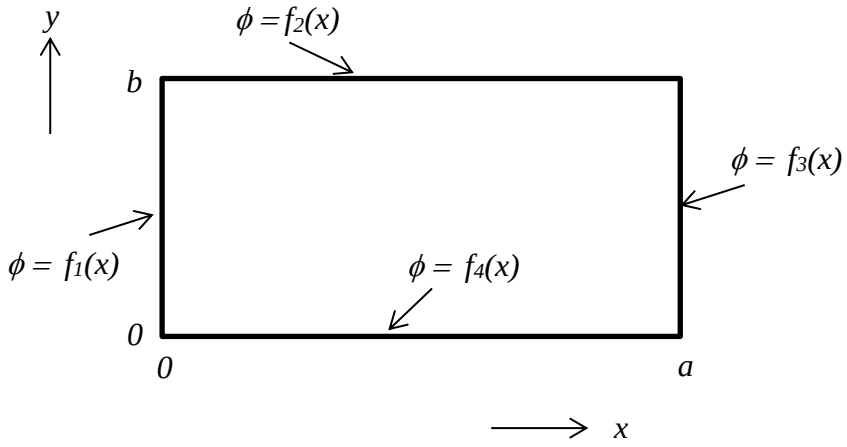
In other words, the general solution to equation (4.27), given the boundary conditions shown in the diagram is:

$$\phi(x, y) = \sum_n E_n \sin\left(\frac{n\pi x}{a}\right)\sinh\left(\frac{n\pi y}{a}\right), \qquad (4.48)$$

where

$$E_n = \frac{2}{a\sinh(n\pi b/a)}\int_0^a f(x)\sin\left(\frac{n\pi x}{a}\right)dx \qquad (4.49)$$

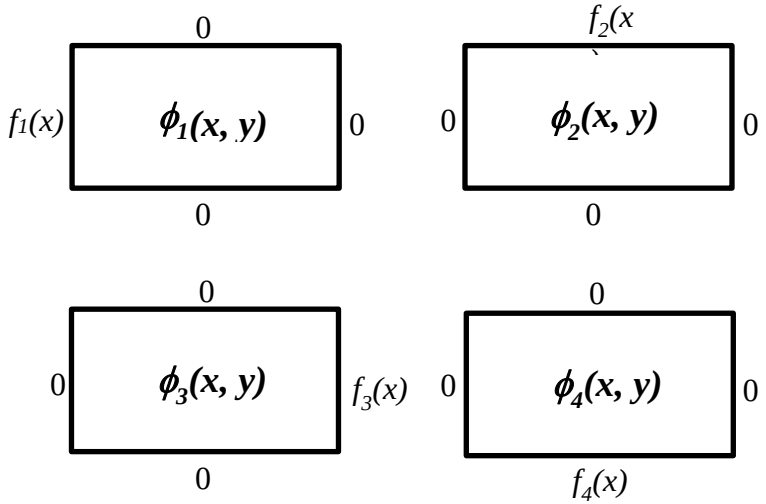
What if we have more general boundary conditions? For example, suppose we had the following profile:



No problem! We can use linearity to write the solution as:

$$\phi(x, y) = \phi_1(x, y) + \phi_2(x, y) + \phi_3(x, y) + \phi_4(x, y), \qquad (4.50)$$

where the ϕ_i satisfy the boundary conditions for the following four situations:



4.3. Solving the Wave Equation for 2D polar co-ordinates

Question: What note(s) do you get when you hit a drum?

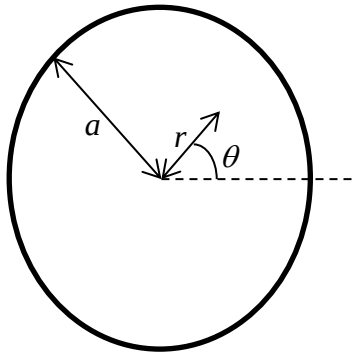
4.3.1. Setting up the equation:

The vibrations of a drum are governed by the wave equation:

$$\nabla^2\Phi = \frac{1}{c^2}\frac{\partial^2\Phi}{\partial t^2}, \qquad (4.51)$$

where Φ describes the amplitude of the vibration and c is the speed of the waves, which is determined by the tension and the mass of the drum-skin.

Consider the case of a circular drum, as shown in the following diagram:



To match the geometry of the problem, we therefore use 2D polar co-ordinates (as in Q7 on Problem Sheet 1).
So equation (4.51) is then written for $\Phi(r, \theta, t)$ as:

$$\frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial \Phi}{\partial r}\right)+\frac{1}{r^2}\frac{\partial^2 \Phi}{\partial \theta^2}=\frac{1}{c^2}\frac{\partial^2 \Phi}{\partial t^2} \qquad (4.52)$$

So we want to solve equation (4.52) for $\Phi(r, \theta, t)$, where Φ represents the displacement of the drum-skin.

4.3.2. Boundary conditions:

There are two types of boundary condition in this problem. The first derives from the fact that if the drum-skin is held rigidly around its perimeter, then the vibration amplitude must go to zero there. This can be expressed mathematically as:

$$\Phi(a, \theta, t)=0, \qquad (4.53)$$

i.e. $\Phi(r, \theta, t)=0$ for $r=a$, for all θ and t.

The other type of boundary condition describes the way in which the vibrations are started. This will typically involve specifying the amplitude and speed of the drum-skin for all r and θ at some instant of time (i.e. the *initial conditions*). However, to determine the frequencies of the drum (i.e. the note(s) it produces), it is not necessary to worry about the initial conditions, and we will leave them unspecified.

4.3.3. Separation of variables 1:

We first separate the spatial (r, θ) and time t variables, and look for a solution of the form:

$$\Phi(r, \theta, t)=F(r, \theta)T(t) \qquad (4.54)$$

How do we know which variables to separate first? Well, it's a combination of trial and error, experience, physical intuition etc, etc. In this case, I happen to know that separating (r, θ) and t first is going to give the right answer! So now substitute equation (4.54) into equation (4.52) to give:

$$\left[\frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial F}{\partial r}\right)+\frac{1}{r^2}\frac{\partial^2 F}{\partial \theta^2}\right]T=\frac{1}{c^2}\frac{d^2T}{dt^2}F \qquad (4.55)$$

$$\frac{1}{F}\left[\frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial F}{\partial r}\right)+\frac{1}{r^2}\frac{\partial^2 F}{\partial \theta^2}\right]=\frac{1}{c^2}\frac{1}{T}\frac{d^2T}{dt^2}=-k^2, \qquad (4.56)$$

function of r and θ only — function of t only

where $-k^2$ is the separation constant.

As usual, it's important to choose sign of the separation constant with care. In this case we want to have sinusoidal solution in the t variable (because vibrations are basically oscillatory in time), and so we have $-k^2$ in equation (4.56).

4.3.4. Equation for *T(t)*:

The equation in *t* in (4.56) is:

$$\frac{d^2T}{dt^2} = -k^2c^2T\,, \tag{4.57}$$

which has solutions

$$T(t) = A_k \sin(kct) + B_k \cos(kct)\,, \tag{4.58}$$

where A_k and B_k are constants that will be fixed by the initial conditions, as described above. Note that these constants have a *k* label. This is because the value of *k* is at the moment arbitrary, and there are infinitely many solutions of the form of equation (4.58), corresponding to different values of *k*.

4.3.5. Separation of variables 2:

The equation for $F(r,\theta)$ from equation (4.56) is

$$\frac{\partial^2 F}{\partial r^2} + \frac{1}{r}\frac{\partial F}{\partial r} + \frac{1}{r^2}\frac{\partial^2 F}{\partial \theta^2} + k^2 F = 0 \tag{4.59}$$

This equation still has two variables, and so we try to separate it again, into *r* and θ parts. We write:

$$F(r,\theta) = R(r)\Theta(\theta) \tag{4.60}$$

When (4.60) is substituted into (4.59), this gives (after multiplying through by r^2 and dividing by $R\Theta$):

$$\frac{1}{R}\left[r^2\frac{d^2R}{dr^2} + r\frac{dR}{dr} + k^2r^2R\right] = -\frac{1}{\Theta}\frac{d^2\Theta}{d\theta^2} = n^2 \tag{4.61}$$

Here n^2 is a second separation constant – its sign has been chosen to ensure that we have a sinusoidal variation in θ (see below).

4.3.6. Equation for *Θ(θ)*:

The equation in θ in equation (4.61) is:

$$\frac{d^2\Theta}{d\theta^2} = -n^2\Theta\,, \tag{4.62}$$

which has solutions

$$\Theta(\theta) = C_n \sin(n\theta) + D_n \cos(n\theta) \tag{4.63}$$

where C_n and D_n are again constants that will be fixed by the initial conditions. Now we apply the requirement that our mathematical description of the drum's vibrations must correspond to a physical reality. As it stands, equation (4.63) has the property that if θ is increased by 2π (and so the spatial co-ordinate returns to the same physical position on the drum-skin) there is no guarantee that our solution remains the same. We must therefore impose the condition that:

$$\Theta(\theta) = \Theta(\theta + 2\pi)\,, \tag{4.64}$$

which, along with equation (4.63), implies that *n must be an integer*.

4.3.7. Equation for *R(r)*:

The equation in *r* in equation (4.61) is:

$$r^2\frac{d^2R}{dr^2} + r\frac{dR}{dr} + \left(k^2r^2 - n^2\right)R = 0 \tag{4.65}$$

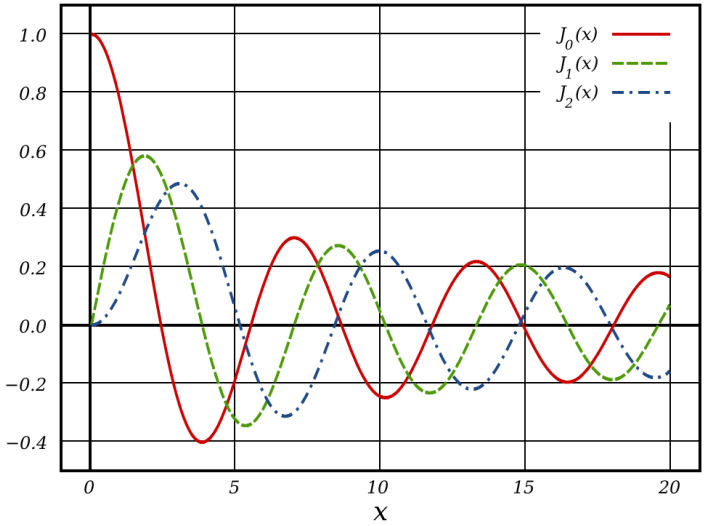
It is convenient to change variables here to $x = kr$, in which case equation (4.65) becomes:

$$x^2\frac{d^2R}{dx^2} + x\frac{dR}{dx} + \left(x^2 - n^2\right)R = 0 \tag{4.66}$$

Equation (4.66) is called **Bessel's Equation**, and often arises in problems with a circular geometry.

We have already seen several examples where the separation of variables reduces a partial differential equation to a number of ordinary differential equations. In all of our previous examples, the ODEs have been very simple, and we have been able to write down their solutions easily. Equation (4.66) is different, however - Bessel's Equation has no simple, analytic solution. We will therefore use graphical methods to represent the solutions.

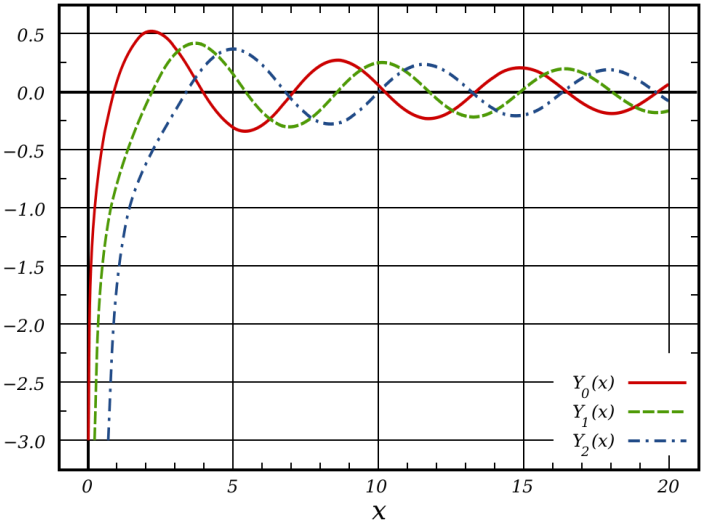
Equation (4.66) has two types of solution for integer values of *n*, which are conventionally labelled $J_n(x)$ and $Y_n(x)$. Both $J_n(x)$ and $Y_n(x)$ are called Bessel functions; they differ in that the J_n solutions are finite at $x=0$, whereas the Y_n solutions are infinite at $x=0$.



Bessel functions of the first kind ($J_n(x)$)

$J_0(x)=0$ for $x=2.405,\ 5.520,\ 8.654.....$

$J_1(x)=0$ for $x=0,\ 3.832,\ 7.016.....$ etc..



Bessel functions of the second kind ($Y_n(x)$)

$Y_0(x)=0$ for $x=0.894,\ 3.958,\ 7.086.....$

$Y_1(x)=0$ for $x=2.197,\ 5.430,\ 8.596.....$ etc..

4.3.8. Using the boundary conditions:

Given that the Y_n solutions diverge at the origin, it is clear that they cannot form part of our solution – infinities do not arise in nature.

The solutions to the *r* equation are therefore $R(x)=J_n(x)$, or:

$$R(r)=J_n(kr) \qquad (4.67)$$

in our original notation.

Referring back to equations (4.54) and (4.60), remember that:

$$\Phi(r,\theta,t)=F(r,\theta)T(t)=R(r)\Theta(\theta)T(t) \qquad (4.68)$$

We now return to the boundary condition given by equation (4.53).

If $\Phi(\mathrm{r}, \theta, t)$ is equal to zero when $r = a$, for any values of θ and t, then we must have

$$R(a) = 0 \tag{4.69}$$

Or, in other words,

$$J_n(ka) = 0\,. \tag{4.70}$$

For each value of n, there are a sequence of x values for which $J_n(x) = 0$, as can be seen in the figure below. Equation (4.70) must therefore fix k to take a set of values, which we can label by

k_{nm} with $n = 0, 1, 2, ...$ and $m = 1, 2, 3, ...$

So $J_n(k_{nm} a) = 0$ fixes the values of the first separation constant $-k^2$ that we first introduced in equation (4.56)).

Note here that the values of n are forced to be integers from the discussion in section (vii), while the values of m are simply labels which denote the different values of k for each value of n that satisfies $J_n(k_{nm} a) = 0$.

4.3.9. The solution:

The full solution can now be put together from equations (4.68), (4.58), (4.63) and (4.67), to give:

$$\Phi(r, \theta, t) = \sum_{n=0,1,2....} \sum_{m=1,2,3....} \left\{ \left[A_{nm} \sin(kct) + B_{nm} \cos(kct) \right] \times \left[C_{nm} \sin(n\theta) + D_{nm} \cos(n\theta) \right] \times J_n(k_{nm} r) \right\} \tag{4.71}$$

This solution takes the form of a sum over a set of *modes of vibration* of the drum, each of which is labelled by two integers n and m:

- The n value determines the θ dependence of each mode and, through J_n, the shape of the drum-skin in the radial direction;
- The m value labels the different allowed modes for each value of n.

In general, all modes will be combined when the drum is hit. The combination in any particular case will be described by the coefficients A_{nm}, B_{nm}, C_{nm} and D_{nm}, which, in turn, will be determined by the particular initial conditions. To give one example, if the drum is hit exactly at its centre, then only modes with $n = 0$ will be included in the solution. *(Can you see why this is the case?)*

So, what note does the drum make? Equation (4.71) shows that each mode has a sinusoidal time dependence, whose period is given by:

$$T_{nm} = \frac{2\pi}{k_{nm} c} \tag{4.72}$$

The frequency of each mode is therefore:

$$f_{nm} = \frac{k_{nm} c}{2\pi}\,. \tag{4.73}$$

So these frequencies, which are fixed by the values of k allowed by the boundary conditions, determine which notes are heard.

5. FOURIER TRANSFORM METHOD FOR SOLVING PDEs

You've already seen an example of solving an ODE using Fourier transforms within the "Fourier Analysis" section of this unit (as an example within Section 3 (p. 47) of the notes for this part of the unit).

Let's look now at an example of how to solve PDEs using this method.

Remember that

$$\mathcal{F}\left[f(t)\right] = F(\omega) = \int_{-\infty}^{\infty} f(t) e^{-i\omega t} dt \qquad (5.1)$$

and

$$\mathcal{F}^{-1}\left[F(\omega)\right] = f(t) = \frac{1}{2\pi}\int_{-\infty}^{\infty} F(\omega) e^{i\omega t} d\omega \qquad (5.2)$$

Similarly,

$$\mathcal{F}\left[f(x)\right] = F(k) = \int_{-\infty}^{\infty} f(x) e^{-ikx} dx \qquad (5.3)$$

and

$$\mathcal{F}^{-1}\left[F(k)\right] = f(x) = \frac{1}{2\pi}\int_{-\infty}^{\infty} F(k) e^{ikx} dk \qquad (5.4)$$

We can now introduce the Fourier transform of $f(x,t)$ with respect to *x* only:

$$\mathcal{F}\left[f(x,t)\right] = F(k,t) = \int_{-\infty}^{\infty} f(x,t) e^{-ikx} dx \qquad (5.5)$$

In effect, we are treating *t* as a constant in this case (we could of course do the converse, and instead consider the Fourier transform of $f(x,t)$ with respect to *t* only).

So let's apply this method to the 1-D diffusion equation again:

$$\frac{\partial^2 \rho}{\partial x^2} = \frac{1}{c}\frac{\partial \rho}{\partial t}, \qquad (5.6)$$

where $\rho(x,t) \to 0$ as $x \to \pm\infty$, and $\rho(x,0) = f(x)$.

We can therefore define the Fourier transform of $\rho(x,t)$ with respect to *x* only as being $P(k,t)$:

$$\mathcal{F}\left[\rho(x,t)\right] = P(k,t) = \int_{-\infty}^{\infty} \rho(x,t) e^{-ikx} dx \qquad (5.7)$$

We can now take the Fourier transform of both sides of equation (5.6) with respect to *x*.

The Fourier transform of the left-hand side of equation (5.6) with respect to *x* is:

$$\mathcal{F}\left[\frac{\partial^2 \rho(x,t)}{\partial x^2}\right] = -k^2 \mathrm{P}(k,t) \qquad (5.8)$$

(using the derivative properties of Fourier transforms).

The Fourier transform of the right-hand side of equation (5.6) with respect to *x* is:

$$\mathcal{F}\left[\frac{1}{c}\frac{\partial \rho}{\partial t}\right] = \frac{1}{c}\frac{\partial \mathrm{P}(k,t)}{\partial t} \qquad (5.9)$$

So we can now equate equations (5.8) and (5.9):

$$-k^2 \mathrm{P}(k,t) = \frac{1}{c}\frac{\partial \mathrm{P}(k,t)}{\partial t}, \qquad (5.10)$$

which can be rewritten as

$$\frac{\partial \mathrm{P}(k,t)}{\partial t} = -k^2 c\,\mathrm{P}(k,t)\,. \qquad (5.11)$$

The Fourier transform method has therefore transformed the original PDE into an ODE, which we can easily solve:

$$\mathrm{P}(k,t) = A\exp\left(-k^2 c t\right). \qquad (5.12)$$

We can now write down the Fourier transform of $\rho(x,0)$ with respect to *x* in two ways. Firstly, substituting $t=0$ into equation (5.7) gives:

$$P(k,0) = \int_{-\infty}^{\infty} \rho(x,0) e^{-ikx} dx = \int_{-\infty}^{\infty} f(x) e^{-ikx} dx \qquad (5.13)$$

Secondly, substituting $t=0$ into equation (5.12) gives:

$$\mathrm{P}(k,0) = A \qquad (5.14)$$

So

$$A = \int_{-\infty}^{\infty} f(x) e^{-ikx} dx = F(k) \qquad (5.15)$$

Substitute this expression for *A* into equation (5.12):

$$\mathrm{P}(k,t) = \exp\left(-k^2 c t\right) F(k) \qquad (5.16)$$

We can now take the inverse Fourier transform of each side of this equation with respect to *x*:

$$\mathcal{F}^{-1}\left[\mathrm{P}(k,t)\right] = \mathcal{F}^{-1}\left[\exp\left(-k^2 c t\right) F(k)\right] \qquad (5.17)$$

We could continue, noting that the right-hand side of this equation is the product of two functions of *k* – so we can use the convolution theorem.

Let's not bother, though! Instead, we can just rewrite equation (5.17) as:

$$\rho(x,t) = \frac{1}{2\pi}\int_{-\infty}^{\infty} \exp\left(-k^2 c t\right) F(k) e^{ikx} dk\,, \qquad (5.18)$$

where

$$F(k) = \int_{-\infty}^{\infty} f(x) e^{-ikx} dx\,, \qquad (5.19)$$

and note the similarity of the form of this solution that we previously obtained (for a finite tube, rather than the infinite tube in this case) in equations (4.19) and (4.20).

6. POWER SERIES SOLUTION METHOD FOR SOLVING ODEs

6.1. Methods for solving ODEs

- For constant coefficients (i.e. $P(x)$ and $Q(x)$ are constants), revisit the methods you learnt in PH10007.
- Laplace and Fourier Transform methods;
- **Power series solutions**.

6.2. Homogeneous ODEs

We've already seen how 2nd order PDEs are transformed into 2nd order ODEs through separation of variables.

The general 2nd order, linear, homogeneous ODE can be written as:

highest derivative is $\frac{d^2}{dx^2}$ — only 1st power of y, no products — each term contains y, or a derivative of y (no terms that are just constants) — x is the only variable

$$\frac{d^2y}{dx^2}+P(x)\frac{dy}{dx}+Q(x)\,y=0, \tag{6.1}$$

where $P(x)$ and $Q(x)$ are arbitrary functions of x.

There are always **two** solutions to this 2nd order ODE, so in general we have a linear combination:

$$y(x)=c_1y_1(x)+c_2y_2(x) \tag{6.2}$$

6.3. Inhomogeneous ODEs

Physical problems can also lead to **inhomogeneous** equations of the form:

$$\frac{d^2y}{dx^2}+P(x)\frac{dy}{dx}+Q(x)\,y=F(x), \tag{6.3}$$

where $F(x)$ might arise from a source term in a PDE.

If $y_p(x)$ is a solution of this inhomogeneous equation, then the general solution is:

$$y(x)=c_1y_1(x)+c_2y_2(x)+y_p(x) \tag{6.4}$$

(referring back to section 1.12 on linear superposition).

Example 1:

If $P(x)=0$ and $Q(x)=\omega^2$, then equation (6.1) becomes:

$$\frac{d^2y}{dx^2}+\omega^2y=0, \tag{6.5}$$

with two distinct solutions: $y_1=A\sin(\omega x)$ and $y_2=B\cos(\omega x)$.

Example 2:

If $P(x)=\frac{1}{x}$ and $Q(x)=\left(1-\frac{n^2}{x^2}\right)$, then equation (6.1) becomes:

$$\frac{d^2y}{dx^2}+\frac{1}{x}\frac{dy}{dx}+\left(1-\frac{n^2}{x^2}\right)y=0, \tag{6.6}$$

This is *Bessel's equation* (compare with equation (4.66)), and so the two distinct solutions are: $y_1=J_n(x)$ and $y_2=Y_n(x)$.

6.4. Power Series Solution of ODEs

Consider again the equation

$$\frac{d^2y}{dx^2} + \omega^2 y = 0, \tag{6.7}$$

and let's try the solution

$$y(x) = x^q \left(a_0 + a_1 x + a_2 x^2 + a_3 x^3 + ...\right) \tag{6.8}$$

$$= \sum_{s=0}^{\infty} a_s x^{s+q},$$

where q is chosen so that $a_0 \neq 0$.

We need to determine q and the coefficients a_s.

From equation (6.8), we have:

$$\frac{dy}{dx} = \sum_{s=0}^{\infty} a_s (s+q) x^{s+q-1} \tag{6.9}$$

$$\frac{d^2y}{dx^2} = \sum_{s=0}^{\infty} a_s (s+q)(s+q-1) x^{s+q-2} \tag{6.10}$$

For the example equation (6.5), this gives:

$$\sum_{s=0}^{\infty} a_s (s+q)(s+q-1) x^{s+q-2} + \omega^2 \sum_{s=0}^{\infty} a_s x^{s+q} = 0 \tag{6.11}$$

Now equation (6.11) must be true for all x. This means that **the coefficients of each and every power of x have to be equal to zero**.

So now look in turn at each of the powers of x in equation (6.11):

6.4.1. Lowest power: indicial equation

The lowest power in equation (6.11) occurs when $s = 0$ in the first series in this equation. So the lowest power is x^{q-2}.

But we know that the coefficients of every power of x have to be equal to zero. So let's set the coefficient of this lowest power of x (i.e. x^{q-2}) to zero:

$$a_0 \, q(q-1) = 0 \tag{6.12}$$

But we already know that $a_0 \neq 0$.

So:

$$q(q-1) = 0 \tag{6.13}$$

Therefore $q = 0$ or $q = 1$.

Equation (6.13) is known as the ***indicial equation***, whose roots determine the possible values of q.

It is always formed by considering the coefficient of the lowest power of the independent variable (here x) in the original equation.

6.4.2. Second lowest power

The next lowest power in equation (6.11) occurs when $s = 1$ in the first series in this equation. So the next lowest power is x^{q-1}.

So the coefficient for the x^{q-1} term is:

$$a_1 (q+1) \, q = 0 \tag{6.14}$$

But we already know that $q = 0$ or $q = 1$.

If $q = 0$, then a_1 is undetermined.

If $q = 1$, then $a_1 = 0$.

6.4.3. Third lowest power

The next lowest power in equation (6.11) occurs when $s=2$ in the first series in this equation. So the next lowest power is x^q.

Looking at the second series in equation (6.11), there is also an x^q term in this series – this occurs for $s=0$ in the second series.

So the coefficient for the x^q term is:

$$a_2\left(q+2\right)\left(q+1\right)+\omega^2 a_0=0 \qquad (6.15)$$

This equation relates the value of a_2 to the values of a_0 and q.

6.4.4. General power: recurrence relation

We can write the general power for x in equation (6.11) as x^{t+q}. This power of x will occur when $s=t+2$ in the first series, and $s=t$ in the second series.

If we set the coefficient of the x^{t+q} term to zero, we therefore find that:

$$a_{t+2}\left(q+t+2\right)\left(q+t+1\right)+\omega^2 a_t=0, \qquad (6.16)$$

which gives:

$$a_{t+2}=\frac{-\omega^2}{\left(q+t+2\right)\left(q+t+1\right)}\,a_t \qquad (6.17)$$

Equation (6.17) is known as a ***recurrence relation***, relating a_t to a_{t+2}, and hence to a_{t+4}, a_{t+6} etc..

Look first at the $q=1$ solution.

In this case $a_1=0$, and so (from equation (6.17)) a_3, a_5, a_7 etc. are also equal to zero.

Therefore only even terms arise in the series for $q=1$, as follows:

$$a_{t+2}=\frac{-\omega^2}{\left(t+3\right)\left(t+2\right)}\,a_t \qquad (6.18)$$

So

$$a_2=\frac{-\omega^2}{3\cdot 2}\,a_0=\frac{-\omega^2}{3!}\,a_0 \qquad (\text{for } t=0) \qquad (6.19)$$

$$a_4=\frac{-\omega^2}{5\cdot 4}\,a_2=\frac{+\omega^4}{5!}\,a_0 \qquad (\text{for } t=2) \qquad (6.20)$$

$$a_6=\frac{-\omega^2}{7\cdot 6}\,a_4=\frac{-\omega^6}{7!}\,a_0 \qquad (\text{for } t=4) \qquad (6.21)$$

etc..

In general,

$$a_{2n}=\frac{\left(-1\right)^n\omega^{2n}}{\left(2n+1\right)!}\,a_0, \text{ where } n=1,\ 2,\ 3.... \qquad (6.22)$$

Recall from equation (6.8) that

$$y\left(x\right)=\sum_{s=0}^{\infty}a_s x^{s+q} \qquad (6.23)$$

So:

$$y\left(x\right)=a_0 x-\frac{\omega^2 a_0 x^3}{3!}+\frac{\omega^4 a_0 x^5}{5!}-..... \qquad (6.24)$$

$$y\left(x\right)=\frac{a_0}{\omega}\left[\,\omega x-\frac{\left(\omega x\right)^3}{3!}+\frac{\left(\omega x\right)^5}{5!}-.....\,\right]=\frac{a_0}{\omega}\sin\left(\omega x\right) \qquad (6.25)$$

Now look at the $q=0$ solution.

(From equation (6.14), we found that a_1 is undetermined for $q = 0$ - ignore this for now!)

Substituting $q = 0$ into equation (6.17) gives:

$$a_{t+2} = \frac{-\omega^2}{(t+2)(t+1)}\, a_t \qquad (6.26)$$

So

$$a_2 = \frac{-\omega^2}{2\cdot 1}\, a_0 = \frac{-\omega^2}{2!}\, a_0 \qquad (\text{for } t = 0) \qquad (6.27)$$

$$a_4 = \frac{-\omega^2}{4\cdot 3}\, a_2 = \frac{+\omega^4}{4!}\, a_0 \qquad (\text{for } t = 2) \qquad (6.28)$$

$$a_6 = \frac{-\omega^2}{6\cdot 5}\, a_4 = \frac{-\omega^6}{6!}\, a_0 \qquad (\text{for } t = 4) \qquad (6.29)$$

etc..

In general,

$$a_{2n} = \frac{(-1)^n \omega^{2n}}{(2n)!}\, a_0 \text{, where } n = 1,\ 2,\ 3.... \qquad (6.30)$$

Again,

$$y(x) = \sum_{s=0}^{\infty} a_s x^{s+q} \qquad (6.31)$$

So:

$$y(x) = a_0 \left[1 - \frac{(\omega x)^2}{2!} + \frac{(\omega x)^4}{4!} - ..... \right] = a_0 \cos(\omega x) \qquad (6.32)$$

So we have now generated two distinct solutions to our 2nd order ODE given in equation (6.5) – these two solutions are given by equations (6.25) and (6.32).

Now go back to look at the odd terms with $q = 0$. The coefficient a_1 is undetermined, but using the recurrence relation (equation (6.26)), we can write:

$$a_3 = \frac{-\omega^2}{3\cdot 2}\, a_1 = \frac{-\omega^2}{3!}\, a_1 \qquad (\text{for } t = 1) \qquad (6.33)$$

$$a_5 = \frac{-\omega^2}{5\cdot 4}\, a_3 = \frac{+\omega^4}{5!}\, a_1 \qquad (\text{for } t = 3) \qquad (6.34)$$

$$a_7 = \frac{-\omega^2}{7\cdot 6}\, a_5 = \frac{-\omega^6}{7!}\, a_1 \qquad (\text{for } t = 5) \qquad (6.35)$$

etc.., which generates the series:

$$y(x) = a_1 x - \frac{\omega^2 a_1 x^3}{3!} + \frac{\omega^4 a_1 x^5}{5!} - ..... \qquad (6.36)$$

$$y(x) = \frac{a_1}{\omega}\left[\omega x - \frac{(\omega x)^3}{3!} + \frac{(\omega x)^5}{5!} - ..... \right] = \frac{a_1}{\omega} \sin(\omega x) \qquad (6.37)$$

But this is the same as the first series solution (i.e. equation (6.25)).

In general, if a coefficient is undetermined (as was the case here for a_1), it can be set to zero.

6.5. Notes on the Power Series Solutions method

- This procedure tends to be long-winded, but can provide solutions when other methods fail.
- You need to rearrange equations so that all powers of *x* appear as multipliers.

- For example, the equation

$$\frac{d^2y}{dx^2}+\frac{x}{\left(1-x^2\right)}\frac{dy}{dx}+\frac{1}{\left(1-x^2\right)}y=0 \qquad (6.38)$$

should be rewritten (for use with this method) as:

$$\left(1-x^2\right)\frac{d^2y}{dx^2}+x\frac{dy}{dx}+y=0 \qquad (6.39)$$

- You can expand about points other than $x=0$, for example:

$$y\left(x\right)=\sum_{s=0}^{\infty}a_s\left(x-x_0\right)^{s+q} \qquad (6.40)$$

- You must check to see whether each series solution converges – if it doesn't, the solution is not valid.
- The method doesn't always work! You must check to see whether each series solution converges – if it doesn't, the solution will not be physically valid.

6.6. Convergence of infinite series

We've seen that the solution of ODEs can be derived in the form of a power series:

$$y\left(x\right)=\sum_{s=0}^{\infty}a_s x^{s+q} \qquad (6.41)$$

Often, this series has infinitely many terms. How can we tell if such infinite series are well-behaved, in the sense that for particular values of *x* they will have a finite sum? This can be quite a difficult problem, but here we will look at some of the issues which arise, and introduce a number of simple methods for determining whether or not a series is convergent.

Consider the series

$$u_1+u_2+u_3+u_4+..... \qquad (6.42)$$

The i^{th} partial sum of this series is defined by

$$s_i=\sum_{n=1}^{i}u_n, \qquad (6.43)$$

and so the infinite sum becomes

$$S=\lim_{i\to\infty}s_i. \qquad (6.44)$$

If this limit is finite, then the series is said to be **convergent**.

For example, the series

$$\sum_{n=0}^{\infty}\frac{1}{n!}=1+1+\frac{1}{2}+\frac{1}{6}+\frac{1}{24}+..... \qquad (6.45)$$

sums to 2.71828…., as it represents the Maclaurin series for e^1.

On the other hand, if $s_i\to\infty$ as $i\to\infty$, then the series is said to be **divergent**.

For example, the series

$$\sum_{n=0}^{\infty}n=1+2+3+4+5+..... \qquad (6.46)$$

is obviously divergent.

It is also possible that the partial sums oscillate, but never converge. An example of this is the series

$$\sum_{n=1}^{\infty}\left(-1\right)^n=-1+1-1+1-1+..... \qquad (6.47)$$

For *i* even, the partial sum $s_i=0$, while for *i* odd, the partial sum $s_i=-1$. Such a series is termed **oscillatory**.

It is important that we can identify whether or not a series is convergent. Infinities should not arise in a mathematical description of nature, and so if we find a divergent series as the solution of a differential equation, it usually means that we need to think a little more. So let's look at some of the rules which can be used to test if a series is convergent.

6.6.1. Infinite series whose terms do not alternate in sign

In the cases of series whose terms do not alternate in sign:

- If $\lim_{n\to\infty} u_n \neq 0$, the series is not convergent. In other words, the series terms must tend to zero.
- The ratio test tells us that:

if		
$\lim_{n\to\infty}\left(\frac{u_{n+1}}{u_n}\right)\begin{cases}<1\\>1\\=1\end{cases}$	<1	the series is convergent;
	>1	the series is divergent;
	$=1$	convergence cannot be determined, and more analysis is needed.

- The comparison test can be used to compare term by term an unknown series with a known one:

  Let $\sum_{k=0}^{\infty} a_k$ and $\sum_{k=0}^{\infty} b_k$ be series with nonnegative terms, and suppose that $a_1 \le b_1$, $a_2 \le b_2$, $a_3 \le b_3$ etc..

(i) If the 'bigger' series $\sum_{k=0}^{\infty} b_k$ converges, then the 'smaller' series $\sum_{k=0}^{\infty} a_k$ also converges.

(ii) If the 'smaller' series $\sum_{k=0}^{\infty} a_k$ diverges, then the 'bigger' series $\sum_{k=0}^{\infty} b_k$ also diverges.

For example, the sum of the series

$$1+\frac{1}{2}+\frac{1}{3}+\frac{1}{4}+\frac{1}{5}+\frac{1}{6}+\frac{1}{7}+\frac{1}{8}+\ldots\ldots\ldots$$
$$=1+\frac{1}{2}+\left(\frac{1}{3}+\frac{1}{4}\right)+\left(\frac{1}{5}+\frac{1}{6}+\frac{1}{7}+\frac{1}{8}\right)+\left(\frac{1}{9}+\ldots\ldots+\frac{1}{16}\right)+\ldots\ldots\ldots$$

is greater than the sum of the series

$$1+\frac{1}{2}+\left(\frac{1}{4}+\frac{1}{4}\right)+\left(\frac{1}{8}+\frac{1}{8}+\frac{1}{8}+\frac{1}{8}\right)+\left(\frac{1}{16}+\ldots\ldots+\frac{1}{16}\right)+\ldots\ldots\ldots$$
$$=1+\frac{1}{2}+\frac{1}{2}+\frac{1}{2}+\ldots\ldots,$$

which is clearly divergent.

So the first series, all of whose terms are greater than or equal to the second series, must also be divergent.

6.6.2. Infinite series whose terms alternate in sign

For series which have terms of alternating signs, we can use the alternating sign test. If the terms in a series are alternately positive and negative, and if $|u_{n+1}| < |u_n|$ for all *n*, then the series is convergent. This can be seen by writing the series in two ways:

$$S = u_1 - u_2 + u_3 - u_4 + \ldots\ldots = (u_1 - u_2) + (u_3 - u_4) + \ldots\ldots$$
$$= u_1 - (u_2 - u_3) - (u_4 - u_5) + \ldots\ldots$$

where $a_n \geq 0$ and $a_{n+1} < a_n$. In this case, the first method of grouping terms shows that $S \geq 0$, while the second shows that $S \leq u_1$. Putting these together gives $0 \leq S \leq u_1$ – in other words, S must be finite.

We finish with two more definitions:

- A series is said to be **absolutely convergent** if $\sum_n u_n$ and $\sum_n |u_n|$ both converge.
- It is conditionally convergent if $\sum_n u_n$ converges, but $\sum_n |u_n|$ diverges. In other words, the series of the positive terms of a conditionally convergent series diverges to positive infinity, and the series of its negative terms diverges to negative infinity.

Only if a series is absolutely convergent can the normal rules of arithmetic be applied to it – for example, if two absolutely convergent series are multiplied together, the resulting series will also be absolutely convergent.

This will not be the case if one or both of the series are only conditionally convergent. In fact, conditionally convergent series are not very helpful in a mathematical description of nature, as they can be re-arranged to given *any* desired value.

For example, the analysis above shows that the series

$$1-\frac{1}{2}+\frac{1}{3}-\frac{1}{4}+\frac{1}{5}-\frac{1}{6}+\frac{1}{7}-\frac{1}{8}+.....$$

is conditionally convergent. The rather strange nature of this series can be seen by re-writing it as follows:

$$1+\left(\frac{1}{2}-1\right)+\frac{1}{3}+\left(\frac{1}{4}-\frac{1}{2}\right)+\frac{1}{5}+\left(\frac{1}{6}-\frac{1}{3}\right)+.....$$

$$=1+\frac{1}{2}+\frac{1}{3}+\frac{1}{4}+\frac{1}{5}+\frac{1}{6}+.....-\left(1+\frac{1}{2}+\frac{1}{3}+\frac{1}{4}+\frac{1}{5}+\frac{1}{6}+.....\right)$$

Thus the series can be written in a form which is basically $\infty-\infty$, which can take any value you like!

6.6.3. Examples of using the ratio test

Example 1:

For what values of *x* does $\sum_{n=1}^{\infty}\frac{x^n}{n!}$ converge?

$u_n = \frac{x^n}{n!}$ and $u_{n+1} = \frac{x^{n+1}}{(n+1)!}$.

So $\frac{u_{n+1}}{u_n} = \frac{x^{n+1}}{x^n}\frac{n!}{(n+1)!} = \frac{x}{n+1}$

So, $\lim_{n\to\infty}\left(\frac{u_{n+1}}{u_n}\right) = 0$ for all finite *x*.

Therefore the series converges for all finite *x*.

Example 2:

The binomial expansion of $\frac{1}{1-x}$ is

$$\frac{1}{1-x} = 1+x+x^2+x^3+x^4+..... = \sum_{n=0}^{\infty}x^n$$

For what values of *x* does this series converge?

$$\lim_{n\to\infty}\left(\frac{u_{n+1}}{u_n}\right)=\lim_{n\to\infty}\left(\frac{x^{n+1}}{x^n}\right)=\lim_{n\to\infty}(x)=x$$

Therefore the series converges for $x<1$, diverges for $x>1$, and is undetermined for $x=1$.

6.7. Ordinary and singular points

Referring back to equation (6.1), the general linear 2nd order ODE can be written as:

$$\frac{d^2y}{dx^2}+P(x)\frac{dy}{dx}+Q(x)y=0 \qquad (6.48)$$

If $P(x)$ and $Q(x)$ remain finite at $x=x_0$, then x_0 is called an **ordinary point**.

Otherwise, if either $P(x)$ or $Q(x)$ diverge (i.e. tend to ∞) as $x\to x_0$, then x_0 is called a **singular point**.

If $(x-x_o)P(x)$ and $(x-x_o)^2Q(x)$ remain finite as $x\to x_0$, then $x=x_0$ is a **regular singular point**.

If either $(x-x_o)P(x)$ or $(x-x_o)^2Q(x)$ approach infinity as $x\to x_0$, then $x=x_0$ is a **irregular singular point**.

If we try to find a power series solution expanded about an ordinary point or a regular singular point, then we will always find at least one solution.

Expansion about an irregular singular point may fail.

Whether we get 1 or 2 solutions depends on the roots of the indicial equation (call these q_1 and q_2):

- If $q_1=q_2$, we get only 1 solution;
- If $q_1-q_2=$ integer, then the larger *q* will give a solution, and the smaller *q* may or may not.
- If $q_1-q_2\neq$ integer, we get 2 solutions.

There are various methods for finding the second solution if the power series method can't.

For example, in the event that $q_1=q_2=q$, so that we get only one solution ($y_1(x)$, say), the second solution has the form

$$y_2(x)=y_1(x)\ln(x)+\sum_{s=1}^{\infty}b_s x^{s+q}, \qquad (6.49)$$

and we can then work through the power series method again, substituting equation (6.49) into the original ODE.

6.8. Examples of power series solutions

6.8.1. Example 1: Ordinary point

Revisit the equation with $P(x)=0$ and $Q(x)=\omega^2$, i.e.

$$\frac{d^2y}{dx^2}+\omega^2y=0 \qquad (6.50)$$

(as already discussed and solved in section 6.4).

In this case, $x=0$ is an *ordinary point*, so we expect the series solution method to work.

Our previous analysis (section 6.4.1) shows that the *indicial equation* is:

$$q(q-1)=0 \qquad (6.51)$$

So $q=0$ or $q=1$; since the roots of the indicial equation differ by an integer, we will obtain at least one solution. In this particular case, our previous analysis showed that the two roots of the indicial equation led to two distinct solutions, i.e. $A\sin(\omega x)$ and $B\cos(\omega x)$.

6.8.2. Example 2: Regular singular point

Now consider the following equation:

$$\frac{d^2y}{dx^2}-\frac{20}{x^2}y=0 \qquad (6.52)$$

So $P(x)=0$ and $Q(x)=\dfrac{-20}{x^2}$.

In this case, $x=0$ is a *regular singular point*, so we expect the series solution to give at least one solution.

We look for a solution of the form

$$y(x)=\sum_{s=0}^{\infty}a_s x^{s+q} \qquad (6.53)$$

where *q* is chosen so that $a_0\neq 0$.

Substituting equation (6.53) into equation (6.52) gives:

$$\sum_{s=0}^{\infty}a_s(s+q)(s+q-1)x^{s+q-2}-\sum_{s=0}^{\infty}20\,a_s x^{s+q-2}=0. \qquad (6.54)$$

The lowest power of x is x^{q-2} (when $s=0$ in both series), and setting the coefficient of this power to zero gives the *indicial equation*:

$$a_0q(q-1)-20a_0=0 \qquad (6.55)$$

So

$$q^2-q-20=0 \quad \Rightarrow \quad q=-4 \text{ or } q=5 \qquad (6.56)$$

The general power of x is x^{t+q}. This arises from the term with $s=t+2$ in both series.

Setting the coefficient of this general power to zero gives:

$$a_{t+2}\left((t+q+2)(t+q+1)-20\right)=0 \qquad (6.57)$$

Note that there is no recurrence relation in this case.

The only solution to equation (6.57) for $t>0$ is $a_{t+2}=0$. This illustrates a case which sometimes arises when the power series stops at a particular term.

The two solutions in this case are simply:

$$y_1(x)=a_0x^5 \qquad \text{and} \qquad y_2(x)=\frac{a_0}{x^4}$$

(Check by substitution back into equation (6.52)).

6.8.3. Example 3: Irregular singular point

Now consider the following equation:

$$\frac{d^2y}{dx^2}-\frac{20}{x^3}y=0 \qquad (6.58)$$

So $P(x)=0$ and $Q(x)=\dfrac{-20}{x^3}$.

In this case, $x=0$ is an *irregular singular point*, and so we can expect some problems with the power series method.

As usual, we look for a solution of the form

$$y(x)=\sum_{s=0}^{\infty}a_s x^{s+q} \tag{6.59}$$

where q is chosen so that $a_0 \neq 0$.

Substituting this into equation (6.58) gives:

$$\sum_{s=0}^{\infty}a_s(s+q)(s+q-1)x^{s+q-2}-\sum_{s=0}^{\infty}20\,a_s x^{s+q-3}=0. \tag{6.60}$$

The lowest power of x is x^{q-3} (when $s=0$ in the second series), and setting the coefficient of this power to zero gives the equation:

$$20a_0=0 \tag{6.61}$$

This contradicts the basic assumption of the power series method (i.e. that $a_0 \neq 0$), and so there are no solutions in this case.

6.8.4. Example 4: Bessel's Equation

As we've already seen in section 4.3.7 (equation (4.66)), Bessel's Equation for $n=0$ is given by:

$$\frac{d^2y}{dx^2}+\frac{1}{x}\frac{dy}{dx}+y=0 \tag{6.62}$$

So $P(x)=\frac{1}{x}$ and $Q(x)=1$.

In this case, $x=0$ is a *regular singular point*, so we expect the series solution to give at least one solution.

We look for a solution of the form

$$y(x)=\sum_{s=0}^{\infty}a_s x^{s+q} \tag{6.63}$$

where q is chosen so that $a_0 \neq 0$.

Substituting this into equation (6.62) gives:

$$\sum_{s=0}^{\infty}a_s(s+q)(s+q-1)x^{s+q-2}+\sum_{s=0}^{\infty}a_s(s+q)x^{s+q-2}+\sum_{s=0}^{\infty}a_s x^{s+q}=0 \tag{6.64}$$

The lowest power of x is x^{q-2} (when $s=0$ in the first two series), and setting the coefficient of this power to zero gives the *indicial equation*:

$$a_0\left[q(q-1)+q\right]=0 \tag{6.65}$$

So

$$q^2=0 \quad \Rightarrow \quad q=0 \tag{6.66}$$

In this case, the indicial equation has only one root, and so we will obtain only one solution.

When $q=0$, equation (6.64) reduces to:

$$\sum_{s=0}^{\infty}a_s s^2 x^{s-2}+\sum_{s=0}^{\infty}a_s x^s=0 \tag{6.67}$$

The general power of x is x^t. This arises from the term with $s=t+2$ in the first series, and the term with $s=t$ in the second series.

Setting the coefficient of this general power to zero gives:

$$a_{t+2}(t+2)^2+a_t=0 \tag{6.68}$$

Or

$$a_{t+2}=\frac{-1}{(t+2)^2}\,a_t \tag{6.69}$$

We can now build up the solution, term by term, as follows:

$$a_2 = \frac{-1}{2^2}\, a_0 \qquad \text{(for } t=0\text{)} \qquad (6.70)$$

$$a_4 = \frac{-1}{4^2}\, a_2 = \frac{1}{4^2 2^2}\, a_0 \qquad \text{(for } t=2\text{)} \qquad (6.71)$$

$$a_6 = \frac{-1}{6^2}\, a_4 = \frac{-1}{6^2 4^2 2^2}\, a_0 \qquad \text{(for } t=4\text{)} \qquad (6.72)$$

etc..

By inspection, the general term is therefore:

$$a_{2n} = \frac{(-1)^n}{2^{2n}(n!)^2}\, a_0 \text{, where } n = 1,\ 2,\ 3.... \qquad (6.73)$$

The series expansion of the solution , $J_0(x)$, which is finite at the origin, is therefore:

$$\begin{aligned} y_1(x) \equiv J_0(x) &= a_0\left(1 - \frac{x^2}{2^2} + \frac{x^4}{4^2 2^2} - \frac{x^6}{6^2 4^2 2^2} + ...\right) \\ &= \sum_{n=0}^{\infty}\left[\frac{(-1)^n}{2^{2n}(n!)^2} a_0\, x^{2n}\right] \end{aligned} \qquad (6.74)$$

The ratio test can be used to show that this series solution is absolutely convergent for all finite values of *x*.

We have only found one solution of Bessel's equation with $q = 0$, however, using the power series method. As we saw earlier in section 4.3.7, there is another solution, namely $Y_0(x)$.

This solution can be derived using equation (6.49):

$$y_2(x) \equiv Y_0(x) = J_0(x) \times \ln(x) + \sum_{s=0}^{\infty} b_s x^s \qquad (6.75)$$

6.8.5. Example 5: Legendre's Equation

Legendre's Equation is:

$$(1-x^2)\frac{d^2y}{dx^2} - 2x\frac{dy}{dx} + ky = 0, \qquad (6.76)$$

where *k* is an arbitrary constant.

So $P(x) = \dfrac{-2x}{(1-x^2)}$ and $Q(x) = \dfrac{k}{(1-x^2)}$.

We will again look for a series solution expanded about $x = 0$, which is an *ordinary point*, so we expect the series solution to give at least one solution. We therefore look for a solution of the form

$$y(x) = \sum_{s=0}^{\infty} a_s x^{s+q} \qquad (6.77)$$

where *q* is chosen so that $a_0 \neq 0$.

Substituting this into equation (6.76) gives:

$$\begin{aligned} &\sum_{s=0}^{\infty} a_s (s+q)(s+q-1) x^{s+q-2} - \sum_{s=0}^{\infty} a_s (s+q)(s+q-1) x^{s+q} \\ &\qquad - \sum_{s=0}^{\infty} 2a_s (s+q) x^{s+q} + \sum_{s=0}^{\infty} k a_s x^{s+q} = 0 \end{aligned} \qquad (6.78)$$

The lowest power of x is x^{q-2} (when $s = 0$ in the first series), and setting the coefficient of this power to zero gives the *indicial equation*:

$$a_0 q(q-1) = 0 \qquad \Rightarrow q = 0 \quad \text{or} \quad q = 1. \qquad (6.79)$$

The next lowest power is x^{q-1} (when $s = 1$ in the first series), which leads to:

$$a_1(q+1)q = 0. \qquad (6.80)$$

If $q=1$, $a_1=0$.

If $q=0$, a_1 is undefined, and can be set to zero.

The general power, x^{t+q}, arises from the term with $s=t+2$ in the first series, and the terms with $s=t$ in the other series.

Setting the coefficient of this general power to zero gives:

$$a_{t+2}(t+q+2)(t+q+1)=a_t\left[(t+q)(t+q-1)+2(t+q)-k\right], \quad (6.81)$$

which becomes:

$$a_{t+2}=\left[\frac{t(t+1)-k}{(t+2)(t+1)}\right]a_t \qquad \text{for } q=0 \qquad (6.82)$$

and

$$a_{t+2}=\left[\frac{(t+1)(t+2)-k}{(t+3)(t+2)}\right]a_t \qquad \text{for } q=1. \qquad (6.83)$$

In conjunction with equation (6.77), these should provide two independent solutions of Legendre's equation.

However, a problem arises when we investigate the convergence of the solutions given in equations (6.82)and (6.83).

Because $a_1=0$ (and hence, from equations (6.82) and (6.83), all other 'odd' *a* coefficients are equal to zero), both of the power series solutions for $q=0$ and $q=1$ only contain 'even' *a* coefficients (i.e. a_0, a_2, a_4 etc. .

So our solutions are:

$$y(x)=\sum_{s=0}^{\infty}a_s x^{s+q}=a_0x^q+a_2x^{q+2}+....+a_sx^{s+q}+a_{s+2}x^{s+q+2}+.... \quad (6.84)$$

So we can write the ratio test for this case as

$$\lim_{n\to\infty}\left(\frac{u_{n+1}}{u_n}\right)=\lim_{s\to\infty}\left(\frac{a_{s+2}x^{s+q+2}}{a_sx^{s+q}}\right)=\lim_{s\to\infty}\left(\frac{a_{s+2}}{a_s}x^2\right) \qquad (6.85)$$

Looking at equations (6.82) and (6.83), we can see that

$$\lim_{s\to\infty}\left(\frac{a_{s+2}}{a_s}\right)=1 \qquad (6.86)$$

So the ratio test in this instance reduces to $\lim_{s\to\infty}\left(x^2\right)$.

Therefore:

If $|x|<1$ the series converge

$|x|>1$ the series diverge

$|x|=1$ the series diverge (we haven't shown this here, but it can be shown)

But physical solutions must include $x=\pm1$. So we must think harder!

Look again at equations (6.82) and (6.83), where *t* is always an even number.

- The $q=0$ series will stop if the constant k is given by $k=l(l+1)$, where *l* is an even integer.
- The $q=1$ series will stop if the constant k is given by $k=l(l+1)$, where *l* is an odd integer.

If the series stop, then the solutions are convergent for all finite *x*. Such solutions are called ***Legendre Polynomials***.

If $l=0$, then the $q=0$ series will stop. In this case, $k=l(l+1)=0$, and Equation (6.82) gives:

$$a_2 = \left[\frac{0(0+1)-0}{(0+2)(0+1)}\right]a_0 = 0 \qquad (6.87)$$

So

$$y(x) = a_0 \qquad (6.88)$$

If $l = 1$, then the $q = 1$ series will stop. In this case, $k = l(l+1) = 2$, and Equation (6.83) gives:

$$a_2 = \left[\frac{(0+1)(0+2)-2}{(0+3)(0+2)}\right]a_0 = \left[\frac{1\cdot 2-2}{3\cdot 2}\right]a_0 = 0 \qquad (6.89)$$

So

$$y(x) = a_0 x \qquad (6.90)$$

If $l = 2$, then the $q = 0$ series will stop. In this case, $k = l(l+1) = 6$, and Equation (6.82) gives:

$$a_2 = \left[\frac{0(0+1)-6}{(0+2)(0+1)}\right]a_0 = -3a_0 \qquad (6.91)$$

$$a_4 = \left[\frac{2(2+1)-6}{(2+2)(2+1)}\right]a_2 = 0 \qquad (6.92)$$

So the series stops here, and

$$y(x) = a_0\left(1-3x^2\right) \qquad (6.93)$$

We can carry on this way for $l = 3,\ 4,\ 5$ etc.

a_0 is usually chosen to make $y(x) = 1$ at $x = 1$, so the Legendre Polynomials become:

$$P_0(x) = 1 \qquad (6.94)$$

$$P_1(x) = x \qquad (6.95)$$

$$P_2(x) = \frac{1}{2}\left(3x^2 - 1\right) \qquad (6.96)$$

$$P_3(x) = \frac{1}{2}\left(5x^3 - 3x\right) \qquad (6.97)$$

Note that the highest power of *x* in the expression for $P_l(x)$ is x^l .

Finally, we can define the associated Legendre Equation:

$$\left(1-x^2\right)\frac{d^2y}{dx^2} - 2x\frac{dy}{dx} + \left[l(l+1) - \frac{m^2}{1-x^2}\right]y = 0 \qquad (6.98)$$

For integer *l* (where *l* = 0, 1, 2….)

Extra term, with *m* an integer

Legendre Polynomials, as defined above

The solutions are

$$P_l^m(x) = \left(1-x^2\right)^{|m|/2}\frac{d^{|m|}P_l(x)}{dx^{|m|}} \qquad (6.99)$$

Associated Legendre functions. These are zero for $|m| > l$. (Because the highest power in the expression for $P_l(x)$ is x^l).

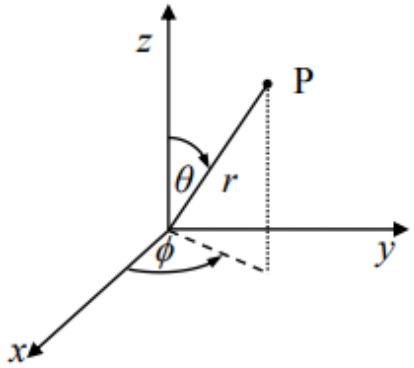
7. SPHERICAL HARMONICS

7.1. Laplace's Equation in Spherical Polars

Reminder of Laplace's Equation:

$$\nabla^2 \Psi = 0$$

Let's now solve this in spherical polar co-ordinates.
Reminder from the vector calculus section of PH20107:



Remember that in this co-ordinate system point P is defined by its radial distance from the origin (r), its polar angle (or latitude) (θ) measured from the z-axis, and its azimuth angle (or longitude) (ϕ).

The ranges for these variables are:

$0 \le r < \infty,\ 0 \le \theta < \pi,\ 0 \le \phi < 2\pi$.

Writing Laplace's Equation in spherical polar co-ordinates gives:

$$\nabla^2\Psi = \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial \Psi}{\partial r}\right) + \frac{1}{r^2\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial\Psi}{\partial\theta}\right) + \frac{1}{r^2\sin^2\theta}\frac{\partial^2\Psi}{\partial\phi^2} = 0 \qquad (7.1)$$

As usual, let's try separation of variables, with

$$\Psi(r,\theta,\phi) = R(r)\,Y(\theta,\phi) \qquad (7.2)$$

$$\Psi(r,\theta,\phi) = R(r)\,\Theta(\theta)\Phi(\phi) \qquad (7.3)$$

Substituting this into the Laplace Equation, dividing through by $\Psi = RY$, and multiplying through by r^2 gives:

$$\frac{1}{R}\frac{d}{dr}\left(r^2\frac{dR}{dr}\right) = -\left(\frac{1}{\Theta\sin\theta}\frac{d}{d\theta}\left(\sin\theta\frac{d\Theta}{d\theta}\right) + \frac{1}{\Phi\sin^2\theta}\frac{d^2\Phi}{d\phi^2}\right) \qquad (7.4)$$

$$\frac{1}{R}\frac{d}{dr}\left(r^2\frac{dR}{dr}\right) = -\frac{1}{Y}\left(\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial Y}{\partial\theta}\right) + \frac{1}{\sin^2\theta}\frac{\partial^2 Y}{\partial\phi^2}\right) \qquad (7.5)$$

Since the left hand side of the equation is a function of r only, while the right hand side is a function of θ and ϕ only, they must each be equal to a separation constant, which we'll call k.

So:

$$\frac{1}{R}\frac{d}{dr}\left(r^2\frac{dR}{dr}\right) = k \qquad (7.6)$$

$$\frac{1}{\Theta\sin\theta}\frac{d}{d\theta}\left(\sin\theta\frac{d\Theta}{d\theta}\right) + \frac{1}{\Phi\sin^2\theta}\frac{d^2\Phi}{d\phi^2} = -k \qquad (7.7)$$

$$\frac{1}{Y}\left(\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial Y}{\partial\theta}\right) + \frac{1}{\sin^2\theta}\frac{\partial^2 Y}{\partial\phi^2}\right) = -k \qquad (7.8)$$

Let's start with the $R(r)$ equation, expanding it out:

$$r^2\frac{d^2R}{dr^2} + 2r\frac{dR}{dr} - kR = 0 \qquad (7.9)$$

Rewrite this using the substitutions $r = \exp(t)$ and $R(r) = S(t)$:

$$\frac{d^2S}{dt^2} + \frac{dS}{dt} - kS = 0 \tag{7.10}$$

This is now a constant coefficient 2nd order ODE, and so is easy to solve:

$$S = A\exp(\lambda_1 t) + B\exp(\lambda_2 t) \tag{7.11}$$

where λ_1 and λ_2 are the two roots of the auxiliary equation

$$\lambda^2 + \lambda - k = 0 \tag{7.12}$$

By inspection, we can therefore see that

$$\lambda_1 + \lambda_2 = -1 \tag{7.13}$$

$$\lambda_1\lambda_2 = -k \tag{7.14}$$

So if we call one of the roots *l*, the other root will be $-(l+1)$.

From equations (7.13) and (7.14), we therefore also now know that

$$k = l(l+1) \tag{7.15}$$

Note that we don't know more than this for now, though. For example, we don't yet know whether or not *l* might have to be an integer.

Our $S(t)$ solution can be written as:

$$S = A\left(\exp(t)\right)^{\lambda_1} + B\left(\exp(t)\right)^{\lambda_2} \tag{7.16}$$

So we can easily transform it back to the $R(r)$ form:

$$R = Ar^{\lambda_1} + Br^{\lambda_2} = Ar^l + Br^{-(l+1)} \tag{7.17}$$

Recap – where have we got to? We know that our solution Ψ is given by

$$\Psi(r,\theta,\phi) = R(r)\,\Theta(\theta)\Phi(\phi) = \left(Ar^l + Br^{-(l+1)}\right)\Theta(\theta)\Phi(\phi) \tag{7.18}$$

$$\Psi(r,\theta,\phi) = R(r)\,Y(\theta,\phi) = \left(Ar^l + Br^{-(l+1)}\right)Y(\theta,\phi) \tag{7.19}$$

We also know that $Y(\theta,\phi)$ must satisfy the equation

$$\frac{1}{\Theta\sin\theta}\frac{d}{d\theta}\left(\sin\theta\frac{d\Theta}{d\theta}\right) + \frac{1}{\Phi\sin^2\theta}\frac{d^2\Phi}{d\phi^2} = -k \tag{7.20}$$

$$\frac{1}{Y}\left(\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial Y}{\partial\theta}\right) + \frac{1}{\sin^2\theta}\frac{\partial^2 Y}{\partial\phi^2}\right) = -k \tag{7.21}$$

where $k = l(l+1)$.

So now we need to separate this equation into its θ and ϕ parts. We write:

$$\frac{1}{Y}\left(\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial Y}{\partial\theta}\right) + \frac{1}{\sin^2\theta}\frac{\partial^2 Y}{\partial\phi^2}\right) = -k \tag{7.22}$$

$$\frac{\sin\theta}{\Theta}\frac{d}{d\theta}\left(\sin\theta\frac{d\Theta}{d\theta}\right) + l(l+1)\sin^2\theta = -\frac{1}{\Phi}\frac{d^2\Phi}{d\phi^2} = m^2 \tag{7.23}$$

The left hand side of the equation is a function of θ only, while the right hand side is a function of ϕ only. So set them both equal to a separation constant m^2. Note the analogy with the circular drum (Section 4.3) – we're setting the separation constant to be negative with respect to the 2nd order ODE in ϕ in order to ensure that we have a sinusoidal variation in ϕ.

The equation in $\Phi(\phi)$ is easy to solve:

$$\Phi(\phi) = C\cos(m\phi) + D\sin(m\phi) \tag{7.24}$$

and because of the 2π-periodic boundary condition in θ, we know that *m* must be an integer.

So we've now just got the $\Theta(\theta)$ equation left:

$$\frac{\sin\theta}{\Theta}\frac{d}{d\theta}\left(\sin\theta\frac{d\Theta}{d\theta}\right)+l(l+1)\sin^2\theta=m^2 \qquad (7.25)$$

To solve this, substitute $x=\cos\theta$ and $y=\Theta(\theta)$ into the first term of this equation:

$$\begin{aligned}
&\frac{\sin\theta}{\Theta}\frac{d}{d\theta}\left(\sin\theta\frac{d\Theta}{d\theta}\right)=\frac{\sin\theta}{y}\frac{d}{d\theta}\left(\sin\theta\frac{dy}{d\theta}\right)\\
&=\frac{\sin\theta}{y}\frac{d}{d\theta}\left(\sin\theta\frac{dy}{dx}\frac{dx}{d\theta}\right)\\
&=\frac{\sin\theta}{y}\frac{d}{d\theta}\left(-\sin^2\theta\frac{dy}{dx}\right)\\
&=\frac{\sin\theta}{y}\frac{d}{dx}\left(-\sin^2\theta\frac{dy}{dx}\right)\frac{dx}{d\theta}\\
&=\frac{-\sin^2\theta}{y}\frac{d}{dx}\left(-\sin^2\theta\frac{dy}{dx}\right)\\
&=\frac{\sin^2\theta}{y}\frac{d}{dx}\left(\sin^2\theta\frac{dy}{dx}\right)\\
&=\frac{\sin^2\theta}{y}\left(2\sin\theta\cos\theta\frac{d\theta}{dx}\frac{dy}{dx}+\sin^2\theta\frac{d^2y}{dx^2}\right)\\
&\vdots\\
&=\frac{\sin^2\theta}{y}\left(-2\cos\theta\frac{dy}{dx}+\sin^2\theta\frac{d^2y}{dx^2}\right)
\end{aligned} \qquad (7.26)$$

So we've now got:

$$\begin{aligned}
&\frac{\sin^2\theta}{y}\left(-2\cos\theta\frac{dy}{dx}+\sin^2\theta\frac{d^2y}{dx^2}\right)+l(l+1)\sin^2\theta=m^2\\
&-2\cos\theta\frac{dy}{dx}+\sin^2\theta\frac{d^2y}{dx^2}+l(l+1)y=\frac{m^2y}{\sin^2\theta}
\end{aligned} \qquad (7.27)$$

So

$$\begin{aligned}
&\sin^2\theta\frac{d^2y}{dx^2}-2\cos\theta\frac{dy}{dx}+\left[l(l+1)-\frac{m^2}{\sin^2\theta}\right]y=0\\
&(1-x^2)\frac{d^2y}{dx^2}-2x\frac{dy}{dx}+\left[l(l+1)-\frac{m^2}{(1-x^2)}\right]y=0
\end{aligned} \qquad (7.28)$$

As if by magic! This is exactly the form of the associated Legendre Equation in equation (6.98)!!

Since we already know that the condition for obtaining convergent solutions to the Legendre Equation for all finite values of *x* is that *l* is a non-negative integer. So this must also be the case for our solution to the Laplace Equation in spherical polar co-ordinates.

We can therefore write the solution to this equation as

$$y(x)=P_l^m(x) \qquad (7.29)$$

where $P_l^m(x)$ is the associated Legendre function for the particular values of *m* and *l*.

However, we were originally trying to solve the $\Theta(\theta)$ equation.

So we now need to undo our previous substitutions ($x=\cos\theta$ and $y=\Theta(\theta)$) in reverse:

$$\Theta(\theta) = P_l^m(\cos\theta) \tag{7.30}$$

where

$$P_l^m(x) = (1-x^2)^{m/2} \frac{d^m P(x)}{dx^m} \tag{7.31}$$

So, finally (!), our full solution is:

$$\Psi(r,\theta,\phi) = R(r)\,\Theta(\theta)\Phi(\phi) \tag{7.32}$$

$$\Psi(r,\theta,\phi) = \left(Ar^l + Br^{-(l+1)}\right) P_l^m(\cos\theta)\left(C\cos(m\phi) + D\sin(m\phi)\right) \tag{7.33}$$

Note that, similarly to Bessel functions, there are two kinds of Legendre functions – Legendre functions of the first kind are conventionally labelled $P_l^m(x)$, and Legendre functions of the second kind are conventionally labelled $Q_l^m(x)$.

Again similarly to Bessel functions, we only need to consider the $P_l^m(x)$ set of solutions, however, as the $Q_l^m(x)$ solutions tend to infinity as x tends to ±1, i.e. as $\cos\theta$ tends to ±1, i.e. as θ tends to 0 or $\pm\pi$. Since physical solutions must be finite on the polar axis, we therefore only need to consider the $P_l^m(x)$ set of solutions, and we can ignore the $Q_l^m(x)$ solutions.

7.2. Spherical Harmonics

Remember that we are looking for a solution to Laplace's Equation $(\nabla^2\Psi = 0)$ in spherical polar co-ordinates, and that our solution is given by:

$$\Psi(r,\theta,\phi) = R(r)\,\Theta(\theta)\Phi(\phi) \tag{7.34}$$

$$\Psi(r,\theta,\phi) = R(r)Y(\theta,\phi) = R(r)\Theta(\theta)\Phi(\phi) \tag{7.35}$$

In other words, any time we solve Laplace's Equation in spherical polar co-ordinates, the angular part of our solution will be:

$$\Theta(\theta)\Phi(\phi) = P_l^m(\cos\theta)\left(C\cos(m\phi) + D\sin(m\phi)\right) \tag{7.36}$$

$$Y(\theta,\phi) = \Theta(\theta)\Phi(\phi) = P_l^m(\cos\theta)\left(C\cos(m\phi) + D\sin(m\phi)\right) \tag{7.37}$$

where

$$P_l^m(x) = (1-x^2)^{m/2} \frac{d^m P(x)}{dx^m} \tag{7.38}$$

These forms of function are known as spherical harmonics, $Y_l^m(\theta,\phi)$, usually defined as:

$$Y_l^m(\theta,\phi) = \Theta(\theta)\Phi(\phi) = (-1)^m \left[\frac{(2l+1)}{4\pi}\frac{(l-m)!}{(l+m)!}\right]^{1/2} P_l^m(\cos\theta)\exp(im\phi) \tag{7.39}$$

$$Y_l^m(\theta,\phi) = (-1)^m \left[\frac{(2l+1)}{4\pi}\frac{(l-m)!}{(l+m)!}\right]^{1/2} P_l^m(\cos\theta)\exp(im\phi) \tag{7.40}$$

This is basically the same as the previous equation, except with the dependence written in complex exponential form, and with the numerical coefficient in the square bracket having been introduced as a normalisation factor.

Remember that we already found the first few Legendre Polynomials for the $m = 0$ example that we solved:

$$P_0(x) = 1 \tag{7.41}$$

$$P_1(x) = x \tag{7.42}$$

$$P_2(x) = \frac{1}{2}\left(3x^2 - 1\right) \tag{7.43}$$

$$P_3(x) = \frac{1}{2}\left(5x^3 - 3x\right) \tag{7.44}$$

In other words, substituting in that $m = 0$ and $x = \cos\theta$:

$$P_0^0(\cos\theta) = 1$$

$$P_1^0(\cos\theta) = \cos\theta$$

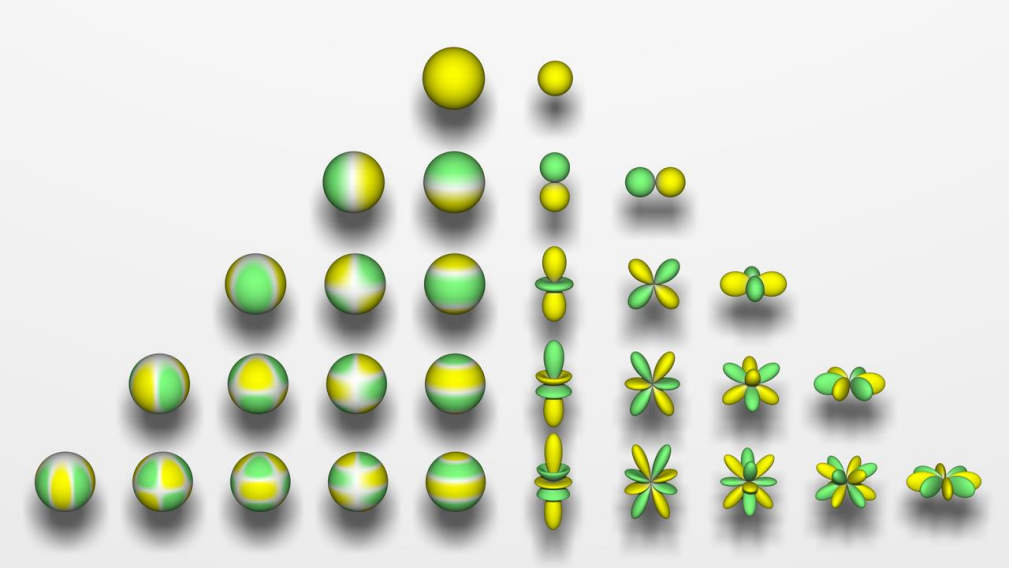
$$P_2^0(\cos\theta) = \frac{1}{2}\left(3\cos^2\theta - 1\right)$$

$$P_3^0(\cos\theta) = \frac{1}{2}\left(5\cos^3\theta - 3\cos\theta\right)$$

We can now generate our spherical harmonic functions $Y_l^m(\theta,\phi)$:

l = 0 (i.e. m = 0):	$Y_0^0(\theta,\phi) = \sqrt{\frac{1}{4\pi}}$
l = 1 (i.e. m = 0, ± 1):	$Y_1^0(\theta,\phi) = \sqrt{\frac{3}{4\pi}}\cos\theta$ $Y_1^{\pm1}(\theta,\phi) = \mp\sqrt{\frac{3}{8\pi}}\sin\theta\exp(\pm i\phi)$
l = 2 (i.e. m = 0, ± 1, ± 2):	$Y_2^0(\theta,\phi) = \sqrt{\frac{5}{16\pi}}\left(3\cos^2\theta - 1\right)$ $Y_2^{\pm1}(\theta,\phi) = \mp\sqrt{\frac{15}{8\pi}}\sin\theta\cos\theta\exp(\pm i\phi)$ $Y_2^{\pm2}(\theta,\phi) = \mp\sqrt{\frac{15}{32\pi}}\sin^2\theta\exp(\pm 2i\phi)$

etc.



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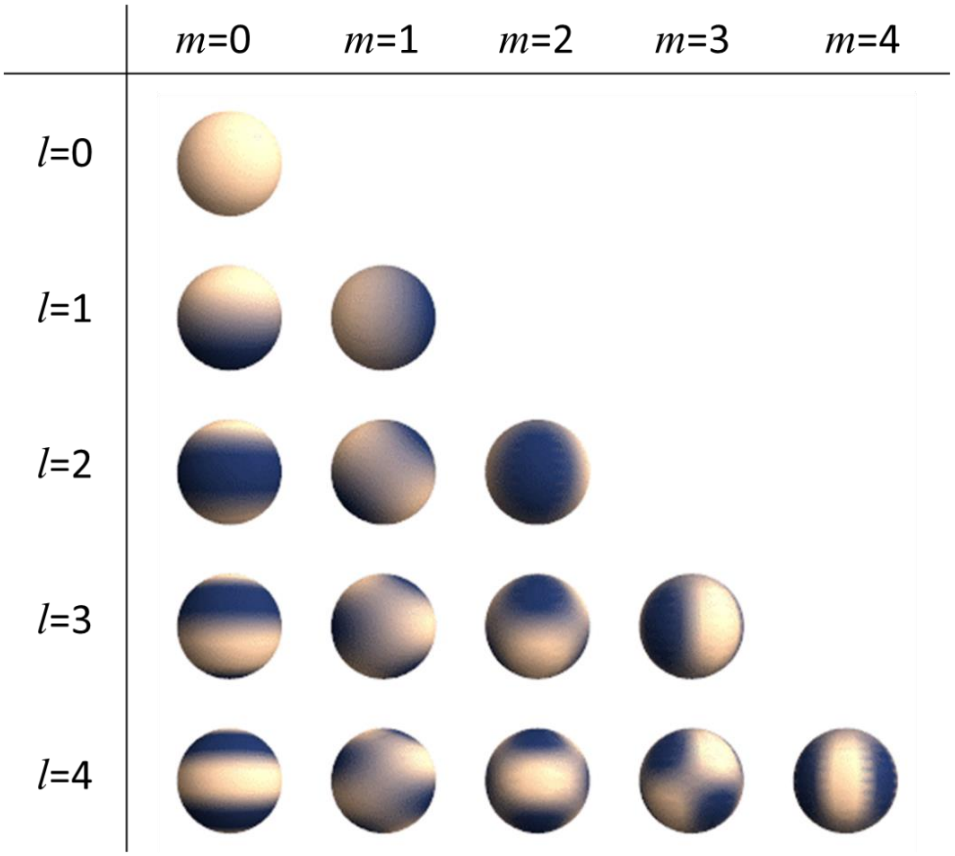

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7.2.1. Properties of Spherical Harmonics

Mutual Orthogonality

Two continuous functions $f(x)$ and $g(x)$ are defined as being *orthogonal* over the interval $[a,b]$ if:

$$\langle f|g\rangle \equiv \int_a^b f^*(x)g(x)dx = 0 \tag{7.45}$$

If, in addition,

$$\langle f|f\rangle \equiv \int_a^b \left[f(x)\right]^2 dx = 1 \tag{7.46}$$

and

$$\langle g|g\rangle \equiv \int_a^b \left[g(x)\right]^2 dx = 1 \tag{7.47}$$

the functions $f(x)$ and $g(x)$ are said to be *orthonormal*.

For example, the sine and cosine functions are examples of sets of orthogonal functions:

$$\int_0^{2\pi} \sin(mx)\sin(nx)dx = \pi\delta_{mn} \tag{7.48}$$

$$\int_0^{2\pi} \cos(mx)\cos(nx)dx = \pi\delta_{mn} \tag{7.49}$$

For $m,n \neq 0$, and where δ_{mn} is the Kronecker delta ($\delta_{mn} = 1$ if $m = n$, or 0 otherwise).

Orthogonal functions can form an infinite basis for a function space, and any complete system of orthogonal functions can be used to express an arbitrary periodic function through harmonic analysis – the mutual orthogonality of the sine and cosine functions is the basis for Fourier analysis.

It can be shown that Legendre polynomials also form a set of orthogonal functions in the interval $[-1,1]$.

For fixed values of *m*, they are mutually orthogonal with respect to *l*:

$$\int_{-1}^{1} P_l^m P_{l'}^m dx = \frac{2(l+m)!}{(2l+1)(l-m)!}\delta_{ll'} \qquad (7.50)$$

Similarly, for fixed values of *l*, they are mutually orthogonal with respect to *m* (with a weighting function of $\frac{1}{1-x^2}$):

$$\int_{-1}^{1} \frac{P_l^m P_l^{m'}}{1-x^2} dx = \frac{(l+m)!}{m(l-m)!}\delta_{mm'} \qquad (7.51)$$

In our notation, the associated Legendre polynomials $P_l^m(\cos\theta)$ are therefore mutually orthogonal within the interval $-1 < \cos\theta < 1$, which corresponds to our full range of $0 \le \theta < \pi$. The $\exp(im\phi)$ functions are also mutually orthogonal, as for sine and cosine, within the range $0 \le \phi < 2\pi$.

The spherical harmonics $Y_l^m(\theta,\phi)$ are therefore mutually orthogonal, and in fact form an orthonormal set, due to the normalisation constant we introduced:

$$\int_{-1}^{1}\int_{0}^{2\pi} \left[Y_l^m(\theta,\phi)\right]^* Y_{l'}^{m'}(\theta,\phi)\, d\phi\, d(\cos\theta) = \delta_{ll'}\delta_{m\,m'} \qquad (7.52)$$

where

$$Y_l^m(\theta,\phi) = \Theta(\theta)\Phi(\phi) \propto P_l^m(\cos\theta)\exp(im\phi) \qquad (7.53)$$

7.3. Example problem

We've already seen that the solution to some PDEs can be expressed in terms of the Fourier series of the boundary function – for example, for our 1D diffusion equation and 2D Laplace equation examples.

Spherical harmonics can be used in an analogous way for boundary value problems in spherical regions. We've already found that the general solution to Laplace's equation in spherical polar co-ordinates is

$$\Psi(r,\theta,\phi) = \left(Ar^l + Br^{-(l+1)}\right)P_l^m(\cos\theta)\left(C\cos(m\phi) + D\sin(m\phi)\right) \qquad (7.54)$$

(for solutions that are finite on the polar axis).

Applying the principle of linear superposition, the full general solution is

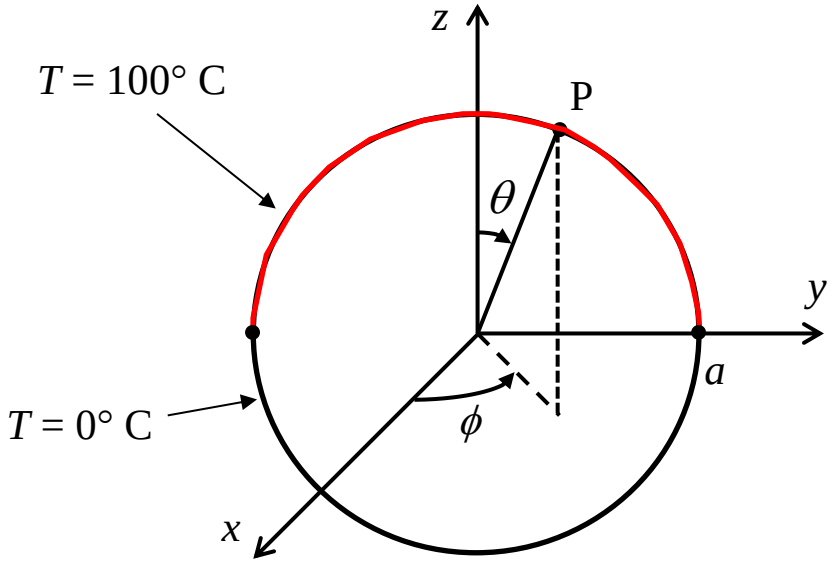
$$\Psi(r,\theta,\phi) = \sum_{l=0}^{\infty}\sum_{m=-l}^{l}\left(A_l r^l + B_l r^{-(l+1)}\right)P_l^m(\cos\theta)\left(C_m\cos(m\phi) + D_m\sin(m\phi)\right)$$

$$= \sum_{l=0}^{\infty}\sum_{m=-l}^{l}\left(A_l r^l + B_l r^{-(l+1)}\right)Y_l^m(\theta,\phi) \qquad (7.55)$$

In other words, we can express our solution as a solution as a (potentially infinite) sum of spherical harmonics or Legendre polynomials.

As usual, the boundary conditions for the particular problem will determine the values of the various coefficients.

For example, consider a sphere of radius *a* centred at the origin. The surfaces of the upper and lower hemispheres are kept at 100° and 0° respectively. Find the steady state temperature $T(r,\theta,\phi)$ inside the sphere.



First note that our boundary conditions are

$$T(a,\theta,\phi)=\begin{cases}100 & \text{for } 0<\theta<\pi/2\\ 0 & \text{for } \pi/2<\theta<\pi\end{cases}$$

They are therefore independent of ϕ in this instance.

This means that $m = 0$ in this instance, and hence we can write our general solution as

$$T(r,\theta,\phi)=\sum_{l=0}^{\infty}\left(A_l r^l + B_l r^{-(l+1)}\right)P_l(\cos\theta) \qquad (7.56)$$

where $P_l(\cos\theta)$ are Legendre polynomials (see equations (7.41) to (7.44) for examples of these polynomials).

The next thing to notice is that we are asked to find the temperature distribution inside the sphere – and that this region includes the origin, i.e. the point where $r = 0$.

So B_l must be zero for all values of l, as otherwise the temperature would tend to infinity at the origin.

Our solution therefore becomes

$$T(r,\theta,\phi)=\sum_{l=0}^{\infty}A_l r^l P_l(\cos\theta) \qquad (7.57)$$

On the surface of the sphere, this becomes

$$T(a,\theta,\phi)=\sum_{l=0}^{\infty}A_l a^l P_l(\cos\theta) \qquad (7.58)$$

In order to find expressions for our coefficients A_l, we need to use the fact that we can express any reasonable function $f(x)$ in the interval $|x|<1$ as an infinite sum of Legendre polynomials:

$$f(x)=\sum_{l=0}^{\infty}a_l P_l(x) \qquad (7.59)$$

where the coefficients a_l are given by

$$a_l=\frac{2l+1}{2}\int_{-1}^{1}f(x)P_l(x)\,dx \qquad (7.60)$$

Comparing this with our solution gives that

$$A_l a^l=\frac{2l+1}{2}\int_{-1}^{1}T(a,\theta,\phi)P_l(u)\,du \qquad (7.61)$$

where we've used the substitution $u=\cos\theta$.

Substituting in our boundary condition for the temperature of the surface of the sphere gives:

$$A_l = \frac{2l+1}{2a^l}\int_0^1 100 P_l(u)\,du \qquad (7.62)$$

We can therefore evaluate these coefficients, using the standard expressions for the Legendre polynomials, and integrating:

$A_0 = 50$

$A_1 = \frac{75}{a}$

$A_2 = 0$

$A_3 = \frac{-175}{a^3}$

etc...

We can now substitute these coefficients into our full solution:

$$T(r,\theta,\phi) = \sum_{l=0}^{\infty} A_l r^l P_l(\cos\theta)$$

$$= 50 r^0 P_0(\cos\theta) + \frac{75}{a} r^1 P_1(\cos\theta) + 0 - \frac{175}{4a^3} r^3 P_3(\cos\theta) + \ldots$$

$$= 50 P_0(\cos\theta) + 75\left(\frac{r}{a}\right) P_1(\cos\theta) - \frac{175}{4}\left(\frac{r}{a}\right)^3 P_3(\cos\theta) + \ldots$$

$$= 50 + 75\left(\frac{r}{a}\right)\cos\theta - \frac{175}{8}\left(\frac{r}{a}\right)^3 \left(5\cos^3\theta - 3\cos\theta\right) + \ldots$$

So this is the temperature profile inside the sphere. If we had instead been asked to find the temperature profile in the full region outside the sphere, we would instead construct the solution as

$$T(r,\theta,\phi) = \sum_{l=0}^{\infty} B_l r^{-(l+1)} P_l(\cos\theta) \qquad (7.63)$$

This is because we need the solution to stay finite as r tends to infinity – and hence our coefficients A_l must be zero for all values of l.

Following through the similar working shows that the temperature distribution in the region outside the sphere is

$$T(r,\theta,\phi) = \sum_{l=0}^{\infty} B_l r^{-(l+1)} P_l(\cos\theta)$$

$$= 50 a r^{-1} P_0(\cos\theta) + 75 a^2 r^{-2} P_1(\cos\theta) + 0 - \frac{175 a^4}{4} r^{-4} P_3(\cos\theta) + \ldots$$

$$= 50\left(\frac{a}{r}\right) P_0(\cos\theta) + 75\left(\frac{a}{r}\right)^2 P_1(\cos\theta) - \frac{175}{4}\left(\frac{a}{r}\right)^4 P_3(\cos\theta) + \ldots$$

$$= 50\left(\frac{a}{r}\right) + 75\left(\frac{a}{r}\right)^2 \cos\theta - \frac{175}{8}\left(\frac{a}{r}\right)^4 \left(5\cos^3\theta - 3\cos\theta\right) + \ldots$$

8. SOLVING THE SCHRÖDINGER EQUATION FOR THE HYDROGEN ATOM

8.1. Separation of Variables

The motion of the electron in a hydrogen atom is governed by Schrödinger's equation:

$$-\frac{\hbar^2}{2m}\nabla^2\Psi(\mathbf{r})+V(\mathbf{r})\,\Psi(\mathbf{r})=E\,\Psi(\mathbf{r}) \tag{8.1}$$

where ħ is Planck's constant, m is the mass of the electron, $\Psi(\mathbf{r})$ is the wavefunction of the electron, E is the energy of the electron, and $V(\mathbf{r})$ is the electrostatic potential between the electron and the proton:

$$V(\mathbf{r})=\frac{-e^2}{4\pi\varepsilon_0 r} \tag{8.2}$$

Here, e is the charge on the electron, and r is the distance between the electron and the proton.

Given the spherical symmetry, we now rewrite Schrödinger's equation in spherical polar co-ordinates:

$$-\frac{\hbar^2}{2m}\left[\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial\Psi}{\partial r}\right)+\frac{1}{r^2\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial\Psi}{\partial\theta}\right)+\frac{1}{r^2\sin^2\theta}\frac{\partial^2\Psi}{\partial\phi^2}\right]+V(r)\,\Psi=E\,\Psi \tag{8.3}$$

As usual, let's try separation of variables, with

$$\Psi(r,\theta,\phi)=R(r)\,Y(\theta,\phi) \tag{8.4}$$

Substituting this into the Laplace Equation, and dividing through by $\Psi = RY$ gives:

$$\frac{1}{R}\frac{d}{dr}\left(r^2\frac{dR}{dr}\right)+\frac{2mr^2}{\hbar^2}\left(E-V(r)\right)=-\frac{1}{Y}\left(\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial Y}{\partial\theta}\right)+\frac{1}{\sin^2\theta}\frac{\partial^2 Y}{\partial\phi^2}\right) \tag{8.5}$$

Again, the left-hand side of the equation is a function of r only, while the right-hand side is a function of θ and ϕ only. So each side must be equal to the same separation constant, which we'll again call k.

So:

$$\frac{1}{R}\frac{d}{dr}\left(r^2\frac{dR}{dr}\right)+\frac{2mr^2}{\hbar^2}\left(E-V(r)\right)=k \tag{8.6}$$

$$\frac{1}{Y}\left(\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial Y}{\partial\theta}\right)+\frac{1}{\sin^2\theta}\frac{\partial^2 Y}{\partial\phi^2}\right)=-k \tag{8.7}$$

This ODE for $Y(\theta,\phi)$ is identical to the equation that we solved already in Section 7. So we already know that $Y(\theta,\phi)$ is our spherical harmonic function:

$$Y_l^m(\theta,\phi)=(-1)^m\left[\frac{(2l+1)}{4\pi}\frac{(l-m)!}{(l+m)!}\right]^{1/2}P_l^m(\cos\theta)\exp(im\phi) \tag{8.8}$$

where

$$P_l^m(x)=\left(1-x^2\right)^{|m|/2}\frac{d^{|m|}P_l(x)}{dx^{|m|}} \tag{8.9}$$

So we now only need to solve the ODE for $R(r)$, and we'll have the full solution to Schrödinger's equation for the hydrogen atom.

We already know that $k = l(l+1)$ – because this was the condition for us to obtain convergent (and hence physically meaningful) solutions to Legendre's Equation (Slide 185).

So we can rewrite the $R(r)$ ODE as:

$$\frac{d}{dr}\left(r^2 \frac{dR}{dr}\right) + \frac{2mr^2}{\hbar^2}\left(E - V(r)\right)R - l(l+1)R = 0 \qquad (8.10)$$

We now need to make some changes of variables in order to simplify this equation.

Let's first introduce a function $f(r)$, which we define as

$$f(r) = rR(r) \qquad (8.11)$$

i.e. $R(r) = \frac{f(r)}{r}$.

Substituting this into our $R(r)$ ODE gives:

$$\frac{d^2 f}{dr^2} + \frac{2m}{\hbar^2}\left(E + \frac{e^2}{4\pi\varepsilon_0 r}\right)f - \frac{l(l+1)}{r^2}f = 0 \qquad (8.12)$$

where we have put in the explicit form for $V(r)$.

This is still pretty messy! The next step is to get rid of all the fundamental constants in this equation.

We first write that

$$a_B = \frac{\hbar^2}{m}\frac{4\pi\varepsilon_0}{e^2} \qquad (8.13)$$

Here, a_B is a quantity that sets the real length scale in the problem; it is called the ***Bohr Radius*** and has the value 0.529 Å.

We can also introduce another two new constants μ and x for convenience, which we define as:

$$\mu^2 = -\frac{\hbar^2}{2ma_B^2 E} \qquad (8.14)$$

and

$$x = \frac{2r}{\mu a_B} \qquad (8.15)$$

Substituting all of these into our previous ODE for $f(x)$ gives:

$$\frac{d^2 f}{dx^2} + \left(\frac{\mu}{x} - \frac{1}{4} - \frac{l(l+1)}{x^2}\right)f = 0 \qquad (8.16)$$

So our problem now reduces to solving this equation for $f(x)$, and then carrying out the reverse substitutions, so that we find the solution to the equation for $R(r)$.

Let's look a bit closer at our equation for $f(x)$.

Our solutions for the radial part of the wavefunction must be finite everywhere – and, in particular, they must not tend towards infinity as r gets larger.

If we look at our equation for $f(x)$, we can seen that when x becomes very large (which, due to the relationship between x and r, corresponds with r also becoming very large), the equation for $f(x)$ reduces to

$$\frac{d^2 f}{dx^2} - \frac{1}{4}f = 0 \qquad (8.17)$$

which has the solutions

$$f(x) \propto \exp\left(\pm\frac{1}{2}x\right) \qquad (8.18)$$

The exponentially increasing solution here is physically unacceptable. So we use another substitution:

$$F(x) = \exp\left(\frac{1}{2}x\right) f(x) \tag{8.19}$$

Substituting this into our equation for $f(x)$ gives

$$\frac{d^2F}{dx^2} - \frac{dF}{dx} + \left(\frac{\mu}{x} - \frac{l(l+1)}{x^2}\right)F = 0 \tag{8.20}$$

Finally (!), we now have an equation which can be tackled using the power series solution method.

8.2. Power series solution of the resulting ODE

We therefore look for a solution of the form

$$F(x) = \sum_{s=0}^{\infty} a_s x^{s+q} \tag{8.21}$$

where q is chosen so that $a_0 \neq 0$.

Substituting this into our equation for $F(x)$ gives:

$$\sum_{s=0}^{\infty} a_s (s+q)(s+q-1)x^{s+q-2} - \sum_{s=0}^{\infty} a_s (s+q)x^{s+q-1} + \mu\sum_{s=0}^{\infty} a_s x^{s+q-1} - l(l+1)\sum_{s=0}^{\infty} a_s x^{s+q-2} = 0 \tag{8.22}$$

The lowest power of x is x^{q-2}, which arises in the first and fourth series when $s=0$.

Setting the coefficient of this power to zero gives the *indicial equation*:

$$a_0\left[q(q-1) - l(l+1)\right] = 0$$

which has solutions

$$q = l+1 \quad \text{or} \quad q = -l$$

Solutions with $q = -l$ are physically unacceptable, since $F(x)$ (and, hence, the radial part of the wavefunction) would diverge to infinity as $x \to 0$ (and hence as $r \to 0$).

We must therefore have $q = l+1$, in which case our power series solution equation reduces to

$$\sum_{s=0}^{\infty} a_s\left[(s+l+1)(s+l) - l(l+1)\right]x^{s+l-1} + \sum_{s=0}^{\infty} a_s\left[\mu - (s+l+1)\right]x^{s+l} = 0 \tag{8.23}$$

Setting the coefficient of the general power, x^{t+l} (which arises from $s = t+1$ in the first series, and $s = t$ in the second series) to zero gives:

$$a_{t+1}\left[(t+l+2)(t+l+1) - l(l+1)\right] = (t+l+1-\mu)a_t \tag{8.24}$$

So the recurrence relation becomes:

$$a_{t+1} = \left[\frac{t+l+1-\mu}{(t+1)(t+2l+2)}\right]a_t \tag{8.25}$$

We might hope that we've now found the solution to our equation for $F(x)$! However, it still isn't quite that straightforward – we still need to consider the convergence of this solution.

Looking at the recurrence relation, we can see that as $t \to \infty$, $a_{t+1} \to \frac{1}{t}a_t$.

Comparing this with the power series solution of exp (x) :

$$e^x = 1 + \frac{x}{1!} + \frac{x^2}{2!} + \frac{x^3}{3!} \ldots\ldots,$$

we can see that our power series solution must diverge like exp (x), which is physically unacceptable.

The only way to get round this is to look for solutions when the power series solution *stops*, giving a solution in the form of a finite polynomial. This will then yield solutions that can go to zero as $x \to \infty$.

Under what conditions will the power series stop? Looking at our recurrence relation, we can see that a_{t+1} will be zero for some value of t provided that μ is an integer which is greater than or equal to l+1.

μ must therefore be an integer which is greater than l.

In other words, we have found that allowed solutions to our equation for $F(x)$ must have

$\mu = n$, where n is an integer and $n>l$.

But remember that we introduced the constant μ, which we defined as:

$$\mu^2 = -\frac{\hbar^2}{2ma_B^2 E} \qquad (8.26)$$

So we can now write that

$$\mathrm{E} = -\frac{\hbar^2}{2ma_B^2 n^2} = -\frac{1}{n^2}\left(\frac{me^4}{32\pi^2\varepsilon_0^2\hbar^2}\right) \qquad (8.27)$$

This equation is (nearly) enough to explain the spectral lines associated with atomic hydrogen.

8.3. Quantum numbers

We are now very nearly there! We have found that:

Physically acceptable solutions to Schrödinger's equation are characterised by three integers (or *quantum numbers*) n, l, m which satisfy:

$$n > l \text{ and } |m| \le l$$

The allowed solutions can therefore be listed as follows:

n	Allowed values of l	Allowed values of m
1	0	0
2	0	0
	1	-1, 0, 1
3	0	0
	1	-1, 0, 1
	2	-2, -1, 0, 1, 2

8.4. Wavefunctions

The final step in the solution is to construct explicit expressions for the wavefunction $\Psi(r,\theta,\phi)$. The angular parts are described by the spherical harmonic functions, so we now just need the radial parts.

Remember that the recurrence relation is $a_{t+1} = \left[\frac{t+l+1-n}{(t+1)(t+2l+2)}\right] a_t$

Example 1: solution (wavefunction) for *n* = 1, *l* = 0, *m* = 0.

In this case for $t = 0$ we have

$$a_1 = \left[\frac{0+0+1-1}{(0+1)(0+2\times 0+2)}\right] a_0 = 0 \tag{8.28}$$

So the power series only has one term.

Remember that

$$F(x) = \sum_{s=0}^{\infty} a_s x^{s+q} = \sum_{s=0}^{\infty} a_s x^{s+l+1} \tag{8.29}$$

So in this case our power series solution is

$$F(x) = a_0 x \tag{8.30}$$

So we've now found a solution for $F(x)$. But we're really looking for a full expression for the wavefunction $\Psi(r,\theta,\phi)$.

So we now need to reverse the substitutions we made earlier (equations (8.4), (8.11), (8.15) and (8.19)), noting that $\mu = n = 1$ for this case:

$$f(x) = F(x)\exp\left(-\frac{x}{2}\right) = a_0 x \exp\left(-\frac{x}{2}\right) \tag{8.31}$$

So

$$f(r) = \frac{2a_0 r}{a_B}\exp\left(-\frac{r}{a_B}\right) \tag{8.32}$$

and

$$R(r) = \frac{f(r)}{r} = \frac{2a_0}{a_B}\exp\left(-\frac{r}{a_B}\right) \tag{8.33}$$

In other words,

$$R(r) \propto \exp\left(-\frac{r}{a_B}\right) \tag{8.34}$$

Remember that the expression for the wavefunction $\Psi(r,\theta,\phi)$ is:

$$\Psi_{nlm}(r,\theta,\phi) = R_{nl}(r)\, Y_l^m(\theta,\phi) \tag{8.35}$$

So

$$\Psi_{100}(r,\theta,\phi) = R_{10}(r)\, Y_0^0(\theta,\phi) \tag{8.36}$$

But we already know that

$$Y_0^0(\theta,\phi) = \sqrt{\frac{1}{4\pi}} \tag{8.37}$$

So

$$\Psi_{100}(r,\theta,\phi) = \sqrt{\frac{1}{4\pi}}\frac{2a_0}{a_B}\exp\left(-\frac{r}{a_B}\right) = A\exp\left(-\frac{r}{a_B}\right) \tag{8.38}$$

where *A* is a normalisation constant.

To find the value of *A* we require

$$\iiint r^2 \sin\theta\, dr\, d\theta\, d\phi \left|\Psi_{100}(r,\theta,\phi)\right|^2 = 1 \tag{8.39}$$

Example 2: solution (wavefunction) for *n* = 2, *l* = 1, *m* = -1, 0, 1.

In this case for $t = 0$ we have

$$a_1 = \left[\frac{0+1+1-2}{(0+1)(0+2\times 1+2)}\right] a_0 = 0 \tag{8.40}$$

So the power series again only has one term.

Since

$$F(x) = \sum_{s=0}^{\infty} a_s x^{s+q} = \sum_{s=0}^{\infty} a_s x^{s+l+1} \tag{8.41}$$

in this case our power series solution is

$$F(x) = a_0 x^2 \tag{8.42}$$

Again, we need to reverse our previous substitutions (noting that $\mu = n = 2$ for this case) to find an expression for the wavefunction $\Psi(r, \theta, \phi)$:

$$f(x) = F(x)\exp\left(-\frac{x}{2}\right) = a_0 x^2 \exp\left(-\frac{x}{2}\right) \tag{8.43}$$

$$f(r) = \frac{a_0 r^2}{a_B^2}\exp\left(-\frac{r}{2a_B}\right) \tag{8.44}$$

$$R(r) = \frac{f(r)}{r} = \frac{a_0 r}{a_B^2}\exp\left(-\frac{r}{2a_B}\right) \tag{8.45}$$

But

$$\Psi_{nlm}(r, \theta, \phi) = R_{nl}(r)\, Y_l^m(\theta, \phi) \tag{8.46}$$

So

$$\Psi_{21-1}(r, \theta, \phi) = R_{21}(r)\, Y_1^{-1}(\theta, \phi) \tag{8.47}$$

$$\Psi_{210}(r, \theta, \phi) = R_{21}(r)\, Y_1^{0}(\theta, \phi) \tag{8.48}$$

$$\Psi_{211}(r, \theta, \phi) = R_{21}(r)\, Y_1^{1}(\theta, \phi) \tag{8.49}$$

But we already know that

$$Y_1^{-1}(\theta, \phi) = \sqrt{\frac{3}{8\pi}}\sin\theta\exp(-i\phi) \tag{8.50}$$

$$Y_1^{0}(\theta, \phi) = \sqrt{\frac{3}{4\pi}}\cos\theta \tag{8.51}$$

$$Y_1^{1}(\theta, \phi) = -\sqrt{\frac{3}{8\pi}}\sin\theta\exp(i\phi) \tag{8.52}$$

So we can now write our full wavefunctions for these values of *n*, *l* and *m* as:

$$\Psi_{21-1}(r, \theta, \phi) = Ar\exp\left(-\frac{r}{2a_B}\right)\sin\theta\exp(-i\phi) \tag{8.53}$$

$$\Psi_{210}(r, \theta, \phi) = Ar\exp\left(-\frac{r}{2a_B}\right)\cos\theta \tag{8.54}$$

$$\Psi_{211}(r, \theta, \phi) = Ar\exp\left(-\frac{r}{2a_B}\right)\sin\theta\exp(i\phi) \tag{8.55}$$

where *A* is a normalisation constant.

9. MATRICES AND VECTOR SPACES

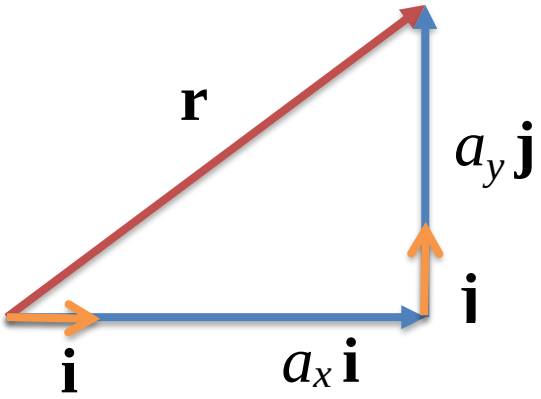
9.1. Vector Spaces

9.1.1. Basis Vectors

In real 3D space we think of a vector as a geometrical object with a magnitude and a direction. This magnitude and direction is fixed – i.e. it's independent of the co-ordinate system we might choose to use to describe it.

For example, take a vector **r** in a 2D Cartesian co-ordinate system:

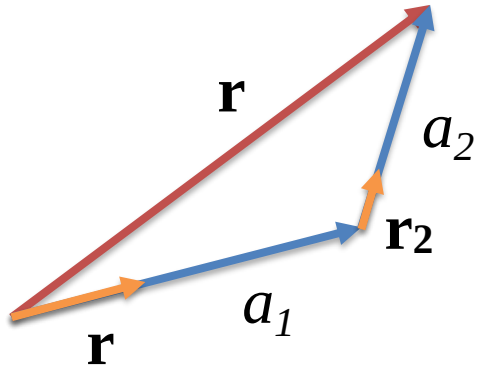
$$\mathbf{r} = a_x\mathbf{i} + a_y\mathbf{j} \tag{9.1}$$



Any vector in the plane can be written as a linear combination of **i** and **j** – they are known as the basis vectors.

Our basis vectors don't have to be orthogonal, however. We could express the same vector **r** in terms of any other two non-collinear (i.e. linearly independent) vectors $\mathbf{r}_1$ and $\mathbf{r}_2$:

$$\mathbf{r} = a_1\mathbf{r}_1 + a_2\mathbf{r}_2 \tag{9.2}$$



There is an infinite choice of basis vectors – for this 2D example, you can choose any two non-collinear vectors to form the basis for **r**.

We could also choose to use more than two basis vectors, but only two are needed for a 2D vector space – any more are redundant. This is because any third vector that you might think to use as an additional basis vector can be constructed from a linear combination of the first two basis vectors – in other words, the third vector is not linearly independent from the first two vectors.

It's important to note that the choice of basis does not affect the vector **r** itself – **r** itself is independent of whichever co-ordinates are used to describe it.

9.1.2. Complex vector spaces

We can now extend our familiar notions of real 2D & 3D vectors spaces to more abstract complex vector spaces. These may have any number of dimensions (although we'll consider only finite dimensionality for now), and the coefficients/components of these vectors may be complex, as opposed to the real numbers that we're used to for real geometric space.

9.1.3. Definition of a vector space

A set of vectors **a**, **b** and **c** is said to form a linear vector space if it satisfies the following:

i. **Commutative & associative addition:**

$$\mathbf{a}+\mathbf{b}=\mathbf{b}+\mathbf{a} \tag{9.3}$$

$$(\mathbf{a}+\mathbf{b})+\mathbf{c}=\mathbf{a}+(\mathbf{b}+\mathbf{c}) \tag{9.4}$$

ii. **Associative multiplication:**

$$\lambda(\mu)\mathbf{a}=(\lambda\mu)\mathbf{a} \tag{9.5}$$

iii. **Distributive addition and multiplication:**

$$\lambda(\mathbf{a}+\mathbf{b})=\lambda\mathbf{a}+\lambda\mathbf{b} \tag{9.6}$$

$$(\lambda+\mu)\mathbf{a}=\lambda\mathbf{a}+\mu\mathbf{a} \tag{9.7}$$

(where λ and μ are arbitrary scalars).

iv. There exists a null vector **0** such that $\mathbf{a}+\mathbf{0}=\mathbf{a}$ for all **a**.

v. Multiplication by unity leaves any vector unchanged, i.e. $1\times\mathbf{a}=\mathbf{a}$.

vi. All vectors have a corresponding negative vector such that $\mathbf{a}+(-\mathbf{a})=\mathbf{0}$. It follows from this that $-\mathbf{a}=(-1)\times\mathbf{a}$.

Now suppose that we have some mathematical entities that obey this set of rules that define a vector space.

Even though these entities might not be anything like what we would normally think of as vectors in ordinary space, if they obey these rules, then we can treat them as if they are vectors.

For example, quantum states can be 'added' and 'multiplied' – not in the same way as our familiar algebraic operations, but nevertheless obeying the rules defining a vector space.

We can therefore treat quantum states as abstract vectors, with all the mathematical tools this brings.

9.1.4. *N*-dimensional vector spaces

Let's now imagine an arbitrary vector **x** lying within an *N*-dimensional vector space (*V*). Any set of *N* linearly independent vectors can be used to form a basis for *V*.

For example, we could choose to use the vectors $\mathbf{e}_1$, $\mathbf{e}_2$, $\mathbf{e}_3$, $\mathbf{e}_4$,…. $\mathbf{e}_N$ as our set of basis vectors.

We would therefore express our vector **x** as a linear combination of these basis vectors:

$$\mathbf{x}=x_1\mathbf{e}_1+x_2\mathbf{e}_2+x_3\mathbf{e}_3+x_4\mathbf{e}_4+.....+x_N\mathbf{e}_N=\sum_{i=1}^{N}x_i\mathbf{e}_i \tag{9.8}$$

However, as we've already noted, *any* set of *N* linearly independent vectors can form a basis for *V*. So we could equally express the same vector **x** as a linear combination of a different set of basis vectors $\mathbf{e}'_1$, $\mathbf{e}'_2$, $\mathbf{e}'_3$, $\mathbf{e}'_4$,…. $\mathbf{e}'_N$. In this case, we would express this same vector **x** as a different linear combination of these different basis vectors:

$$\mathbf{x}=x'_1\mathbf{e}'_1+x'_2\mathbf{e}'_2+x'_3\mathbf{e}'_3+x'_4\mathbf{e}'_4+.....+x'_N\mathbf{e}'_N=\sum_{i=1}^{N}x'_i\mathbf{e}'_i \tag{9.9}$$

9.1.5. The inner product

In real 3D space, the scalar product (or dot product) is defined as

$\mathbf{a}\cdot\mathbf{b}=|\mathbf{a}||\mathbf{b}|\cos\theta$, where θ is the angle between the vectors **a** and **b**.

We can generalise this concept to define the *inner product* of two vectors in a complex *N*-dimensional vector space *V*. The inner product is written as $\langle \mathbf{a} | \mathbf{b} \rangle$, and it maps our vectors **a** and **b** to a scalar.

As we might expect, two vectors in *V* are defined to be orthogonal if

$$\langle \mathbf{a} | \mathbf{b} \rangle = 0 \tag{9.10}$$

In a similar way, the *norm* of a vector **a** is defined as

$$\|\mathbf{a}\| = \langle \mathbf{a} | \mathbf{a} \rangle^{1/2} \tag{9.11}$$

This is analogous to our definition of the modulus $|\mathbf{a}|$ (i.e. the length) of a vector **a** in 3D. Since we would like to associate the norm of a vector with the intuitive geometrical concept of 'length/size', we therefore want it to be a real positive number.

Although the inner product for two complex vectors is related to our standard dot product, we therefore can't say that the inner product $\langle \mathbf{a} | \mathbf{b} \rangle$ is just equal to $\mathbf{a} \cdot \mathbf{b}$, if the vectors **a** and **b** are complex.

This is because if we were to define the inner product to be $\langle \mathbf{a} | \mathbf{b} \rangle = \mathbf{a} \cdot \mathbf{b}$ for complex vectors, we would end up with the norm of a complex vector being a complex number.

Now remember that the modulus of a complex number *z* can be defined as $|z| = \left(z z^* \right)^{1/2}$. Comparing this with our expression for the norm of a complex vector, we can therefore define the inner product for a complex vector to be:

$$\langle \mathbf{a} | \mathbf{b} \rangle = \mathbf{a}^* \cdot \mathbf{b} \tag{9.12}$$

This will then give us a non-negative real value for the norm of a complex vector.

Now let's consider an orthonormal basis $\hat{\mathbf{e}}_1, \hat{\mathbf{e}}_2, \hat{\mathbf{e}}_3, \hat{\mathbf{e}}_4 \ldots\ldots \hat{\mathbf{e}}_N$ $\hat{\mathbf{e}}_1, \hat{\mathbf{e}}_2, \hat{\mathbf{e}}_3 \ldots\ldots \hat{\mathbf{e}}_N$ - in other words, a basis in which the basis vectors are mutually orthogonal, and each has unit norm. This can be expressed mathematically as

$$\langle \hat{\mathbf{e}}_i | \hat{\mathbf{e}}_j \rangle = \delta_{ij} \tag{9.13}$$

where δ_{ij} is the Kronecker delta symbol, defined as

$$\delta_{ij} = \begin{cases} 1 & \text{for } i = j \\ 0 & \text{for } i \neq j \end{cases} \tag{9.14}$$

We can therefore write two vectors **a** and **b** in this orthonormal basis as:

$$\mathbf{a} = a_1 \hat{\mathbf{e}}_1 + a_2 \hat{\mathbf{e}}_2 + a_3 \hat{\mathbf{e}}_3 + \ldots\ldots\ldots a_N \hat{\mathbf{e}}_N \tag{9.15}$$

$$\mathbf{b} = b_1 \hat{\mathbf{e}}_1 + b_2 \hat{\mathbf{e}}_2 + b_3 \hat{\mathbf{e}}_3 + \ldots\ldots\ldots b_N \hat{\mathbf{e}}_N \tag{9.16}$$

and their inner product is:

$$\langle \mathbf{a} | \mathbf{b} \rangle = \langle a_1 \hat{\mathbf{e}}_1 + a_2 \hat{\mathbf{e}}_2 + a_3 \hat{\mathbf{e}}_3 + \ldots\ldots\ldots a_N \hat{\mathbf{e}}_N \, | \, b_1 \hat{\mathbf{e}}_1 + b_2 \hat{\mathbf{e}}_2 + b_3 \hat{\mathbf{e}}_3 + \ldots\ldots\ldots b_N \hat{\mathbf{e}}_N \rangle \tag{9.17}$$

We can now expand this using the properties listed above to give:

$$\langle \mathbf{a} | \mathbf{b} \rangle = \sum_{i=1}^{N} a_i^* b_i \langle \hat{\mathbf{e}}_i | \hat{\mathbf{e}}_i \rangle + \sum_{i=1}^{N} \sum_{j \neq i}^{N} a_i^* b_j \langle \hat{\mathbf{e}}_i | \hat{\mathbf{e}}_j \rangle = \sum_{i=1}^{N} a_i^* b_i \tag{9.18}$$

This is as expected from our expression $\langle \mathbf{a} | \mathbf{b} \rangle = \mathbf{a}^* \cdot \mathbf{b}$ above, and is the generalisation of the expression for the inner/dot product of vectors in real 3D space, where the dot product of vectors $\mathbf{a} = a_1 \mathbf{i} + a_2 \mathbf{j} + a_3 \mathbf{k}$ and $\mathbf{b} = b_1 \mathbf{i} + b_2 \mathbf{j} + b_3 \mathbf{k}$ is $a_1 b_1 + a_2 b_2 + a_3 b_3$.

9.1.6. Properties of the inner product

The inner product has the following properties:

$$\langle \mathbf{a}|\mathbf{b}\rangle = \langle \mathbf{b}|\mathbf{a}\rangle^* \tag{9.19}$$

$$\langle \mathbf{a}+\mathbf{b}|\mathbf{c}\rangle = \langle \mathbf{a}|\mathbf{c}\rangle + \langle \mathbf{b}|\mathbf{c}\rangle \tag{9.20}$$

$$\langle \mathbf{a}|\mathbf{b}+\mathbf{c}\rangle = \langle \mathbf{a}|\mathbf{b}\rangle + \langle \mathbf{a}|\mathbf{c}\rangle \tag{9.21}$$

$$\langle \mathbf{a}|c\,\mathbf{b}\rangle = c\langle \mathbf{a}|\mathbf{b}\rangle \tag{9.22}$$

$$\langle c\,\mathbf{a}|\mathbf{b}\rangle = c^*\langle \mathbf{a}|\mathbf{b}\rangle \tag{9.23}$$

9.2. Linear Operators

An operator A associates every vector $\mathbf{x}$ with another vector $\mathbf{y}$:

$$\mathbf{y} = A\mathbf{x} \tag{9.24}$$

The action of A is to transform one geometrical entity (a vector) into another one.

9.2.1. Properties of linear operators (compare with Section 1.5):

- Distributive and associative addition and multiplication:

$$(A+B)\mathbf{x} = A\mathbf{x} + B\mathbf{x} \tag{9.25}$$

$$(\lambda A)\mathbf{x} = \lambda(A\mathbf{x}) \tag{9.26}$$

$$(AB)\mathbf{x} = A(B\mathbf{x}) \tag{9.27}$$

(where A and B are operators, and λ is a scalar constant).

- As we saw earlier, the product of two linear operators is not in general commutative. In other words, in general $AB\mathbf{x} \neq BA\mathbf{x}$.
- Two operators A and B are equal if $A\mathbf{x} = B\mathbf{x}$ for all vectors $\mathbf{x}$.
- The identity operator I is defined as $I\mathbf{x} = \mathbf{x}$.
- If there exists an operator A^{-1} such that $AA^{-1} = A^{-1}A = I$, then this operator A^{-1} is the inverse of A.

Reminder of our previous general definition of a linear operator L acting on functions:

$$L(a\psi + b\Phi) = aL(\psi) + bL(\Phi) \tag{9.28}$$

Similarly, our linear operator A acting on vectors has the property:

$$A(\lambda\mathbf{a} + \mu\mathbf{b}) = \lambda A\mathbf{a} + \mu A\mathbf{b} \tag{9.29}$$

Just as the actual vectors $\mathbf{a}$ and $\mathbf{b}$ are independent of the basis in which they are expressed, the transformational action of operator A is also independent of the basis.

Let's choose a particular basis $\mathbf{e}_1, \mathbf{e}_2, \mathbf{e}_3 \ldots \mathbf{e}_N$ for our N-dimensional complex linear vector space.

The action of operator A on each of these basis vectors is to produce a new linear combination of them:

$$A\mathbf{e}_j = \sum_{i=1}^{N} A_{ij}\mathbf{e}_i \tag{9.30}$$

Here A_{ij} is the i^{th} component of the vector $A\mathbf{e}_j$ in this basis, and collectively the numbers A_{ij} are called the components of the linear operator A in the $\mathbf{e}_i$ basis.

We can therefore write our relation $\mathbf{y} = A\mathbf{x}$ in component form as

$$\mathbf{y} = \sum_{i=1}^{N} y_i \mathbf{e}_i = A\left(\sum_{j=1}^{N} x_j \mathbf{e}_j\right) = \sum_{j=1}^{N} x_j \left(A\mathbf{e}_j\right) = \sum_{j=1}^{N} x_j \sum_{i=1}^{N} A_{ij} \mathbf{e}_i \quad (9.31)$$

So the relationship between the components of **x** and **y**, as expressed in this basis, is:

$$y_i = \sum_{j=1}^{N} A_{ij} x_j \quad (9.32)$$

For this example we chose $\mathbf{e}_1, \mathbf{e}_2, \mathbf{e}_3 \ldots \mathbf{e}_N$ as our basis, and we expressed **x** in component form as $\mathbf{x} = \sum_{i=1}^{N} x_i \mathbf{e}_i$, and **y** (the result of *A* acting on **x**) as $\mathbf{y} = \sum_{i=1}^{N} y_i \mathbf{e}_i$.

However, it's important to remember that there is an infinite choice of basis vectors, but that **x**, **y** and *A* are independent of the choice of basis. The *components* of **x** and **y** will be different in a different basis.

If we now choose $\mathbf{e}_1', \mathbf{e}_2', \mathbf{e}_3' \ldots \mathbf{e}_N'$ as an alternative basis, we will now have that

$$\mathbf{x} = \sum_{i=1}^{N} x_i' \mathbf{e}_i' \quad (9.33)$$

and

$$\mathbf{y} = \sum_{i=1}^{N} y_i' \mathbf{e}_i' \quad (9.34)$$

In this case, the relationship between the components of **x** and **y**, as expressed in this new basis, becomes

$$y_i' = \sum_{j=1}^{N} A_{ij}' x_j' \quad (9.35)$$

9.3. Matrices

Let's continue thinking about our operator expression $\mathbf{y} = A\mathbf{x}$. As we've just seen, both the vectors **x** and **y** and the operator *A* can be expressed in terms of their components with respect to the particular basis/bases chosen, i.e. in terms of x_i, y_i and A_{ij}.

These components may be expressed as matrices. These are column matrices for **x** and **y**. (NB: I'm going to use the term "column matrix", rather than "column vector", to emphasise the distinction between the actual vectors and their representation in a particular basis).

Let's suppose that vector **x** is in an *N*-dimensional vector space for which we have chosen a particular basis $\mathbf{e}_1, \mathbf{e}_2, \mathbf{e}_3 \ldots \mathbf{e}_N$. The components of vector **x** with respect to this basis are x_i, and can be represented by the following column matrix x:

$$\mathsf{x} = \begin{pmatrix} x_1 \\ x_2 \\ x_3 \\ \vdots \\ x_N \end{pmatrix} \quad (9.36)$$

Vector **y** may be in the same vector space as **x**, but more generally it may be in a different *M*-dimensional vector space, and represented in a different basis $\mathbf{f}_1, \mathbf{f}_2, \mathbf{f}_3 \ldots \mathbf{f}_M$. The components of **y** with respect to this basis would then be represented by the following column matrix y:

$$\mathsf{y} = \begin{pmatrix} y_1 \\ y_2 \\ y_3 \\ \vdots \\ y_M \end{pmatrix} \quad (9.37)$$

Operator A therefore transforms vectors from an N-dimensional vector space with basis $\mathbf{e}_1, \mathbf{e}_2, \mathbf{e}_3 \ldots \mathbf{e}_N$ to an M-dimensional vector space with basis $\mathbf{f}_1, \mathbf{f}_2, \mathbf{f}_3 \ldots \mathbf{f}_M$. It can be represented by the following M x N matrix:

$$\mathsf{A} = \begin{pmatrix} A_{11} & A_{12} & \cdots & A_{1N} \\ A_{21} & A_{22} & \cdots & A_{2N} \\ \vdots & \vdots & \ddots & \vdots \\ A_{M1} & A_{M2} & \cdots & A_{MN} \end{pmatrix} \tag{9.38}$$

The component A_{ij} of operator A can therefore also be written as the matrix element $(\mathsf{A})_{ij}$.

If vectors **x** and **y** are in the same vector space, then operator A will be represented by a square matrix A.

9.3.1. Reminder of basic matrix algebra

You should remember from PH10007 how to:

- Add and subtract two matrices
- Multiply a matrix by a scalar
- Find the transpose of a matrix
- Multiply two matrices together
- Find the determinant of a matrix
- Find the inverse of a matrix.

9.3.2. Complex and Hermitian conjugates

The complex conjugate of a matrix A is the matrix obtained by taking the complex conjugate of each of the elements of A, and is denoted as A^*. In other words,

$$\left(\mathsf{A}^*\right)_{ij} = \left(A_{ij}\right)^* \tag{9.39}$$

The Hermitian conjugate of a matrix A is the transpose of its complex conjugate (or, alternatively the complex conjugate of its transpose), and is denoted as $\mathsf{A}^\dagger$. In other words,

$$\mathsf{A}^\dagger = \left(\mathsf{A}^*\right)^{\mathrm{T}} = \left(\mathsf{A}^{\mathrm{T}}\right)^* \tag{9.40}$$

We can use the definition of the Hermitian conjugate to derive an alternative expression for the inner product of two matrices.

Suppose we have vectors **a** and **b**, which are represented in a particular orthonormal basis by the matrices a and b, as follows:

$$\mathsf{a} = \begin{pmatrix} a_1 \\ a_2 \\ a_3 \\ \vdots \\ a_N \end{pmatrix} \text{ and } \mathsf{b} = \begin{pmatrix} b_1 \\ b_2 \\ b_3 \\ \vdots \\ b_N \end{pmatrix}.$$

The Hermitian conjugate of a is

$$\mathsf{a}^\dagger = \begin{pmatrix} a_1^* & a_2^* & a_3^* & \cdots & a_N^* \end{pmatrix} \tag{9.41}$$

We can therefore write that

$$\mathsf{a}^\dagger \mathsf{b} = \begin{pmatrix} a_1^* & a_2^* & a_3^* & \cdots & a_N^* \end{pmatrix} \begin{pmatrix} b_1 \\ b_2 \\ b_3 \\ \vdots \\ b_N \end{pmatrix} = \sum_{i=1}^{N} a_i^* b_i \tag{9.42}$$

But this is the same expression that we found for the inner product earlier:

$$\langle \mathbf{a} | \mathbf{b} \rangle = \mathbf{a}^* \cdot \mathbf{b} \tag{9.43}$$

So, for an orthonormal basis, we can say that

$$\langle \mathbf{a} | \mathbf{b} \rangle = \mathbf{a}^* \cdot \mathbf{b} = \mathsf{a}^\dagger \mathsf{b} \tag{9.44}$$

where a and b are the matrices representing vectors **a** and **b** in this particular orthonormal basis.

9.3.3. Properties of determinants

$$|\mathsf{A}^{\mathrm{T}}| = |\mathsf{A}| \tag{9.45}$$

$$|\mathsf{A}^*| = |\mathsf{A}|^* \tag{9.46}$$

$$|\mathsf{A}^\dagger| = |\mathsf{A}|^* \tag{9.47}$$

9.3.4. Properties of inverse matrices

$$\left(\mathsf{A}^{-1}\right)^{-1} = \mathsf{A} \tag{9.48}$$

$$\left(\mathsf{A}^{\mathrm{T}}\right)^{-1} = \left(\mathsf{A}^{-1}\right)^{\mathrm{T}} \tag{9.49}$$

$$\left(\mathsf{A}^\dagger\right)^{-1} = \left(\mathsf{A}^{-1}\right)^\dagger \tag{9.50}$$

9.3.5. Properties of products of matrices

$$|\mathsf{AB}| = |\mathsf{A}||\mathsf{B}| = |\mathsf{BA}| \tag{9.51}$$

$$(\mathsf{AB})^* = \mathsf{A}^*\mathsf{B}^* \tag{9.52}$$

$$(\mathsf{AB})^{\mathrm{T}} = \mathsf{B}^{\mathrm{T}}\mathsf{A}^{\mathrm{T}} \tag{9.53}$$

$$(\mathsf{AB})^{-1} = \mathsf{B}^{-1}\mathsf{A}^{-1} \tag{9.54}$$

$$(\mathsf{AB})^\dagger = \mathsf{B}^\dagger\mathsf{A}^\dagger \tag{9.55}$$

(Note the reversal of the order of A and B in equations (9.53) to (9.55)).

9.4. Special types of square matrix

9.4.1. Diagonal matrices

$$\mathsf{D} = \begin{pmatrix} A_{11} & 0 & \cdots & 0 \\ 0 & A_{22} & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & A_{NN} \end{pmatrix} \tag{9.56}$$

All non-leading diagonal elements must be zero.

9.4.2. Identity matrix

$$\mathrm{I} = \begin{pmatrix} 1 & 0 & \cdots & 0 \\ 0 & 1 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & 1 \end{pmatrix} \tag{9.57}$$

Diagonal matrix for which all leading diagonal elements are equal to 1.

$$(\mathrm{I})_{ij} = \delta_{ij} = \begin{cases} 1 & \text{for } i = j \\ 0 & \text{for } i \neq j \end{cases} \tag{9.58}$$

The identity matrix has the property that $\mathsf{A}\mathsf{A}^{-1} = \mathrm{I}$.

9.4.3. Upper/lower triangular matrices

$$\mathsf{U} = \begin{pmatrix} A_{11} & A_{12} & A_{13} & \cdots & A_{1N} \\ 0 & A_{22} & A_{23} & \cdots & A_{2N} \\ 0 & 0 & A_{33} & \cdots & A_{3N} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & \cdots & A_{NN} \end{pmatrix} \tag{9.59}$$

$$\mathsf{L} = \begin{pmatrix} A_{11} & 0 & 0 & \cdots & 0 \\ A_{21} & A_{22} & 0 & \cdots & 0 \\ A_{31} & A_{32} & A_{33} & \cdots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ A_{N1} & A_{N2} & A_{N3} & \cdots & A_{NN} \end{pmatrix} \qquad (9.60)$$

9.4.4. Symmetric and anti-symmetric matrices

A symmetric matrix A has the property that $\mathsf{A} = \mathsf{A}^T$, where A^T is the transpose of A. In other words, $A_{ij} = A_{ji}$.

Example of a symmetric matrix:

$$\mathsf{A} = \begin{pmatrix} 3 & i & 2 \\ i & 5-i & -4 \\ 2 & -4 & 2i \end{pmatrix}$$

An anti-symmetric matrix A has the property that $\mathsf{A} = -\mathsf{A}^T$, where A^T is the transpose of A. In other words, $A_{ij} = -A_{ji}$, which means that all leading diagonal elements must be equal to zero.

Example of an anti-symmetric matrix:

$$\mathsf{A} = \begin{pmatrix} 0 & i & -2 \\ -i & 0 & 4 \\ 2 & -4 & 0 \end{pmatrix}$$

Any N x N matrix A can be written as the sum of a symmetric and an anti-symmetric matrix:

$$\mathsf{A} = \frac{1}{2}\left(\mathsf{A} + \mathsf{A}^T\right) + \frac{1}{2}\left(\mathsf{A} - \mathsf{A}^T\right) = \mathsf{B} + \mathsf{C} \qquad (9.61)$$

where $\mathsf{B} = \frac{1}{2}\left(\mathsf{A} + \mathsf{A}^T\right)$ is a symmetric matrix, and $\mathsf{C} = \frac{1}{2}\left(\mathsf{A} - \mathsf{A}^T\right)$ is an anti-symmetric matrix.

9.4.5. Hermitian and anti-Hermitian matrices

A Hermitian matrix A has the property that $\mathsf{A} = \mathsf{A}^\dagger$, where $\mathsf{A}^\dagger$ is the Hermitian conjugate of A. In other words, $A_{ij} = A_{ji}^*$.

Example of a Hermitian matrix:

$$\mathsf{A} = \begin{pmatrix} 3 & i & 2-i \\ -i & 5 & -4 \\ 2+i & -4 & 2 \end{pmatrix}$$

An anti-Hermitian matrix A has the property that $\mathsf{A} = -\mathsf{A}^\dagger$. . In other words, $A_{ij} = -A_{ji}^*$, which again means that all leading diagonal elements must be equal to zero.

Example of an anti-Hermitian matrix:

$$\mathsf{A} = \begin{pmatrix} 0 & i & 2-i \\ i & 0 & -4 \\ -2-i & 4 & 0 \end{pmatrix}$$

Any N x N matrix A can be written as the sum of a Hermitian and an anti-Hermitian matrix:

$$\mathsf{A} = \frac{1}{2}\left(\mathsf{A} + \mathsf{A}^\dagger\right) + \frac{1}{2}\left(\mathsf{A} - \mathsf{A}^\dagger\right) = \mathsf{B} + \mathsf{C} \qquad (9.62)$$

where $\mathsf{B} = \frac{1}{2}\left(\mathsf{A} + \mathsf{A}^\dagger\right)$ is a Hermitian matrix, and $\mathsf{C} = \frac{1}{2}\left(\mathsf{A} - \mathsf{A}^\dagger\right)$ is an anti- Hermitian matrix.

9.4.6. Orthogonal matrices

An orthogonal matrix A is a non-singular matrix (i.e. a matrix with a non-zero determinant) which has the property that $\mathsf{A}^{\mathrm{T}} = \mathsf{A}^{-1}$, i.e. its transpose is also its inverse.

In general, $\mathsf{A}\mathsf{A}^{-1} = \mathrm{I}$. Therefore, for an orthogonal matrix:

$$\mathsf{A}\mathsf{A}^{T} = \mathrm{I} \tag{9.63}$$

But remember that $\left|\mathsf{A}^{\mathrm{T}}\right| = \left|\mathsf{A}\right|$ (for any matrix A).

So for an orthogonal matrix:

$$\left|\mathsf{A}^{-1}\right| = \left|\mathsf{A}\right| \tag{9.64}$$

Hence:

$$\left|\mathsf{A}\right|^2 = \left|\mathsf{A}\right|\left|\mathsf{A}\right| = \left|\mathsf{A}\right|\left|\mathsf{A}^{-1}\right| = \left|\mathsf{A}\mathsf{A}^{-1}\right| = \left|\mathrm{I}\right| = 1 \tag{9.65}$$

So the determinant of an orthogonal matrix is $\left|\mathsf{A}\right| = \pm 1$.

9.4.7. Unitary matrices

A unitary matrix A is a non-singular matrix (i.e. a matrix with a non-zero determinant) which has the property that $\mathsf{A}^{\dagger} = \mathsf{A}^{-1}$, i.e. its Hermitian conjugate is also its inverse.

In general, $\mathsf{A}\mathsf{A}^{-1} = \mathrm{I}$. Therefore, for a unitary matrix:

$$\mathsf{A}\mathsf{A}^{\dagger} = \mathrm{I} \tag{9.66}$$

But remember that $\left|\mathsf{A}^{\dagger}\right| = \left|\mathsf{A}\right|^{*}$ (for any matrix A).

So for a unitary matrix

$$\left|\mathsf{A}\mathsf{A}^{\dagger}\right| = \left|\mathsf{A}\right|\left|\mathsf{A}^{\dagger}\right| = \left|\mathsf{A}\right|\left|\mathsf{A}\right|^{*} \tag{9.67}$$

Combining this with equation (9.66) gives:

$$\left|\mathsf{A}\right|\left|\mathsf{A}\right|^{*} = \left|\mathsf{A}\mathsf{A}^{\dagger}\right| = \left|\mathrm{I}\right| = 1 \tag{9.68}$$

So the determinant of a unitary matrix has a modulus (i.e. a norm, 'magnitude' or 'length') of 1.

Let's look at what this means in terms of our previous operator expression $\mathbf{y} = A\mathbf{x}$, expressed in some basis by the matrix equation

$$\mathsf{y} = \mathsf{A}\,\mathsf{x} \tag{9.69}$$

Let's now suppose that A is a unitary matrix. Since the rows and columns of a unitary matrix form an orthonormal basis (we're not going to prove this here), we can therefore use the following expression (from equation (9.44)) for the inner product:

$$\langle \mathbf{a} | \mathbf{b} \rangle = \mathbf{a}^{*} \cdot \mathbf{b} = \mathsf{a}^{\dagger}\mathsf{b} \tag{9.70}$$

We can therefore write that

$$\langle \mathbf{y} | \mathbf{y} \rangle = \mathsf{y}^{\dagger}\mathsf{y} \tag{9.71}$$

Combining this with equation (9.69) gives:

$$\langle \mathbf{y} | \mathbf{y} \rangle = \mathsf{y}^{\dagger}\mathsf{y} = \left(\mathsf{A}\,\mathsf{x}\right)^{\dagger}\mathsf{A}\mathsf{x} = \mathsf{x}^{\dagger}\mathsf{A}^{\dagger}\mathsf{A}\mathsf{x} \tag{9.72}$$

But A is a unitary matrix, and so $\mathsf{A}^{\dagger} = \mathsf{A}^{-1}$.

Substituting this into equation (9.72) gives:

$$\langle \mathbf{y} | \mathbf{y} \rangle = \mathsf{x}^{\dagger}\mathsf{A}^{\dagger}\mathsf{A}\mathsf{x} = \mathsf{x}^{\dagger}\mathsf{A}^{-1}\mathsf{A}\mathsf{x} = \mathsf{x}^{\dagger}\mathsf{x} = \langle \mathbf{x} | \mathbf{x} \rangle \tag{9.73}$$

Hence, the action of a linear operator A that is represented by a unitary matrix does not change the norm of a complex vector – the norm of vector **y** is equal to the norm of vector **x**.

9.4.8. Normal matrices

A normal matrix A is a matrix that commutes with its Hermitian conjugate. In other words $\mathsf{A}\mathsf{A}^\dagger = \mathsf{A}^\dagger\mathsf{A}$.

Hermitian matrices and unitary matrices are examples of normal matrices.

If A is a normal matrix, its inverse A^{-1} is also normal. We can show this as follows (using the general rules in section 9.3):

$$\mathsf{A}^{-1}\left(\mathsf{A}^{-1}\right)^\dagger = \mathsf{A}^{-1}\left(\mathsf{A}^\dagger\right)^{-1} = \left(\mathsf{A}^\dagger\mathsf{A}\right)^{-1} \tag{9.74}$$

But A is a normal matrix, and so $\mathsf{A}\mathsf{A}^\dagger = \mathsf{A}^\dagger\mathsf{A}$.

So

$$\mathsf{A}^{-1}\left(\mathsf{A}^{-1}\right)^\dagger = \left(\mathsf{A}\mathsf{A}^\dagger\right)^{-1} = \left(\mathsf{A}^{-1}\right)^\dagger\mathsf{A}^{-1} = \left(\mathsf{A}^\dagger\right)^{-1}\mathsf{A}^{-1} = \left(\mathsf{A}^{-1}\right)^\dagger\mathsf{A}^{-1} \tag{9.75}$$

In other words, if A is a normal matrix, its inverse A^{-1} is also normal.

9.5. Eigenvectors and eigenvalues

Let's again consider our previous operator expression $\mathbf{y} = A\mathbf{x}$, expressed in some basis by the matrix equation $\mathsf{y} = \mathsf{A}\mathsf{x}$. Let's also consider the possibility that there exist some vectors **x** for which the effect of linear operator *A* acting on them in an *N*-dimensional vector space is to turn them into multiples of themselves. These vectors would then have to satisfy the equation

$$A\mathbf{x} = \lambda\mathbf{x} \tag{9.76}$$

where λ is a scalar.

Any non-zero vector **x** that satisfies this equation is called an eigenvector of operator *A*, and λ is the eigenvalue corresponding to this eigenvector.

In general, there will be *N* solutions to this equation, corresponding to *N* independent eigenvectors $\mathbf{x}^i$ (note that the *i* is a superscript, not a power), each of which has an eigenvalue λ_i (although the eigenvalues may not all be distinct).

As usual, we can choose a particular basis in the vector space, and hence write this equation in terms of the matrix components of *A* and **x** with respect to this basis:

$$\mathsf{A}\mathsf{x} = \lambda\mathsf{x} \tag{9.77}$$

The column matrices x that satisfy this equation are the eigenvectors of matrix A, and represent the eigenvectors **x** of *A* in our chosen basis.

If x is an eigenvector of A, with eigenvalue λ, then any scalar multiple of x will also be an eigenvector of A, with the same eigenvalue.

We will therefore usually use normalised eigenvectors, for which

$$\langle\mathbf{x}|\mathbf{x}\rangle = \mathsf{x}^\dagger\mathsf{x} = 1 \tag{9.78}$$

9.5.1. Eigenvectors and eigenvalues of normal matrices

Remember that a normal matrix A is a matrix that commutes with its Hermitian conjugate, so that $\mathsf{A}\mathsf{A}^\dagger = \mathsf{A}^\dagger\mathsf{A}$, and that Hermitian matrices and unitary matrices are examples of normal matrices.

Suppose that x is an eigenvector of a normal matrix A, with eigenvalue λ:

$$\mathsf{A}\mathsf{x} = \lambda\mathsf{x} \tag{9.79}$$

So

$$\left(\mathsf{A} - \lambda\mathrm{I}\right)\mathsf{x} = 0 \tag{9.80}$$

We can now take the Hermitian conjugate of this equation:

$$\left(\left(\mathsf{A} - \lambda\mathrm{I}\right)\mathsf{x}\right)^\dagger = 0 \tag{9.81}$$

Using the general matrix identities in section 9.3, we can now write:

$$\mathbf{x}^\dagger (\mathbf{A} - \lambda \mathbf{I})^\dagger = 0 \tag{9.82}$$

Multiplying equations (9.80) and (9.82) together gives

$$\mathbf{x}^\dagger (\mathbf{A} - \lambda \mathbf{I})^\dagger (\mathbf{A} - \lambda \mathbf{I}) \mathbf{x} = 0 \tag{9.83}$$

Now let's think about the middle two brackets, i.e. $(\mathbf{A} - \lambda \mathbf{I})^\dagger (\mathbf{A} - \lambda \mathbf{I})$.

$$\begin{aligned} (\mathbf{A} - \lambda \mathbf{I})^\dagger (\mathbf{A} - \lambda \mathbf{I}) &= (\mathbf{A}^\dagger - \lambda^* \mathbf{I})(\mathbf{A} - \lambda \mathbf{I}) \\ &= \mathbf{A}^\dagger \mathbf{A} - \lambda^* \mathbf{A} - \lambda \mathbf{A}^\dagger + \lambda^* \lambda \end{aligned} \tag{9.84}$$

But $\mathbf{A}$ is normal, and so $\mathbf{A}^\dagger \mathbf{A} = \mathbf{A}\mathbf{A}^\dagger$. Therefore:

$$\begin{aligned} (\mathbf{A} - \lambda \mathbf{I})^\dagger (\mathbf{A} - \lambda \mathbf{I}) &= \mathbf{A}\mathbf{A}^\dagger - \lambda^* \mathbf{A} - \lambda \mathbf{A}^\dagger + \lambda^* \lambda \\ &= (\mathbf{A} - \lambda \mathbf{I})(\mathbf{A}^\dagger - \lambda^* \mathbf{I}) \end{aligned} \tag{9.85}$$

But

$$(\mathbf{A}^\dagger - \lambda^* \mathbf{I}) = (\mathbf{A} - \lambda \mathbf{I})^\dagger \tag{9.86}$$

Combining equations (9.85) and (9.86) gives that

$$(\mathbf{A} - \lambda \mathbf{I})^\dagger (\mathbf{A} - \lambda \mathbf{I}) = (\mathbf{A} - \lambda \mathbf{I})(\mathbf{A} - \lambda \mathbf{I})^\dagger \tag{9.87}$$

In other words, we have shown that if $\mathbf{A}$ is normal, $\mathbf{A} - \lambda \mathbf{I}$ will also be normal.

Now let's return to equation (9.83). Because $\mathbf{A} - \lambda \mathbf{I}$ is normal, we can rewrite this as:

$$\mathbf{x}^\dagger (\mathbf{A} - \lambda \mathbf{I})(\mathbf{A} - \lambda \mathbf{I})^\dagger \mathbf{x} = 0 \tag{9.88}$$

Using the general identities in section 9.3, we can then rearrange this as

$$\left((\mathbf{A} - \lambda \mathbf{I})^\dagger \mathbf{x}\right)^\dagger \left((\mathbf{A} - \lambda \mathbf{I})^\dagger \mathbf{x}\right) = 0 \tag{9.89}$$

But remember that the norm of a vector is given by $\langle \mathbf{x} | \mathbf{x} \rangle = \mathbf{x}^\dagger \mathbf{x}$.

So we have found that the norm of $(\mathbf{A} - \lambda \mathbf{I})^\dagger \mathbf{x}$ is equal to 0, and hence that:

$$(\mathbf{A} - \lambda \mathbf{I})^\dagger \mathbf{x} = 0 \tag{9.90}$$

Rearranging this gives:

$$(\mathbf{A}^\dagger - \lambda^* \mathbf{I}) \mathbf{x} = 0 \tag{9.91}$$

So our eigenvector equation for $\mathbf{A}^\dagger$ is

$$\mathbf{A}^\dagger \mathbf{x} = \lambda^* \mathbf{x} \tag{9.92}$$

In other words, for a normal matrix $\mathbf{A}$, the eigenvalues of $\mathbf{A}^\dagger$ are the complex conjugates of the eigenvalues of $\mathbf{A}$.

Let's now think about two eigenvectors $\mathbf{x}^i$ and $\mathbf{x}^j$ of a normal matrix $\mathbf{A}$, corresponding to two different eigenvalues λ_i and λ_j:

$$\mathbf{A}\mathbf{x}^i = \lambda_i \mathbf{x}^i \tag{9.93}$$

$$\mathbf{A}\mathbf{x}^j = \lambda_j \mathbf{x}^j \tag{9.94}$$

We can now multiply both sides of equation (9.94) by $(\mathbf{x}^i)^\dagger$:

$$(\mathbf{x}^i)^\dagger \mathbf{A}\mathbf{x}^j = \lambda_j (\mathbf{x}^i)^\dagger \mathbf{x}^j \tag{9.95}$$

However, we have just found (equation (9.92)) that $\mathbf{A}^\dagger \mathbf{x}^i = \lambda_i^* \mathbf{x}^i$, and we also remember the general identity that $(\mathbf{A}\mathbf{B})^\dagger = \mathbf{B}^\dagger \mathbf{A}^\dagger$.

So:

$$(\mathbf{x}^i)^\dagger \mathbf{A} = (\mathbf{A}^\dagger \mathbf{x}^i)^\dagger = (\lambda_i^* \mathbf{x}^i)^\dagger = \lambda_i (\mathbf{x}^i)^\dagger \tag{9.96}$$

Substituting this into equation (9.95) gives:

$$\lambda_i \left(\mathbf{x}^i\right)^\dagger \mathbf{x}^j = \lambda_j \left(\mathbf{x}^i\right)^\dagger \mathbf{x}^j \qquad (9.97)$$

Rearranging gives:

$$\left(\lambda_i - \lambda_j\right)\left(\mathbf{x}^i\right)^\dagger \mathbf{x}^j = 0 \qquad (9.98)$$

Thus, if $\lambda_i \neq \lambda_j$, $\left(\mathbf{x}^i\right)^\dagger \mathbf{x}^j = 0$.

But remember that $\left(\mathbf{x}^i\right)^\dagger \mathbf{x}^j$ represents the inner product of the eigenvectors $\mathbf{x}^i$ and $\mathbf{x}^j$. Since this inner product is equal to 0, this means that the eigenvectors $\mathbf{x}^i$ and $\mathbf{x}^j$ must be orthogonal.

So we've found two important properties of normal matrices:

i. The eigenvalues of $\mathbf{A}^\dagger$ are the complex conjugates of the eigenvalues of $\mathbf{A}$, i.e. if $\mathbf{A}\mathbf{x} = \lambda\mathbf{x}$, then $\mathbf{A}^\dagger\mathbf{x} = \lambda^*\mathbf{x}$.

ii. If all N eigenvalues of a normal matrix $\mathbf{A}$ are distinct, then all N eigenvectors of $\mathbf{A}$ are mutually orthogonal. These N eigenvectors provide a basis for the N-dimensional vector space, and so any arbitrary vector $\mathbf{y}$ can be expressed as a linear combination of these eigenvectors:
$\mathbf{y} = \sum_{i=1}^{N} a_i \mathbf{x}^i$, where $a_i = \left(\mathbf{x}^i\right)^\dagger \mathbf{y}$.
The eigenvectors therefore form an orthogonal basis for the vector space, and this can be made an orthonormal basis by normalising the eigenvectors, so that $\left(\mathbf{x}^i\right)^\dagger \mathbf{x}^i = 1$.

9.5.2. Eigenvectors and eigenvalues of Hermitian and anti-Hermitian matrices

We've just shown that for a normal matrix, if $\mathbf{A}\mathbf{x} = \lambda\mathbf{x}$, then $\mathbf{A}^\dagger\mathbf{x} = \lambda^*\mathbf{x}$.

Now consider two cases:

i. If this normal matrix is also Hermitian, then $\mathbf{A} = \mathbf{A}^\dagger$. So we can then write that $\mathbf{A}\mathbf{x} = \lambda^*\mathbf{x}$, and hence that $\lambda = \lambda^*$. This can only be the case if λ is real.

ii. Alternatively, if our normal matrix is anti-Hermitian, then $\mathbf{A} = -\mathbf{A}^\dagger$. So we can then write that $\mathbf{A}\mathbf{x} = -\lambda^*\mathbf{x}$, and hence that $\lambda = -\lambda^*$. This can only be the case if λ is imaginary.

We've therefore found some important properties of Hermitian and anti-Hermitian matrices:

i. The eigenvalues of a Hermitian matrix are real.

ii. The eigenvalues of an anti-Hermitian matrix are imaginary.

iii. Since Hermitian and anti-Hermitian matrices are examples of normal matrices, their eigenvectors are also mutually orthogonal, and hence can form an orthonormal basis.

9.5.3. Eigenvectors and eigenvalues of unitary matrices

For a unitary matrix, $\mathbf{A}^\dagger = \mathbf{A}^{-1}$, and we also know the general identity $\mathbf{A}\mathbf{A}^{-1} = \mathbf{A}^{-1}\mathbf{A} = \mathbf{I}$.

So we can then write that

$$\mathbf{x}^\dagger \mathbf{x} = \mathbf{x}^\dagger \mathbf{I} \mathbf{x} = \mathbf{x}^\dagger \mathbf{A}^\dagger \mathbf{A} \mathbf{x}$$

But we also know that $\mathbf{A}\mathbf{x} = \lambda \mathbf{x}$, and taking the Hermitian conjugate of this equation gives $(\mathbf{A}\mathbf{x})^\dagger = (\lambda \mathbf{x})^\dagger$, which we can expand as $\mathbf{x}^\dagger \mathbf{A}^\dagger = \lambda^* \mathbf{x}^\dagger$.

Substituting these into our expression above gives

$$\mathbf{x}^\dagger \mathbf{x} = (\lambda^* \mathbf{x}^\dagger)(\lambda \mathbf{x}) = \lambda^* \lambda \mathbf{x}^\dagger \mathbf{x}$$

So we can deduce that $\lambda^* \lambda = |\lambda^2| = 1$, or in other words, that the eigenvalues of a unitary matrix all have unit modulus.

9.5.4. Eigenvectors and eigenvalues of a general square matrix

If a general *N* x *N* square matrix is not normal, there will not in general be anything special about its eigenvectors and eigenvalues. The *N* eigenvectors will not all be mutually orthogonal, and may not all be linearly independent.

9.6. Commuting matrices

An important question arises when we consider two different *N* x *N* normal matrices $\mathbf{A}$ and $\mathbf{B}$. Under what conditions can these matrices have the same set of eigenvectors?

The answer is that they will have the same set of eigenvectors if and only if they commute – i.e. if $\mathbf{AB} = \mathbf{BA}$. We'll prove this in two parts:

i. **'If they commute':** We start by considering two general matrices that commute, and show that they have the same set of eigenvectors.

ii. **'Only if they commute':** We then consider two general matrices with the same set of eigenvectors, and show that they must commute.

9.6.1. If they commute:

Let's start by considering two normal matrices $\mathbf{A}$ and $\mathbf{B}$ that commute – we're aiming to prove that $\mathbf{A}$ and $\mathbf{B}$ must then have the same set of eigenvectors.

We start with defining the eigenvector equation for $\mathbf{A}$ as $\mathbf{A}\mathbf{x}^i = \lambda_i \mathbf{x}^i$, where $\mathbf{x}^i$ is the i^{th} eigenvector of $\mathbf{A}$, with corresponding eigenvalue λ_i.

Because $\mathbf{A}$ and $\mathbf{B}$ commute, we can write that

$$\mathbf{AB}\mathbf{x}^i = \mathbf{BA}\mathbf{x}^i \tag{9.99}$$

But

$$\mathbf{A}\mathbf{x}^i = \lambda_i \mathbf{x}^i \tag{9.100}$$

So this gives that

$$\mathbf{AB}\mathbf{x}^i = \mathbf{BA}\mathbf{x}^i = \mathbf{B}\lambda_i \mathbf{x}^i = \lambda_i \mathbf{B}\mathbf{x}^i \tag{9.101}$$

So

$$\mathbf{A}(\mathbf{B}\mathbf{x}^i) = \lambda_i (\mathbf{B}\mathbf{x}^i) \tag{9.102}$$

This is a new eigenvector equation, which states that $\mathbf{B}\mathbf{x}^i$ is an eigenvector of $\mathbf{A}$, with corresponding eigenvalue λ_i.

But $\mathbf{A}$ is a normal vector, and hence we know that it has *N* linearly independent mutually orthogonal eigenvectors, which we defined via the equation $\mathbf{A}\mathbf{x}^i = \lambda_i \mathbf{x}^i$, with $i = 1, 2, 3 \ldots N$.

These N eigenvectors form a complete set, which are unique (apart from that each of them could be scaled by a constant factor).

So this means that if $\mathsf{B}\mathbf{x}^i$ is an eigenvector of A, as we've just found that it is, then $\mathsf{B}\mathbf{x}^i$ must be equal to $\mathbf{x}^i$, or a scalar multiple of $\mathbf{x}^i$. In other words, $\mathsf{B}\mathbf{x}^i = \mu_i \mathbf{x}^i$, where μ_i is a scalar.

But this is just an eigenvector equation for B, which tells us that $\mathbf{x}^i$ is an eigenvector of B, as well as being an eigenvector of A.

We can extend this to every value of i, from 1 to N, and we could also swap the order of matrices A and B to show that every eigenvector of A is also an eigenvector of B.

In other words, we've shown that if matrices A and B commute, every eigenvector of B is an eigenvector of A, and vice versa.

9.6.2. Only if they commute:

To complete our 'if and only if' proof, we now need to show the converse – i.e. if two matrices A and B have all the same eigenvectors, that they therefore commute.

If two matrices A and B have all the same eigenvectors, then we can write the following for each of their i^{th} eigenvectors $\mathbf{x}^i$:

$\mathsf{A}\mathbf{x}^i = \lambda_i \mathbf{x}^i$ and $\mathsf{B}\mathbf{x}^i = \mu_i \mathbf{x}^i$.

The N eigenvectors form a complete orthogonal/orthonormal basis, and any arbitrary vector $\mathbf{x}$ can therefore be expressed as a linear combination of them:

$$\mathbf{x} = \sum_{i=1}^{N} c_i \mathbf{x}^i \qquad (9.103)$$

Let's now substitute this into the expression for $\mathsf{AB}\mathbf{x}$:

$$\mathsf{AB}\mathbf{x} = \mathsf{AB}\sum_{i=1}^{N} c_i \mathbf{x}^i \qquad (9.104)$$

Now substitute in that $\mathsf{B}\mathbf{x}^i = \mu_i \mathbf{x}^i$ and $\mathsf{A}\mathbf{x}^i = \lambda_i \mathbf{x}^i$:

$$\begin{aligned} \mathsf{ABx} &= \mathsf{AB}\sum_{i=1}^{N} c_i \mathbf{x}^i \\ &= \mathsf{A}\sum_{i=1}^{N} c_i \mu_i \mathbf{x}^i \qquad (9.105) \\ &= \sum_{i=1}^{N} c_i \lambda_i \mu_i \mathbf{x}^i \end{aligned}$$

We can now carry out the equivalent working on the expression for $\mathsf{BA}\mathbf{x}$:

$$\begin{aligned} \mathsf{BAx} &= \mathsf{BA}\sum_{i=1}^{N} c_i \mathbf{x}^i \\ &= \mathsf{B}\sum_{i=1}^{N} c_i \lambda_i \mathbf{x}^i \qquad (9.106) \\ &= \sum_{i=1}^{N} c_i \mu_i \lambda_i \mathbf{x}^i \end{aligned}$$

Comparing equations (9.105) and (9.106) shows that

$$\mathsf{ABx} = \mathsf{BAx} \qquad (9.107)$$

and hence that

$$(\mathsf{AB} - \mathsf{BA})\mathbf{x} = 0 \qquad (9.108)$$

In other words, we've shown that if two matrices A and B have all the same eigenvectors, that they therefore commute.

9.7. Infinite dimensional vector spaces

Suppose we have some well-behaved functions $f(x)$, $g(x)$, $h(x)$ within an interval $a \le x \le b$, and that these functions form a linear vector space (referring back to our previous definition in section 9.1.3).

Remember back to when we expressed an arbitrary vector **x** lying within an *N*-dimensional vector space (*V*) in terms of a linear combination of *N* linearly independent basis vectors:

$$\mathbf{x} = x_1\mathbf{e}_1 + x_2\mathbf{e}_2 + x_3\mathbf{e}_3 + x_4\mathbf{e}_4 + \ldots\ldots\ldots + x_N\mathbf{e}_N = \sum_{i=1}^{N} x_i\mathbf{e}_i \quad (9.109)$$

By analogy with this, we can now introduce an infinite set of linearly independent basis functions $y_n(x)$ (where $n = 0,1,2\ldots\infty$), such that our function $f(x)$ can be expressed as a linear sum of these basis functions:

$$f(x) = \sum_{n=0}^{\infty} c_n y_n(x) \quad (9.110)$$

Again similarly to our previous working, any linearly independent set of functions can form a basis, and so we can equally well express the same function $f(x)$ using a different basis $u_n(x)$:

$$f(x) = \sum_{n=0}^{\infty} d_n u_n(x) \quad (9.111)$$

where the d_n are a different set of coefficients.

Recall that the inner product of two vectors **a** and **b** is:

$$\langle \mathbf{a} | \mathbf{b} \rangle = \sum_{i=1}^{N} a_i^* b_i \quad (9.112)$$

In a similar way, we can define the inner product for our functions as

$$\langle f|g\rangle = \int_a^b f^*(x)\,g(x)\rho(x)\,dx \qquad (9.113)$$

where $\rho(x)$ is a weight function, which is real and non-negative over our full range for *x*.

If the weight function is unity for all *x*, as it often is, the inner product becomes:

$$\langle f|g\rangle = \int_a^b f^*(x)\,g(x)\,dx \qquad (9.114)$$

Two functions are said to be orthogonal in the interval $[a,b]$ if

$$\langle f|g\rangle = \int_a^b f^*(x)\,g(x)\rho(x)\,dx = 0 \qquad (9.115)$$

Again, remember that we defined the *norm* (i.e. the 'size') of a vector **a** as $\|\mathbf{a}\| = \langle \mathbf{a}|\mathbf{a}\rangle^{1/2}$.

Similarly, we define the norm of a function $f(x)$ as

$$\begin{aligned}\|f\| &= \langle f\,|\,f\rangle^{1/2} \\ &= \left[\int_a^b f^*(x)\,f(x)\rho(x)\,dx\right]^{1/2} \\ &= \left[\int_a^b |f(x)|^2\,\rho(x)\,dx\right]^{1/2}\end{aligned} \qquad (9.116)$$

So a normalised function $\hat{f}$ (i.e. a function with unit norm) can be expressed as $\hat{f} = \dfrac{f}{\|f\|}$.

An infinite-dimensional vector space of functions, for which an inner product is defined, is known as a Hilbert space.

9.8. Orthonormal basis functions

Just as we saw previously, it is often helpful to choose an orthonormal set of functions as a basis.

Refer back to section 9.7, where we used an infinite set of linearly independent (but not necessarily orthonormal) functions $y_n(x)$ as the basis for our Hilbert space:

$$f(x) = \sum_{n=0}^{\infty} c_n y_n(x) \qquad (9.117)$$

Now suppose we want instead to express our Hilbert space in terms of an orthonormal set of basis functions $\hat{\phi}_n(x)$ (where $n = 0,1,2...\infty$), i.e. a set of functions for which

$$\left\langle \hat{\phi}_i \middle| \hat{\phi}_j \right\rangle = \int_a^b \hat{\phi}_i^*(x)\,\hat{\phi}_j(x)\rho(x)\,dx = \delta_{ij} \qquad (9.118)$$

We can use a method called Gram-Schmidt orthogonalisation to generate a set of orthogonal linearly independent functions $\phi_n(x)$ from a set of non-orthogonal linearly independent functions $y_n(x)$:

$$\begin{aligned}\phi_0 &= y_0 \\ \phi_1 &= y_1 - \hat{\phi}_0\left\langle \hat{\phi}_0 \middle| y_1 \right\rangle \\ \phi_2 &= y_2 - \hat{\phi}_1\left\langle \hat{\phi}_1 \middle| y_2 \right\rangle - \hat{\phi}_0\left\langle \hat{\phi}_0 \middle| y_2 \right\rangle \\ &\ldots \\ \phi_n &= y_n - \hat{\phi}_{n-1}\left\langle \hat{\phi}_{n-1} \middle| y_n \right\rangle - \ldots\ldots - \hat{\phi}_0\left\langle \hat{\phi}_0 \middle| y_n \right\rangle\end{aligned} \qquad (9.119)$$

The set of functions $\phi_n(x)$ generated this way will be orthogonal and linearly independent. To turn them into an orthornomal set $\hat{\phi}_n(x)$, we then just need to normalise each function, by dividing it by its norm.

9.9. Hermitian operators

An operator L is defined as being Hermitian, if the following condition holds over the interval $[a, b]$:

$$\int_a^b f^*(x)\left[Lg(x)\right]dx = \int_a^b \left[Lf(x)\right]^* g(x)dx \qquad (9.120)$$

We've already shown that the eigenvalues of Hermitian matrices are real, and that their eigenfunctions are orthogonal (for distinct eigenvalues).

In a similar way, the eigenvalues of Hermitian operators are real, and their eigenfunctions can be chosen to be orthogonal.

Because of this, Hermitian operators are frequently used in quantum mechanics. Their eigenvalues give the only possible measured values of an observable quantity (such as energy or angular momentum). These observable quantities must be real – this fits with the eigenvalues of Hermitian operators being real.

The infinite set of eigenfunctions of a Hermitian operator form a complete basis set over the interval in question, so that we can expand any function $y(x)$ as an infinite series of eigenfunctions over this interval:

$$y(x) = \sum_{n=0}^{\infty} c_n y_n(x) \qquad (9.121)$$

Again, this fits with the formulation of quantum mechanics, where the wavefunction for a particle in an infinite potential well (for example) can be written as a linear combination of the infinite set of eigenfunctions, each weighted by a coefficient c_n.

9.10. Revisiting Dirac notation

Reminder from PH20013:

Dirac notation denotes a quantum state with wavefunction ψ as $|\psi\rangle$. Since ψ belongs to a vector space of functions, $|\psi\rangle$ is known as a ket vector, or a state vector. What we put inside the $|\ \rangle$ is a label of the state.

The Dirac notation for the Hermitian conjugate of the ket vector $|\psi\rangle$ is called the bra vector $\langle\psi|$. The wavefunction describing this state is ψ^*, the complex conjugate of ψ.

So the inner product of two wavefunctions ψ and ϕ is then written as:

$$\langle\psi|\phi\rangle = \int \psi^*(x)\phi(x)dx \qquad (9.122)$$

For a normalised state

$$\langle\psi|\psi\rangle = \int \psi^*(x)\psi(x)dx = 1 \qquad (9.123)$$

Multiplying a ket vector by a scalar doesn't change the state. Applying an operator, however, may alter the state.

For example, if we have a state ψ whose wavefunction is $\psi(x) = \sin(x)$ and if L is the differential operator $\partial/\partial x$, then

$$|\psi_1\rangle = L|\psi\rangle \equiv |L\psi\rangle = \cos(x) \qquad (9.124)$$

In other words, the effect of operator L acting upon the ket vector $|\psi\rangle$ is to transform it into a ket describing a different state, $|\psi_1\rangle$.

Now let's consider the expression $\langle\phi|L|\psi\rangle$. We already know that

$$L|\psi\rangle = |\psi_1\rangle \tag{9.125}$$

So

$$\langle\phi|L|\psi\rangle = \langle\phi|\psi_1\rangle \tag{9.126}$$

In other words, $\langle\phi|L|\psi\rangle$ represents the inner product of $|\psi_1\rangle$ and $|\phi\rangle$, where $|\psi_1\rangle$ is the resultant of operator L acting on $|\psi\rangle$.

Going back to our definition of a Hermitian operator:

$$\int_a^b f^*(x)\left[Lg(x)\right]dx = \int_a^b \left[Lf^*(x)\right]g(x)dx \tag{9.127}$$

We can now rewrite this in Dirac notation:

$$\langle f|Lg\rangle = \langle Lf|g\rangle = \langle f|L|g\rangle \tag{9.128}$$

9.11. Commutation

As we already know, the product of two linear operators is not in general commutative.

In other words, in general $AB|\psi\rangle \neq BA|\psi\rangle$.

As an example, suppose that A is the differential operator $\partial/\partial x$, and B is the operator 'multiply by x'.

In this case:

$$AB|\psi\rangle = \frac{\partial}{\partial x}(x\psi) = \psi + x\frac{\partial\psi}{\partial x} \tag{9.129}$$

$$BA|\psi\rangle = x\frac{\partial\psi}{\partial x} \tag{9.130}$$

So $AB|\psi\rangle \neq BA|\psi\rangle$.

If $AB|\psi\rangle = BA|\psi\rangle$ for all ket vectors $|\psi\rangle$, then operators A and B are said to commute. If this is not the case, they are said to be non-commuting operators.

The commutator of two linear operators is denoted $[A,B]$, and defined as

The commutator of two linear operators is denoted $[A,B]$, and defined as

$$[A,B]|\psi\rangle = AB|\psi\rangle - BA|\psi\rangle \tag{9.131}$$

The commutator for two commuting operators is equal to zero.

For our previous example

$$\begin{aligned}[A,B]|\psi\rangle &= AB|\psi\rangle - BA|\psi\rangle \\ &= \left(\psi + x\frac{\partial\psi}{\partial x}\right) - x\frac{\partial\psi}{\partial x} \\ &= \psi \\ &= |\psi\rangle\end{aligned} \tag{9.132}$$

In other words, for our example, $[A,B]=1$.

10. APPENDIX: FOURIER SINE AND COSINE SERIES FOR FINITE-RANGE FUNCTIONS

Remember from the Fourier part of unit PH20107 that if an infinite periodic function $f(t)$ has a period T and $\omega_0 = 2\pi / T$, then its Fourier series is:

$$f(t) = \frac{a_0}{2} + \sum_{n=1}^{\infty} a_n \cos(n\omega_0 t) + b_n \sin(n\omega_0 t), \qquad (10.1)$$

where

$$a_n = \frac{2}{T}\int_{t_0}^{t_0+T} f(t)\cos(n\omega_0 t)\,dt \qquad n = 0,\ 1,\ 2,\ 3..... \qquad (10.2)$$

and

$$b_n = \frac{2}{T}\int_{t_0}^{t_0+T} f(t)\sin(n\omega_0 t)\,dt \qquad n = 1,\ 2,\ 3..... \qquad (10.3)$$

Remember also that for an odd function, $a_n = 0$, so that:

$$f(t) = \sum_{n=1}^{\infty} b_n \sin(n\omega_0 t) \qquad (10.4)$$

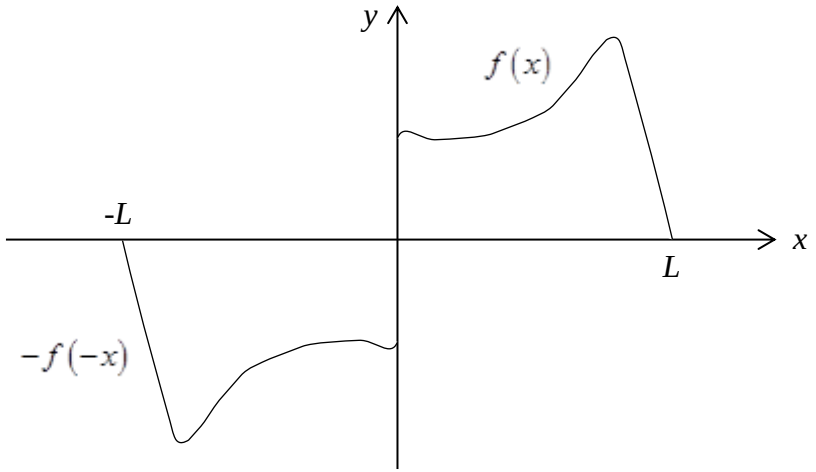
Similarly, for an even function, $b_n = 0$, so that:

$$f(t) = \frac{a_0}{2} + \sum_{n=1}^{\infty} a_n \cos(n\omega_0 t) \qquad (10.5)$$

When solving PDEs we will often need to represent a function that is defined over a finite interval as a Fourier series containing only either sine or cosine terms.

Suppose that we want to represent a function $f(x)$ defined within a finite interval $0 \le x \le L$ as a Fourier series that contains only sine terms.

As outlined in Appendix C of your lecture notes for the Fourier part of PH20107, we can do this by imagining that we artificially extend $f(x)$ to negative *x* as an odd function, as shown in the diagram below:



We can then imagine repeating this unit (i.e. the odd function which now extends over the interval $-L \le x \le L$) with a period $T = 2L$, to give an infinite periodic odd function.

By comparison with equations (10.4) and (10.3), we can therefore write the Fourier series for $f(x)$ in the finite interval $0 \le x \le L$ as:

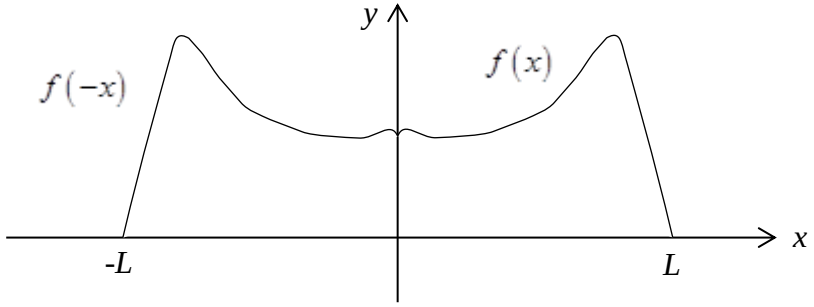
$$f(x) = \sum_{n=1}^{\infty} b_n \sin(n\omega_0 x) = \sum_{n=1}^{\infty} b_n \sin\left(\frac{n\pi x}{L}\right), \qquad (10.6)$$

where

$$b_n = \frac{2}{T}\int_{-L}^{L} f(x)\sin(n\omega_0 x)\,dx = \frac{2}{L}\int_{0}^{L} f(x)\sin\left(\frac{n\pi x}{L}\right)dx \quad (10.7)$$

Similarly, we might instead want to represent the same function $f(x)$, defined over the same finite interval as a Fourier series that contains only cosine terms.

In this case, we now imagine artificially extending $f(x)$ to negative x as an even function, as shown in the diagram below:



Again, we then imagine repeating this unit with a period $T = 2L$, to give an infinite periodic even function.

By comparison with equations (10.5) and(10.2), we can therefore write the Fourier series for $f(x)$ in the finite interval $0 \le x \le L$ as:

$$f(x) = \frac{a_0}{2} + \sum_{n=1}^{\infty} a_n \cos(n\omega_0 x) = \frac{a_0}{2} + \sum_{n=1}^{\infty} a_n \cos\left(\frac{n\pi x}{L}\right), \quad (10.8)$$

where

$$a_n = \frac{2}{T}\int_{-L}^{L} f(x)\cos(n\omega_0 x)\,dx = \frac{2}{L}\int_{0}^{L} f(x)\cos\left(\frac{n\pi x}{L}\right)dx$$