Physical Mathematics 2010

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Abstract

These are the lecture notes to accompany the Physical Mathematics lecture course. They are a modified version of the previous years notes which written by Dr Alisdair Hart.

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1 Organisation

Online notes & tutorial sheets

`www.ph.ed.ac.uk/~paboyle/Teaching/PhysicalMathematics/`

1.1 Books

There are many books covering the material in this course. Good ones include:

- "Mathematical Methods for Physics and Engineering", K.F. Riley, M.P. Hobson and S.J. Bence (Cambridge University Press)
  - The main textbook.
  - Available at a discount from the Teaching Office.
- "Mathematical Methods in the Physical Sciences", M.L. Boas (Wiley)
- "Mathematical Methods for Physicists", G. Arfken (Academic Press)

These, and plenty more besides, are available **for free** in the JCMB library.

1.2 On the web

There are some useful websites for quick reference, including:

- `http://mathworld.wolfram.com`,
- `http://en.wikipedia.org`,
- `http://planetmath.org`.

1.3 Workshops

Workshops run from week 2 through week 11.
Sign up for *one* of the two sessions at Teaching Office:

- Tuesday 11:10-12:00 (room 1206C JCMB)
- Tuesday 14:00-15:50 (room 3217 JCMB)

In week 11, I will set a 60 minute mock exam, then for the final 60 minutes answers will be distributed and you will mark your neighbours script (or your own if you prefer).
The mark will *not* contribute to your course mark, but serves as useful practice and diagnostic.

2 The wave equation

We can the transverse displacement of a stretched string using a function $u(x,t)$ which tells us how far the infinitesimal element of string at (longitudinal) position x has been (transversely) displaced at time t. The function $u(x,t)$ satisfies a partial differential equation (PDE) known as the wave equation:

$$\frac{\partial^2 u}{\partial x^2} = \frac{1}{c^2}\,\frac{\partial^2 u}{\partial t^2} \tag{2.1}$$

where c is a constant,and has units of length over time (i.e. of velocity) and is, in fact, the speed of propagation of travelling waves on the string.
In the absence of boundaries, the general solution can be seen by noting:

$$\begin{aligned}\frac{\partial^2 u}{\partial x^2} - \frac{1}{c^2}\frac{\partial^2 u}{\partial t^2} &= \left(\frac{\partial}{\partial x} - \frac{1}{c}\frac{\partial}{\partial t}\right)\left(\frac{\partial}{\partial x} + \frac{1}{c}\frac{\partial}{\partial t}\right) u \\ &= \left(\frac{\partial}{\partial x} + \frac{1}{c}\frac{\partial}{\partial t}\right)\left(\frac{\partial}{\partial x} - \frac{1}{c}\frac{\partial}{\partial t}\right) u\end{aligned}$$

This is solved by

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

where f and g are arbitrary functions of a single variable. This represents the superposition of arbitrary left and right propagating waves.

2.1 Separation of variables

Our equation of motion in Eqn. (2.1) is perhaps the simplest second order partial differential equation (PDE) imaginable – it doesn't contain any mixed derivatives (e.g. $\frac{\partial^2 u}{\partial x \partial t}$). We call such a differential equation a *separable* one, or say that it is of *separable form*.
We can seek particular solutions in which variations with space and time are *independent*. Such are *standing waves* of the of the *seperable* form:

$$u(x,t) = X(x)\,T(t)\ .$$

This really is a *restriction* of the class of possible solutions and there are certainly solutions to the wave equation that are *not* of separated form (e.g. travelling waves as above).
However, we shall see *all* solutions of the wave equation (separated form or not) can be written as a linear combination of solutions of separated form, so this restriction is not a problem.
Differentiating, we get

$$\begin{aligned}\frac{\partial u}{\partial x} &= \frac{dX}{dx}\,T \equiv X'T \qquad &\Rightarrow \qquad \frac{\partial^2 u}{\partial x^2} &= X''T \\ \frac{\partial u}{\partial t} &= X\,\frac{dT}{dt} \equiv X\dot{T} \qquad &\Rightarrow \qquad \frac{\partial^2 u}{\partial t^2} &= X\ddot{T}\end{aligned}$$

Substituting this into the PDE:

$$X''(x)T(t) = \frac{1}{c^2}X(x)\ddot{T}(t)\ ,$$

Thus,

$$\frac{X(x)''}{X(x)} = \frac{1}{c^2}\,\frac{\ddot{T}(t)}{T(t)}$$

Now

$$\frac{\partial}{\partial t}LHS = \frac{\partial}{\partial x}RHS = 0$$

Hence both LHS and RHS must be equal to the same constant and we may write

$$\frac{X''}{X} = \frac{1}{c^2}\frac{\ddot{T}}{T} = -k^2 \qquad \text{(say)},$$

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

EXAM TIP: You will lose marks here if you do not write "Seeking solutions of separated form", and explain something equivalent to the above discussion.
Now we have *separated* our PDE in two variables into two simple second order ordinary differential equations (ODEs) in one variable each:

$$\begin{aligned}\frac{d^2X}{dx^2} &= -k^2X(x)\\ \frac{d^2T}{dt^2} &= -\omega_k^2T(t)\end{aligned}$$

where the angular frequency $\omega_k = ck$. This is the interpretation of c for standing waves: it is the constant of proportionality that links the wavenumber k to the angular frequency ω_k.
These have the form of an eigenvalue problem, where $X(x)$ must be an eigenfunction of $\frac{d^2}{dx^2}$ with eigenvalue $-k^2$. Similarly $T(t)$ must be an eigenfunction of $\frac{d^2}{dt^2}$ with eigenvalue $-\omega_k^2 = -c^2k^2$.

2.2 Solving the ODE's

We can now solve the two ODEs separately. The solutions to these are familiar from simple harmonic motion, and we can just write down the solutions:

$$\begin{aligned}X(x) &= A_k \sin kx + B_k \cos kx\\ T(t) &= C_k \sin \omega_k t + D_k \cos \omega_k t\\ \Rightarrow u(x,t) &= (A_k \sin kx + B_k \cos kx)\,(C_k \sin \omega_k t + D_k \cos \omega_k t)\end{aligned}$$

where A_k, B_k, C_k, and D_k are arbitrary constants. The subscript denotes that they can take different values for different values of k. At this stage there is no restriction on the values of k: each values provides a separate solution to the ODEs.
Note that a propagating wave, of the form

$$\cos(kx - \omega_k t) = \cos kx \cos \omega_k t + \sin kx \sin \omega_k t$$

and so a propagating wave can be written as a linear combination of standing waves.

2.3 Boundary and initial conditions

The details of a specific physical system may involve the boundary conditions (BCs) solutions must satisfy. For example, what happens at the ends of the string and what were the initial conditions.
The string weight & tension on a guitar determine c.
The length (& frets) of a guitar determine the boundary conditions.
The plucking of the guitar determines the initial conditions.

2.3.1 BCs & orthogonality of normal modes

Physicists tend to be somewhat lazy (or perhaps unclear?) about decomposing general functions into eigenfunctions of a given differential operator.
Sturm–Liouville theory describes a class of problem and gives some useful results. We will not go into a complete discussion of Sturm-Liouville problems, but note that the ODE equations we consider in this course in fact satisfy the Sturm-Liouville conditions. We summarise some of the precise statements made possible.
Suppose X_1 and X_2 are eigenfunctions of $\frac{d^2}{dx^2}$, with eigenvalues $-\lambda_1$ and $-\lambda_2$, and satisfy some BCs at $x = a$ and $x = b$.

$$\ddot{X}_1 = -\lambda_1 X_1$$
$$\ddot{X}_2 = -\lambda_2 X_2$$

Observe:

$$\frac{d}{dx}(\dot{X}_1 X_2 - X_1 \dot{X}_2) = \ddot{X}_1 X_2 - X_1 \ddot{X}_2$$

Thus,

$$\begin{aligned} \int_a^b \left(\ddot{X}_1 X_2 - X_1 \ddot{X}_2\right) dx &= \left[\dot{X}_1 X_2 - X_1 \dot{X}_2\right]_a^b \\ &= (\lambda_2 - \lambda_1) \int_a^b X_1 X_2 dx \end{aligned} \tag{2.2}$$

Now, for many standard boundary conditions the *Wronskian* $\left[\dot{X}_1 X_2 - X_1 \dot{X}_2\right]_a^b = 0$, for example:

Dirichlet $X_1(a) = X_1(b) = X_2(a) = X_2(b) = 0$

Neumann $\dot{X}_1(a) = \dot{X}_1(b) = \dot{X}_2(a) = \dot{X}_2(b) = 0$

Periodic $\dot{X}_1(a) = \dot{X}_1(b)\,; \dot{X}_2(a) = \dot{X}_2(b)\,; X_1(a) = X_1(b)\,; X_2(a) = X_2(b)$

In these boundary conditions, eigenfunctions with distinct eigenvalues are *orthogonal* under the scalar (dot) product defined by:

$$X_1 \cdot X_2 = \int_a^b X_1 X_2 dx$$

If $\lambda_1 = \lambda_2$, then we are not guaranteed orthogonality, however, if X_1 and X_2 are genuinely different (linearly independent) then the Gramm-Schmidt procedure in section 4.1 allows us to construct an orthonormal basis in any case.

2.3.2 Completeness of normal modes

Proof of completeness is beyond the scope of this course. However, we can state two theorems regarding different *meanings* of "completeness":

Uniform convergence:

if a function f has continuous first and second derivatives on $[a, b]$ and f satisfies the boundary conditions then f can be exactly represented by a sum of eigenmodes: it will match at *every* point. That is the *maximum* deviation between $f(x)$ and the sum $S(x) = \sum_n a_n X_n$ of eigenmodes becomes zero as the number of modes included tends to ∞.

$$\max_{x \in a,b} |f(x) - S(x)|^2; \to 0 \tag{2.3}$$

Any solution of the differential equation satisfying the boundary conditions can be written as a sum of eigenmodes.

L_2 convergence:

If the function $f(x)$ has $\int_a^b |f(x)|^2 dx$ finite it can be approximated by a sum $S(x) = \sum_n a_n X_n$ of eigenmodes in the weaker sense

$$\int_a^b |f(x) - S(x)|^2 dx \to 0 \tag{2.4}$$

(2.4) means that the sum $S(x)$ can deviate from $f(x)$ at certain points, and the maximum error can remain non-zero. However, not for anything other than an *inifinitessimal* distance asotherwise it would contribute something to the integral.
Thus the basis is complete it can describe and only differs infinitessimally close to discontinuities and violations of the boundary conditions.

any bounded function on the interval $[a, b]$ can be described away from discontinuities & boundaries

2.3.3 Boundary conditions (in x)

Consider the guitar example above.
Assume the string is stretched between $x = 0$ and $x = L$, then the BCs in this case are that $u(x = 0, t) = u(x = L, t) = 0$ for all t. Because these BCs hold for all times at specific x, they affect $X(x)$ rather than $T(t)$. We find

$$\begin{aligned} u(0,t) = 0 \quad &\Rightarrow \quad B_k = 0 \,, \\ u(L,t) = 0 \quad &\Rightarrow \quad k_n = n\pi/L \,, \qquad n = 0, 1, 2 \ldots \end{aligned}$$

Here, BCs have restricted the allowed values of k and thus the allowed frequencies of oscillation. Different boundary conditions will have different allowed values. Restriction of eigenvalues by boundary conditions is a very general property in physics:

finite boundaries $\Rightarrow$ discrete (quantised) eigenvalue spectrum.

Each n value corresponds to a *normal mode* of the string:

$$u(x,t) = A_n \sin k_n x \{C_n \sin \omega_n t + D_n \cos \omega_n t\}$$

A normal mode is an excitation of the string that obeys the BCs and oscillates with a single, normal mode frequency. We sometimes call these *eigenmodes* of the system, with associated *eigenfrequencies* $\omega_n = \omega_{k_n}$.

2.3.4 Normal mode decomposition

Just like any vector can be represented as a linear combination of basis vectors, so the *general solution* to the wave equation is a linear superposition of (normal) eigenmode solutions:

$$\begin{aligned} u(x,t) &= \sum_{n=1}^{\infty} A_n \sin k_n x \{C_n \sin \omega_n t + D_n \cos \omega_n t\} \\ &\equiv \sum_{n=1}^{\infty} \sin k_n x \{E_n \sin \omega_n t + F_n \cos \omega_n t\} \end{aligned} \tag{2.5}$$

As before $\omega_n = ck_n$. We sum only from $n = 1$ because $\sin k_0 x = 0$, and we do not need to include negative n because $\sin \frac{-n\pi x}{L} = -\sin \frac{n\pi x}{L}$. Constants A_n, C_n, D_n are all unknown, so we can merge them together to give $E_n = A_n C_n$ and $F_n = A_n D_n$.
We also see that the way we have ensured that $u(0,t) = 0$ is by making it an *odd function* in x: $u(-x,t) = -u(x,t) \Rightarrow u(0,t) = 0$.

2.3.5 Initial conditions (in t)

As we have a second order temporal ODE, we need two sets of initial conditions to solve the problem. Typically these are the the shape $f(x)$ and velocity profile $g(x)$ of the string at $t = 0$:

$$\begin{aligned} u(x,0) = f(x) &= \sum_{n=1}^{\infty} F_n \sin k_n x \\ \dot{u}(x,0) = g(x) &= \sum_{n=1}^{\infty} \omega_n E_n \sin k_n x \end{aligned}$$

These conditions determine unique values for each of the E_n and F_n. Having got these, we can substitute them back into the general solution to obtain $u(x,t)$ and thus describing the motion for all times.
Consider the equation for F_n. Let's choose to calculate one, specific constant out of this set i.e. F_m for some specific m. To do this, multiply both sides by $\sin k_m x$ and integrate over the whole string (in this case $x = 0...L$) giving:

$$\int_0^L dx\ f(x) \sin k_m x = \sum_{n=1}^{\infty} F_n \int_0^L dx\ \sin k_n x\ \sin k_m x\ .$$

Now we note that the sine functions form an *orthogonal set*:

$$\begin{aligned} \int_0^L dx\ \sin k_n x\ \sin k_m x &= \frac{1}{2}\int_0^L dx\ [\cos(k_n x - k_m x) - \cos(k_n x + k_m x)] \\ &= \frac{1}{2}\begin{cases} \left[\frac{\sin(k_n x - k_m x)}{k_n - k_m} - \frac{\sin(k_n x + k_m x)}{k_n + k_m}\right]_0^L & ;\quad n \neq m \\ \left[x - \frac{\sin(k_n x + k_m x)}{k_n + k_m}\right]_0^L & ;\quad n = m \end{cases} \\ &= \frac{L}{2}\delta_{mn} \end{aligned}$$

where δ_{mn} is the Kronecker delta, giving zero for $m \neq n$ So:

$$\begin{aligned}\int_0^L dx\ f(x)\sin k_m x =& \sum_{n=1}^{\infty} F_n \int_0^L dx\ \sin k_n x\ \sin k_m x \\ =& \frac{L}{2}\sum_{n=1}^{\infty} F_n \delta_{mn} \\ =& \frac{L}{2} F_m\end{aligned}$$

using the sifting property. Therefore, after relabelling $m \to n$:

$$\begin{aligned}F_n =& \frac{2}{L}\int_0^L dx\ f(x)\sin k_n x \\ E_n =& \frac{2}{L\omega_n}\int_0^L dx\ g(x)\sin k_n x\ .\end{aligned} \tag{2.6}$$

We are given f and g, so as long as we can do the integrals on the RHS, we have determined all the unknown constants and therefore know the motion for all times.
The solution written as a sum of sine waves is an example of a Fourier series.

2.3.6 A quick example

Suppose the initial conditions are that the string is initially stretched into a sine wave $f(x) = a\sin(3\pi x/L)$ (for some a) and at rest, i.e. $g(x) = 0$.
The latter immediately gives $E_n = 0$ for all n. The former gives:

$$\begin{aligned}F_n =& \frac{2}{L}\int_0^L dx\ f(x)\sin k_n x \\ =& \frac{2a}{L}\int_0^L dx\ \sin\frac{3\pi x}{L}\sin\frac{n\pi x}{L} = \frac{2a}{L}\times\frac{L}{2}\delta_{n3}\end{aligned}$$

using the above relation. So all the F_n are zero except $F_3 = a$. So the motion is described by

$$u(x,t) = a\sin\frac{3\pi x}{L}\cos\frac{3\pi ct}{L}\ .$$

The answer is very simple. If the system starts as a pure *normal mode* of the system, it will remain as one.

3 Fourier Series

3.1 Overview

Fourier series are a way of decomposing a function as a sum of sine and cosine waves. We can decompose almost any function in this way as discussed in section 2.3.2
Fourier serieas are particularly useful if we are looking at system that satisfies a wave equation, because sinusoids are the *normal mode* oscillations which have simple time dependence. We can use this decomposition to understand more complicated excitations of the system.
Fourier series describe a *finite interval* of a function, typically $-L \to L$ or $0 \to L$. If the size of the system is infinite we instead need to use Fourier transforms which we will learn later in Sec. 5.
Outside this range a Fourier series is periodic (repeats itself) because all the sine and cosine waves are themselves periodic. The Fourier series *periodically extends* the function outside the range.
Fourier series are useful in the following contexts:

- The function really is periodic e.g. a continuous square wave
- We are only interested in what happens inside the expansion range.

Fourier modes Consider the wave equation on an interval $[-L, L]$ with periodic boundary conditions

$$\frac{d^2X(x)}{dx^2} = -k^2X(x)$$
$$X(x+2L) = X(x)$$

The solutions look like

$$X(x) = a_k\psi_k(x) + b_k\phi_k(x) \ ,$$
$$\text{where} \quad \psi_k(x) \equiv \cos kx \ ,$$
$$\phi_k(x) \equiv \sin kx \ .$$

a_k, b_k are unknown constants. Now, periodicity condition means $\cos k(x+2L) = \cos kx$ and $\sin k(x+2L) = \sin kx$. This is satisfied if $2kL = 2n\pi$ or

$$k = \frac{n\pi}{L}$$

for n an integer.

3.2 The Fourier expansion

The set of Fourier modes $\{\psi_{n\geq 0}(x), \phi_{n\geq 1}(x)\}$ are therefore defined as:

$$\psi_n(x) = \cos\frac{n\pi x}{L} \ ,$$
$$\phi_n(x) = \sin\frac{n\pi x}{L} \tag{3.1}$$

Between $-L \leq x \geq L$ we can write a general real function as a *linear combination* of these Fourier modes:

$$f(x) = \sum_{n=0}^{\infty} a_n\psi_n(x) + \sum_{n=1}^{\infty} b_n\phi_n(x)$$
$$= a_0 + \sum_{n=1}^{\infty} \left(a_n\psi_n(x) + b_n\phi_n(x)\right) \tag{3.2}$$

where a_n and b_n are (real-valued) *Fourier coefficients*.

3.3 Orthogonality

Having written a function as a sum of Fourier modes, we would like to be able to calculate the components. This is made easy because the Fourier mode functions are *orthogonal* i.e.

$$\begin{aligned}\int_{-L}^{L} dx\ \psi_m(x)\psi_n(x) &= N_n^{\psi}\delta_{mn}\ ,\\ \int_{-L}^{L} dx\ \phi_m(x)\phi_n(x) &= N_n^{\phi}\delta_{mn}\ ,\\ \int_{-L}^{L} dx\ \psi_m(x)\phi_n(x) &= 0\ .\end{aligned}$$

$N^{\psi}_{n\geq 0}$ and $N^{\phi}_{n\geq 1}$ are *normalisation constants* which we find by doing the integrals using the trig. identities in Eqn. (3.3) below. It turns out that $N_n^{\psi} = N_n^{\phi} = L$ for all n, except $n = 0$ when $N_0^{\psi} = 2L$.

ASIDE: useful trig. relation To prove the orthogonality, the following double angle formulae are useful:

$$\begin{aligned}2\cos A\cos B &= \cos(A+B)+\cos(A-B)\\ 2\sin A\cos B &= \sin(A+B)+\sin(A-B)\\ 2\sin A\sin B &= -\cos(A+B)+\cos(A-B)\\ 2\cos A\sin B &= \sin(A+B)-\sin(A-B)\end{aligned} \tag{3.3}$$

3.4 Calculating the Fourier coefficients

The orthogonality proved above allows us to calculate the Fourier coefficients as follows:

$$a_m = \begin{cases}\dfrac{1}{2L}\displaystyle\int_{-L}^{L} dx\ \psi_m(x)f(x) & m=0\ ,\\ \dfrac{1}{L}\displaystyle\int_{-L}^{L} dx\ \psi_m(x)f(x) & m>0\ ,\end{cases}$$

$$\text{Similarly,}\quad b_m = \frac{1}{L}\int_{-L}^{L} dx\ \phi_m(x)f(x)\ .$$

Proof: suppose $f(x) = \sum_k a_k\psi_k + b_k\phi_k$, then

$$\begin{aligned}\frac{1}{N_j^{\psi}}\int_{-L}^{L}\psi_j f(x)dx &= \sum_k \frac{a_k}{N_j^{\psi}}\int_{-L}^{L}\psi_k + \frac{b_k}{N_j^{\psi}}\int_{-L}^{L}\phi_k dx\\ &= \sum_k a_k\delta_{jk} + b_k\times 0\\ &= a_j\end{aligned}$$

The proof for b_k is very similar.

3.5 Even and odd expansions

What if the function we wish to expand is even:$f(-x) = f(x)$, or odd: $f(-x) = -f(x)$? Because the Fourier modes are also even ($\psi_n(x)$) or odd ($\phi_n(x)$), we can simplify the Fourier expansions.

3.5.1 Expanding an even function

Consider first the case that $f(x)$ is even:

$$b_m = \frac{1}{L}\int_{-L}^{L} dx\ \phi_m(x)f(x) = \frac{1}{L}\int_{0}^{L} dx\ \phi_m(x)f(x) + \frac{1}{L}\int_{-L}^{0} dx\ \phi_m(x)f(x)$$

In the second integral, make a change of variables $y = -x \Rightarrow dy = -dx$. The limits on y are $L \to 0$, and use this minus sign to switch them round to $0 \to L$. $f(x) = f(-y) = +f(y)$ because it is an even function, whereas $\phi_m(x) = \phi_m(-y) = -\phi_m(y)$ as it is odd. Overall, then:

$$b_m = \frac{1}{L}\int_{0}^{L} dx\ \phi_m(x)f(x) - \frac{1}{L}\int_{0}^{L} dy\ \phi_m(y)f(y) = 0$$

i.e. the Fourier decomposition of an even function contains only even Fourier modes. Similarly, we can show that

$$a_m = \frac{1}{L}\int_{0}^{L} dx\ \psi_m(x)f(x) + \frac{1}{L}\int_{0}^{L} dy\ \psi_m(y)f(y) = \frac{2}{L}\int_{0}^{L} dx\ \psi_m(x)f(x)$$

for $m > 0$ and

$$a_0 = \frac{1}{L}\int_{0}^{L} dx\ \psi_{m=0}(x)f(x)\ .$$

3.5.2 Expanding an odd function

For an odd function we get a similar result: all the a_m vanish, so we only get odd Fourier modes, and we can calculate the b_m by doubling the result from integrating from $0 \to L$:

$$a_m = 0$$
$$b_m = \frac{2}{L}\int_{0}^{L} dx\ \phi_m(x)f(x)$$

We derive these results as before: split the integral into regions of positive and negative x; make a transformation $y = -x$ for the latter; exploit the symmetries of $f(x)$ and the Fourier modes $\psi_m(x)$, $\phi_m(x)$.

3.6 Periodic extension, or what happens outside the range?

We call the original function $f(x)$, possibly defined for all x, and the Fourier series expansion $f_{\rm FS}(x)$. Inside the expansion range $f_{\rm FS}(x)$ is guaranteed to agree exactly with $f(x)$. Outside this range, the Fourier expansion $f_{\rm FS}(x)$ need not, in general, agree with $f(x)$ which is after all an arbitrary function.

Consider function $f(x) = x^2$ between $-L$ and L. This is an *even* function so we know $b_n = 0$. The other coefficients are:

$$a_0 = \frac{1}{2L}\int_{-L}^{L} dx\ x^2 = \frac{1}{L}\int_{0}^{L} dx\ x^2 = \frac{1}{L}\ \frac{L^3}{3} = \frac{L^2}{3}$$

We need to do the integral

$$a_m = \frac{2}{L}\int_{0}^{L} dx\ x^2 \cos\frac{m\pi x}{L}$$

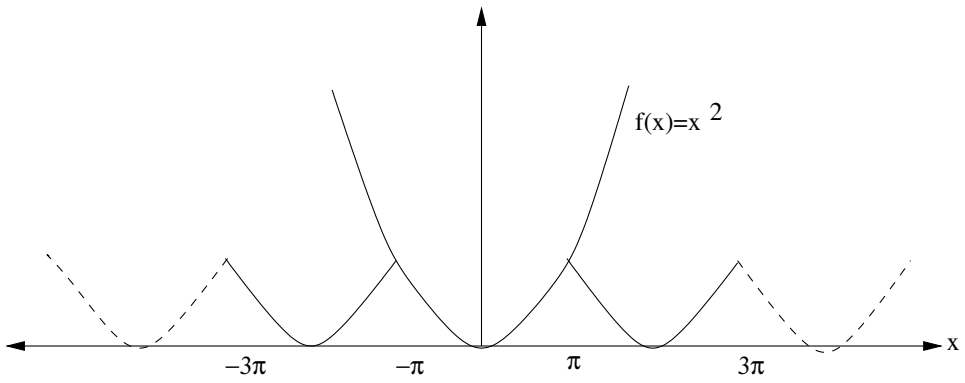


Figure 3.1: $f(x) = x^2$ as a periodic function.

The first stage is to make a substitution that simplifies the argument of the cosine function:

$$y = \frac{m\pi x}{L} \quad \Rightarrow \quad dy = \frac{m\pi}{L} dx$$

which also changes the upper integration limit to $m\pi$. So

$$a_m = \frac{2}{L} \int_0^{m\pi} \frac{L}{n\pi} dy \, \frac{L^2 y^2}{m^2\pi^2} \cos y = \frac{2L^2}{m^3\pi^3} \int_0^{m\pi} dy \, y^2 \cos y \, .$$

We now solve this simplified integral by integrating by parts. An easy way of remembering integration by parts is

$$\int u.dv = uv - \int v.du$$

and in this case we will make $u = y^2$ and $dv = \cos y$. Because y^2 is an integer power, repeat differentiation will eventually yield a constant and we can do the integral.

$$\int dy \, y^2 \cos y = y^2 \sin y - \int dy \, 2y \sin y \, .$$

We now repeat the process for the integral on the RHS, setting $u = 2y$ for the same reason:

$$\int dy \, y^2 \cos y = y^2 \sin y - \left[-2y \cos y + \int dy \, 2 \cos y \right] = y^2 \sin y + 2y \cos y - 2 \sin y \, .$$

So, using $\sin m\pi = 0$ and $\cos m\pi = (-1)^m$:

$$a_m = \frac{2L^2}{m^3\pi^3} \left[y^2 \sin y + 2y \cos y - 2 \sin y \right]_0^{m\pi} = \frac{2L^2}{m^3\pi^3} \times 2m\pi(-1)^m = \frac{4L^2(-1)^m}{m^2\pi^2} \tag{3.4}$$

So, overall our Fourier series is

$$f_{\rm FS}(x) = \frac{L^2}{3} + \frac{4L^2}{\pi^2} \sum_{n=1}^{\infty} \frac{(-1)^n}{n^2} \cos \frac{n\pi x}{L} \, . \tag{3.5}$$

$f_{\rm FS}(x)$ agrees exactly with the original function $f(x)$ inside the expansion range. *Outside*, however in general it need not. The Fourier series has *periodically extended* the function $f(x)$ outside the expansion range, Fig. 3.1. Only if $f(x)$ itself has the same periodicity will $f_{\rm FS}(x)$ agree with $f(x)$ for all x.

A plot of the coefficients, $\{c_n\}$ versus n, is known as the *spectrum* of the function: it tells us how much of each frequency is present in the function. The process of obtaining the coefficients is often known as *spectral analysis*. We show the spectrum for $f(x) = x^2$ in Fig. 3.2.

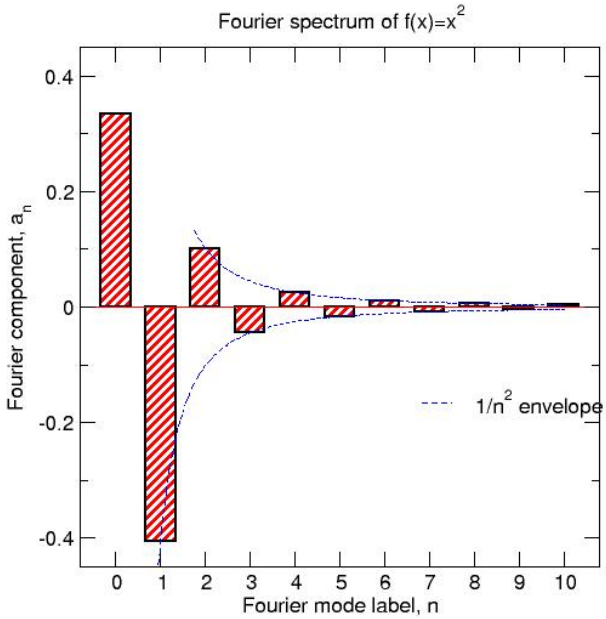


Figure 3.2: The Fourier spectrum a_n (with y-axis in units of L^2) for function $f(x) = x^2$.

3.7 Complex Fourier Series

Sines and cosines are one Fourier basis i.e. they provide one way to expand a function in the interval $[-L, L]$. Another, related basis is that of complex exponentials.

$$f(x) = \sum_{n=-\infty}^{\infty} c_n \varphi_n(x) \quad \text{where} \quad \varphi_n(x) = e^{-ik_n x} = e^{-in\pi x/L} \tag{3.6}$$

This is a *complex Fourier series*, because the expansion coefficients, c_n, are in general complex numbers even for a real-valued function $f(x)$ (rather than being purely real as before). Note that the sum over n runs from $-\infty$ in this case.
These basis functions are also orthogonal and the orthogonality relation in this case is

$$\int_{-L}^{L} dx\ \varphi_m^*(x)\varphi_n(x) = \int_{-L}^{L} dx\ e^{i(k_m - k_n)x} = \left\{ \begin{array}{ll} [x]_{-L}^{L} & = 2L \quad (\text{if } n = m) \\ \left[\frac{\exp(i(k_m - k_n)x)}{i(k_m - k_n)}\right]_{-L}^{L} & = 0 \quad (\text{if } n \neq m) \end{array} \right\} = 2L\ \delta_{mn}$$

Note the complex conjugation of $\varphi_m(x)$. For the case $n \neq m$, we note that $m - n$ is a non-zero integer (call it p) and

$$\exp[i(k_m - k_n)L] - \exp[i(k_m - k_n)(-L)] = \exp[ip\pi] - \exp[-ip\pi] = (\exp[i\pi])^p - (\exp[-i\pi])^p = (-1)^p - (-1)^p = 0$$

For $p = m - n = 0$ the denominator is also zero, hence the different result.
We can use (and need) this orthogonality to find the coefficients. If we decide we want to calculate c_m for some chosen value of m, we multiply both sides by *the complex conjugate of* $\varphi_m(x)$ and

integrate over the full range:

$$\int_{-L}^{L} dx\ \varphi_m(x)^* f(x) = \sum_{n=-\infty}^{\infty} c_n \int_{-L}^{L} dx\ \varphi_m(x)^* \varphi_n(x) = \sum_{n=-\infty}^{\infty} c_n . 2L\delta_{mn} = c_m . 2L$$

$$\Rightarrow \quad c_m = \frac{1}{2L}\int_{-L}^{L} dx\ \varphi_m(x)^* f(x) = \frac{1}{2L}\int_{-L}^{L} dx\ e^{ik_m x} f(x)$$

As before, the integral of a sum is the same as a sum of integrals, that c_n are constants.

3.7.1 Example

Go back to our example of expanding $f(x) = x^2$ for $x \in [-L, L]$ (we could choose $L = \pi$ if we wished).
We decide to calculate component c_m for a particular value of m, which involves an integral as above. In fact, we can generalise and calculate *all* the different m values using two integrals: one for $m = 0$ and another for generic $m \neq 0$:

$$c_{m=0} = \frac{1}{2L}\int_{-L}^{L} dx\ x^2 = \frac{L^2}{3}$$

$$c_{m\neq 0} = \frac{1}{2L}\int_{-L}^{L} dx\ x^2 e^{-im\pi x/L} = \frac{2L^2(-1)^m}{2m^2\pi^2}$$

See below for details of how to do the second integral. We notice that in this case all the c_m are real, but this is not the case in general.

ASIDE: doing the integral We want to calculate

$$c_m \equiv \frac{1}{2L}\int_{-L}^{L} dx\ x^2 e^{im\pi x/L}$$

To make life easy, we should change variables to make the exponent more simple (whilst keeping y real) i.e. set $y = m\pi x/L$, for which $dy = dx.m\pi/L$. The integration limits become $\pm m\pi$:

$$c_m = \frac{1}{2L}\int_{-m\pi}^{m\pi} dy\ \frac{L}{m\pi} \times \frac{L^2 y^2}{m^2\pi^2} e^{iy} = \frac{L^2}{2m^3\pi^3}\int_{-m\pi}^{m\pi} dy\ y^2 e^{iy}$$

Again we integrate by parts. We set $u = y^2 \ \Rightarrow\ du = 2y$ and $dv = e^{iy} \ \Rightarrow\ v = e^{iy}/i = -ie^{iy}$. So

$$c_m = \frac{L^2}{2m^3\pi^3}\left\{\left[-iy^2 e^{iy}\right]_{-m\pi}^{m\pi} - \int_{-m\pi}^{m\pi} dy\ 2y.(-i)e^{iy}\right\} = \frac{L^2}{2m^3\pi^3}\left\{\left[-iy^2 e^{iy}\right]_{-m\pi}^{m\pi} + 2i\int_{-m\pi}^{m\pi} dy\ ye^{iy}\right\}$$

Repeating, this time with $u = y \ \Rightarrow\ du = 1$ to get:

$$\begin{aligned} c_m &= \frac{L^2}{2m^3\pi^3}\left\{\left[-iy^2 e^{iy}\right]_{-m\pi}^{m\pi} + 2i\left(\left[-iye^{iy}\right]_{-m\pi}^{m\pi} - \int_{-m\pi}^{m\pi} dy\ (-i)e^{iy}\right)\right\} \\ &= \frac{L^2}{2m^3\pi^3}\left\{\left[-iy^2 e^{iy}\right]_{-m\pi}^{m\pi} + 2i\left(\left[-iye^{iy}\right]_{-m\pi}^{m\pi} + i\left[-ie^{iy}\right]_{-m\pi}^{m\pi}\right)\right\} \\ &= \frac{L^2}{2m^3\pi^3}\left[-iy^2 e^{iy} - 2i.i.ye^{iy} + 2i.i.(-i).e^{iy}\right]_{-m\pi}^{m\pi} \\ &= \frac{L^2}{2m^3\pi^3}\left[-iy^2 e^{iy} + 2ye^{iy} + 2ie^{iy}\right]_{-m\pi}^{m\pi} \end{aligned}$$

We can now just substitute the limits in, using $e^{im\pi} = e^{-im\pi} = (-1)^m$. Alternately, we can note that the first and third terms are even under $y \to -y$ and therefore we will get zero when we evaluate between *symmetric* limits $y = \pm m\pi$ (N.B. this argument only works for symmetric limits). Only the second term, which is odd, contributes:

$$\begin{aligned} c_m &= \frac{L^2}{2m^3\pi^3}\left[2ye^{iy}\right]_{-m\pi}^{m\pi} = \frac{L^2}{2m^3\pi^3}\left(2m\pi e^{-im\pi} - (-2m\pi)e^{im\pi}\right) \\ &= \frac{L^2}{2m^3\pi^3} \times 4m\pi(-1)^m = \frac{2L^2(-1)^m}{m^2\pi^2} \end{aligned} \tag{3.7}$$

3.8 Comparing real and complex Fourier expansions

There is a strong link between the real and complex Fourier basis functions, because cosine and sine can be written as the sum and difference of two complex exponentials:

$$\varphi_n(x) = \psi_n(x) - i\phi_n(x) \quad \Rightarrow \quad \begin{cases} \psi_n(x) = \dfrac{1}{2}[\varphi_{-n}(x) + \varphi_n(x)] \\ \\ \phi_n(x) = \dfrac{1}{2i}[\varphi_{-n}(x) - \varphi_n(x)] \end{cases}$$

so we expect there to be a close relationship between the real and complex Fourier coefficients. Staying with the example of $f(x) = x^2$, we can rearrange the complex Fourier series by splitting the sum as follows:

$$f_{\text{FS}}(x) = c_0 + \sum_{n=1}^{\infty} c_n e^{-in\pi x/L} + \sum_{n=-1}^{-\infty} c_n e^{in\pi x/L}$$

we can now relabel the second sum in terms of $n' = -n$:

$$f_{\text{FS}}(x) = c_0 + \sum_{n=1}^{\infty} c_n e^{-in\pi x/L} + \sum_{n'=1}^{\infty} c_{-n'} e^{in'\pi x/L}$$

Now n and n' are just dummy summation indices with no external meaning, so we can now relabel $n' \to n$ and the second sum now looks a lot like the first. Noting from Eqn. (3.7) that in this case $c_{-m} = c_m$, we see that the two sums combine to give:

$$f_{\text{FS}}(x) = c_0 + \sum_{n=1}^{\infty} c_n \left(\varphi_n(x) + \varphi_{-n}(x)\right) = c_0\psi_0 + \sum_{n=1}^{\infty} 2c_n\psi_n(x)$$

So, this suggests that our real and complex Fourier expansions are identical with $a_0 = c_0$ and $a_{n>0} = 2c_{n>0}$ (and $b_n = 0$). Comparing our two sets of coefficients in Eqns. (3.4) and (3.7), we see this is true.

3.9 Differentiation and integration

If the Fourier series of $f(x)$ is differentiated or integrated, *term by term*, the new series is the Fourier series for $f'(x)$ or $\int dx\, f(x)$, respectively. This means that we do not have to do a second expansion to, for instance, get a Fourier series for the derivative of a function.

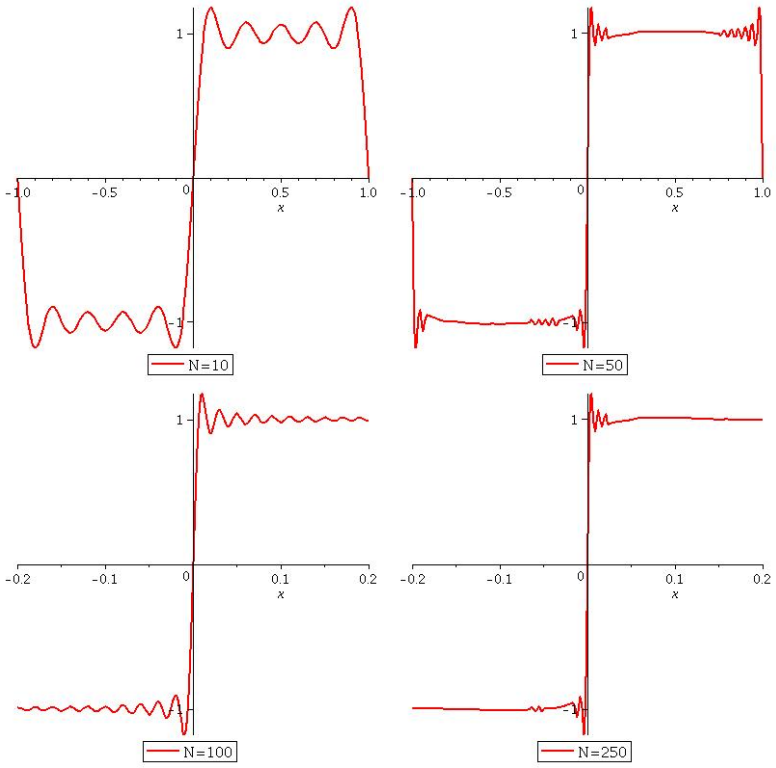


Figure 3.3: The Gibbs phenomenon for truncated Fourier approximations to the signum function Eqn. 3.8. Note the different x-range in the lower two panels.

3.10 Gibbs phenomenon

An interesting case is when we try to describe a function with a finite discontinuity (i.e. a jump) using a truncated Fourier series. Consider the signum function which picks out the sign of a variable:

$$f(x) = \text{signum}\, x = \begin{cases} -1 & \text{if } x < 0\ , \\ +1 & \text{if } x \geq 0\ , \end{cases} \tag{3.8}$$

We saw in section 2.3.2 that the Fourier series will describe only guarantee to describe a discontinuous function in the sense of the integrated mean-square difference tending to zero as the number of terms included is increased.
In Fig. 3.3 we plot the original function $f(x)$ and the truncated Fourier series $f_n(x)$ for various numbers of terms N in the series. We find that the truncated sum works well, except near the discontinuity. Here the function overshoots the true value and then has a "damped oscillation". As we increase N the oscillating region gets smaller, but the overshoot determining the *maximum deviation* remains roughly the same size (about 18%).
The *average* error decreases to zero, however, because the width of the overshoot shrinks to zero. Thus deviations between $f_N(x)$ and $f(x)$ can be large, and is concentrated at those certain values of x where the discontinuity in $f(x)$ lies.
Note that for any finite number of terms $f_n(x)$ *must* be continuous, because it is a sum of a finite number of continuous functions. Describing discontinuities is naturally challenging.
The overshoot is known as the Gibbs phenomenon or as a "ringing artefact". For the interested, there are some more details at `http://en.wikipedia.org/wiki/Gibbs_phenomenon`.

4 Functions as vectors

4.1 Linear spaces

Formally, both unit vectors and eigenfunctions can be used to form *linear spaces*.
That is given a set of *things* $\{v_i\}$, a linear space is formed by taking all possible linear combinations of these *things*. This set of all linear combinations is the span of $\{v_i\}$.
The *things* could be unit vectors in the coordinate axes for vectors (the a_k are coordinates), or equally well, the eigenfunctions of a differential equation, and the a_k are Fourier coefficients.
Providing the addition of *things* follows simple axioms such as:

$$(a_i v_i) + (b_j v_j) = (a_i + b_i)v_i$$

and there is a well defined scalar product we can infer quite a lot.
We call $\{v_i\}$ linearly independent if

$$a_i v_i = \mathbf{0} \Rightarrow a_i = 0.$$

If this is the case, then none of the v_i can be written as a linear combination of the others.
(If a set of vectors span the linear space but are not linearly independent, we can reduce the size of the set until we do have a linearly independent set that spans the space. The size of this reduced set is the dimension d of the space.)

4.1.1 Gramm-Schmidt orthogonalisation

We now consider make use of the *dot* product. We can normalise the first vector as $e_0 = \frac{1}{|v_0|}v_0$.
We can orthogonalise all the $d-1$ other vectors with respect to e_0

$$v_i' = v_i - (v_i \cdot e_0)e_0.$$

As the vectors are linearly independent, v_i' must be non-zero, and we can normalise v_1' to form e_1.
The process can now be repeated to eliminate components parallel to e_1 from the $d-2$ other vectors.
When this process terminates there will be d orthonormal basis vectors, and thus an orthonormal basis for a linear space can *always* be found.

4.1.2 Matrix mechanics

In the early days of quantum mechanics Heisenberg worked on *matrix mechanics*, while Schroedinger worked with the wavefunctions solving his equation.
The relation between the two is actually simple and relevant here. Heisenberg described a quantum state as a *state vector* of coefficients describing the linear combination of *eigenfunctions*. Thus was a coordinate in the linear space spanned by the eigenfunctions.
Heisenberg operators were then matrices which acted on these vectors.

4.2 Scalar product of functions

In physics we often make the transition:

$$\text{discrete picture} \rightarrow \text{continuous picture}.$$

Take N particles of mass $m = \frac{M}{N}$ evenly spaced on a massless string of length L, under tension T.
The transverse displacement of the n^{th} particle is $u_n(t)$. As there are N coordinates we can think of the motion as occurring in an N-dimensional space.
The gap between particles is $a = L/(N+1)$, and we can label the n^{th} particle with $x = x_n \equiv na$.
We can also write $u_n(t)$, the transverse displacement of the n^{th} particle, as $u(x_n, t)$.

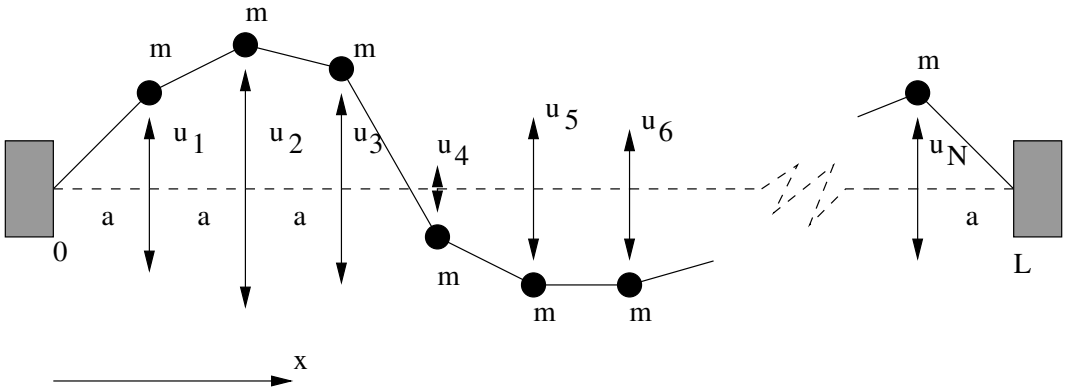


Figure 4.1: Transverse vibrations of N masses m attached to a stretched string of length L.

Transition to the continuum Let the number of masses N become infinite, while holding $L = Na$ and $M = Nm$ fixed. We go from thinking about motion of masses on a massless string to oscillations of a massive string. As $N \to \infty$, we have $a \to 0$ and $x_n \equiv na \to x$: a continuous variable. The N-component displacement vector $u(x_n, t)$ becomes a continuous function $u(x, t)$.

4.2.1 Scalar product → integral

In N-dimensions the inner product of vectors $\boldsymbol{f} = \{f_1, f_2, \ldots f_N\}$ and $g = \{g_1, g_2, \ldots g_N\}$, is:

$$\boldsymbol{f} \cdot \boldsymbol{g} = f_1^* g_1 + f_2^* g_2 + \ldots + f_N^* g_N = \sum_{n=1}^{N} f_n^* g_n$$

$$\equiv \sum_{n=1}^{N} f(x_n)^* g(x_n)$$

Again, we have moved the n dependence inside the brackets for convenience.
In an interval $x \to x + dx$ there are $\Delta n = dx/a$ particles. So, for large N we can replace a sum over n by an integral with respect to dx/a: the sum becomes a definite integral. Multiplying through by this factor of a ,

$$a\boldsymbol{f} \cdot \boldsymbol{g} \equiv a \sum_{n=1}^{N} f(x_n)^* g(x_n) \underset{N\to\infty}{\longrightarrow} \int_0^L dx\ f(x)^*\ g(x)$$

The conclusion is that there is a strong link between the inner product of two vectors and the inner product of two functions.

4.3 Inner products, orthogonality, orthonormality and Fourier series

We want the inner product of a function with itself to be *positive-definite*, i.e. $f \cdot f \geq 0$ meaning it is a real, non-negative number and that $|f|^2 = f \cdot f = 0 \Rightarrow f(x) = 0$.
That is, the *norm* of a function is only zero if the function $f(x)$ is zero everywhere.
For real-valued functions of one variable (e.g $f(x)$, $g(x)$) we *choose to define* the inner product as

$$f \cdot g \equiv \int dx\ f(x).g(x)$$

$$= g \cdot f$$

and for complex-valued functions

$$\begin{aligned} f \cdot g &\equiv \int dx\ f(x)^*.g(x) \\ &= (g \cdot f)^* \neq g \cdot f \end{aligned}$$

The integration limits are chosen according to the problem we are studying. For Fourier analysis we use $-L \to L$. For the special case of waves on a string we used $0 \to L$.

Normalised: We say a function is *normalised* if the inner product of the function with itself is 1, i.e. if $f \cdot f = 1$.

Orthogonal: We say that two functions are *orthogonal* if their inner product is zero, i.e. if $f \cdot g = 0$. If we have a set of functions for which any pair of functions are orthogonal, we call it an *orthogonal set*, i.e. if $\phi_m \cdot \phi_n \propto \delta_{mn}$ for all m, n.

Orthonormal: If all the functions in an orthogonal set are normalised, we call it an *orthonormal set* i.e. if $\phi_m \cdot \phi_n = \delta_{mn}$.

4.3.1 Example: complex Fourier series

An example of an orthogonal set is the set of complex Fourier modes $\{\varphi_n\}$. We define the inner product as

$$f \cdot g = \int_{-L}^{L} dx\ f(x)^* g(x)$$

and we see the orthogonality:

$$\varphi_m \cdot \varphi_n \equiv \int_{-L}^{L} dx\ \varphi_m(x)^* \varphi_n(x) = N_n\ \delta_{mn}$$

with normalisation $N_n \equiv \varphi_n \cdot \varphi_n = 2L$. This makes for a handy notation for writing down the Fourier component calculations that we looked at before:

$$f(x) = \sum_{n=-\infty}^{\infty} c_n \varphi_n(x) \qquad \Rightarrow \quad c_n = \frac{\varphi_n \cdot f}{\varphi_n \cdot \varphi_n}$$

In more detail, the numerator is

$$\varphi_n \cdot f \equiv \int_{-L}^{L} dx\ \varphi_n^*(x) f(x)$$

Note that the order of the functions is *very important*: the basis function comes first.
In each case, we can *projected out* the relevant Fourier component by exploiting the fact that the *basis functions* formed an *orthogonal set*. The same can be done for the real Fourier series which we leave as an exercise.

4.3.2 Normalised basis functions

Consider the complex Fourier series. If we define some new functions

$$\widehat{\varphi}_n(x) \equiv \frac{1}{\sqrt{\varphi_n \cdot \varphi_n}}\,\varphi_n(x) = \frac{\varphi_n(x)}{\sqrt{2L}}$$

then it should be clear that

$$\widehat{\varphi}_m \cdot \widehat{\varphi}_n = \delta_{mn}$$

giving us an *orthonormal set*. The inner product is defined exactly as before.
We can *choose* to use these *normalised* functions as a Fourier basis, with new expansion coefficients C_n:

$$f(x) = \sum_{n=-\infty}^{\infty} C_n \widehat{\varphi}_n(x) \qquad \Rightarrow \quad C_n = \widehat{\varphi}_n \cdot f$$

because the denominator $\widehat{\varphi}_n \cdot \widehat{\varphi}_n = 1$.
Coefficients C_n and c_n are closely related:

$$C_n = \widehat{\varphi}_n \cdot f = \frac{\varphi_n \cdot f}{\sqrt{\varphi_n \cdot \varphi_n}} = \sqrt{\varphi_n \cdot \varphi_n}\,\frac{\varphi_n \cdot f}{\varphi_n \cdot \varphi_n} = \sqrt{\varphi_n \cdot \varphi_n}\,c_n = \sqrt{2L}\,c_n$$

We can do the same for real Fourier series, defining $\widehat{\psi}_n$ and $\widehat{\phi}_n$ and associated Fourier coefficients A_n and B_n. The relationship to a_n and b_n can be worked out in exactly the same way.

5 Fourier transforms

Fourier transforms (FTs) are an extension of Fourier series that can be used to describe functions on an infinite interval. A function $f(x)$ and its Fourier transform $F(k)$ are related by:

$$F(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} dx\ f(x)\ e^{ikx}\ , \tag{5.1}$$

$$f(x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} dk\ F(k)\ e^{-ikx}\ . \tag{5.2}$$

We say that $F(k)$ is the FT of $f(x)$, and that $f(x)$ is the inverse FT of $F(k)$.
FTs include all wavenumbers $-\infty < k < \infty$ rather than just a discrete set.

EXAM TIP: If you are asked to state the relation between a function and it's Fourier transform (for maybe 3 or 4 marks), it is sufficient to quote these two equations. If they want you to repeat the derivation in Sec. 5.4, they will ask explicitly for it.

5.0.3 Relation to Fourier Series

Fourier series only include modes with $k_n = \frac{2n\pi}{L}$. This constraint on k arose from imposing periodicity on the eigenfunctions of the wave equation. Adjacent modes were separated by $\delta k = \frac{2\pi}{L}$.
Now, as $L \to \infty$, $\delta k \to 0$ and the Fourier Series turns into the Fourier Transform.
We'll show this in more detail in Sec. 5.4.

5.0.4 FT conventions

Eqns. (5.1) and (5.2) are the definitions we will use for FTs throughout this course. Unfortunately, there are many different conventions in active use for FTs. These can differ in:

- The sign in the exponent
- The placing of the 2π prefactor(s)
- Whether there is a factor of 2π in the exponent

You will probably come across different conventions at some point in your career and it is important to always check and match conventions.

5.1 Some simple examples of FTs

In this section we'll find the FTs of some simple functions.

EXAM TIP: Looking at past papers, you are very often asked to define and sketch $f(x)$ in each case, and also to calculate and sketch $F(k)$.

5.1.1 The top-hat

A top-hat function $\Pi(x)$ of height h and width $2a$ (a assumed positive), centred at $x = d$ is defined by:

$$\Pi(x) = \begin{cases} h, & \text{if } d-a < x < d+a\ , \\ 0, & \text{otherwise}\ . \end{cases} \tag{5.3}$$

The function is sketched in Fig. 5.1.
Its FT is:

$$F(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} dx\ \Pi(x)\ e^{ikx} = \frac{h}{\sqrt{2\pi}} \int_{d-a}^{d+a} dx\ e^{ikx} = \sqrt{\frac{2a^2h^2}{\pi}}\ e^{ikd}\ \operatorname{sinc} ka \tag{5.4}$$

The derivation is given below. The function $\operatorname{sinc} x \equiv \frac{\sin x}{x}$ is sketched in Fig. 5.2 (with notes on how to do this also given below). $F(k)$ will look the same (for $d = 0$), but the nodes (zeros) will now be at $k = \pm\frac{n\pi}{a}$ and the intercept will be $\sqrt{\frac{2a^2h^2}{\pi}}$ rather than 1. You are very unlikely to have to sketch $F(k)$ for $d \neq 0$.

Deriving the FT:

$$F(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} dx\ \Pi(x)\ e^{ikx} = \frac{h}{\sqrt{2\pi}} \int_{d-a}^{d+a} dx\ e^{ikx}$$

Now we make a substitution $u = x - d$ (which now centres the top-hat at $u = 0$), and have $du = dx$.. The integration limits become $u = \pm a$. This gives

$$\begin{aligned} F(k) &= \frac{h}{\sqrt{2\pi}} \cdot e^{ikd} \int_{-a}^{a} du\ e^{iku} = \frac{h}{\sqrt{2\pi}} \cdot e^{ikd} \left[\frac{e^{iku}}{ik}\right]_{-a}^{a} = \frac{h}{\sqrt{2\pi}} \cdot e^{ikd} \left(\frac{e^{ika} - e^{-ika}}{ik}\right) \\ &= \frac{h}{\sqrt{2\pi}} \cdot e^{ikd} \cdot \frac{2a}{ka} \cdot \frac{e^{ika} - e^{-ika}}{2i} = \sqrt{\frac{4a^2h^2}{2\pi}} \cdot e^{ikd} \cdot \frac{\sin ka}{ka} = \sqrt{\frac{2a^2h^2}{\pi}}\ e^{ikd}\ \operatorname{sinc} ka \end{aligned}$$

Note that we conveniently multiplied top and bottom by $2a$ midway through.

Sketching sinc x: You should think of $\operatorname{sinc} x \equiv \frac{\sin x}{x}$ as a $\sin x$ oscillation (with nodes at $x = \pm n\pi$ for integer n), but with the amplitude of the oscillations dying off as $1/x$. Note that $\operatorname{sinc} x$ is an even function, so it is symmetric when we reflect about the y-axis.
The only complication is at $x = 0$, when $\operatorname{sinc} 0 = \frac{0}{0}$ which appears undefined. Instead of thinking about $x = 0$, we should think about the limit $x \to 0$ and use **l'Hôpital's Rule** (see below):

$$\lim_{x\to 0} \operatorname{sinc} x = \lim_{x\to 0} \left[\frac{\frac{d}{dx}\sin x}{\frac{d}{dx}x}\right] = \lim_{x\to 0} \left[\frac{\cos x}{1}\right] = 1$$

The final sketch is given in Fig. 5.2.

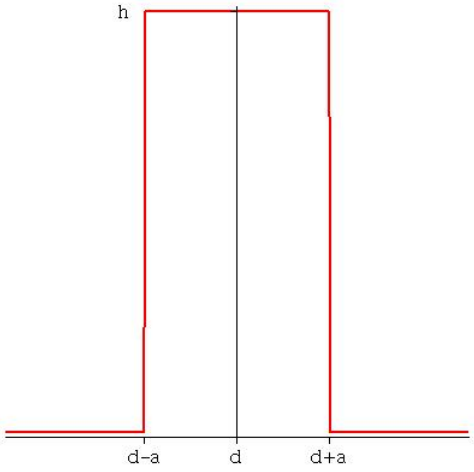


Figure 5.1: Sketch of top-hat function defined in Eqn. (5.3)

EXAM TIP: Make sure you can sketch this, and that you label all the zeros and intercepts.

Revision: l'Hôpital's Rule: If (and only if!) $f(x) = g(x) = 0$ for two functions at some value $x = c$, then

$$\lim_{x\to c}\left[\frac{f(x)}{g(x)}\right] = \lim_{x\to c}\left[\frac{f'(x)}{g'(x)}\right] \ , \tag{5.5}$$

where primes denote derivatives. Note that we differentiate the top and bottom separately rather than treating it as a single fraction.
If (and only if!) both $f'(x = c) = g'(x = c) = 0$ as well, we can repeat this to look at double derivatives and so on...

5.2 The Gaussian

The Gaussian curve is also known as the bell-shaped or normal curve. A Gaussian of width σ centred at $x = d$ is defined by:

$$f(x) = N\exp\left(-\frac{x^2}{2\sigma^2}\right) \tag{5.6}$$

where N is a normalisation constant, which is often set to 1. We can instead define the *normalised* Gaussian, where we choose N so that the area under the curve to be unity i.e. $N = 1/\sqrt{2\pi\sigma^2}$ (derived below).

5.2.1 Gaussian integral

Gaussian integrals occur regularly in physics. We are interested in

$$I = \int_{-\infty}^{\infty} \exp -x^2 dx$$

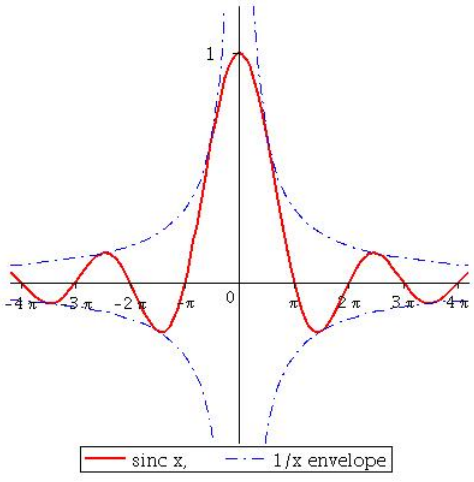


Figure 5.2: Sketch of $\mathrm{sinc}\, x \equiv \frac{\sin x}{x}$

This can be solved via a trick in polar coordinates: observe

$$\begin{aligned} I^2 &= \int_{-\infty}^{\infty} \exp -x^2 dx \int_{-\infty}^{\infty} \exp -y^2 dy \\ &= \int_{-\infty}^{\infty} dx \int_{-\infty}^{\infty} dy \exp -(x^2+y^2) \\ &= \int_0^{\infty} dr 2\pi r \exp -r^2 \\ &= \pi \int_0^{\infty} du \exp -u \\ &= \pi \left[-\exp -u \right]_0^{\infty} \\ &= \pi \end{aligned}$$

Thus,

$$I = \int_{-\infty}^{\infty} \exp -x^2 dx = \sqrt{\pi}$$

5.2.2 Fourier transform of Gaussian

The Gaussian is sketched for two different values of the width parameter σ. Fig. 5.3 has $N = 1$ in each case, whereas Fig. 5.4 shows normalised curves. Note the difference, particularly in the intercepts.
The FT is

$$F(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} dx \; N \exp\left(-\frac{x^2}{2\sigma^2} \right) \; e^{ikx} = N\sigma \exp\left(-\frac{k^2\sigma^2}{2} \right) \; , \tag{5.7}$$

i.e. the FT of a Gaussian is another Gaussian (this time as a function of k).

Deriving the FT For notational convenience, let's write $a = \frac{1}{2\sigma^2}$, so

$$F(k) = \frac{N}{\sqrt{2\pi}} \int_{-\infty}^{\infty} dx \; \exp\left(-\left[ax^2 - ikx \right] \right)$$

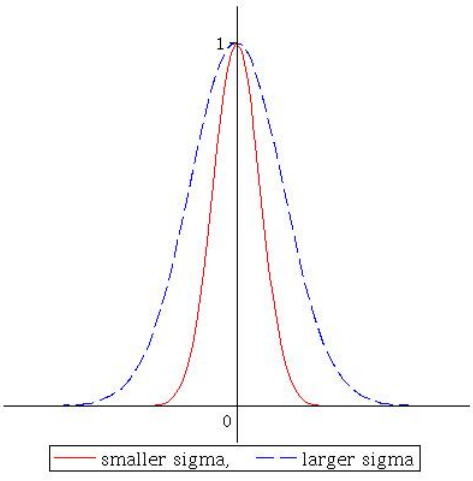


Figure 5.3: Sketch of Gaussians with $N = 1$

Now we can complete the square inside [. . .]:

$$-ax^2 + ikx = -\left(x\sqrt{a} - \frac{ik}{2\sqrt{a}}\right)^2 - \frac{k^2}{4a}$$

giving

$$F(k) = \frac{N}{\sqrt{2\pi}} e^{-k^2/4a} \int_{-\infty}^{\infty} dx \ \exp\left(-\left[x\sqrt{a} - \frac{ik}{2\sqrt{a}}\right]^2\right) .$$

We then make a change of variables:

$$u = x\sqrt{a} - \frac{ik}{2\sqrt{a}} .$$

This does not change the limits on the integral, and the scale factor is $dx = du/\sqrt{a}$, giving

$$F(k) = \frac{N}{\sqrt{2\pi a}} \ e^{-k^2/4a} \int_{-\infty}^{\infty} du \ e^{-u^2} = N\sqrt{\frac{1}{2a}} \cdot e^{-k^2/4a} .$$

Finally, we change back from a to σ.

5.3 Reciprocal relations between a function and its F.T

These examples illustrate a general *and very important* property of FTs: there is a reciprocal (i.e. inverse) relationship between the width of a function and the width of its Fourier transform. That is, narrow functions have wide FTs and wide functions have narrow FTs.
This important property goes by various names in various physical contexts, e.g.:

- Uncertainty principle: the width of the wavefunction in position space (Δx) and the width of the wavefunction in momentum space (Δp) are inversely related: $\Delta x \cdot \Delta p \simeq \hbar$.
- Bandwidth theorem: to create a very short-lived pulse (small Δt), you need to include a very wide range of frequencies (large $\Delta\omega$).
- In optics, this means that big objects (big relative to wavelength of light) cast sharp shadows (narrow F.T. implies closely spaced maxima and minima in the interference fringes).

We discuss some explicit examples:

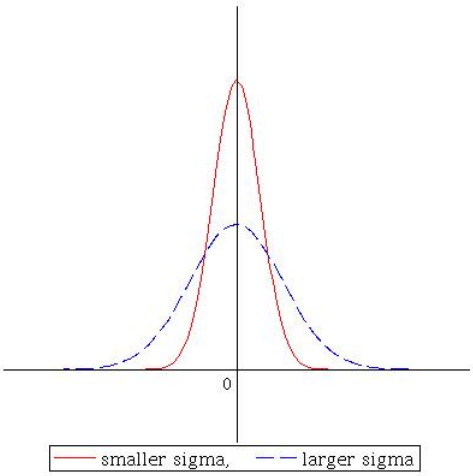


Figure 5.4: Sketch of normalised Gaussians. The intercepts are $f(0) = \frac{1}{\sqrt{2\pi\sigma^2}}$.

The top-hat: The width of the top-hat as defined in Eqn. (5.3) is obviously $2a$.
For the FT, whilst the $\mathrm{sinc}\, ka$ function extends across all k, it dies away in amplitude, so it does have a width. Exactly how we define the width does not matter; let's say it is the distance between the first nodes $k = \pm\pi/a$ in each direction, giving a width of $2\pi/a$.
Thus the width of the function is proportional to a, and the width of the FT is proportional to $1/a$.

The Gaussian: Again, the Gaussian extends infinitely but dies away, so we can define a width. Choosing a suitable definition, the width of $f(x)$ is σ (other definitions will differ by a numerical factor).
Comparing the form of FT in Eqn. (5.7) to the original definition of the Gaussian in Eqn. (5.6), if the width of $f(x)$ is σ, the width of $F(k)$ is $1/\sigma$ by the same definition.
Again, we have a reciprocal relationship between the width of the function and that of its FT.

The "spike" function: We shall see in section 5.6.6 that the extreme case of an infinitely *narrow* spike has an infinitely *broad* (i.e. constant as a function of k) Fourier transform.

5.4 FTs as generalised Fourier series

As we mentioned above, FTs are the natural extensions of Fourier Series that are used to describe functions in an infinite interval rather than one of size L or $2L$.
We know that any function $f(x)$ defined on the interval $-L < x < L$ can be represented by a complex Fourier series

$$f(x) = \sum_{n=-\infty}^{\infty} C_n e^{-ik_n x}, \tag{5.8}$$

where the coefficients are given by

$$C_n = \frac{1}{2L} \int_{-L}^{L} dx\ f(x)\ e^{ik_n x}\ . \tag{5.9}$$

where the allowed wavenumbers are $k = \frac{n\pi}{L}$. Now we want to investigate what happens if we let L tend to infinity.
At finite L, the separation of adjacent wavenumbers (i.e. for $n \to n+1$) is $\delta k = \frac{\pi}{L}$. As $L \to \infty$, $\delta k \to 0$.
Now we do a common trick in mathematical physics and multiply both sides of Eqn. (5.8) by 1. The trick is that we just multiply by 1 on the LHS, but on the RHS we exploit the fact that $L\delta k/\pi = 1$ and multiply by that instead:

$$f(x) = \sum_{n=-\infty}^{\infty} \delta k\ \left(\frac{L}{\pi} C_n\right) e^{-ik_n x}\ . \tag{5.10}$$

Now, what is the RHS? It is the sum of the areas of a set of small rectangular strips of width δk and height $\left(\frac{L}{\pi} C_n\right) e^{-ik_n x}$. As we take the limit $L \to \infty$ and δk tends to zero, we have exactly defined an integral rather than a sum: $\sum_n \delta k \to \int dk$. The wavenumber k_n becomes a continuous variable k and C_n becomes a function $C(k)$.
For convenience, let's define a new function:

$$F(k) = \sqrt{2\pi} \times \lim_{L\to\infty} \left(\frac{L}{\pi} C_n\right)$$

and Eqn. (5.10) becomes the FT as defined in Eqn. (5.2).

For the inverse FT, we multiply both sides of Eqn. (5.9) by $\frac{L}{\pi} \times \sqrt{2\pi}$:

$$\sqrt{2\pi}\left(\frac{L}{\pi}\right) C_n = \frac{1}{\sqrt{2\pi}} \int_{-L}^{L} dx\ f(x)\ e^{ik_n x}\ . \tag{5.11}$$

The limit $L \to \infty$ is more straightforward here: $k_n \to k$ and the LHS becomes $F(k)$. This is then exactly the inverse FT defined in Eqn. (5.1).

EXAM TIP: You are often asked to explain how the FT is the limit of a Fourier Series (for perhaps 6 or 7 marks), so make sure you can reproduce the stuff in this section.

5.5 Differentiating Fourier transforms

As we shall see, F.T.s are very useful in solving PDEs. This is because the F.T. of a differential is related to the F.T $F(k)$ of the original function by a factor of ik. It is simple to show by replacing $f(x)$ with the the inverse F.T. of F(k):

$$f'(x) = \frac{d}{dx}\frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} F(k)e^{-ikx} = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty}(-ik)F(k)e^{-ikx},$$

and in general:

$$f^{(p)}(x) = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty}(-ik)^p F(k)e^{-ikx}. \tag{5.12}$$

5.6 The Dirac delta function

The Dirac delta function is a very useful tool in physics, as it can be used to represent something very localised or instantaneous which retains a measurable total effect. It is easier to think of it as an infinitely narrow (and tall) spike, and defining it necessarily involves a limiting process such that it is "narrower" than "anything else".

5.6.1 Definition

The Dirac delta function $\delta(x-d)$ is defined by *two* expressions. First, it is zero everywhere except at the point $x = d$ where it is infinite:

$$\delta(x-d) = \begin{cases} 0 & \text{for } x \neq d\ , \\ \to \infty & \text{for } x = d\ . \end{cases} \tag{5.13}$$

Secondly, it tends to infinity at $x = d$ in such a way that the area under the Dirac delta function is unity:

$$\int_{-\infty}^{\infty} dx\ \delta(x-d) = 1\ . \tag{5.14}$$

i.e. if the integration range contains the spike we get 1, otherwise we get 0. In many cases the upper and lower limits are infinite ($a = -\infty$, $b = \infty$) and then we always get 1.

EXAM TIP: When asked to define the Dirac delta function (maybe for 3 or 4 marks), make sure you write *both* Eqns. (5.13) *and* (5.14).

5.6.2 Sifting property

The *sifting property* of the Dirac delta function is that, given some function $f(x)$:

$$\int_{-\infty}^{\infty} dx\ \delta(x-d)\ f(x) = f(d) \tag{5.15}$$

i.e. the delta function picks out the value of the function at the position of the spike (so long as it is within the integration range).
Of course, the integration limits don't technically need to be infinite in the above formulæ. If we integrate over a finite range $a < x < b$ the expressions become:

$$\int_{a}^{b} dx\ \delta(x-d)\ f(x) = \begin{cases} f(d) & \text{for } a < d < b\ , \\ 0 & \text{otherwise.} \end{cases}$$

That is, we get the above results if the position of the spike is inside the integration range, and zero otherwise.

EXAM TIP: If you are asked to state the sifting property, it is sufficient to write Eqn. (5.15). You do not need to prove the result as in Sec. 5.6.4 unless they specifically ask you to.

5.6.3 The delta function as a limiting case

It is sometimes hard to work with the delta function directly and it is easier to think of it as the limit of a more familiar function. The exact shape of this function doesn't matter, except that it should look more and more like a (normalised) spike as we make it narrower.
Two possibilities are the top-hat as the width $a \to 0$ (normalised so that $h = 1/(2a)$), or the normalised Gaussian as $\sigma \to 0$. We'll use the top-hat here, just because the integrals are easier.
Let $\Pi_a(x)$ be a normalised top-hat of width $2a$ centred at $x = 0$ as in Eqn. (5.3) — we've made the width parameter obvious by putting it as a subscript here. The Dirac delta function can then be defined as

$$\delta(x) = \lim_{a\to 0} \Pi_a(x)\ . \tag{5.16}$$

5.6.4 Proving the sifting property

We can use the limit definition of the Dirac delta function [Eqn. (5.16)] to prove the sifting property given in Eqn. (5.15):

$$\int_{-\infty}^{\infty} dx\ f(x)\ \delta(x) = \int_{-\infty}^{\infty} dx\ f(x) \lim_{a\to 0} \Pi_a(x) = \lim_{a\to 0} \int_{-\infty}^{\infty} dx\ f(x)\ \Pi_a(x)\ .$$

Substituting for $\Pi_a(x)$, the integral is only non-zero between $-a$ and a.

$$\int_{-\infty}^{\infty} dx\ f(x)\ \delta(x) = \lim_{a\to 0} \frac{1}{2a} \int_{-a}^{a} dx\ f(x)\ .$$

Now, $f(x)$ is an arbitrary function so we can't do much more. Except that we know we are going to make a small, so we can Taylor expand the function around $x = 0$ (i.e. the position of the centre of the spike) knowing this will be a good description of the function for small enough a:

$$\int_{-\infty}^{\infty} dx\ f(x)\ \delta(x) = \lim_{a\to 0} \frac{1}{2a} \int_{-a}^{a} dx\ \left[f(0) + x f'(0) + \frac{x^2}{2!} f''(0) + \dots \right]\ .$$

The advantage of this is that all the $f^{(n)}(0)$ are constants, which makes the integral easy:

$$\begin{aligned}\int_{-\infty}^{\infty} dx\ f(x)\ \delta(x) &= \lim_{a\to 0}\frac{1}{2a}\left(f(0)\,[x]_{-a}^{a} + f'(0)\left[\frac{x^2}{2}\right]_{-a}^{a} + \frac{f''(0)}{2!}\left[\frac{x^3}{3}\right]_{-a}^{a} + \dots\right)\\ &= \lim_{a\to 0}\left(f(0) + \frac{a^2}{6}f''(0) + \dots\right)\\ &= f(0)\ .\end{aligned}$$

which gives the sifting result.

EXAM TIP: It is a common exam question to ask you to derive the sifting property in this way. Make sure you can do it.
Note that the odd terms vanished after integration. This is special to the case of the spike being centred at $x = 0$. It is a useful exercise to see what happens if the spike is centred at $x = d$ instead.

5.6.5 Some other properties of the Dirac function

These include:

$$\begin{aligned}\delta(-x) &= \delta(x)\\ \delta(ax) &= \frac{\delta(x)}{|a|}\\ \delta(x^2 - a^2) &= \frac{\delta(x-a) + \delta(x+a)}{2|a|}\end{aligned} \tag{5.17}$$

For the last two observe:

$$\int_{-\infty}^{\infty} f(x)\delta(ax)dx = \int_{-\infty}^{\infty} f(\frac{u}{|a|})\delta(u)\frac{du}{|a|} = \frac{f(0)}{|a|}$$

and

$$\delta(x^2 - a^2) = \delta([x-a][x+a]) = \delta([x-a]2a) + \delta(-2a[x+a]) = \frac{\delta([x-a]) + \delta([x+a])}{2|a|}$$

5.6.6 FT and integral representation of $\delta(x)$

The Dirac delta function is very useful when we are doing FTs. The FT of the delta function follows easily from the sifting property:

$$F(k) = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} dx\ \delta(x-d)\ e^{ikx} = \frac{e^{ikd}}{\sqrt{2\pi}}\ .$$

In the special case $d = 0$, we get $F(k) = 1/\sqrt{2\pi}$.

Extreme case reciprocal relation:

F.T. of infinitely *narrow* spike is infinitely *broad*

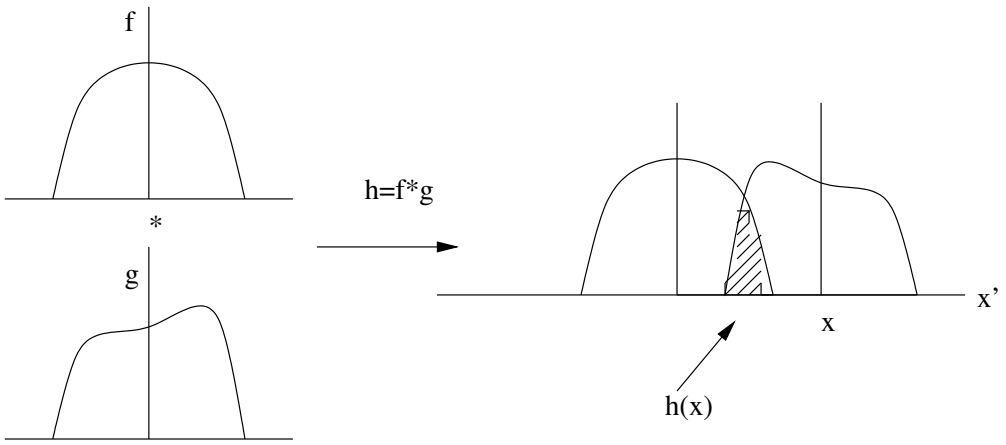


Figure 5.5: Illustration of the convolution of two functions.

The inverse FT gives us the *integral representation* of the delta function:

$$\delta(x-d) = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} dk\ F(k)e^{-ikx} = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} dk\ \left(\frac{e^{ikd}}{\sqrt{2\pi}}\right)e^{-ikx}$$
$$= \frac{1}{2\pi}\int_{-\infty}^{\infty} dk\ e^{-ik(x-d)}\ .$$

$$\boxed{\int_{-\infty}^{\infty} dk\ e^{-ik(x)} = 2\pi\delta(x)}$$

Note the prefactor of 2π rather than $\sqrt{2\pi}$.
In the same way that we have defined a delta function in x, we can also define a delta function in k. This would, for instance, represent a signal composed of oscillations of a single frequency or wavenumber K.

5.7 Convolution

Convolution combines two (or more) functions in a way that is useful for describing physical systems (as we shall see). A particular benefit of this is that the FT of the convolution is easy to calculate. The convolution of two functions $f(x)$ and $g(x)$ is defined to be

$$f(x) * g(x) = \int_{-\infty}^{\infty} dx'\ f(x')g(x-x')\ ,$$

The result is also a function of x, meaning that we get a different number for the convolution for each possible x value. Note the positions of the dummy variable x' (a common mistake in exams). We can interpret the convolution process graphically. Imagine we have two functions $f(x)$ and $g(x)$ each positioned at the origin. By "positioned" we mean that they both have some distinctive feature that is located at $x = 0$. To convolve the functions for a given value of x:

1. On a graph with x' on the horizontal axis, sketch $f(x')$ positioned (as before) at $x' = 0$,
2. Sketch $g(x')$, but displaced to be positioned at $x' = x$,
3. Flip the sketch of $g(x')$ left-right,
4. Then $f * g$ tells us about the resultant overlap.

This is illustrated in Fig. 5.5.

5.7.1 Examples of convolution

1. Gaussian smearing or blurring is implemented in most Photograph processing software *convolves* the image with a Gaussian of some width.

2. Convolution of a general function $f(x)$ with a delta function $\delta(x-a)$.

$$\delta(x-a) * f(x) = \int_{-\infty}^{\infty} dx'\ \delta(x'-a) f(x-x') = f(x-a).$$

using the sifting property of the delta function

- In words: convolving $f(x)$ with $\delta(x-a)$ has the effect of shifting the function from being positioned at $x=0$ to position $x=a$.

EXAM TIP: It is *much* easier to work out $\delta(x-a) * f(x)$ than $f(x) * \delta(x-a)$. We know they are the same because the convolution is commutative. Unless you are specifically asked to prove it, you can assume this commutativity in an exam and swap the order.

3. Making double-slits: to form double slits of width a separated by distance $2d$ between centres:

$$[\delta(x+d) + \delta(x-d)] * \Pi(x)\ .$$

We can form diffraction gratings with more slits by adding in more delta functions.

5.8 The convolution theorem

States that the Fourier transform of a *convolution* is a *product* of the individual Fourier transforms:

$$f(x) * g(x) = \sqrt{2\pi}\left(\frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} dk F(k)G(k)e^{-ikx}\right)$$

$$f(x)\ g(x) = \frac{1}{\sqrt{2\pi}}\left(\frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} F(k) * G(k)\ e^{-ikx} dk\right)$$

where $F(k)$, $G(k)$ are the F.T.s of $f(x)$, $g(x)$ respectively.

Proof

$$\begin{aligned}
f(x) * g(x) &= \int dx' f(x') g(x - x\prime) \\
&= \frac{1}{2\pi}\int dk \int dk' \int dx' F(k)G(k')e^{-ikx'}e^{-ik(x-x\prime)} \\
&= \frac{1}{2\pi}\int dk \int dk' F(k)G(k')e^{-ikx}\int dx' e^{-i(k-k')x'} \\
&= \frac{1}{2\pi}\int dk \int dk' F(k)G(k')e^{-ikx} 2\pi\delta(k-k') \\
&= \sqrt{2\pi}\left(\frac{1}{\sqrt{2\pi}}\int dk F(k)G(k)e^{-ikx}\right)
\end{aligned}$$

We define

$$F(k) * G(k) \equiv \int_{-\infty}^{\infty} dq\ F(q)\ G(k-q)$$

so

$$\begin{aligned}
\frac{1}{2\pi}\int_{-\infty}^{\infty} F(k) * G(k)e^{-ikx}dk &= \frac{1}{2\pi}\int_{-\infty}^{\infty} dq \int_{-\infty}^{\infty} dk F(q)G(k-q)e^{-ikx} \\
&= \frac{1}{(2\pi)^2}\int_{-\infty}^{\infty} dx'' \int_{-\infty}^{\infty} dx' \int_{-\infty}^{\infty} dq \int_{-\infty}^{\infty} dk f(x'')g(x')e^{iqx''}e^{(k-q)x'}e^{-ikx} \\
&= \frac{1}{(2\pi)^2}\int_{-\infty}^{\infty} dx'' \int_{-\infty}^{\infty} dx' \int_{-\infty}^{\infty} dq \int_{-\infty}^{\infty} dk f(x'')g(x')e^{ik(x'-x)}e^{q(x''-x')} \\
&= \frac{1}{(2\pi)^2}\int_{-\infty}^{\infty} dx'' \int_{-\infty}^{\infty} dx' f(x'')g(x')2\pi\delta(x'-x)2\pi\delta(x''-x') \\
&= f(x)g(x)
\end{aligned}$$

5.8.1 Examples of the convolution theorem

1. Double-slit interference: two slits of width a and spacing $2d$

$$\begin{aligned}
F.T.[\{\delta(x+d)+\delta(x-d)\} * \Pi(x)] &= \sqrt{2\pi}\ F.T.[\{\delta(x+d)+\delta(x-d)\}]\ F.T.[\Pi(x)] \\
&= \sqrt{2\pi}\ \{F.T.[\delta(x+d)] + F.T.[\delta(x-d)]\}\ F.T.[\Pi(x)] \\
&= \sqrt{2\pi}\ \frac{e^{-ikd}+e^{ikd}}{\sqrt{2\pi}}\ \frac{\operatorname{sinc}\frac{ka}{2}}{\sqrt{2\pi}} \\
&= \frac{2}{\sqrt{2\pi}}\cos(kd)\operatorname{sinc}\left(\frac{ka}{2}\right)
\end{aligned}$$

   (We'll see *why* this is the diffraction pattern in Sec. 5.9.1).

2. Fourier transform of the triangular function of base width $2a$.

   - We know that triangle is a convolution of top hats:

$$\Delta(x) = \Pi(x) * \Pi(x)\ .$$

   - Hence by the convolution theorem:

$$F.T.[\Delta] = \sqrt{2\pi}(F.T.[\Pi(x)])^2 = \sqrt{2\pi}\left(\frac{1}{\sqrt{2\pi}}\operatorname{sinc}\frac{ka}{2}\right)^2$$

5.9 Physical applications of Fourier transforms

F.T.s arise naturally in many areas of physics, especially in optics and quantum mechanics, and can also be used to solve PDEs.

5.9.1 Far-field optical diffraction patterns

If we shine monochromatic (wavelength λ), coherent, collimated (i.e. plane wavefronts) light on an optical grating, light only gets through in certain places. We can describe this using a *transmission*

function $t(x)$ whose values are positive or zero. Zero represents no light getting through at point x. We often normalise the transmission function so that

$$\int_{-\infty}^{\infty} dx\ t(x) = 1$$

A single slit of finite width therefore has a top-hat transmission function $t(x) = \Pi(x)$, where x measures the distance across the grating (perpendicular to the direction of the slit), relative to some arbitrary, but fixed, origin.
The far-field diffraction pattern for light passing through this grating is related to the F.T. of the transmission function.

- Using Huygen's principle, each point on the grating x is a source of secondary, spherical wavelets.
- The amplitude of the electric field associated with each set of spherical wavelets $E(x) \propto t(x)$.
- Place a detector a long way away (relative to the size of the grating), so that all light reaching it effectively left the grating at the same angle θ to the normal. This is the *far-field* limit.
- The observed electric field $E(\theta)$ is given by summing the contributions from each position on the grating x, allowing for the path difference $\delta x = x \sin\theta$ (relative to the arbitrary, but fixed, choice of origin).

  The wavelet from position x contributes

  $$E(x) \sim t(x)\ e^{i\frac{2\pi}{\lambda}(\delta x)} \equiv t(x)\ e^{i\frac{2\pi}{\lambda}x\sin\theta}\ .$$

- Because the light is coherent, the total observed electrical field is

  $$E(\theta) = \int_{-\infty}^{\infty} dx\ E(x) \propto \int_{-\infty}^{\infty} dx\ t(x)\ e^{i\frac{2\pi}{\lambda}x\sin\theta}\ .$$

- Writing $v = \frac{2\pi}{\lambda}\sin\theta$, we have

  $$E(\theta) \propto \int_{-\infty}^{\infty} dx\ t(x)\ e^{ivx}\ ;$$

- i.e the electric field is (proportional to) the Fourier transform of the transmission function (using v as the F.T. variable rather than k).
- The observed intensity is $I(\theta) \propto |E(\theta)|^2$.

E.g. Ideal double-slit diffraction I.e. two infinitely narrow slits distance a apart, which we can represent in the transmission function as a pair of delta-functions at $x = \pm a/2$:

$$t(x) = \frac{1}{2}\left[\delta\left(x - \frac{a}{2}\right) + \delta\left(x + \frac{a}{2}\right)\right]$$

The far-field diffraction pattern (i.e. the Fourier transform) is given by

$$\begin{aligned} E(\theta) &\propto \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} dx\ \frac{1}{2}\left[\delta\left(x - \frac{a}{2}\right) + \delta\left(x + \frac{a}{2}\right)\right]\ e^{ivx} \\ &\propto \frac{1}{2\sqrt{2\pi}}\left(e^{iva/2} + e^{-iva/2}\right) \\ &\propto \frac{1}{\sqrt{2\pi}}\ \cos\left(\frac{va}{2}\right). \end{aligned}$$

The observed intensity pattern is the well known 'cos-square fringes'.

6 Vectors (review)

6.1 Scalars and Vectors

Scalar : Quantity specified by a single number
Vector : Quantity specified by a number (magnitude) and direction

e.g. speed s is a scalar, velocity $\boldsymbol{v}$ is a vector, $s = |\boldsymbol{v}|$.

6.2 Why vector notation

We could of course always right out the laws of physics in component form, however this is tedious and it is easier to use vector notation. The laws of physics are simplified when expressed in vector notation.
Adding two vectors must give the same result regardless of the coordinate system, while the rule for addition will depend on the coordinate system. So, vectors have a geometrical interpetation, that is more fundamental than, and independent of any choice of coordinate system.

6.3 Scalar product

The scalar product of $\boldsymbol{a}$ and $\boldsymbol{b}$ is written $\boldsymbol{a} \cdot \boldsymbol{b}$. This is often called the "dot" product. Note,

$$\boldsymbol{a} \cdot \boldsymbol{b} = |a||b| \cos\theta,$$

where θ is the angle between the vectors. In particular

$$\boldsymbol{a} \cdot \boldsymbol{a} = |a|^2.$$

6.4 Cartesian coordinates

We will use orthogonal unit basis vectors $\{\boldsymbol{e}_i\} = \{\boldsymbol{e}_1, \boldsymbol{e}_2, \boldsymbol{e}_3\} \equiv \hat{x}, \hat{y}, \hat{z}$. These represent unit vectors in some set of coordinate axes, and we identify $1, 2, 3$ with x, y, z.
Our basis vectors are taken as *orthogonal*

$$\boldsymbol{e}_i \cdot \boldsymbol{e}_j = 0; i \neq j.$$

They also taken as unit vectors, and orthogonal and normalised basis is called *orthonormal* and satisfies:

$$\boldsymbol{e}_i \cdot \boldsymbol{e}_j = \delta_{ij},$$

where the Kronecker δ symbol is

$$\delta_{ij} = \begin{cases} 1; & i = j \\ 0; & i \neq j \end{cases}$$

A general vector can be expressed as a linear combination of these *basis* vectors:

$$\boldsymbol{a} = \sum_i \boldsymbol{a}_i e_i = a_x\hat{x} + a_y\hat{y} + a_z\hat{z}$$

This is often be expressed as the coordinates (a_x, a_y, a_z).
The scalar product of two vectors is

$$\boldsymbol{a} \cdot \boldsymbol{b} = a_i b_i = a_x b_x + a_y b_y + a_z b_z,$$

where we have introduced *Einstein summation convention* where a repeated index is implicitly summed over its range.

6.4.1 Example: parallel and perpendicular pieces

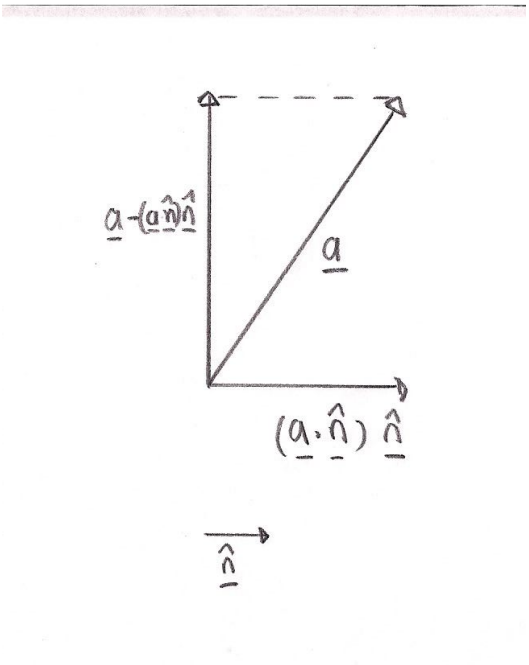
If a vector $\hat{n}$ is a *unit* vector then the dot product

$$\boldsymbol{a}_{||} = (\boldsymbol{a} \cdot \hat{n})\hat{n}$$

gives the component of $\boldsymbol{a}$ that is parallel to $\hat{n}$.
Also,

$$\boldsymbol{a}_{\perp} = [\boldsymbol{a} - (\boldsymbol{a} \cdot \hat{n})\hat{n}]$$

gives the component of $\boldsymbol{a}$ that is perpendicular to $\hat{n}$.



6.4.2 Example: uniform gravitational field

Using vector expressions allows to write simple physical formulae without having to carefully align the axes with the symmetries of our problem. For example, The gravitational potential energy is commonly written as

$$P.E. = mgh$$

However, this could equally be expressed in terms of the coordinate vector $\boldsymbol{r}$ and the downwards pointing gravitational field vector $\boldsymbol{g}$:

$$P.E. = -m(\boldsymbol{g} \cdot \boldsymbol{r}).$$

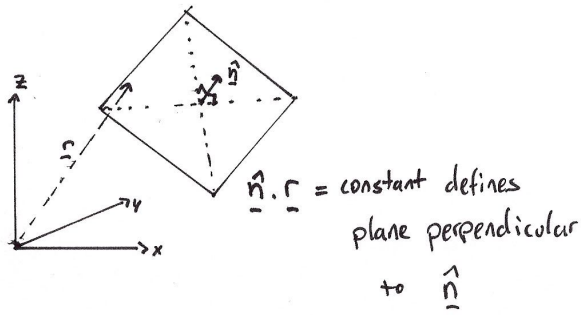
An equipotential is then defined by $-m\boldsymbol{g} \cdot \boldsymbol{r} = P.E. = \text{constant}$.

6.4.3 Example: Equation of a plane

This is just

$$g_1 x + g_2 y + g_3 z = -\frac{P.E.}{m}, \tag{6.18}$$

which is the general equation for a plane. There is little intuition gained from staring at the general component form (6.18).



However, if we write $\hat{n} = \frac{-\boldsymbol{g}}{|g|}$ (remember the gravitational field points down, so $\hat{n}$ now points up) then $\hat{n}$ is a unit vector and the equivalent equation

$$\hat{n} \cdot \boldsymbol{r} = \frac{P.E.}{m|g|},. \tag{6.19}$$

makes this clear that the equipotential of a uniform gravitational field is a simple a horizontal plane of constant height $z = \frac{P.E.}{m|g|}$ – if we align the coordinate system with $\hat{z} = \hat{n}$.
Alignment is natural and possible when there is a single "physics" direction such as the gravitational force. However, when there are multiple directions in a problem writing everything out in terms of components becomes self-defeating.

6.4.4 Example: Plane waves

A one dimensional travelling wave is normally written

$$W(x,t) = A\cos(\omega t - kx)$$

where the angular frequency $\omega = 2\pi f$, and the wavenumber $k = 2\pi\lambda$.
In two or more dimensions a travelling plane wave is extended in the direction perpendicular to its direction of travel. This can be written rather compactly as

$$W(\boldsymbol{x},t) = A\cos(\omega t - \boldsymbol{k}\cdot\boldsymbol{x}).$$

Here, $\boldsymbol{k} = k\hat{n}$ encodes both the direction $\hat{n}$ and wavenumber k. All points lying in the same plane perpendicular to $\hat{n}$ yield the same value for $\boldsymbol{k}\cdot\boldsymbol{x}$ and thus oscillate in phase.
A complex valued wave takes the form

$$Ae^{i(\omega t - \boldsymbol{k}\cdot\boldsymbol{x})}$$

6.5 Cross product

The vector, or cross, product of two vectors

$$\boldsymbol{c} = \boldsymbol{a} \times \boldsymbol{b}$$

is defined via

$$c_i = \epsilon_{ijk} a_j b_k.$$

Here, the Levi-Civita symbol ϵ_{ijk} is the totally antisymmetric tensor:

$$\epsilon_{ijk} = \begin{cases} +1 & ijk \text{ is an } \textit{even} \text{ permutation of } 123 \\ -1 & ijk \text{ is an } \textit{odd} \text{ permutation of } 123 \\ 0 & \text{otherwise (i.e. two or more indices the same} \end{cases} \tag{6.20}$$

Evaluating a cross product is typically taught via the "determinant" approach. This is rather tedious and, in my view, the simplest procedure to evaluate $\boldsymbol{c} = \boldsymbol{a} \times \boldsymbol{b}$is based on the above rule for ϵ_{ijk}, and the cyclic shifts give a positive sign; a shift and permute gives a negative sign.
Write down:

$$\hat{x}, \hat{y}, \hat{z}, \hat{x}, \hat{y}, \hat{z}$$

The cross product consecutive pairs of unit vectors become the next element of the list. Thus:

$$\begin{aligned} \hat{x} \times \hat{y} &= \hat{z} \\ \hat{y} \times \hat{z} &= \hat{x} \\ \hat{z} \times \hat{x} &= \hat{y} \end{aligned} \tag{6.21}$$

If you need to reverse order to match, then there is a minus sign:

$$\begin{aligned} \hat{y} \times \hat{x} &= -\hat{z} \\ \hat{z} \times \hat{y} &= -\hat{x} \\ \hat{x} \times \hat{z} &= -\hat{y} \end{aligned} \tag{6.22}$$

Therefore the cross product

$$\begin{aligned} (a_x\hat{x} + a_y\hat{y} + a_z\hat{z}) \times (b_x\hat{x} + b_y\hat{y} + b_z\hat{z}) \times &= (a_y b_z - a_z b_y)\hat{x} + (a_z b_x - a_x b_z)\hat{y} + (a_x b_y - a_y b_x)\hat{z} \\ &\equiv (a_y b_z - a_z b_y, a_z b_x - a_x b_z, a_x b_y - a_y b_x). \end{aligned} \tag{6.23}$$

7 Vector calculus

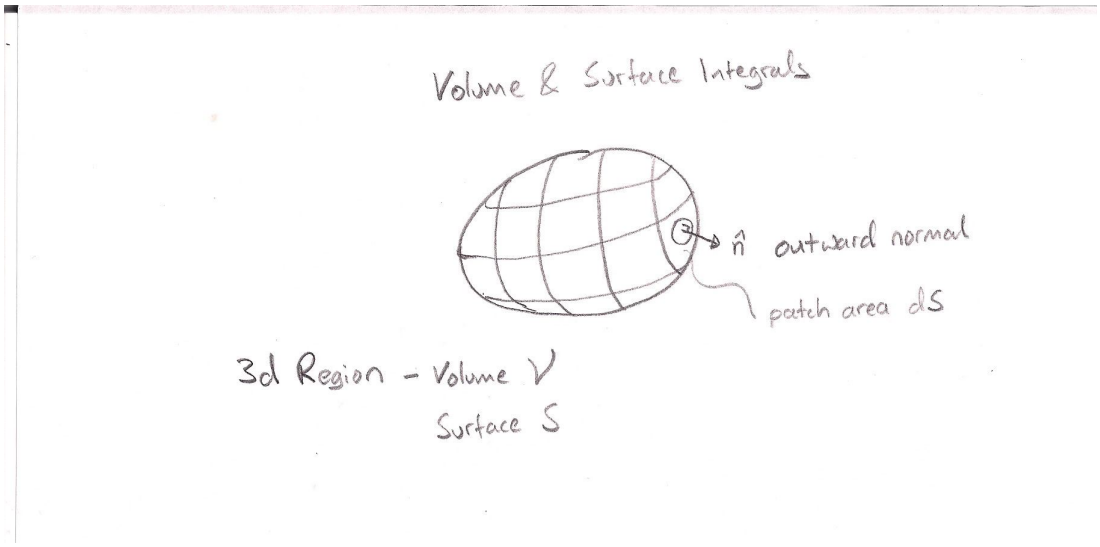
In this section we revise volume, line and surface integrals, introduce the vector differential operator $\boldsymbol{\nabla}$ and its' action on scalar and vector valued functions of three dimensions.
The mathematics introduced lies behind all physical laws, and is necessary in all be the very simplest of situations. The integral theorems are fundamental to electromagnetism. You will fail both electromagnetism and this course if you do not learn vector calculus.
In what follows, these functions will be assumed continuous, and differentiable.

7.1 Volume, Surface, and Line integrals

Volume, line and surface integrals crop up everywhere in physics, especially in the mathematical treatment of electromagnetism based on Maxwell's equations.
We first of all define what we mean by volume, surface and line integrals.

7.1.1 Volume integral

In this section we will repeatedly consider simply connected three-dimensional "chunks" of space, which we call a volume $\mathcal{V}$. The boundary of this volume represents a two dimensional *closed* surface $\mathcal{S}$.



Integrals of some scalar function $f(x, y, z)$ can be performed over the whole volume. This we denote

$$\int_{\mathcal{V}} f(\boldsymbol{x}) d\mathcal{V} \tag{7.24}$$

For example, the integral over a cube of side L is

$$\int_0^L dx \int_0^L dy \int_0^L dz f(x, y, z)$$

For irregular shapes, the integration limits for y will depend on x, and the limits for z will depend on both x and on y. However, when considering a general integral we use the notation (7.24).

Example volume integral Integrate a charge density $\rho(x) = x + y + z$ over the cube of side L to find the total charge enclosed.

$$\begin{aligned}
\int_0^L dx \int_0^L dy \int_0^L dz(x+y+z) &= \int_0^L dx \int_0^L dy \left[xz + yz + \frac{z^2}{2}\right]_0^L \\
&= \int_0^L dx \int_0^L dy xL + yL + \frac{L^2}{2} \\
&= \int_0^L dx \int_0^L dy \left[xLy + \frac{y^2}{2}L + \frac{L^2}{2}y\right]_0^L \\
&= \int_0^L dx xL^2 + L^3 \\
&= \left[\frac{x^2}{2}L^2 + L^3 x\right]_0^L \\
&= \frac{3L^4}{2} \qquad (7.25)
\end{aligned}$$

Example irregular volumes FIXME parametric bounds.

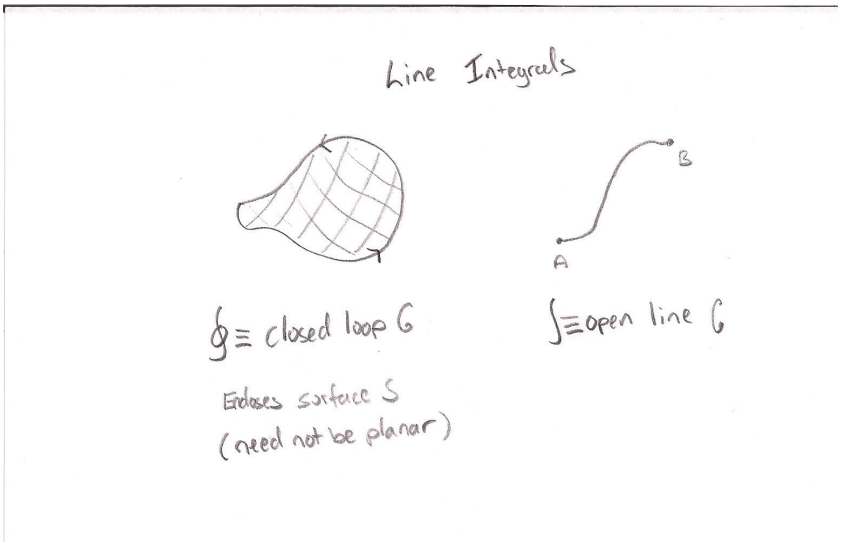
7.2 Line integrals in physics

A line integral of a vector field $\boldsymbol{v}$ over some curve $\mathcal{C}$ is the integral long the line of the component of the vector parallel to the tangential to the curve:

$$\int_{\mathcal{C}} \boldsymbol{v} \cdot d\boldsymbol{l}$$

Here the differential $d\vec{l}$ can be thought of as $dl\hat{t}$ and where dl a scalar integration variable representing the distance along the line, while $\hat{t}$ is the unit vector in the direction of the tangent to the line. If the curve $\mathcal{C}$ is a closed loop (e.g. the boundary of some open surface), this is written as

$$\oint_{\mathcal{C}} \boldsymbol{v} \cdot d\boldsymbol{l}.$$



7.2.1 Example: work done

If an object is moved in the presence of a force, the work done is "force times distance". More precisely, the work done is the product of the force and the distance travelled *in the direction of the force.*
So, in moving from position vector $\boldsymbol{r} = (x, y, z)$ to position vector $\boldsymbol{r} + d\boldsymbol{r}$, with $d\boldsymbol{r} = (dx, dy, dz)$, against a position-dependent force $\boldsymbol{F}(\boldsymbol{r})$, the work done is $\boldsymbol{F}(\boldsymbol{r}) \cdot d\boldsymbol{r}$.
If we move along a path described by a contour $\mathcal{C}$ (which could be open or closed), the total work done is

$$\int_{\mathcal{C}} \boldsymbol{F}(\boldsymbol{r}) \cdot d\boldsymbol{r}$$

which is an example of a line integral.

7.2.2 Strategy for evaluating line integrals

A line integral looks very compact, but to actually calculate the answer we need to unpack it:

1. Express the force components. This is usually just given to you.
2. Break the path up into sections, each of which is easy to express.
3. For each section, find an expression for $d\boldsymbol{r}$ in terms of one integration variable. For instance:
   - If we are integrating (i.e. moving) along a line parallel to the x-axis, so $d\boldsymbol{r} = (dx, 0, 0)$.
   - If we are integrating along the parabola $y = x^2$ at fixed $z = c$, then $dy = 2x\ dx$ and $dz = 0$, so $d\boldsymbol{r} = (dx, 2x\ dx, 0)$.
   - If we are integrating along the line defined parametrically: $x = 2t^3$, $y = t^2$, $z = t$ between $t = 0$ and $t = 1$ then $d\boldsymbol{r} = (6t^2 dt, 2t\ dt, dt)$.
4. Substitute the definition of the line into the equation for the force so that it only involved the integration variable. For instance, if the force is $\boldsymbol{F}(\boldsymbol{r}) = (x^3, 2yz, x)$:
   - and we are integrating along the parabola $y = x^2$ at fixed $z = c$, then on that line $\boldsymbol{F}(\boldsymbol{r}) = (x^3, 2(x^2)c, x)$.

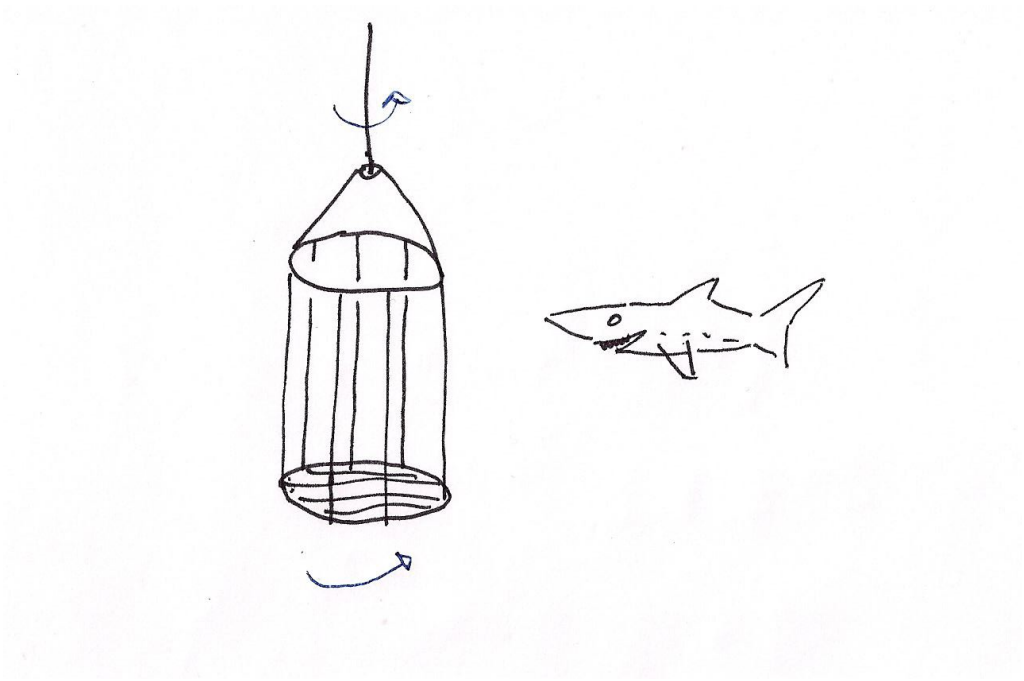
- or if we are integrating along the line defined parametrically: $x = 2t^3$, $y = t^2$, $z = t$, then on the line $\boldsymbol{F}(\boldsymbol{r}) = ((2t^3)^3, 2(t^2)t, 2t^3)$.

5. Expand the dot product and calculate the resulting integral for that line section. Repeat the above proces for all line sections and sum up the results.

If we reverse the direction of a line integral, keeping the same contour and swapping the start and end points, we just get minus the original answer.

7.2.3 Example: Chief Brody's shark cage

Chief Brody is cowering in a very light cylindrical shark cage, radius r suspended in the ocean currents. The cage is free to rotate in a horizontal plane.



If the flow is uniform and fast, Chief Brody will simply be pressed up against the cage wall. If the flow swirls, however, the cage will rotate at a rate determined by the difference in the velocity on the two sides and poor Chief Brody will become rather dizzy.
The drag force per-unit length is $b\boldsymbol{v}\cdot\hat{t}$ where $\hat{t}$ is the unit tangent vector $\hat{z}$ to the surface of the cage. The section associated pie slice of width $d\theta$ has length $rd\theta$. The force on this section is $brd\theta\boldsymbol{v}\cdot\hat{t}$. Writing this as a *line integral* we have a vector differential $d\boldsymbol{l}$, and

$$\begin{aligned}\tau &= b\oint \boldsymbol{v}\cdot\hat{t}rd\theta \\ &= b\oint \boldsymbol{v}\cdot d\boldsymbol{l}\end{aligned} \tag{7.26}$$

This torque will vanish if the (very light) cage rotates at an angular velocity $\omega = \frac{\oint \boldsymbol{v}\cdot d\boldsymbol{l}}{2\pi r^2}$.
Unsurprisingly, we conclude that the bars of the cage rotate with speed

$$s = r\omega = \frac{\oint \boldsymbol{v}\cdot d\boldsymbol{l}}{2\pi r}$$

which is just the mean tangential speed of the water flow averaged around the perimeter.

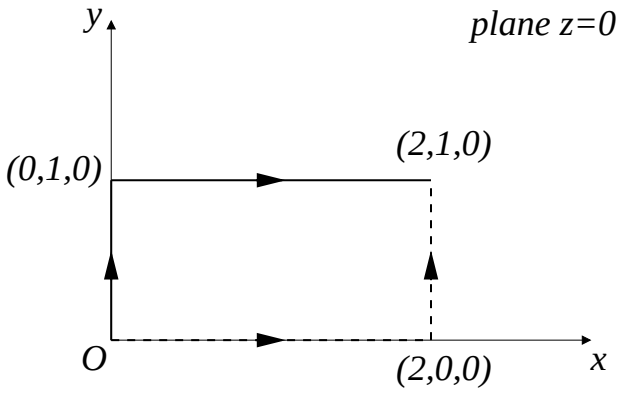


Figure 7.6: Two line integral contours with the same start and end points.

7.2.4 Example: Line integral

As an example, if $\boldsymbol{F}(\boldsymbol{r}) = (xy, -y^2, 0)$ and we move from point $\boldsymbol{r} = (0,0,0)$ to $(2,1,0)$ by first moving up the y-axis to $(0,1,0)$ and then parallel to the x-axis to $(2,1,0)$. These two sections are shown as solid lines in Fig. 7.6.
We are given the force in Cartesian coordinates. We split the line integral into two parts. For the first part, $d\boldsymbol{r} = (0, dy, 0)$ and we integrate dy from $y = 0$ to $y = 1$. Along this line, $x = z = 0$, so $\boldsymbol{F} = (0, -y^2, 0)$ and the contribution to the line integral is:

$$\int_0^1 \begin{pmatrix} 0 \\ -y^2 \\ 0 \end{pmatrix} \cdot \begin{pmatrix} 0 \\ dy \\ 0 \end{pmatrix} = \int_0^1 dy \ -y^2 = -\frac{1}{3} \, .$$

Along the second part, $d\boldsymbol{r} = (dx, 0, 0)$ and we integrate dx from $x = 0$ to $x = 2$. Along this line, $y = 1$ and $z = 0$, so $\boldsymbol{F} = (x, -1, 0)$ and the contribution to the line integral is:

$$\int_0^2 \begin{pmatrix} x \\ -1 \\ 0 \end{pmatrix} \cdot \begin{pmatrix} dx \\ 0 \\ 0 \end{pmatrix} = \int_0^2 dx \ x = 2 \, .$$

So the final answer for the line integral is $I_1 = -\frac{1}{3} + 2 = \frac{5}{3}$.
Now consider a new problem: the same force and the same start and end points, but a moving between them on a different contour: first moving along the x-axis (the line $y = 0$) from $(0,0,0)$ to $(2,0,0)$ and then up the line $x = 2$ from $(2,0,0)$ to $(2,1,0)$. This is shown as dashed lines in Fig. 7.6. The answer is:

$$I_2 = \int_0^2 \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix} \cdot \begin{pmatrix} dx \\ 0 \\ 0 \end{pmatrix} + \int_0^1 \begin{pmatrix} 2y \\ -y^2 \\ 0 \end{pmatrix} \cdot \begin{pmatrix} 0 \\ dy \\ 0 \end{pmatrix} = 0 + \int_0^1 dy \ -y^2 = -\frac{1}{3} \, .$$

In general, the work done is a path-dependent quantity, so $I_1 \neq I_2$ even for the same force.
Because the start and end points are the same, if we go out on the dashed contour and back on the solid, we end up where we started. Reversing the direction we traverse the solid contour switches the sign of the line integral. So the net work done in moving around the closed path built of straight lines $(0,0,0) \to (2,0,0) \to (2,1,0) \to (0,1,0) \to (0,0,0)$ is $I_2 - I_1 = -\frac{1}{3} - \frac{5}{3} = -2$.
The answer is not zero because the line integral is path dependent. In many cases this is physically sensible: if we push a washed-up refrigerator around a closed path on a sandy beach, we do a lot of work in getting back to where we started.
A line integral around a closed contour is often written using $\oint$ instead of $\int$, but it means the same thing.

7.3 Surface integrals

The flux of a vector valued function of position (vector field) through a surface can be computed as a surface integral. The surface is divided into infinitessimal area elements $d\mathcal{S}$.
A direction through the surface is chosen as positive flux. The *normal* $\hat{n}$ defined such that at any point on the surface $\hat{n}$ is the unit vector pointing in this direction.
For a closed surface this is most naturally the outward direction, and for a open surface with a perimeter we are normally interested in a direction around its perimeter (e.g. Faradays law). In this case the right hand rule chooses the direction.
The surface integral of a vector $\boldsymbol{v}(x, y, z)$, is

$$\int_{\mathcal{S}} \boldsymbol{v} \cdot \hat{n} d\mathcal{S}.$$

For example, if light shines on a surface, the amount of photons crossing the surface per unit time is proportional to the intensity of light times the area. More carefully, we need to worry at which angle the light is incident on the surface.
Given an element of surface dS whose *outward* normal is the unit vector $\hat{\boldsymbol{n}}$, we can define $d\boldsymbol{S} = \hat{\boldsymbol{n}}\, dS$. In general $d\boldsymbol{S}(\boldsymbol{r})$ will be position dependent.
If we describe the flow of photons by a current (a vector $\boldsymbol{J}(\boldsymbol{r})$ which might be position dependent), the flux across an element of surface is $\boldsymbol{J}(\boldsymbol{r}) \cdot d\boldsymbol{S}$. Integrating over the complete surface S (which could be open or closed), gives the total flux:

$$\int_S \boldsymbol{J} \cdot d\boldsymbol{S}$$

which is an example of a surface integral.

7.3.1 Strategy for evaluating surface integrals

As with the line integral, to actually evaluate this we have to break this neat expression down into something calculable:

1. Express the current components. This is usually just given to you.
2. Break the surface up into sections, each of which is easy to express mathematically.
3. For each section, identify the normal vector $\hat{\boldsymbol{n}}$ and find an expression for dS in terms of one integration measure. For instance:
   - If we are integrating over a surface in the xy-plane, the normal vector is parallel to the z-axis and $dS = dx\, dy$.
   - For most common surfaces, the normal vector is easy to construct from a sketch. Or we can exploit the fact that is our surface can be described by a function $\phi(\boldsymbol{r}) =$ constant, then the normal is parallel to $\boldsymbol{\nabla}\phi$, e.g.:
     - A sphere of radius a centred on the origin has surface $x^2 + y^2 + z^2 = a^2$, so $\phi = x^2 + y^2 + z^2 =$ constant. $\boldsymbol{\nabla}\phi = (2x, 2y, 2z) = 2\boldsymbol{r}$ so the unit normal vector is $\hat{\boldsymbol{n}} = \hat{\boldsymbol{r}}$. The surface element dS is best expressed in spherical polar coordinates: $dS = a^2 d\theta d\phi$.

– For a cylinder of radius a, the curved surface is $x^2+y^2=a^2$ and $\hat{\boldsymbol{n}}=(x,y,0)/\sqrt{x^2+y^2}$. The surface element is best expressed in cylindrical polar coordinates: $dS=ad\phi dz$. For the flat ends of the cylinder, $z=$ constant, so the unit normal vector is $(0,0,\pm1)$. Why "$\pm$"? $\hat{\boldsymbol{n}}$ should be the *outward* normal vector, so for the top of the cylinder it is $(0,0,1)$ and for the bottom $(0,0,-1)$. In each case $dS=dx\ dy$ in Cartesian coordinates, or $dS=\rho d\rho\ d\phi$ in cylindrical polars.

4. Expand the dot product and calculate the resulting double integral for that line section. Repeat for all surface sections and sum up the results.

Clearly the flux across the surface is minus the flux in the opposite direction. This is because $\hat{\boldsymbol{n}}$ switches sign because the *outward* for the surface is opposite in each case.

7.3.2 Example: surface integral over cube

The surface integral over the cube has terms from the six faces

$$\begin{aligned}\int_{\mathcal{S}} \boldsymbol{v}\cdot\hat{n}d\mathcal{S} &= \int_0^L dy\int_0^L dz\boldsymbol{v}(L,y,z)\cdot\hat{x}-\int_0^L dy\int_0^L dz\boldsymbol{v}(0,y,z)\cdot\hat{x}\\ &+\int_0^L dx\int_0^L dz\boldsymbol{v}(x,L,z)\cdot\hat{y}-\int_0^L dx\int_0^L dz\boldsymbol{v}(x,0,z)\cdot\hat{y}\\ &+\int_0^L dx\int_0^L dy\boldsymbol{v}(x,y,L)\cdot\hat{z}-\int_0^L dx\int_0^L dy\boldsymbol{v}(x,y,0)\cdot\hat{z}\end{aligned}\tag{7.27}$$

If $\boldsymbol{v}$ is a uniform flow (independent of position), then the opposite sign integrals cancel, and we get zero: as much flows into the box as flows out of the box under constant flow.
If we take $\boldsymbol{x}=(y,z,x)$ then we get

$$\begin{aligned}\int_{\mathcal{S}} \boldsymbol{v}\cdot\hat{n}d\mathcal{S} &= \int_0^L dy\int_0^L dzL-0\\ &+\int_0^L dx\int_0^L dzL-0\\ &+\int_0^L dx\int_0^L dyL-0\\ &=3L^3\end{aligned}\tag{7.28}$$

7.4 Partial derivatives

If $f(x,y)$ is a function of two variables, we can define partial derivatives with respect to each variable.

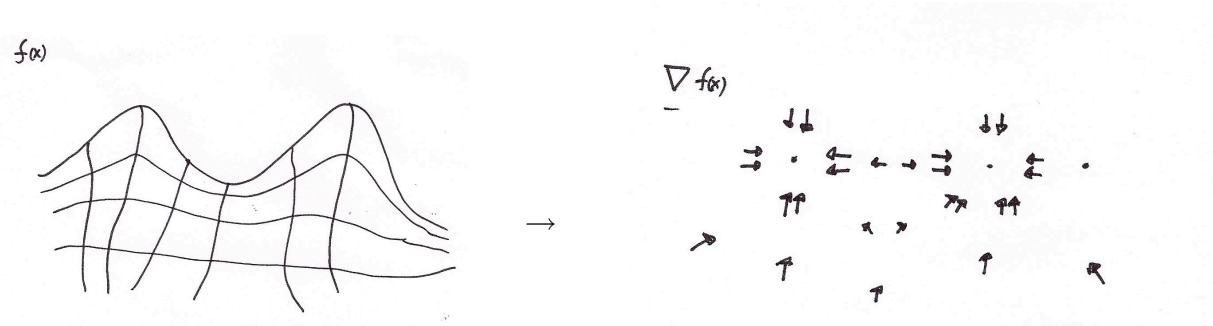
$$\begin{aligned}\frac{\partial}{\partial_x}f(x,y) &= \lim_{\epsilon\to 0}\frac{f(x+\epsilon,y)-f(x,y)}{\epsilon}\\ \frac{\partial}{\partial_y}f(x,y) &= \lim_{\epsilon\to 0}\frac{f(x,y+\epsilon)-f(x,y)}{\epsilon}\end{aligned} \tag{7.29}$$

7.5 Gradient operator

We define the gradient operator *grad* as:

$$\boldsymbol{\nabla} = \frac{\partial}{\partial_x}\hat{x} + \frac{\partial}{\partial_y}\hat{y} + \frac{\partial}{\partial_z}\hat{z} \tag{7.30}$$

In two dimensions this is very familiar. If $f(x,y)$ is a function of two variables (a height as a function of map coordinates), then $\boldsymbol{\nabla} f(x,y)$ is just a two component vector indicating the steepness and direction of slope.



7.5.1 Example: Electrostatic field

The electric field in one dimension is given by $E(x) = -\frac{dV(x)}{dx}$.
In three dimensions this clearly generalises as follows:

$$\begin{aligned}E_x(x,y,z) &= -\frac{\partial V(x,y,z)}{\partial_x}\\ E_y(x,y,z) &= -\frac{\partial V(x,y,z)}{\partial_y}\\ E_z(x,y,z) &= -\frac{\partial V(x,y,z)}{\partial_z}.\end{aligned} \tag{7.31}$$

This is rather succintly written as

$$\boldsymbol{E} = -\boldsymbol{\nabla} V = -(\frac{\partial V(x,y,z)}{\partial_x}, \frac{\partial V(x,y,z)}{\partial_y}, \frac{\partial V(x,y,z)}{\partial_z})$$

Here, V is a scalar, $\boldsymbol{\nabla}$ is a vector indexed differential operator, and the result $\boldsymbol{E}$ is vector.
The direction of the gradient $\boldsymbol{\nabla}$ of a function picks out the direction of steepest upwards slope (i.e. the opposite direction to a skiers "fall-line") automatically.

7.5.2 Example: Gravitational field

Let's revisit our gravitational potential example

$$P.E.(\boldsymbol{r}) = -m(\boldsymbol{g} \cdot \boldsymbol{r}).$$

Then the gradient is a vector and picks out the gravitational field direction:

$$-\boldsymbol{\nabla} P.E.(\boldsymbol{r}) = m\boldsymbol{g}$$

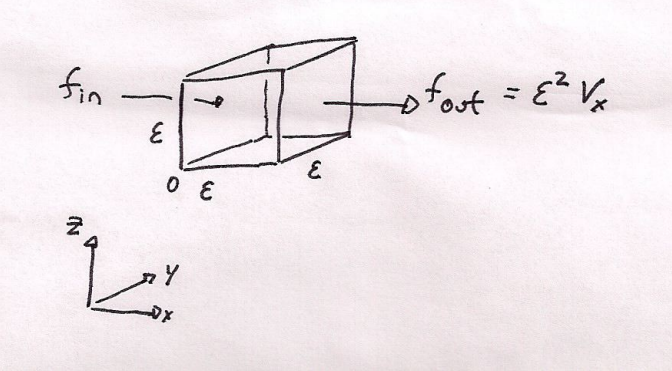
7.6 Divergence of a vector function

Consider a *vector field* $\boldsymbol{v}(x, y, z) = \boldsymbol{v}(\boldsymbol{x})$.
The divergence of a vector field is the scalar product

$$\boldsymbol{\nabla} \cdot \boldsymbol{v}(\boldsymbol{x}) = \frac{\partial}{\partial_x} v_x + \frac{\partial}{\partial_y} v_y + \frac{\partial}{\partial_z} v_z + .$$

7.6.1 Example: Oil from a well

To illustrate the meaning of *divergence* consider an idealised blow-out preventer as a tiny pipe releasing crude oil into the Gulf stream.
We denote the velocity field $\boldsymbol{v}(\boldsymbol{x})$, and consider a cubical box of side ϵ, volume ϵ^3, containing the outlet. The box is taken sufficiently small that Taylor expansion of the $\boldsymbol{v}(\boldsymbol{x})$ works.



If we consider the $\hat{x}$ faces first, the inflow (for positive v_x), in $m^3 s^1$, through face-A is

$$f_{\text{in}} = \epsilon^2 v_x(0, \frac{\epsilon}{2}, \frac{\epsilon}{2}) + O(\epsilon)^4).$$

We can always take ϵ small enough that this is a good approximation. The net outflow through face-B is is

$$f_{\text{out}} = \epsilon^2 v_x(\epsilon, \frac{\epsilon}{2}, \frac{\epsilon}{2}) + O(\epsilon)^4) = \epsilon^2 [v_x(0, \frac{\epsilon}{2}, \frac{\epsilon}{2}) + \epsilon \frac{\partial}{\partial_x} v_x(0, \frac{\epsilon}{2}, \frac{\epsilon}{2})]$$

Thus the net outflow from these faces is

$$f_{\text{out}} - f_{\text{in}} = \epsilon^3 \frac{\partial}{\partial_x} v_x(0, \frac{\epsilon}{2}, \frac{\epsilon}{2}).$$

The other directions are similar and the net outflow per unit volume is

$$\frac{\partial}{\partial_x} v_x + \frac{\partial}{\partial_y} v_y + \frac{\partial}{\partial_z} v_z = \boldsymbol{\nabla} \cdot \boldsymbol{v}.$$

Thus we can identify the divergence of a vector field as the *outflow per unit volume.*

7.6.2 Vector identities

The "simplifications at the abstract level" mentioned above come from using vector identities like:

$$\boldsymbol{\nabla} \cdot \boldsymbol{\nabla} f = \nabla^2 f \quad (\text{"div grad = Laplacian"}) \tag{7.32}$$
$$\boldsymbol{\nabla} \times \boldsymbol{\nabla} f = 0 \quad (\text{"curl grad = 0"}) \tag{7.33}$$
$$\boldsymbol{\nabla} \cdot (\boldsymbol{\nabla} \times \boldsymbol{J}) = 0 \quad (\text{"div curl = 0"}) \tag{7.34}$$
$$\boldsymbol{\nabla} \times (\boldsymbol{\nabla} \times \boldsymbol{J}) = \boldsymbol{\nabla}(\boldsymbol{\nabla} \cdot \boldsymbol{J}) - \nabla^2 \boldsymbol{J} \quad (\text{"curl curl = grad div - Laplacian"}) \tag{7.35}$$
$$\boldsymbol{\nabla} \cdot (f\, \boldsymbol{J}) = f(\boldsymbol{\nabla} \cdot \boldsymbol{J}) + \boldsymbol{J} \cdot (\boldsymbol{\nabla} f) \tag{7.36}$$
$$\boldsymbol{\nabla} \times (f\, \boldsymbol{J}) = f(\boldsymbol{\nabla} \times \boldsymbol{J}) - \boldsymbol{J} \times (\boldsymbol{\nabla} f) \tag{7.37}$$

where f and J are arbitrary scalar and vector quantities.
You should be able to prove these expressions (using index notation). Because they all involve vectors, if you prove them for Cartesian coordinates (the simplest), you know (and can just state) that they must be true in all coordinate systems.
The trick to proving these is not to forget to write in f or $\boldsymbol{J}$, so you don't miss any cross terms. Within each term, each derivative acts on *everything* to the right of it.

7.7 Integral theorems

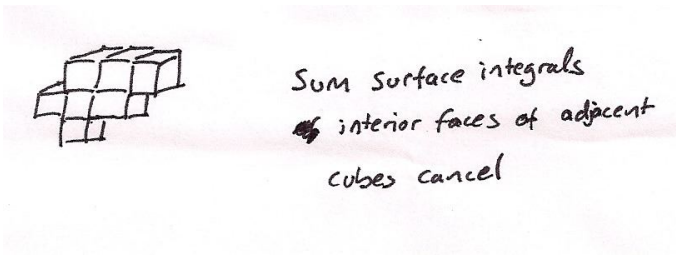
The following two theorems are fundamental to most of physics!

7.7.1 Divergence theorem

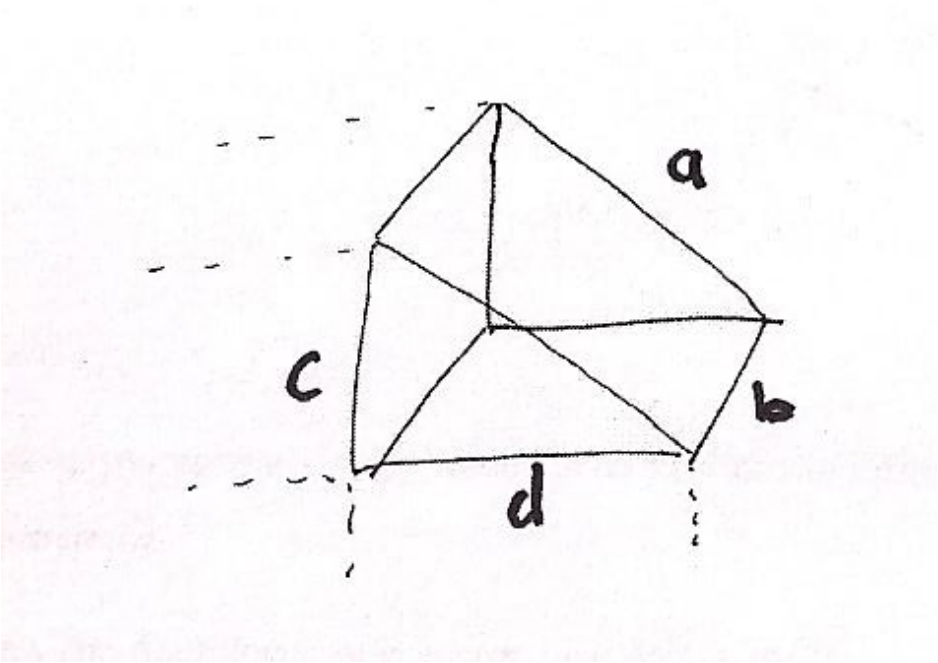
The divergence theorem (also known as Gauss' theorem) states that the integral of the divergence of a vector $\boldsymbol{v}$ over a generic volume $\mathcal{V}$, is equal to the integral over the bounding surface $\mathcal{S}$ of the dot product of $\boldsymbol{v}$ with the unit outward facing normal vector.

$$\boxed{\int_{\mathcal{V}} \boldsymbol{\nabla} \cdot \boldsymbol{v} d\mathcal{V} = \int_{\mathcal{S}} \boldsymbol{v} \cdot \hat{n} d\mathcal{S}}$$

Since we proved this above for an infinitessimal volume element, the theorem can easily be proved by considering the volume as filled with a Lego-stack of infinitessimal volume elements.



The total volume integral of the divergence is just the sum of the infinitessimal divergence contributions.
In summing the surface integrals from the volume elements, the *interior* face contributions from neighbouring elements must cancel, as the field is the same, while the outward normal reverses sign. The *exterior* faces can always be reduced to plane segments like:



Consider the sloped face: its normal is just

$$\hat{n} = (\frac{c}{a}, \frac{d}{a}, 0)$$

Here the flow through that tracks the exterior surface is

$$\begin{aligned} ab\hat{n} \cdot \boldsymbol{v} &= ab(v_x \frac{c}{a} + v_y \frac{d}{a}) \\ &= bcv_x + bdv_y \end{aligned} \tag{7.38}$$

and this is therefore the sum of the flows over the two faces (having drop terms of order ϵ from the coordinate dependence of $\boldsymbol{v}$).
Thus, at the very boundary, the jagged lego edges are equivalent to the smooth surface when we use small boxes, and the sum of the surface integrals of the volume elements is equal to the overall surface integral for the whole region.
This proves the divergence theorem!

7.8 Curl of a vector function

The vector cross product can also be used to define the *curl* of a vector. The name *curl* was coined by James Clerk Maxwell.

$$\boldsymbol{\nabla} \times \boldsymbol{v} = (\frac{\partial}{\partial_y} v_z - \frac{\partial}{\partial_z} v_y, \frac{\partial}{\partial_z} v_x - \frac{\partial}{\partial_x} v_z, \frac{\partial}{\partial_x} v_y - \frac{\partial}{\partial_y} v_x)$$

Example: Chief Brody's shark cage (again)

To illustrate the meaning of the curl of a vector field, we will again consider the velocity field of shark infested sea water. Now, we will make the cage infinitessimally small... anything can happen in Hollywood!

We now show that the line integral of velocity is related to the z-component of the curl of the water velocity.
Consider the line integral around the small triangle ABC:

$$\begin{aligned}\oint_{ABC} \boldsymbol{v}d\boldsymbol{l} &= \int_{AB} \boldsymbol{v}d\boldsymbol{l} \int_{BC} \boldsymbol{v}d\boldsymbol{l} \int_{CA} \boldsymbol{v}d\boldsymbol{l} \\ &= \int_0^1 v_x(at,0)adt + \int_0^1 [v_y(a(1-t),bt)b - v_x(a(1-t),bt)a]dt - \int_0^1 v_y bdt\end{aligned}$$

For small distances, the velocity field is describes by

$$\boldsymbol{v}(x,y) = \boldsymbol{v}(0,0) + x\frac{\partial}{\partial_x}\boldsymbol{v}(0,0) + y\frac{\partial}{\partial_y}\boldsymbol{v}(0,0)$$

Thus, for a small triangle oriented in the x-y plane

$$\begin{aligned}\oint_{ABC} \boldsymbol{v}d\boldsymbol{l} &= \int_0^1 [v_x(0,0) + at\frac{\partial}{\partial_x}v_x(0,0)]adt \\ &\quad + \int_0^1 [v_y(0,0) + a(1-t)\frac{\partial}{\partial_x}v_y(0,0) + bt\frac{\partial}{\partial_y}v_y(0,0)]bdt \\ &\quad - \int_0^1 [v_x(0,0) + a(1-t)\frac{\partial}{\partial_x}v_x(0,0) + bt\frac{\partial}{\partial_y}v_x(0,0)]adt \\ &\quad - \int_0^1 [v_y(0,0) + bt\frac{\partial}{\partial_y}v_x(0,0)]bdt\end{aligned}$$

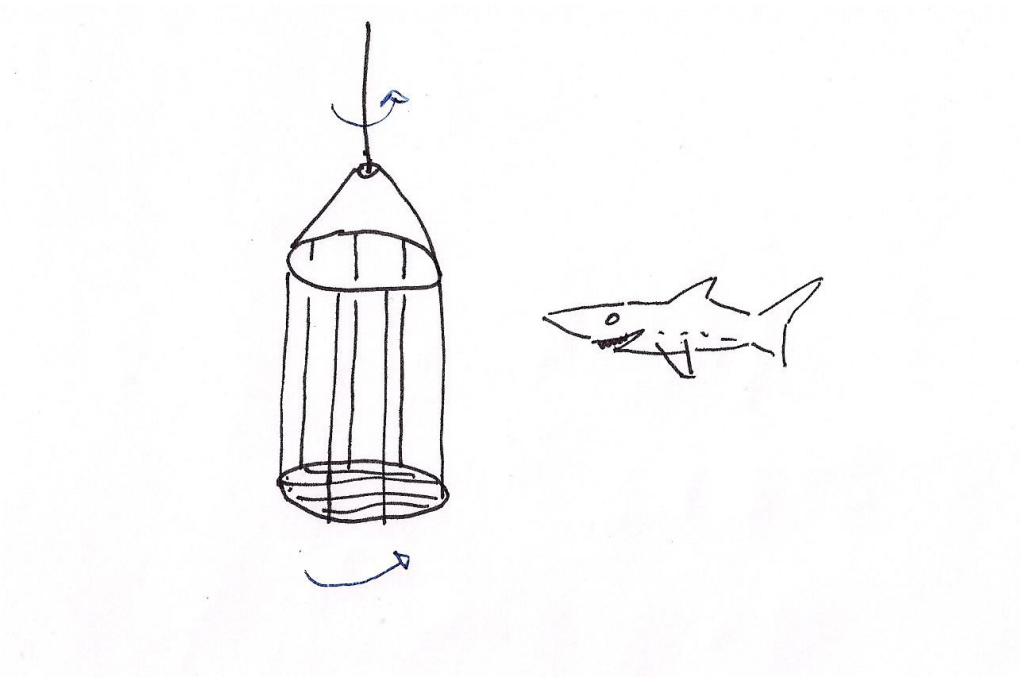
$$\begin{aligned}\oint_{ABC} \boldsymbol{v}d\boldsymbol{l} &= \cancel{v_x(0,0)(a-a) + v_x(0,0)(b-b)} \\ &+ \cancel{\frac{1}{2}(a^2-a^2)\frac{\partial}{\partial_x}v_x(0,0) + \frac{1}{2}(b^2-b^2)\frac{\partial}{\partial_y}v_y(0,0)} \\ &+ \frac{1}{2}ab\frac{\partial}{\partial_x}v_y(0,0) - \frac{1}{2}ab\frac{\partial}{\partial_y}v_x(0,0) \\ &= \frac{1}{2}ab(\boldsymbol{\nabla}\times\boldsymbol{v})_z\end{aligned}$$

This is just the product of the area $d\mathcal{S}$ with the normal unit vector $\hat{n}$ to the triangle "dotted" with the curl of $\boldsymbol{v}$:

$$\boldsymbol{\nabla}\times\boldsymbol{v}\cdot\hat{n}d\mathcal{S}$$

The normal is defined such the direction of the line integral follows the right handed rule (fingers point in direction of integral, thumb defines normal vector to surface).
Now, if two triangles are placed edge to edge, the line integral around the perimeter of the two, is equal to the sum of the line integrals: the interior line enters the individual line integrals for each triangle with opposite sign such that it vanishes in the sum.

Now, our infinitessimal circular line integral can be inferred by tiling with (even more!) infinitessimal triangles. This is just the area multiplied by the curl of the velocity, and we have the angular velocity is $\omega = \frac{\pi r^2 \boldsymbol{\nabla} \times \boldsymbol{v}}{2\pi r^2} = \frac{1}{2} \boldsymbol{\nabla} \times \boldsymbol{v}$.



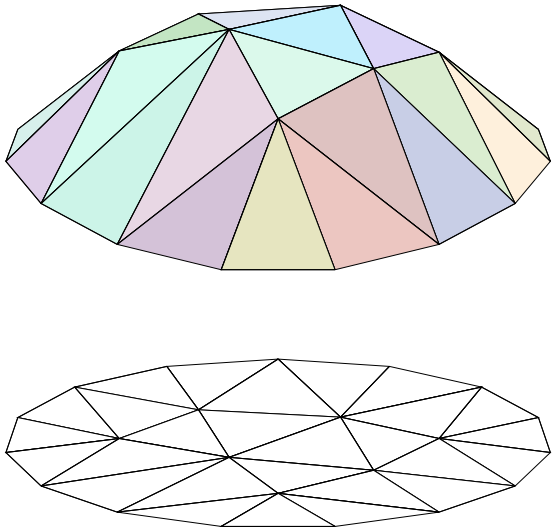
Thus, a simple interpretation of the curl of a vector field is as determining the rate at which Chief Brody's cage will rotate while he is waiting for Jaws to eat him.

7.8.1 Stoke's theorem

Stoke's theorem states that the line integral of a vector $\boldsymbol{v}$ around a closed curve $\mathcal{C}$ is equal to the surface integral of $\boldsymbol{v}$ over any area $\mathcal{S}$ bounded by that curve.

$$\boxed{\int_{\mathcal{S}} \boldsymbol{\nabla} \times \boldsymbol{v} d\mathcal{S} = \oint_{\mathcal{C}} \boldsymbol{v} \cdot dl}$$

Given the above proof for an infinitessimal triangle and circle, the result is easy. We simply tile *any* curved surface area bounded by the line $\mathcal{S}$ with a "spider web" composed of infinitessimal triangles.



The surface integral is the sum of the area integrals from each infinitessimal triangle.
This has to be equal to the sum of the line integrals around each triangle. However, the interior line segments of the spider web are always traversed twice, and in opposite directions from the two triangles on either side, and we are left only with the line integral around the perimiter which is traversed once.
This proves the result.

7.9 Conservatism, irrotationalism and the scalar potential

If a vector field $\boldsymbol{F}$ is *irrotational*, i.e. its curl is zero at all points in space, then the line integral around a closed contour is zero. This in turn implies that the line integral of $\boldsymbol{F}$ along an open contour is path-independent. When we use a line integral to calculate work done and we have path independence, we say the force is *conservative* (with a small "c"). Gravity is a conservative force (as well as it being fictitious), but friction is not conservative.
Since "curl grad = 0", if $\boldsymbol{\nabla} \times \boldsymbol{F} = 0$, there must exist a *scalar potential* $\phi(\boldsymbol{r})$ such that the vector field $\boldsymbol{F} = -\boldsymbol{\nabla}\phi$. The minus sign is just a convention. ϕ is a scalar field, so it just has one value (and no direction) at each point in space. In many cases, ϕ is the potential energy of the system.
As grad of a constant is zero, we have the freedom to vary ϕ by a constant.In the case of potentials, we often choose this constant so that $\phi \to 0$ as $|\boldsymbol{r}| \to \infty$.
If you need to calculate ϕ, in simple cases you can do this by hand: think of a function such that each component of $-\boldsymbol{\nabla}\phi$ gives the same component of $\boldsymbol{F}$. A more systematic way is to calculate a line integral of $\boldsymbol{F}$ from some reference point (often ∞) to position $\boldsymbol{r}$ (of course, the path taken between these points doesn't matter). You can find details of this in most relevant textbooks, including Boas.

7.10 Laplacian

The Laplacian operator acting on a scalar function f is

$$\boldsymbol{\nabla}^2 f = \boldsymbol{\nabla} \cdot (\boldsymbol{\nabla} f) = (\frac{\partial^2}{\partial_x^2} + \frac{\partial^2}{\partial_y^2} + \frac{\partial^2}{\partial_z^2}) f,$$

.

We define the Laplacian of a vector function $\boldsymbol{v}$ as

$$\boldsymbol{\nabla}^2\boldsymbol{v} = (\boldsymbol{\nabla}^2\boldsymbol{x}, \boldsymbol{\nabla}^2\boldsymbol{y}, \boldsymbol{\nabla}^2\boldsymbol{z})$$

Exercise: show that

$$\boldsymbol{\nabla}^2\boldsymbol{v} = \boldsymbol{\nabla}(\boldsymbol{\nabla}\cdot\boldsymbol{v}) - \boldsymbol{\nabla}\times(\boldsymbol{\nabla}\times\boldsymbol{v})$$

I call this the "gdmcc" rule as an aide memoir. This is essential in the derivation of electromagnetic plane waves from Maxwell's equations.

7.11 Physical applications examples

We now illustrate some of the most common applications

7.11.1 Action on a plane wave

Suppose a function is a complex plane wave. This could be, for example, a quantum mechanical wave function.

$$f(\boldsymbol{x}) = e^{i(\boldsymbol{k}\cdot\boldsymbol{x}-\omega t)}$$

Then

$$\boldsymbol{\nabla}f(\boldsymbol{x}) = i\boldsymbol{k}e^{i(\boldsymbol{k}\cdot\boldsymbol{x}-\omega t)} = i\boldsymbol{k}f(\boldsymbol{x})$$

and

$$\boldsymbol{\nabla}^2 f(\boldsymbol{x}) = -k^2 e^{i(\boldsymbol{k}\cdot\boldsymbol{x}-\omega t)} = -k^2 f(\boldsymbol{x})$$

For a vector function:

$$\boldsymbol{v}(x) = \boldsymbol{v}_0 e^{i(\boldsymbol{k}\cdot\boldsymbol{x}-\omega t)}$$

we have

$$\boldsymbol{\nabla}\cdot\boldsymbol{v}(x) = (\boldsymbol{k}\cdot\boldsymbol{v}_0)e^{i(\boldsymbol{k}\cdot\boldsymbol{x}-\omega t)} = \boldsymbol{k}\cdot\boldsymbol{v}(x)$$

and

$$\boldsymbol{\nabla}\times\boldsymbol{v}(x) = (\boldsymbol{k}\times\boldsymbol{v}_0)e^{i(\boldsymbol{k}\cdot\boldsymbol{x}-\omega t)} = \boldsymbol{k}\times\boldsymbol{v}(x)$$

$$\boldsymbol{\nabla}^2\boldsymbol{v}(x) = \left[\boldsymbol{k}(\boldsymbol{k}\cdot\boldsymbol{v}_0) - \boldsymbol{k}\times(\boldsymbol{k}\times\boldsymbol{v}_0)\right]e^{i(\boldsymbol{k}\cdot\boldsymbol{x}-\omega t)} = \boldsymbol{k}\cdot\boldsymbol{v}(x)$$

This last relation is essential in the derivation of electromagnetic plane waves from Maxwell's equations.

7.11.2 Gaussian pill boxes

Then there is a high degree of symmetry, a common technique is apply the divergence theorem to surface chosen to align with the symmetries of the problem.
For example, consider Gauss' Law

$$\boldsymbol{\nabla}\cdot\boldsymbol{E}(\boldsymbol{x}) = \frac{\rho(\boldsymbol{x})}{\epsilon_0}$$

The divergence theorem of course implies that the integral of the flux crossing a surface is the volume integral of the charge density – i.e. total charge enclosed – divided by ϵ_0.
Consider the infinite parallel plate capacitor.
In a metal, the electrons are mobile and move in response to any electric field until that field is cancelled. The symmetry under $y \leftrightarrow -y$ means that $E_y = E_z = 0$.

Thus, for the Gaussian pill box show, only face A is crossed by a field $E_x = V/d$.
The volume integral of charge density is the total charge contained: $Q = \epsilon^2\tilde{\rho}$ where we denote the charge per unit area $\tilde{\rho}$.
The surface integral is $\int_{\mathcal{S}} \boldsymbol{E} \cdot \hat{n} d\boldsymbol{\mathcal{S}} = \epsilon^2 \frac{V}{d}$
And, so

$$\tilde{\rho} = \epsilon_0 \frac{V}{d}$$

And the famous relation

$$Q = \frac{A\epsilon_0}{d} V$$

Now, here there is an interesting aspect to the idealisation that will be important later:
The total charge in our Gaussian pill box is a fixed, finite number. However, this finite charge lies in an *infinitely narrow* sheet at the surface. The volume density $\rho(\vec{x})$ must be infinite while $\int_{\mathcal{V}} \rho d\mathcal{V}$ has a definite value.
Our mathematical idealisation must be treated carefully - if we take an infinitessimal width ϵ, negligibly smaller than any other length scale in the problem, and the charge density to be

$$\rho(\boldsymbol{x}) = \begin{cases} 0 & ; \quad x < x_0 \\ \frac{\tilde{\rho}}{\epsilon} & ; \quad x_0 < x < x_0 + \epsilon \\ 0 & ; \quad x > x_0 + \epsilon \end{cases} ,$$

then the problem goes away.

$$\begin{aligned} \int \rho(\boldsymbol{x}) dx &= \tilde{\rho} \\ \int \rho(\boldsymbol{x}) dx dy dz &= \int \tilde{\rho} dy dz = Q \end{aligned} \tag{7.39}$$

This problem is better treated, however, by introducing the Dirac delta function $\delta(x)$. It is defined to be zero whenever $x \neq 0$, have unit integral

$$\int \delta(x) dx = 0$$

and the infinitessimal width so narrower that any other function we care to use looks constant over this width, thus

$$\int f(x)\delta(x - x_0) dx = f(x_0)$$

We now simply take

$$\rho(\boldsymbol{x}) = \tilde{\rho}\delta(x - x_0)$$

as a sheet of charge, with surface density $\tilde{\rho}$ per unit area, and extending in the y-z plane at $x = x_0$. The volume density is infinite, courtesy of the δ-function, but has a finite volume integral over our pill-box as required.

7.11.3 Point charges & δ-functions

The density corresponding to a point charge at $\boldsymbol{x}_0 = (x_0, y_0, z_0)$ is now rather easy to define:

$$\rho(x) = Q\delta(x - x_0)\delta(y - y_0)\delta(z - z_0) = Q\delta^3(\boldsymbol{x} - \boldsymbol{x}_0)$$

Then, as expected

$$\begin{aligned}\int dx \int dy \int dz \rho(x) &= Q \int \delta(x-x_0)dx \int \delta(y-y_0)dy \int \delta(z-z_0)dz \\ &= Q \end{aligned} \tag{7.40}$$

Gauss' law can also be applied to this charge distribution.
This is simple when the region considered is a sphere centered at the point charge. Otherwise, the calculation is somewhat more complicated, and we will discuss the general case later in this course. For the spherical volume radius r and charge at the origin the electric field is by symmetry radial, and of the form

$$E(\boldsymbol{x}) = E(|\boldsymbol{x}|)\hat{x}$$

.
Gauss' law gives

$$\begin{aligned}\frac{1}{\epsilon_0}\int_{\mathcal{V}} \rho(\boldsymbol{x})d\mathcal{V} &= \int_{\mathcal{S}} \boldsymbol{E}(\boldsymbol{x})\cdot\hat{n}d\mathcal{S} \\ \frac{Q}{\epsilon_0} &= E(|\boldsymbol{x}|)\int_{\mathcal{S}} \hat{x}\cdot\hat{x}d\mathcal{S} \\ &= E(r)\int_{\mathcal{S}} d\mathcal{S} \\ &= E(r)4\pi r^2 \end{aligned} \tag{7.41}$$

and thus, as we all know,

$$\boldsymbol{E}(\boldsymbol{r}) = \frac{Q}{4\pi\epsilon_0 r^2}\hat{r}.$$

As we all know $E(\boldsymbol{r}) = -\boldsymbol{\nabla}V(r)$, and

$$V(r) = \frac{Q}{4\pi\epsilon_0 r}. \tag{7.42}$$

Example: show that

$$-\boldsymbol{\nabla}V(r) = \frac{Q}{4\pi\epsilon_0 r^2}\hat{r},$$

and for $r \neq 0$,

$$\boldsymbol{\nabla}^2 V(r) = 0$$

(A)

$$\begin{aligned}\boldsymbol{\nabla}\frac{Q}{4\pi\epsilon_0 r} &= \frac{Q}{4\pi\epsilon_0}\boldsymbol{\nabla}\frac{1}{r} \\ &= \frac{Q}{4\pi\epsilon_0} - \frac{1}{r^2}\boldsymbol{\nabla}r \\ &= \frac{Q}{4\pi\epsilon_0} - \frac{1}{r^2}\hat{\boldsymbol{r}} \\ &= -\frac{Q}{4\pi\epsilon_0 r^2}\hat{\boldsymbol{r}} \end{aligned}$$

(B)

$$\begin{aligned}
\boldsymbol{\nabla}^2 V(r) &= -\frac{Q}{4\pi\epsilon_0}\boldsymbol{\nabla}\cdot\frac{\boldsymbol{r}}{r^3} \\
&= -\frac{Q}{4\pi\epsilon_0}\left[-\frac{3}{r^4}(\boldsymbol{\nabla}r)\cdot\boldsymbol{r}+\frac{1}{r^3}(\boldsymbol{\nabla}\cdot\boldsymbol{r})\right] \\
&= -\frac{Q}{4\pi\epsilon_0}\left[-\frac{3}{r^3}+\frac{1}{r^3}(3)\right] \\
&= 0
\end{aligned}$$

The result (7.41) is interesting: the divergence theorem now implies that

$$\boldsymbol{\nabla}^2 V = \frac{Q}{\epsilon_0}\delta^3(\boldsymbol{r}),$$

and so,

$$\boldsymbol{\nabla}^2 \frac{1}{4\pi r} = \delta^3(\boldsymbol{r}).$$

This is an example of a Green function. In general for a general differential operator $\mathcal{D}$, the corresponding Green function $G(\boldsymbol{x})$ is defined as the solution of:

$$\mathcal{D}G(\boldsymbol{x}) = \delta^n(\boldsymbol{x})$$

Here, the dimension $n \in \{1, 2, 3\}$ depending on whether the differential operator acts in one, two or three dimensions.

$$G^H(\boldsymbol{x}) = \frac{1}{4\pi|\boldsymbol{x}|}$$

This is the three dimensional Helmholtz Green function G^H of the differential operator $\boldsymbol{\nabla}^2$.
We can use the Green function to immediately solve the related inhomogenous differential equation for any source $S(x)$

$$\mathcal{D}F(\boldsymbol{x}) = S(x)$$

In plain english, this means we can now solve Poisson's equation for an *any* charge distribution $\rho(x)$:

$$\boldsymbol{\nabla}^2 V(\boldsymbol{r}) = \frac{\rho(x)}{\epsilon_0}$$

The solution is:

$$V(\boldsymbol{x}) = \int d^3\boldsymbol{y} G^H(\boldsymbol{x}-\boldsymbol{y})\frac{\rho(\boldsymbol{y})}{\epsilon_0} \tag{8.43}$$

The form of integral (8.43) is a convolution of the Green function G^H with the charge density ρ. We can check this is a solution of Poisson's equation:

$$\begin{aligned}\boldsymbol{\nabla}_x^2 V(\boldsymbol{x}) &= \int d^3\boldsymbol{y}\boldsymbol{\nabla}_x^2 G^H(\boldsymbol{x}-\boldsymbol{y})\frac{\rho(\boldsymbol{y})}{\epsilon_0} \\ &= \int d^3\boldsymbol{y}\delta^3(\boldsymbol{x}-\boldsymbol{y})\frac{\rho(\boldsymbol{y})}{\epsilon_0} = \frac{\rho(\boldsymbol{x})}{\epsilon_0}\end{aligned}$$

Now, consider the potential arising from a set of point charges:

$$\rho(\boldsymbol{x}) = Q_1\delta^3(\boldsymbol{x}-\boldsymbol{x}_1) + Q_2\delta^3(\boldsymbol{x}-\boldsymbol{x}_1) + Q_3\delta^3(\boldsymbol{x}-\boldsymbol{x}_1)$$

Then,

$$\begin{aligned} V(\boldsymbol{x}) &= \int d^3\boldsymbol{y} G^H(\boldsymbol{x}-\boldsymbol{y})\frac{\rho(\boldsymbol{y})}{\epsilon_0} \\ &= \frac{Q_1}{\epsilon_0}\int d^3\boldsymbol{y} G^H(\boldsymbol{x}-\boldsymbol{y})\delta^3(\boldsymbol{y}-\boldsymbol{x}_1) \\ &+ \frac{Q_2}{\epsilon_0}\int d^3\boldsymbol{y} G^H(\boldsymbol{x}-\boldsymbol{y})\delta^3(\boldsymbol{y}-\boldsymbol{x}_2) \\ &+ \frac{Q_3}{\epsilon_0}\int d^3\boldsymbol{y} G^H(\boldsymbol{x}-\boldsymbol{y})\delta^3(\boldsymbol{y}-\boldsymbol{x}_3) \\ &= \frac{Q_1}{\epsilon_0}G^H(\boldsymbol{x}-\boldsymbol{x}_1)+\frac{Q_2}{\epsilon_0}G^H(\boldsymbol{x}-\boldsymbol{x}_2)+\frac{Q_3}{\epsilon_0}G^H(\boldsymbol{x}-\boldsymbol{x}_3) \\ &= \frac{Q_1}{4\pi\epsilon_0|\boldsymbol{x}-\boldsymbol{x}_1|}+\frac{Q_2}{4\pi\epsilon_0|\boldsymbol{x}-\boldsymbol{x}_2|}+\frac{Q_3}{4\pi\epsilon_0|\boldsymbol{x}-\boldsymbol{x}_3|} \end{aligned} \tag{8.44}$$

This is the usual rule for the addition of the potentials due to a number of charges.
This style of solution works for the Green functions of generic differential operators.

8.1 Fourier Transforms in $2D$ and $3D$

This section will make more sense when we have looked at higher dimensional PDEs later in the course. It is included here for completeness.
The extension of the F.T. to higher dimensions is straightforward:

$$F.T.[f(\boldsymbol{x})] = F(\boldsymbol{k}) = \left(\frac{1}{\sqrt{2\pi}}\right)^d \int d^d x\ f(\boldsymbol{x})\ e^{i\boldsymbol{k}\cdot\boldsymbol{x}}$$

where $\boldsymbol{k}$ and $\boldsymbol{x}$ are vectors in d-dimensional space and $d^d x$ is the corresponding volume element.

EXAMPLE: $d = 2$ in cartesians.

$$F(\boldsymbol{k}) = F(k_x, k_y) = \frac{1}{(\sqrt{2\pi})^2}\int_{-\infty}^{\infty} dx \int_{-\infty}^{\infty} dy\ f(x,y)\ e^{i(k_x x + k_y y)}\ .$$

Fourier transforms of vector fields For vector functions of position $\boldsymbol{v}(\boldsymbol{x})$, we can define the Fourier transform of each component seperately in the usual way for a scalar. However, this is equivalent to defining vector valued Fourier coefficients:

$$F.T.[\boldsymbol{v}(\boldsymbol{x})] = \boldsymbol{V}(\boldsymbol{k}) = \left(\frac{1}{\sqrt{2\pi}}\right)^d \int d^d x\ \boldsymbol{v}(\boldsymbol{x})\ e^{i\boldsymbol{k}\cdot\boldsymbol{x}}$$

8.1.1 Derivatives of Fourier Transforms

We consider the action of differential operators on a function represented as a Fourer transform.
This is particularly simple because the basic function e^{ikx} is an eigenfunction of the derivative: $\frac{d}{dx}e^{ikx} = ike^{ikx}$.
We consider both scalar, $f(\boldsymbol{x})$ and vector $\boldsymbol{v}(\boldsymbol{x})$ functions of $\boldsymbol{x}$.

$$f(\boldsymbol{x}) = \left(\frac{1}{\sqrt{2\pi}}\right)^d \int d^d k\ F(\boldsymbol{k})\ e^{-i\boldsymbol{k}\cdot\boldsymbol{x}}$$

$$\boldsymbol{v}(\boldsymbol{x}) = \left(\frac{1}{\sqrt{2\pi}}\right)^d \int d^d k\ \boldsymbol{V}(\boldsymbol{k})\ e^{-i\boldsymbol{k}\cdot\boldsymbol{x}}$$

Then,

$$\begin{aligned}
\boldsymbol{\nabla} f(\boldsymbol{x}) &= \left(\frac{1}{\sqrt{2\pi}}\right)^d \int d^d k\ (-i\boldsymbol{k}) F(\boldsymbol{k})\ e^{-i\boldsymbol{k}\cdot\boldsymbol{x}} \\
\boldsymbol{\nabla}^2 f(\boldsymbol{x}) &= \left(\frac{1}{\sqrt{2\pi}}\right)^d \int d^d k\ (-k^2) F(\boldsymbol{k})\ e^{-i\boldsymbol{k}\cdot\boldsymbol{x}} \\
\boldsymbol{\nabla}\cdot v(\boldsymbol{x}) &= \left(\frac{1}{\sqrt{2\pi}}\right)^d \int d^d k\ (-i\boldsymbol{k})\cdot\boldsymbol{V}(\boldsymbol{k})\ e^{-i\boldsymbol{k}\cdot\boldsymbol{x}} \\
\boldsymbol{\nabla}\times v(\boldsymbol{x}) &= \left(\frac{1}{\sqrt{2\pi}}\right)^d \int d^d k\ (-i\boldsymbol{k})\times\boldsymbol{V}(\boldsymbol{k})\ e^{-i\boldsymbol{k}\cdot\boldsymbol{x}} \\
\boldsymbol{\nabla}^2 v(\boldsymbol{x}) &= \left(\frac{1}{\sqrt{2\pi}}\right)^d \int d^d k\ -[\boldsymbol{k}(\boldsymbol{k}\cdot\boldsymbol{V}(\boldsymbol{k})) - \boldsymbol{k}\times\boldsymbol{k}\times\boldsymbol{V}(\boldsymbol{k})]\ e^{-i\boldsymbol{k}\cdot\boldsymbol{x}}
\end{aligned} \tag{8.45}$$

Where for the last, we used the "gdmcc" rule.

8.2 Solving PDE's by Fourier transform

We can now look at solving a PDE by Fourier transform. For example, consider Poisson's equation

$$\boldsymbol{\nabla}^2 f(x) = \rho(x)$$

We insert Fourier transforms for both $f(x)$ and $\rho(x)$,

$$f(x) = \left(\frac{1}{\sqrt{2\pi}}\right)^d \int d^d k\ F(\boldsymbol{k})\ e^{-i\boldsymbol{k}\cdot\boldsymbol{x}}$$

$$\rho(x) = \left(\frac{1}{\sqrt{2\pi}}\right)^d \int d^d k\ \varrho(\boldsymbol{k})\ e^{-i\boldsymbol{k}\cdot\boldsymbol{x}}$$

and we have

$$I(x) = \left(\frac{1}{\sqrt{2\pi}}\right)^d \int d^d k\ \left[-|k|^2 F(\boldsymbol{k}) - \varrho(\boldsymbol{k})\right]\ e^{-i\boldsymbol{k}\cdot\boldsymbol{x}} = 0$$

We can now remove the k-integral by considering

$$\begin{aligned}
0 &= \left(\frac{1}{\sqrt{2\pi}}\right)^d \int d^d x e^{i\boldsymbol{k}'\cdot\boldsymbol{x}} I(x) \\
&= \int d^d k\ \left[-|k|^2 F(\boldsymbol{k}) - \varrho(\boldsymbol{k})\right] \times \left(\frac{1}{2\pi}\right)^d \int d^d x e^{i(\boldsymbol{k}'-\boldsymbol{k})\cdot\boldsymbol{x}} \\
&= \int d^d k\ \left[-|k|^2 F(\boldsymbol{k}) - \varrho(\boldsymbol{k})\right] \delta^d(\boldsymbol{k}-\boldsymbol{k}') \\
0 &= \left[-|k'|^2 F(\boldsymbol{k}') - \varrho(\boldsymbol{k}')\right]
\end{aligned} \tag{8.46}$$

We could have chosen *any* k', and so this is true for *every* k'.
We can therefore conclude:

$$F(\boldsymbol{k}) = -\frac{\varrho(\boldsymbol{k}')}{k^2}$$

Inverse of a differential operator The differential operator $\boldsymbol{\nabla}^2$ is *simple* in Fourier space

$$\boldsymbol{\nabla}^2 F(\boldsymbol{k}) \equiv -k^2 F(\boldsymbol{k})$$

We can think of the operator as possessing Fourier transform:

$$\boldsymbol{\nabla}^2(\boldsymbol{k}) \equiv -k^2$$

The inverse of the operator therefore has Fourier space representation

$$\left[\boldsymbol{\nabla}^2\right]^{-1}(\boldsymbol{k}) = \frac{-1}{k^2}$$

We can therefore solve the equation

$$\boldsymbol{\nabla}^2 f(\boldsymbol{x}) = \rho(\boldsymbol{x})$$

via

$$F(\boldsymbol{k}) = \left[\boldsymbol{\nabla}^2\right]^{-1}(\boldsymbol{k})\boldsymbol{\nabla}^2(\boldsymbol{k})F(\boldsymbol{k}) = \left[\boldsymbol{\nabla}^2\right]^{-1}(\boldsymbol{k})\varrho(\boldsymbol{k})$$

8.3 Relation to Green function solution

Let's revisit our Green function approach to solving Poisson's equation.

$$\boldsymbol{\nabla}^2 G(\boldsymbol{x}) = \delta^n(\boldsymbol{x})$$

If we write $G(\boldsymbol{x})$ and $\delta^n(\boldsymbol{x})$ in terms of their Fourier components this is

$$\begin{aligned} \boldsymbol{\nabla}^2 \left(\frac{1}{\sqrt{2\pi}}\right)^d \int d^d k\, G(\boldsymbol{k})\, e^{-i\boldsymbol{k}\cdot\boldsymbol{x}} &= \left(\frac{1}{\sqrt{2\pi}}\right)^d \int d^d k\, e^{-i\boldsymbol{k}\cdot\boldsymbol{x}} \\ -k^2 G(\boldsymbol{k}) &= 1 \\ G(\boldsymbol{k}) &= \frac{-1}{k^2} \end{aligned} \tag{8.47}$$

Thus, we can identify the Green's function with the inverse of the differential operator.
The multiplication in Fourier space, is equivalently a convolution in coordinate space and the previously discussed Green's function convolution technique is *identical* to our Fourier transform solution.

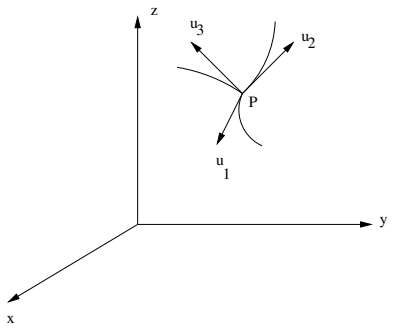


Figure 9.1: Orthogonal curvilinear coordinates in three dimensions.

9 Curvilinear coordinate systems

We now consider vector calculus in alternate coordinates systems which use some combination angles and distances.
Specifically we consider orthogonal curvilinear coordinate systems (fig. 9.1). Such coordinate systems can be particularly useful when the functions we are considering have symmetries, such as cylindrical or spherical symmetry.
In plain English these are orthogonal curvilinear coordinate systems systems that have perpendicular directions $\boldsymbol{e}_i$, but which rotate in some position dependent way, which we choose to track some symmetry of the physics.
The directions at each point are selected by the infinitessimal change in $\boldsymbol{x}$ generated by an infinitessimal change in each of the *curvilinear coordinates*.
We must be able to translate the differential equations of physics appropriately. If we label the curvilinear coordinates (ξ_1, ξ_2, ξ_3) the local axes are given by

$$\frac{\partial \boldsymbol{x}}{\partial \xi_i} = h_i \boldsymbol{e}_i$$

Here, $h_i = \left|\frac{\partial \boldsymbol{x}}{\partial \xi_i}\right|$ is a scale factor with that ensures $\boldsymbol{e_i}$ is a unit vector.
It is useful to consider a *locally* defined cartesian coordinate system

$$\tilde{\boldsymbol{x}}_i = \boldsymbol{x} \cdot \boldsymbol{e}_i$$

9.1 Circular (or plane) polar coordinates

Plane polar coordinates (r, ϕ) are defined by:

$$x = r\cos\phi\ , \qquad y = r\sin\phi\ , \tag{9.1}$$

The radial coordinate r (sometimes written as r) can range from 0 to ∞. The angular coordinate ϕ (sometimes written as θ) ranges from 0 to 2π.

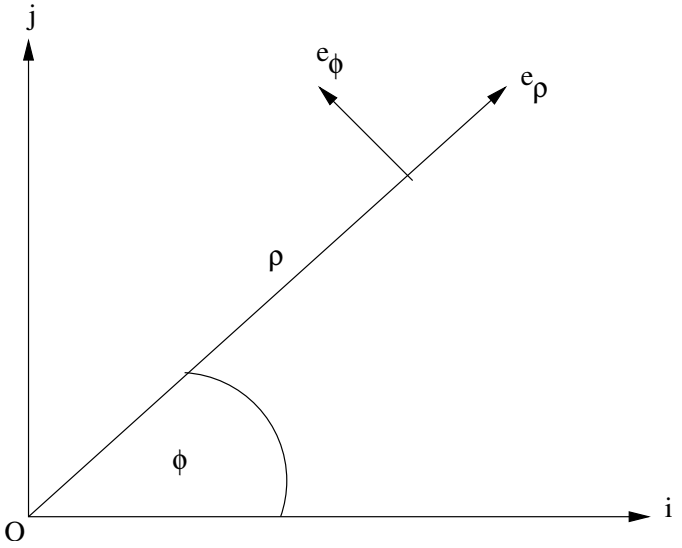


Figure 9.2: Plane polar coordinates.

The *local* orthonormal basis generated by polar coordinates is:

$$\begin{aligned}
\frac{\partial \boldsymbol{x}}{\partial r} &= (\cos\phi, \sin\phi) \\
\frac{\partial \boldsymbol{x}}{\partial \phi} &= r(-\sin\phi, \cos\phi) \\
h_r &= 1 \\
h_\phi &= r \\
e_r &= (\cos\phi, \sin\phi) \\
e_\phi &= (-\sin\phi, \cos\phi)
\end{aligned} \tag{9.2}$$

Exercise Show that this system is *orthogonal* by verifying that $(\frac{\partial \boldsymbol{x}}{\partial r}) \cdot (\frac{\partial \boldsymbol{x}}{\partial \phi}) = 0$

9.1.1 Area integrals

When we change coordinates in an integral, we have to include a scale factor in the integration variable.
As we increase each coordinate by an infinitesimal amount, we sweep out a small area which we call $d\mathcal{A}$. Now, as we chose *orthogonal* curvilinear coordinates we know $\boldsymbol{e}_r$ and $\boldsymbol{e}_\phi$ are perpendicular, and the area is

$$\begin{aligned}
d\mathcal{A} &= d\tilde{x}_r d\tilde{x}_\phi \\
&= h_r dr h_\phi d\phi \\
&= r dr d\phi
\end{aligned} \tag{9.3}$$

Example: area of circle Consider

$$\int_0^R dr \int_0^{2\pi} r d\phi = 2\pi \int_0^R r dr = \pi R^2$$

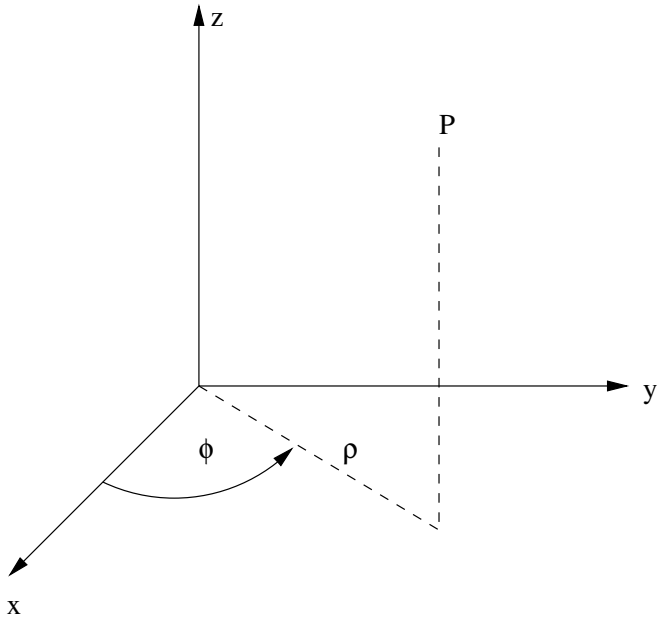


Figure 9.3: Cylindrical polar coordinates.

9.2 Cylindrical polar coordinates

An simple extension of plane polar coordinates into the third dimension: see Fig. 9.3.

$$x = r\cos\phi\,, \qquad y = r\sin\phi\,, \qquad z = z \tag{9.4}$$

- radius $r \in [0, \infty]$, angle $\phi \in [0, 2\pi]$, and z coordinate $z \in [-\infty, \infty]$.
- Scale factors: $h_r = 1$, $h_\phi = r$, $h_z = 1$.

Example: volume of a cylinder Consider

$$\int_0^L dz \int_0^R dr \int_0^{2\pi} r d\phi = 2\pi L \int_0^R r dr = \pi R^2 L$$

9.3 Spherical polar coordinates

Useful when there is spherical symmetry: see Figure 9.4.

$$x = r\sin\theta\cos\phi, \qquad y = r\sin\theta\sin\phi, \qquad z = r\cos\theta \tag{9.5}$$

- radius $r \in [0, \infty]$, angle $\theta \in [0, \pi]$, angle $\phi \in [0, 2\pi]$.

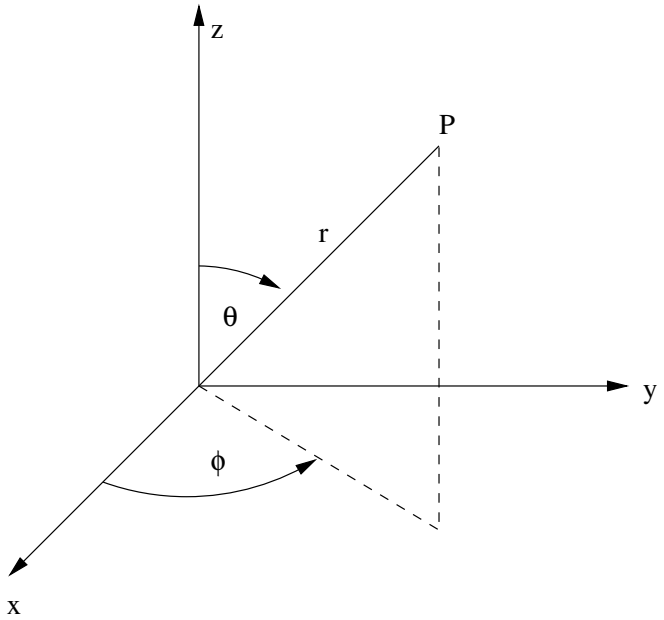


Figure 9.4: Spherical polar coordinates.

$$\begin{aligned}
\frac{\partial \boldsymbol{x}}{\partial r} &= (\sin\theta\cos\phi, \sin\theta\sin\phi, \cos\theta) \\
\frac{\partial \boldsymbol{x}}{\partial \theta} &= r(\cos\theta\cos\phi, \cos\theta\sin\phi, -\sin\theta) \\
\frac{\partial \boldsymbol{x}}{\partial \phi} &= r(-\sin\theta\sin\phi, \sin\theta\cos\phi, 0) \\
h_r &= 1 \\
h_\theta &= r \\
h_\phi &= r\sin\theta
\end{aligned} \tag{9.6}$$

Example : volume of sphere

$$\begin{aligned}
\int_0^R dr \int_0^\pi r d\theta \int_0^{2\pi} r\sin\theta d\phi &= 2\pi \int_0^R r^2 dr \int_0^\pi \sin\theta d\theta \\
&= 2\pi \left[\frac{r^3}{3}\right]_0^R [-\cos\theta]_0^\pi \\
&= \frac{4}{3}\pi R^3
\end{aligned} \tag{9.7}$$

Example : area of sphere

$$\begin{aligned}
\int_0^\pi R d\theta \int_0^{2\pi} R\sin\theta d\phi &= 2\pi R^2 \int_0^\pi \sin\theta d\theta \\
&= 2\pi R^2 [-\cos\theta]_0^\pi \\
&= 4\pi R^2
\end{aligned} \tag{9.8}$$

9.4 Differential operators

9.4.1 Gradient

In the *local* coordinate system the gradient operator is

$$\sum_i \frac{\partial}{\partial \tilde{x}_i} \boldsymbol{e}_i = \sum_i \frac{1}{h_i} \frac{\partial}{\partial \tilde{\xi}_i} \boldsymbol{e}_i$$

Circular polars

$$\begin{aligned} \boldsymbol{\nabla} f &= \frac{\partial f}{\partial \tilde{x}_r} \boldsymbol{e}_r + \frac{\partial f}{\partial \tilde{x}_\phi} \boldsymbol{e}_\phi \\ &= \frac{\partial f}{h_r \partial r} \boldsymbol{e}_r + \frac{\partial f}{h_\phi \partial \phi} \boldsymbol{e}_\phi \\ &= \frac{\partial f}{\partial r} \boldsymbol{e}_r + \frac{1}{r} \frac{\partial f}{\partial \phi} \boldsymbol{e}_\phi \end{aligned} \tag{9.9}$$

Cylindrical polars

$$\boldsymbol{\nabla} = \frac{\partial f}{\partial r} \boldsymbol{e}_r + \frac{1}{r} \frac{\partial f}{\partial \phi} \boldsymbol{e}_\phi + \frac{\partial f}{\partial z} \hat{z}$$

Spherical polars

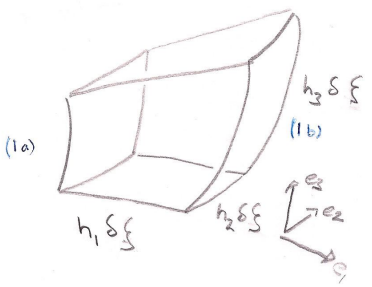
$$\boldsymbol{\nabla} = \frac{\partial f}{\partial r} \boldsymbol{e}_r + \frac{1}{r} \frac{\partial f}{\partial \theta} \boldsymbol{e}_\theta + \frac{1}{r \sin\theta} \frac{\partial f}{\partial \phi} \boldsymbol{e}_\phi$$

9.4.2 Divergence

For the divergence we must be a little bit more careful. The coordinate dependence of the scale factors themselves must be taken into account.

$$\boldsymbol{\nabla} \cdot \boldsymbol{v} = \lim_{V \to 0} \frac{\int_{\mathcal{A}} \boldsymbol{v} \cdot \hat{\boldsymbol{n}} d\mathcal{A}}{V}$$

Consider the infinitessimal cube



Flux through (1a) is $F_1 = v_1\ h_2\ d\xi_2\ h_3\ d\xi_3$.
Net flux difference between (1a) and (1b) is $\frac{\partial F_1}{\partial \xi_1} \delta\xi_1$.
Thus, summing over all pairs of faces

$$\begin{aligned} \boldsymbol{\nabla} \cdot \boldsymbol{v} &= \frac{1}{h_1 h_2 h_3 \delta\xi_1 \delta\xi_2 \delta\xi_3} \left[\frac{\partial F_1}{\partial \xi_1} \delta\xi_1 + \frac{\partial F_2}{\partial \xi_2} \delta\xi_2 + \frac{\partial F_3}{\partial \xi_3} \delta\xi_3 \right] \\ &= \frac{1}{h_1 h_2 h_3} \left[\frac{\partial h_2 h_3 v_1}{\partial \xi_1} + \frac{\partial h_3 h_1 v_2}{\partial \xi_2} + \frac{\partial h_1 h_2 v_3}{\partial \xi_3} \right] \end{aligned} \tag{9.10}$$

Circular polars

$$\boldsymbol{\nabla}\cdot\boldsymbol{v}=\frac{1}{r}\frac{\partial}{\partial r}(rv_r)+\frac{1}{r}\frac{\partial}{\partial\phi}v_\phi$$

Cylindrical polars

$$\boldsymbol{\nabla}\cdot\boldsymbol{v}=\frac{1}{r}\frac{\partial}{\partial r}(rv_r)+\frac{1}{r}\frac{\partial}{\partial\phi}v_\phi+\frac{\partial}{\partial z}v_z$$

Spherical polars

$$\boldsymbol{\nabla}\cdot\boldsymbol{v}=\frac{1}{r^2}\frac{\partial}{\partial r}(r^2v_r)+\frac{1}{r\sin\theta}\frac{\partial}{\partial\theta}(\sin\theta v_\theta)+\frac{1}{r\sin\theta}\frac{\partial}{\partial\phi}v_\phi$$

9.4.3 Laplacian

We can now form the Laplacian as simply the divergence of the gradient, combining the results of the previous two subsections:

$$\boldsymbol{\nabla}^2 f=\boldsymbol{\nabla}\cdot\boldsymbol{\nabla}f$$

leading to:

Circular polars

$$\nabla^2 f=\frac{1}{r}\frac{\partial}{\partial r}(r\frac{\partial f}{\partial r})+\frac{1}{r^2}\frac{\partial^2 f}{\partial\phi^2}$$

Cylindrical polars

$$\nabla^2 f=\frac{1}{r}\frac{\partial}{\partial r}(r\frac{\partial f}{\partial r})+\frac{1}{r^2}\frac{\partial^2 f}{\partial\phi^2}+\frac{\partial^2 f}{\partial z^2}$$

Spherical polars

$$\nabla^2 f=\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial f}{\partial r}\right)+\frac{1}{r^2\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\,\frac{\partial f}{\partial\theta}\right)+\frac{1}{r^2\sin^2\theta}\frac{\partial^2 f}{\partial\phi^2}. \tag{9.11}$$

Note, that there are no mixed second order derivatives and that these equations are seperable.

10 Wave equation in circular polars

Equivalently, solving the wave equation for a circular drum

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

In this section we shall use r for the radial coordinate. As before, we consider solutions of separated form: $u(r,\phi,z,t)=R(r)\Phi(\phi)T(t)$. Substitute into wave equation and divide across by $u=R\Phi T$.

$$\frac{1}{R}\frac{\partial^2 R}{\partial r^2}+\frac{1}{rR}\frac{\partial R}{\partial r}+\frac{1}{r^2\Phi}\frac{\partial^2\Phi}{\partial\phi^2}=\frac{1}{c^2T}\frac{\partial^2 T}{\partial t^2}\ .$$

First separation: time equation: $\mathrm{LHS}(r,\phi,z)=\mathrm{RHS}(t)=\text{constant}$

$$\frac{1}{c^2}\frac{1}{T}\frac{d^2T}{dt^2}=-k^2.$$

The solutions to this are of the form $T(t) = G_k \cos \omega_k t + H_k \sin \omega_k t$ with $\omega_k \equiv ck$.

Second separation: Multiply through by r^2 and separate again:

$$\text{LHS}(r) = \text{RHS}(\phi) = \text{a constant.}$$

For the angular dependence:

$$\frac{1}{\Phi}\frac{d^2\Phi}{d\phi^2} = -n^2;$$

The solution is $\Phi = C\cos n\phi + D \sin n\phi$.
We want the solution to the wave equation to be *single valued*, so $\Phi(\phi + 2\pi) = \Phi(\phi)$, forcing n to be integer-valued: $n = 0, \pm 1, \pm 2 \ldots$
The equation describing the radial dependence is the only difficult one to solve:

$$\frac{d^2R}{dr^2} + \frac{1}{r}\frac{dR}{dr} - \frac{n^2}{r^2}R + k^2 R = 0 \, .$$

Multiply across by r^2 and rewrite

$$r^2R'' + rR' + (k^2r^2 - n^2)R = 0 \, . \tag{10.12}$$

This is known as *Bessel's equation of order n.* The solutions are known as Bessel functions. Being a quadratic ODE, there are two independent solutions called $J_n(kr)$ and $Y_n(kr)$. Note we have labelled the solutions with integer n.

10.0.4 Method of Froebenius

We can solve Bessel's equation by substituting a general *Laurent series* as a trial solution. A Laurent series is a generalisation of a Taylor series to possibly include negative power terms (called poles).
We try a solution

$$R(r) = \sum_{i=0}^{\infty} C_i r^{i+m}$$

where c_i and m are unknowns. m represents the lowest power of r that occurs in the solution, and where it arises $c_i = 0$ for $i < 0$ because otherwise m would *not* represent the lowest power of r.
Differentiating we get

$$R'(r) = \sum_{i=0}^{\infty}(i+m)C_i r^{i+m-1}$$

$$rR'(r) = \sum_{i=0}^{\infty}(i+m)C_i r^{i+m}$$

$$r^2R''(r) = \sum_{i=0}^{\infty}(i+m)(i+m-1)C_i r^{i+m}$$

Bessel's equation becomes a relation between coefficients:

$$\sum_{i=0}^{\infty}(i+m)C_i r^{i+m} + (i+m)(i+m-1)C_i r^{i+m} - n^2 C_i r^{i+m} + k^2 C_{i-2} r^{i+m}$$

Since this must be true for all r, then we have the *indicial equation*

$$\left[(i+m) + (i+m)(i+m-1) - n^2\right] C_i + k^2 C_{i-2} = 0$$

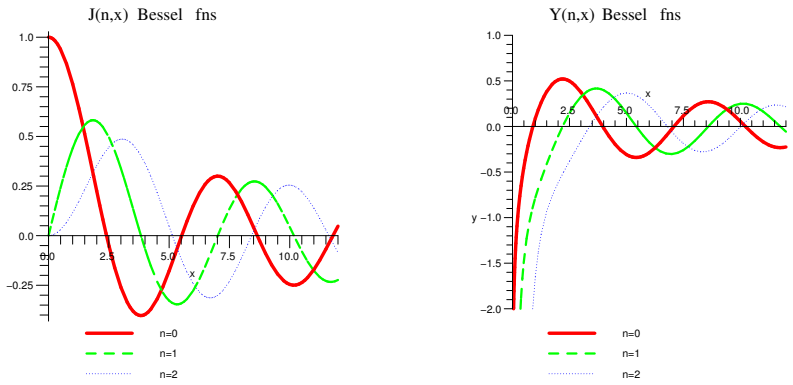


Figure 10.5: The first three Bessel functions of integral order.

The series *switches on* when $C_{-2} = 0$ and $C_0 \neq 0$. Then,

$$m^2 = n^2.$$

We are interested in the case where $m \geq 0$ so that the solutions are finite at $r = 0$.
Next, we are interested in forming a recurrence relation between coefficients. The above indicial equation suggests

$$C_i = \frac{k^2}{n^2 - (i+m)^2} C_{i-2}$$

If we consider the Bessel function $J_0(r)$, we take $n = m = 0$ and have (up to normalisation)

$$\begin{aligned} C_0 &= 1 \\ C_2 &= -\frac{k^2}{4} \\ C_4 &= +\frac{k^4}{4.16} \\ C_6 &= -\frac{k^6}{4.16.36} \\ &\ldots \end{aligned} \tag{10.13}$$

The series is

$$1 - \frac{(kr)^2}{4} + \frac{(kr)^4}{4.16} - \frac{(kr)^6}{4.16.36} \ldots$$

and is purely a function of (kr). As the sign oscillates we have many turning points.

10.0.5 Roots of Bessel functions

The first few J_n and Y_n functions are plotted in Fig. 10.5. The Y_n functions diverge at the origin and so are not suitable for describing oscillations of a drumskin.
The Bessel functions $J_n(x)$ have a series of zeros ("nodes" or "roots") which we label α_{n1}, α_{n2}, α_{n3}. For the function $\sin nx$, the nodes occur at $x = \alpha_{nm} = m\pi$ are equally spaced. For Bessel functions, however, they are not. The nodes must be found numerically, in practice either looked up in tables or calculated using packages such as Maple.

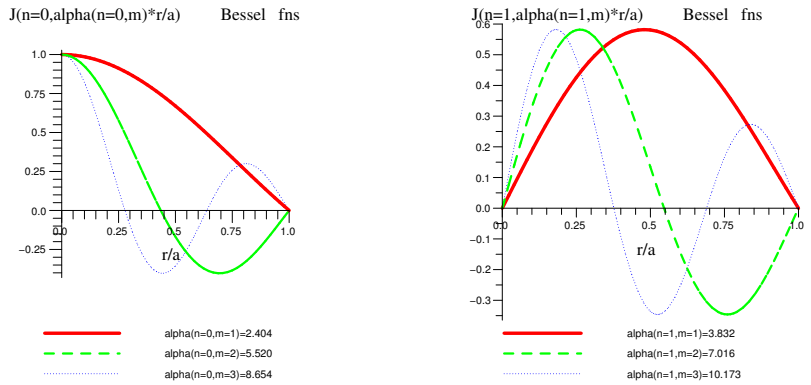


Figure 10.6: Rescaling the J_0 and J_1 Bessel functions so that one of the nodes lies at $r = a$

10.0.6 Spatial BCs and normal modes

Our solution can be written as

$$u(r, \phi, t) = J_n(kr)\ (C\cos n\phi + D\sin n\phi)\ (G\cos\omega_k t + H\sin\omega_k t)$$

with $\omega_k = ck$ and currently no restriction on k.
We now apply spatial boundary conditions. Recall periodicity in ϕ quantised n. In the radial direction we require that the drumskin does not move at the rim:

$$u(r = a, \phi, t) = 0 \text{ for all } \phi \text{ and } t.$$

We therefore want the edge of the drum to coincide with one of the nodes of the Bessel function. The m^{th} node of the Bessel function of order n occurs when the argument of the Bessel function takes value α_{nm}, and we rescale the Bessel function so that one of these zeros coincides with $r = a$. It doesn't matter which node we choose to lie at $r = a$, so we have different normal mode solutions depending on which m we choose. The allowed values of k are therefore

$$k_{nm}a = \alpha_{nm}.$$

Quantising k also quantises ω_k. This is like we fond for the harmonics, but the normal mode frequencies are here not equally spaced (because the α_{nm} are not evenly spaced). This proves why the drum is not as harmonious as the guitar.
Some examples of rescaling for $n = 0$ and $n = 1$ are shown in Fig. 10.6.
Our normal mode solutions are therefore

$$u(r, \phi, t) = J_n\left(\alpha_{nm}\frac{r}{a}\right)\ (C_{nm}\cos n\phi + D_{nm}\sin n\phi)\ (G_{nm}\cos\omega_{nm}t + H_{nm}\sin\omega_{nm}t)\ .$$

Each normal mode is labelled by n and m and will have different constants so we label them appropriately. k depends on n and m via α_{nm}, so we also change the label on ω.

10.0.7 Zeros and nodal lines

Only J_0 is zero at the origin (e.g. Fig. 10.5) so $u = 0$ at $r = 0$ for all t if $n > 0$.
Nodal lines are other points on the drumskin that remain stationary for this normal mode:

- We find $(m-1)$ nodal lines in r: they occur at $\alpha_{nm}r/a = \alpha_{nm'} \implies r = a\alpha_{nm'}/\alpha_{nm}$ for $m' = 1, 2 \ldots (m-1)$. (See Fig. 10.6.)

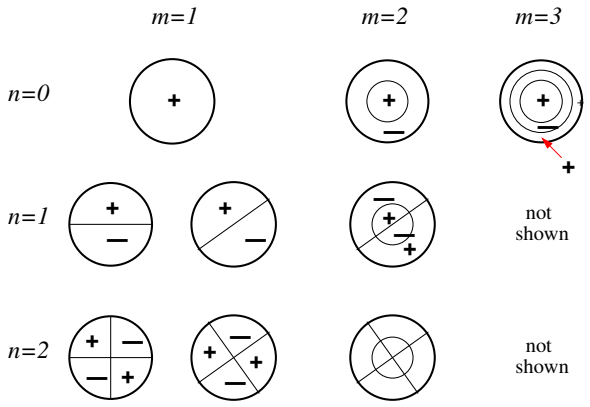


Figure 10.7: Some normal modes for a round drum.

- $2n$ nodal lines in ϕ: occur at intervals $\delta\phi = \pi/n$ for $n \neq 0$. N.B. do not need to start at $\phi = 0$.

Some low-lying modes are shown in Fig. 10.7. Note that the wave equation had rotational symmetry. This does not mean that the solutions have to have rotational symmetry ($n = 1, 2 \ldots$ do not). It means that if we take normal mode solution and then rotate it, it is still a solution of the wave equation.

10.0.8 The general solution

The general solution is a linear superposition of all allowed modes:

$$u(r,\phi,t) = \sum_{n=0}^{\infty}\sum_{m=1}^{\infty} J_n\left(\alpha_{nm}\frac{r}{a}\right)\,(C_{nm}\cos n\phi + D_{nm}\sin n\phi)\,(G_{nm}\cos\omega_{nm}t + H_{nm}\sin\omega_{nm}t) \quad (10.14)$$

Each (n, m) term contains *two* normal modes ($\cos n\phi$ and $\sin n\phi$), and there are four unknown constants. Two unknowns per mode is what we expect for a second order differential equation.
We will use initial conditions to fix the unknowns, but before that we need to learn a bit more about the properties of Bessel functions. In particular we need an orthogonality relation.

10.0.9 Orthogonality and completeness

We state one orthogonality relation without proof. For given, fixed n

$$\int_0^a dr\; J_n\left(\alpha_{nm}\frac{r}{a}\right) J_n\left(\alpha_{nl}\frac{r}{a}\right) r = \frac{a^2}{2}[J_{n+1}(\alpha_{nm})]^2\delta_{m,l}\;, \quad (10.15)$$

where $J_n(\alpha_{nm}) = 0$, i.e. α_{nm} is the m^{th} root of the Bessel function of integral order n.
The extra factor of r compared with Fourier orthogonality arises *mathematically* because Bessel's equation contained first order derivatives in r.
The extra factor of r compared with Fourier orthogonality arises *physically* because Bessel's equation arose in the radial direction of two dimensional wave equation. It is a *vestigial circumference* factor $2\pi r$, turning a line integral into an area integral that is appropriate for a 2D orthogonality relation.
The set of Bessel functions $\{J_n(\alpha_{nm}x)\;;\; m = 1\ldots\infty\}$ for fixed n form a complete set, so any function can be expanded in the interval $0 \leq r \leq a$ as a *Bessel* (or Fourier-Bessel) *series*:

$$f(r) = \sum_{m=1}^{\infty} A_{nm} J_n\left(\alpha_{nm}\frac{r}{a}\right), \quad (10.16)$$

The coefficients are determined using the orthogonality condition in the usual way, as we shall now see.

10.0.10 Initial conditions for the drumskin

The general solution for the displacement of a circular drumskin of radius a was given in Eqn. (10.14). Combining constants we have:

$$f(r,\phi,t) = \sum_{n=0}^{\infty}\sum_{m=1}^{\infty} J_n\left(\frac{\alpha_{nm}r}{a}\right)(A_{nm}\cos n\phi + B_{nm}\sin n\phi)\cos(\omega_{nm}t + \varepsilon_{nm})$$

Typical initial conditions are that the drumskin is initially at rest (implying $\varepsilon_{nm} = 0$) and described by given function $p(r,\phi)$:

$$f(r,\phi,t=0) \equiv \sum_{n=0}^{\infty}\sum_{m=1}^{\infty} A_{nm}J_n\left(\frac{\alpha_{nm}r}{a}\right)\cos n\phi + B_{nm}J_n\left(\frac{\alpha_{nm}r}{a}\right)\sin n\phi = p(r,\phi)\ . \tag{10.17}$$

Given initial conditions $p(r,\phi)$ we can find the coefficients A_{nm} and B_{nm} via our orthogonality relations. We rewrite the initial condition equation as

$$\sum_{n=0}^{\infty}\sum_{m=1}^{\infty}(A_{nm}\Psi_{nm}(r,\phi) + B_{nm}\Phi_{nm}(r,\phi)) = p(r,\phi)\ . \tag{10.18}$$

where we have basis functions

$$\Psi_{nm}(r,\phi) = J_n\left(\frac{\alpha_{nm}r}{a}\right)\ \cos n\phi\ , \qquad \Phi_{nm}(r,\phi) = J_n\left(\frac{\alpha_{nm}r}{a}\right)\ \sin n\phi\ . \tag{10.19}$$

Define the inner product of two of these basis functions as

$$S\cdot T \equiv \int dA\ S\ T = \int dr\ \int d\phi\ r\ S(r,\phi)\ T(r,\phi)\ ,$$

and we find that $\{\Psi_{nm},\Phi_{nm}\}$ form an orthogonal set:

$$\begin{aligned}
\Psi_{uv}\cdot\Psi_{nm} &= \frac{a^2\pi}{2}(1+\delta_{u0})[J_u(\alpha_{uv})]^2\ \delta_{un}\ \delta_{vm}\\
\Psi_{uv}\cdot\Phi_{nm} &= 0\\
\Phi_{uv}\cdot\Phi_{nm} &= \frac{a^2\pi}{2}[J_u(\alpha_{uv})]^2\ \delta_{un}\ \delta_{vm}
\end{aligned}$$

We might term such functions the (unnormalised) *Circular Harmonics*. They are orthogonal, but not orthonormal. Note that the extra r is just what we get when we transform an area integral from Cartesian to circular polar coordinates. Note also that the angular orthogonality ensures we only compare Bessel functions of the same order (which is all Eqn. (10.15) covered).
We can use this orthogonality to obtain the coefficients from Eqn. (10.17). Applying $(\Psi_{uv}\cdot)$ or $(\Phi_{uv}\cdot)$ to both sides we get

$$\begin{aligned}
A_{uv} &= \frac{2}{a^2\pi(1+\delta_{u0})[J_u(\alpha_{uv})]^2}\times\int_0^a dr\ \int_0^{2\pi} d\phi\ r\ \Psi_{uv}(r,\phi)\ p(r,\phi)\\
B_{uv} &= \frac{2}{a^2\pi[J_u(\alpha_{uv})]^2}\times\int_0^a dr\ \int_0^{2\pi} d\phi\ r\ \Phi_{uv}(r,\phi)\ p(r,\phi)
\end{aligned}$$

We probably have to do these integrals numerically.

11 Wave equation in spherical polar coordinates

We now look at solving problems involving the Laplacian in spherical polar coordinates. The angular dependence of the solutions will be described by *spherical harmonics*.
We take the wave equation as a special case:

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

The Laplacian given by Eqn. (9.11) can be rewritten as:

$$\nabla^2 u = \underbrace{\frac{\partial^2 u}{\partial r^2} + \frac{2}{r}\frac{\partial u}{\partial r}}_{\text{radial part}} + \underbrace{\frac{1}{r^2 \sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial u}{\partial\theta}\right) + \frac{1}{r^2\sin^2\theta}\frac{\partial^2 u}{\partial\phi^2}}_{\text{angular part}} . \tag{11.1}$$

11.1 Separating the variables

We consider solutions of separated form

$$u(r,\theta,\phi,t) = R(r)\,\Theta(\theta)\,\Phi(\phi)\,T(t) .$$

Substitute this into the wave equation and divide across by $u = R\Theta\Phi T$:

$$\frac{1}{R}\frac{d^2R}{dr^2} + \frac{2}{rR}\frac{dR}{dr} + \frac{1}{r^2}\frac{1}{\Theta\sin\theta}\frac{d}{d\theta}\left(\sin\theta\frac{d\Theta}{d\theta}\right) + \frac{1}{r^2\sin^2\theta}\frac{1}{\Phi}\frac{d^2\Phi}{d\phi^2} = \frac{1}{c^2}\frac{1}{T}\frac{d^2T}{dt^2}.$$

11.1.1 First separation: r, θ, ϕ versus t

$$\text{LHS}(r,\theta,\phi) = \text{RHS}(t) = \text{constant} = -k^2.$$

This gives the T equation:

$$\frac{1}{c^2}\frac{1}{T}\frac{d^2T}{dt^2} = -k^2 \tag{11.2}$$

which is easy to solve.

11.1.2 Second separation: θ, ϕ versus r

Multiply LHS equation by r^2 and rearrange:

$$-\frac{1}{\Theta\sin\theta}\frac{d}{d\theta}\left(\sin\theta\frac{d\Theta}{d\theta}\right) - \frac{1}{\sin^2\theta}\frac{1}{\Phi}\frac{d^2\Phi}{d\phi^2} = \frac{r^2}{R}\frac{d^2R}{dr^2} + \frac{2r}{R}\frac{dR}{dr} + k^2r^2 . \tag{11.3}$$

$$\text{LHS}(\theta,\phi) = \text{RHS}(r) = \text{constant} = \lambda$$

We choose the separation constant to be λ. For later convenience, it will turn out that $\lambda = l(l+1)$ where l has to be integer.
Multiplying the RHS equation by R/r^2 gives the R equation:

$$\frac{d^2R}{dr^2} + \frac{2}{r}\frac{dR}{dr} + \left[k^2 - \frac{\lambda}{r^2}\right]R = 0. \tag{11.4}$$

This can be turned into Bessel's equation; we'll do this later.

11.1.3 Third separation: θ versus ϕ

Multiply LHS of Eqn. (11.3) by $\sin^2\theta$ and rearrange:

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

$$\text{LHS}(\theta)=\text{RHS}(\phi)=\text{constant}=-m^2\ .$$

The RHS equation gives the Φ equation without rearrangement:

$$\frac{d^2\Phi}{d\phi^2}=-m^2\Phi\ . \tag{11.5}$$

Multiply the LHS by $\Theta/\sin^2\theta$ to get the Θ equation:

$$\frac{1}{\sin\theta}\frac{d}{d\theta}\left(\sin\theta\frac{d\Theta}{d\theta}\right)+\left[\lambda-\frac{m^2}{\sin^2\theta}\right]\Theta=0\ . \tag{11.6}$$

11.2 Solving the separated equations

Now we need to solve the ODEs that we got from the original PDE by separating variables.

11.2.1 Solving the T equation

Eqn. (11.2) is of simple harmonic form and solved as before, giving sinusoids as solutions:

$$\frac{d^2T}{dt^2}=-c^2k^2T\equiv-\omega_k^2T\ ,$$

with $\omega_k=ck$.

11.2.2 Solving the Φ equation

Eqn. (11.5) is easily solved. Rather than using cos and sin, it is more convenient to use complex exponentials:

$$\Phi(\phi)=e^{\pm im\phi}$$

Note that we have to include both positive and negative values of m.
As ϕ is an angular coordinate, we expect our solutions to be *single-valued*, i.e. unchanged as we go right round the circle $\phi\to\phi+2\pi$:

$$\Phi(\phi+2\pi)=\Phi(\phi)\qquad\Rightarrow\qquad e^{i2\pi m}=1\qquad\Rightarrow\qquad m=\text{integer.}$$

This is another example of a BC (periodic in this case) quantising a separation constant.
In principle m can take any integer value between $-\infty$ and ∞. In practise, we will see that it is restricted to the range $-l\le m\le l$.

11.2.3 Solving the Θ equation

Starting from Eqn. (11.6), make a change of variables $w = \cos\theta$:

$$\frac{d}{dw} = \frac{d\theta}{dw}\,\frac{d}{d\theta} = \left(\frac{dw}{d\theta}\right)^{-1}\frac{d}{d\theta} = -\frac{1}{\sin\theta}\,\frac{d}{d\theta}\,,$$
$$(1-w^2)\frac{d}{dw} = -\frac{1-\cos^2\theta}{\sin\theta}\,\frac{d}{d\theta} = -\frac{\sin^2\theta}{\sin\theta}\,\frac{d}{d\theta} = -\sin\theta\,\frac{d}{d\theta}\,,$$
$$\frac{d}{dw}(1-w^2)\frac{d}{dw} = -\frac{1}{\sin\theta}\,\frac{d}{d\theta}\left[-\sin\theta\,\frac{d}{d\theta}\right] = \frac{1}{\sin\theta}\,\frac{d}{d\theta}\left[\sin\theta\,\frac{d}{d\theta}\right]\,.$$

Eqn. (11.6) becomes

$$\left(\frac{d}{dw}(1-w^2)\frac{d}{dw} + \lambda - \frac{m^2}{1-w^2}\right)\Theta(w) = 0\,.$$

which is known as the *Associated Legendre Equation*. Solutions of the Associated Legendre Equation are the Associated Legendre Polynomials.
In this course we will only solve this equation for $m = 0$.
It will turn out that there are smart ways to generate solutions for $m \neq 0$ from the solutions for $m = 0$ using angular momentum ladder operators (see quantum mechanics of hydrogen atom). So it would be unnecessarily "heroic" to directly solve this equation for $m \neq 0$.
For $m = 0$ we can write the special case as the *Legendre Equation*:

$$\left((1-w^2)\frac{d^2}{dw^2} - 2w\frac{d}{dw} + \lambda\right)\Theta(w) = 0\,.$$

We apply the method of Froebenius by taking

$$\Theta(w) = \sum_{i=0}^{\infty} c_i w^i$$

Then

$$\sum_{i=0}^{\infty} c_i i(i-1)(w^{i-2} - w^i) - 2c_i i w^i + \lambda c_i w^i = 0$$

and rearranging the series to always refer the power w^i,

$$\sum_{i=0}^{\infty} \left[c_{i+2}(i+2)(i+1) + c_i(\lambda - i(i-1) - 2i\right] w^i = 0$$

Since this is true for all w, it is true term by term, and the indicial equation is

$$c_{i+2}\left((i+2)(i+1)\right) = c_i\left(i(i+1) - \lambda\right)$$

The series "switches on" when $C_0 \times 0 = 0$ admits $C_0 \neq 0; C_{-2} = 0$, or when $C_1 \times 0 = 0$ admits $C_1 \neq 0; C_{-1} = 0$.
Note, however $c_{i+2} \simeq C_i$ for large i. This gives an ill convergent series and for finite solutions the series must terminate at some value of i, which we call l. Thus,

$$\lambda = l(l+1)$$

for some (quantised) integer value l. It will turn out in quantum mechanics that l is the orbital angular momentum quantum number. We denote the solutions the Legendre polynomials

$$P_l(w) \equiv P_l(\cos\theta)$$

P_0 starts, and terminates with a single term C_0.
P_1 starts, and terminates with a single term C_1.
P_2 starts, with C_0 and terminates on C_2.
etc...
The first few are

$$\begin{aligned} P_0(w) &= 1 \\ P_1(w) &= w \\ P_2(w) &= \frac{1}{2}(3w^2-1) \\ P_3(w) &= \frac{1}{2}(5w^3-3w) \end{aligned}$$

The orthogonality relation is

$$\int_{-1}^{1} P_m(w)P_n(w)dw = \int_0^{\pi} P_m(\cos\theta)P_n(\cos\theta)\sin\theta d\theta = N_m\delta_{mn}$$

where N_m is a normalisation factor that we do not need here.
In quantum mechanics this is already sufficient to cover S, P , D and F orbitals.
As mentioned the associated Legendre polynomials can be produced from Legendre polynomials in quantum mechanics using angular momentum ladder operators. Consequently, it suffices here to state that the associated Legendre polynomials are written as

$$P_l^m(w)\ ; m \in \{-l, \ldots, 0, \ldots + l\}$$

And,

$$P_l^0(w) = P_l(w)$$

11.2.4 General angular solution

Putting aside the radial part for the moment, the rest of the general solution is:

$$\Theta(\theta)\Phi(\phi)T(t) = \sum_{n=0}^{\infty}\sum_{m=-n}^{n} P_n^m(\cos\theta)\ e^{im\phi}\ (E_{mn}\cos\omega_k t + F_{mn}\sin\omega_k t)$$

The angular dependence is given by the combination:

$$P_n^m(\cos\theta)\ e^{im\phi} \propto Y_m^n(\theta,\phi)$$

These are known as the *spherical harmonics* (once we include a normalisation constant). We'll discuss these more in Sec. 11.3.
What we have not yet established is the link between the value of k (and hence ω_k) and the values of m and n. To do this, we need to solve the radial equation for various special cases.

11.2.5 Parity

The Legendre polynomials have the following property under $w \to -w$:

$$P_l(-w) = (-1)^l P_l(w)\ ,$$

so we say the Legendre polynomial $P_l(x)$ has parity $(-1)^l$.

11.3 The spherical harmonics

Spherical harmonics $\{Y_n^m(\theta,\phi)\}$ provide a complete, orthonormal basis for expanding the angular dependence of a function.
They crop up a lot in physics because they are the normal mode solutions to the angular part of the Laplacian.
They are defined as:

$$Y_n^m(\theta,\phi) = \frac{(-1)^m}{\sqrt{2\pi}}\sqrt{\frac{2n+1}{2}\cdot\frac{(n-m)!}{(n+m)!}}P_n^m(\cos\theta)e^{im\phi} \ .$$

The extra factor of $(-1)^m$ introduced is just a convention and does not affect the orthonormality of the functions.

11.3.1 Orthonormality

The spherical harmonics satisfy an orthogonality relation:

$$\int_0^{2\pi} d\phi \int_0^{\pi} d\theta \ \sin\theta \ \left[Y_{n_1}^{m_1}(\theta,\phi)\right]^* Y_{n_2}^{m_2}(\theta,\phi) = \delta_{n_1,n_2}\delta_{m_1,m_2} \ .$$

Note that they are orthonormal, not just orthogonal, as the constant multiplying the product of Kronecker deltas is unity.

Details The orthonormality came from considering $Z_n^m(\theta,\phi) \equiv P_n^m(\cos\theta)\Phi_m(\phi)$, where $\Phi_m(\phi) = e^{im\phi}$. This implies:

$$\begin{aligned}\int_0^{\pi} d\theta \int_{-\pi}^{\pi} d\phi \ \sin\theta \ [Z_{n_1}^{m_1}(\theta,\phi)]^* Z_{n_2}^{m_2}(\theta,\phi) &= \left[\int_0^{\pi} d\theta \ \sin\theta \ P_{n_1}^{m_1}(\cos\theta)P_{n_2}^{m_2}(\cos\theta)\right]\times \\ &\qquad \left[\int_{-\pi}^{\pi} d\phi \ \Phi_{m_1}(\phi)^*\Phi_{m_2}(\phi)\right] \\ &= \frac{2}{2n_1+1}\cdot\frac{(n_1+m_1)!}{(n_1-m_1)!}\delta_{n_1,n_2}\times 2\pi\delta_{m_1,m_2} \ .\end{aligned}$$

To create orthonormal functions, we divide Z_n^m by the square root of the normalisation factor to get Y_n^m.

11.3.2 Completeness and the Laplace expansion

The completeness property means that any function $f(\theta,\phi)$ evaluated over the surface of the unit sphere can be expanded in the double series known as the *Laplace series*:

$$\begin{aligned} f(\theta,\phi) &= \sum_{n=0}^{\infty}\sum_{m=-n}^{n} a_{nm}Y_n^m(\theta,\phi) \ , \\ \Rightarrow \qquad a_{mn} &= \int_0^{\pi} d\theta \int_{-\pi}^{\pi} d\phi \ \sin\theta \ [Y_n^m(\theta,\phi)]^* f(\theta,\phi) \ . \end{aligned}$$

Note that the sum over m only runs from $-n$ to n, because the associated Laplace polynomials P_n^m are zero outside this range.
In Quantum Mechanics, we associate n with the total angular momentum quantum number and m with the z-component of the angular momentum. In this case $-n \le m \le n$ makes physical sense: the z-component cannot be larger than the total length of the vector.

11.4 Time independent Schroedinger equation in central potential

Consider

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

We consider solutions of separated form: $\psi(r,\theta,\phi)=R(r)\Theta(\theta)\Phi(\phi)$. Substitute into Schroedinger equation and divide across by $\psi=R\Theta\Phi$.

$$\frac{2m}{\hbar^2}\left(V(r)-E\right)-\frac{1}{R}\frac{1}{r^2}\frac{\partial}{\partial r}r^2\frac{\partial}{\partial r}R=\frac{1}{\Theta}\frac{1}{r^2\sin\theta}\frac{\partial}{\partial\theta}\sin\theta\frac{\partial}{\partial\theta}\Theta+\frac{1}{\Phi}\frac{1}{r^2\sin^2\theta}\frac{\partial^2}{\partial\phi^2}\Phi$$

Multiplying through by r^2

$$r^2\frac{2m}{\hbar^2}\left(V(r)-E\right)-\frac{1}{R}\frac{\partial}{\partial r}r^2\frac{\partial}{\partial r}R=\frac{1}{\Theta}\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\sin\theta\frac{\partial}{\partial\theta}\Theta+\frac{1}{\Phi}\frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2}\Phi$$

First separation: radial & angular dependence

$$\mathrm{LHS}(r)=\mathrm{RHS}(\theta,\phi)=\text{constant}=-l(l+1).$$

Consider the LHS radial equation:

$$\left[-\frac{\partial}{\partial r}r^2\frac{\partial}{\partial r}+l(l+1)+r^2\frac{2m}{\hbar^2}(V(r)-E)\right]R=0$$

The differential equation is simplified by a substitution,

$$\begin{aligned}u(r) &= rR(r)\\ u'(r) &= R(r)+rR'(r)\\ u''(r) &= 2R'(r)+rR''(r)=\frac{1}{r}\frac{\partial}{\partial r}r^2\frac{\partial}{\partial r}R\end{aligned}$$

and so

$$\left[-\frac{d^2}{dr^2}+\frac{l(l+1)}{r^2}+\frac{2m}{\hbar^2}(V(r)-E)\right]u(r)=0$$

We take a Coulomb potential and will be considering bound states, with $E<0$. It is convenient to rewrite in terms of the modulus $|E|$ and introduce explicit negative sign. We also change variables to $\rho=\frac{\sqrt{2m|E|}}{\hbar}r$

$$V(r)=\frac{-e^2}{4\pi\epsilon_0 r}=\frac{-e^2\sqrt{2m|E|}}{4\pi\epsilon_0\hbar\rho},$$

and so

$$\left[\frac{d^2}{d\rho^2}-1-\frac{l(l+1)}{\rho^2}+\frac{e^2}{4\pi\epsilon_0\hbar\rho}\sqrt{\frac{2m}{|E|}}\right]u(\rho)=0$$

We define $\lambda=\frac{e^2}{4\pi\epsilon_0\hbar}\sqrt{\frac{2m}{|E|}}=\alpha\sqrt{\frac{2mc^2}{|E|}}$, where $\alpha=\frac{e^2}{4\pi\epsilon_0\hbar c}\simeq\frac{1}{137}$ is the fine structure constant. This gives us

$$\left[\frac{d^2}{d\rho^2}-1-\frac{l(l+1)}{\rho^2}+\frac{\lambda}{\rho}\right]u(\rho)=0$$

We are now (almost!) ready to apply the method of Froebenius. In principle it could immediately be applied and we would get a an infinite Taylor series that indeed solves the equation. However, a

closed form solution can be obtained with one extra transformation that removes an over exponential dependence on ρ.
Observe that this equation for large ρ tends to

$$\rightarrow \left[\frac{d^2}{d\rho^2} - 1\right] u(\rho)$$

which has as a normalisable solution $u(\rho) \rightarrow e^{-\rho}$, and in addition a non-normalisable solution $u(\rho) \rightarrow e^{+\rho}$ which we ignore. Applying Froebenius now would give rise to an infinite Taylor series describing the exponential, and we can do rather better by taking a trial solution:

$$u(\rho) = e^{-\rho} f(\rho).$$

Then,

$$u'' = e^{-\rho} \left[f''(\rho) - 2f'(\rho) + f(\rho)\right].$$

Now,

$$\left[\frac{d^2}{d\rho^2} - 2\frac{d}{d\rho} + \cancel{1} - \cancel{1} - \frac{l(l+1)}{\rho^2} + \frac{\lambda}{\rho}\right] f(\rho) = 0$$

We now apply the method of Froebenius substituting $f(\rho) = \sum_{i=0}^{\infty} c_i \rho^{i+m}$,

$$\sum_{i=0}^{\infty} c_i(i+m)(i+m-1)\rho^{i+m-2} - 2c_i(i+m)\rho^{i+m-1} - l(l+1)c_i\rho^{i+m-2} + \lambda c_i \rho^{i+m-1}$$

Thus, reexpressing so that all terms are of equal power ρ^{i+m-1}

$$\sum_{i=-1}^{\infty} c_{i+1}(i+m+1)(i+m)\rho^{i+m-1} - 2c_i(i+m)\rho^{i+m-1} - l(l+1)c_{i+1}\rho^{i+m-1} + \lambda c_i \rho^{i+m-1}$$

and we have the indicial equation,

$$c_{i+1}\left[(i+m+1)(i+m) - l(l+1)\right] = c_i\left[2(i+m) - \lambda\right]$$

The series "switches on" for c_0 when $m(m-1) = l(l+1)$. Thus, $m = (l+1)$, and

$$c_{i+1}\left[(i+l+2)(i+l+1) - l(l+1)\right] = c_i\left[2(i+l+1) - \lambda\right]$$

If $\lambda = 2(i+l+1) = n$ then the series "switches off" after i terms. If the series does not terminate, then $c_{i+1} \rightarrow \frac{2c_i}{i}$, and this looks like the non-renormalisable exponential $u(\rho) \simeq e^{\rho}$ which we do not seek.
Thus, the series terminates for the bound states with $\lambda = 2(i+l+1) = n$. We call n the principal quantum number, and the energy is

$$\alpha\sqrt{\frac{2mc^2}{|E|}} = 2n$$

Thus

$$|E| = \frac{\alpha^2 mc^2}{2n^2}$$

Note that for any given l, then $n \geq l+1$.

11.4.1 Wavefunctions

We denote the radial solution for $L = l$, and principle quantum number $n \geq l + 1$ as R_{nl}.

	$n = 1, l = 0$	$n = 2, l = 0$	$n = 2, l = 1$
c_0	1	1	1
c_1	-		-
c_2	-	-	-

12 Complex analysis

We often consider complex valued functions of a complex variable.

$$f(z) = u(x, y) + iv(x, y).$$

For example, one might consider the complex analog of a simple polynomial:

$$f(z) = 1 + z + z^2$$

It is natural to generalise the differentiation rules we know from real variables x to apply to complex variables z

$$f'(z) = 1 + 2z.$$

12.1 Cauchy-Riemann equations

However, in principle we could evaluate either

$$\lim_{\epsilon \to 0} \frac{f(z+\epsilon) - f(z)}{\epsilon} = \frac{\partial u(x,y)}{\partial x} + i\frac{\partial v(x,y)}{\partial x}$$

or

$$\lim_{\epsilon \to 0} \frac{f(z+i\epsilon) - f(z)}{i\epsilon}. = \frac{\partial v(x,y)}{\partial y} - i\frac{\partial u(x,y)}{\partial y}$$

For complex differentiation to be conistent we require these be the same. Thus, if we think of $z = x + iy$ in terms of real and imaginary parts we require

$$\begin{aligned} \frac{\partial}{\partial x}u(x,y) &= \frac{\partial}{\partial y}v(x,y) \\ \frac{\partial}{\partial y}u(x,y) &= -\frac{\partial}{\partial x}v(x,y). \end{aligned} \tag{12.7}$$

(12.7) are called the Cauchy-Riemann equations.
If the C-R equations are satisfied through some patch of the complex plane, $f(z)$ is said (by mathematicians!) to be *holomorphic* on that patch.

12.2 Contour integrals

We introduce a complex line integral, which we call a *contour integral*.
We parameterise by $t \in [0, 1]$, such that z(t) sweeps along the line in a continuous fashion with $z(0)$ lying at the start of the line, and $z(1)$ being the end of the line.

Example integral around circle
We define $z(t) = re^{i2\pi t}$.
The contour integral is just

$$\oint f(z)dz = \int_0^1 f(z(t))\frac{dz}{dt}dt = 2\pi i \int_0^1 f(re^{i2\pi t})re^{i2\pi t}dt$$

The factor $\frac{dz}{dt}$ makes this integral independent of the particular parameterisation chosen.

12.2.1 Relation to Gauss and Stokes theorems

If we consider $\boldsymbol{a} = (u, -v, 0) \equiv f^*(z)$ as a 3d vector, then this implies that

$$\partial_y a_x - \partial_x a_y = (\boldsymbol{\nabla} \times \boldsymbol{a})_z = 0.$$

We also have that

$$\partial_x a_x + \partial_y a_y = \boldsymbol{\nabla} \cdot \boldsymbol{a} = 0.$$

Perhaps there is an interesting connection to our vector calculus here. If we consider a closed contour and the Cauchy Riemann equations are satisfied, it turns out we can apply both Stoke's and Gauss's theorems simultaneously!

$$\begin{aligned}
\oint f(z)dz &= \oint f(z(t))\frac{dz(t)}{dt}dt && (12.8)\\
&= \int_{t=0}^{1} [u(x(t), y(t)) + iv(x(t), y(t))] \left[\frac{dx(t)}{dt} + i\frac{dy(t)}{dt}\right] dt && (12.9)\\
&= \int_{t=0}^{1} \left[u(x(t), y(t))\frac{dx(t)}{dt} - v(x(t), y(t))\frac{dy(t)}{dt}\right] dt && (12.10)\\
&+ i\int_{t=0}^{1} \left[v(x(t), y(t))\frac{dx(t)}{dt} + u(x(t), y(t))\frac{dy(t)}{dt}\right] dt && (12.11)\\
&= \oint \boldsymbol{a} \cdot d\boldsymbol{l} + i(\oint \boldsymbol{a} \cdot (d\boldsymbol{l} \times \hat{z})) && (12.12)\\
&= \int_{\mathcal{A}} (\boldsymbol{\nabla} \times \boldsymbol{a})_z d\mathcal{A} + i\int_{\mathcal{A}} \boldsymbol{\nabla} \cdot \boldsymbol{a} d\mathcal{A} && (12.13)\\
&= 0 && (12.14)
\end{aligned}$$

This is wonderful: our vector calculus can be applied to $\boldsymbol{a}(x, y) \equiv f^*(z)$ and we conclude that if the Cauchy Riemann equations are satisfied the result is zero.
Above we made use of the fact that $d\boldsymbol{l} \times \hat{z}$ gives the normal $dl\hat{n}$, and then we can take an infinitessimal volume extending in the $\hat{z}$ direction with the same cross section as the area $\mathcal{A}$

12.3 Analytic continuation

The Cauchy Riemann conditions relate derivatives in the imaginary direction to those in the real direction. This is sufficient constraint that we can generalise analytic real functions of real variables in a unique way to be holomorphic complex functions of complex variables. This is known as analytic continuation.
For a physicist this shouldn't be surprising - if $\boldsymbol{a}$ were electrostatic field, in a region containing no charges and no varying magnetic fields the electric field in the interior has to be uniquely determined by it's boundary conditions.
In complex analysis, $\boldsymbol{\nabla} \cdot \boldsymbol{a} = 0$ and $(\boldsymbol{\nabla} \times \boldsymbol{a})_z = 0$ introduce similar constraints that allow the $f(z)$ on the "interior" to be determined by a small patch.
For example, this can be done by taking a Taylor expansion of the real function and simply substituting z, wherever x occurs. A polynomial of x,

$$f(x) = 1 + x + x^2$$

turns into the same polynomial of z.

$$f(z) = 1 + z + z^2$$

A polynomial function is holomorphic on the whole complex plane.

12.4 Poles & residues

Consider the function $f(z) = C(z - z_0)^n$.
Clearly for $n < 0$ it is *infinite* for $z = z_0$, but holomorphic everywhere else. Mathematicians call such a function *meromorphic*.
If $n = -1$ we call this a *single pole*. We define the residue of $f(z)$ at z_0 to be to be the coefficient for a *single pole* at z_0, $\text{res}(f(z), z_0) = C$.
If $n = -2$ we call this a double pole, and it has $\text{res}(f(z), z_0) = 0$. and so on for $n = -3, -4, -5 \ldots$.
Now consider the real function:

$$f(x) = \frac{1}{1 + x^2}.$$

This, of course, when continued to be a complex function is

$$f(z) = \frac{1}{1 + z^2} = \frac{1}{(z - i)(z + i)}$$

$f(x)$ was finite, continuous and differentiable for all real x.
Over the complex plane f(z) has two *poles* (infinities), at $z = i$ and $z = -i$.
We therefore generalise the *Taylor* series to the *Laurent series*.

12.4.1 Laurent series

The Laurent series takes the form

$$\sum f(z) = \sum_{i=0}^{\infty} C_i (z - z_0)^{i+m},$$

it is a generalisation of the Taylor series expansion about the point z_0, that allows $m < 0$, and so can have *poles*.
Let's revisit

$$f(z) = \frac{1}{1 + z^2} = \frac{1}{(z - i)(z + i)}$$

if we expand this around $z_0 = i$ we have

$$\begin{aligned} f(z) &= \frac{1}{(2i)(z - i)(1 + \frac{(z-i)}{2i})} \\ &= \frac{1}{2i}\frac{1}{z - i}\left[1 - \left(\frac{(z - i)}{2i}\right) + \left(\frac{(z - i)}{2i}\right)^2 - \ldots\right] \\ &= \sum_{n=-1}^{\infty} \frac{1}{2i}\left(\frac{-1}{2i}\right)^{n+1} (z - i)^n \end{aligned}$$

The residue is $\text{res}(f(z), z_0 = i) = \frac{1}{2i}$.
The residue for the pole at $z = -i$ is $\frac{-1}{2i}$.
Some rules can save the tedium of evaluating the Laurent series in the fashion above.

- if $f(z)$ is holomorphic then

$$\text{res}(\frac{f(z)}{z - z_0}, z_0) = f(z_0).$$

- if $f(z)$ has a single pole at z_0 then

$$\text{res}(f(z), z_0) = \lim_{z \to z_0} (z - z_0) f(z).$$

- if $f(z)$ vanishes linearly in $z - z_0$ then

$$\text{res}(\frac{1}{f(z)}, z_0) = \frac{1}{f'(z_0)}.$$

12.4.2 Contour integral around a pole

Consider the contour integral around the unit circle centered on z_0 of $f(z) = C(z - z_0)^n$. We change variables to $z = z_0 + e^{i\theta}; dz = ie^{i\theta} d\theta$.

$$\begin{aligned}
\oint C(z - z_0)^n dz &= C \int_0^{2\pi} e^{in\theta} i e^{i\theta} d\theta \\
&= iC \int_0^{2\pi} e^{i(n+1)\theta} d\theta \\
&= C \begin{cases} \frac{1}{n+1} \left[e^{i(n+1)\theta} \right]_0^{2\pi} & ; \quad n \neq -1 \\ 2\pi i & ; \quad n = -1 \end{cases} \\
&= \begin{cases} 0 & ; \quad n \neq -1 \\ 2\pi i C & ; \quad n = -1 \end{cases}
\end{aligned} \tag{12.15}$$

The intergral picks only one term, $n = -1$, out a Laurent series and has value $2\pi i \times C$, where C is the residue of $f(z)$ at z_0.
So if $f(z)$ has a Laurent series expansion about z_0, we can find any of the terms by multiplying $f(z)$ by a power of $(z - z_0)$ and integrating around a closed circle contour centered at z_0:

$$C_i = \frac{1}{2\pi i} \oint \frac{f(z)}{(z - z_0)^{n+1}} dz$$

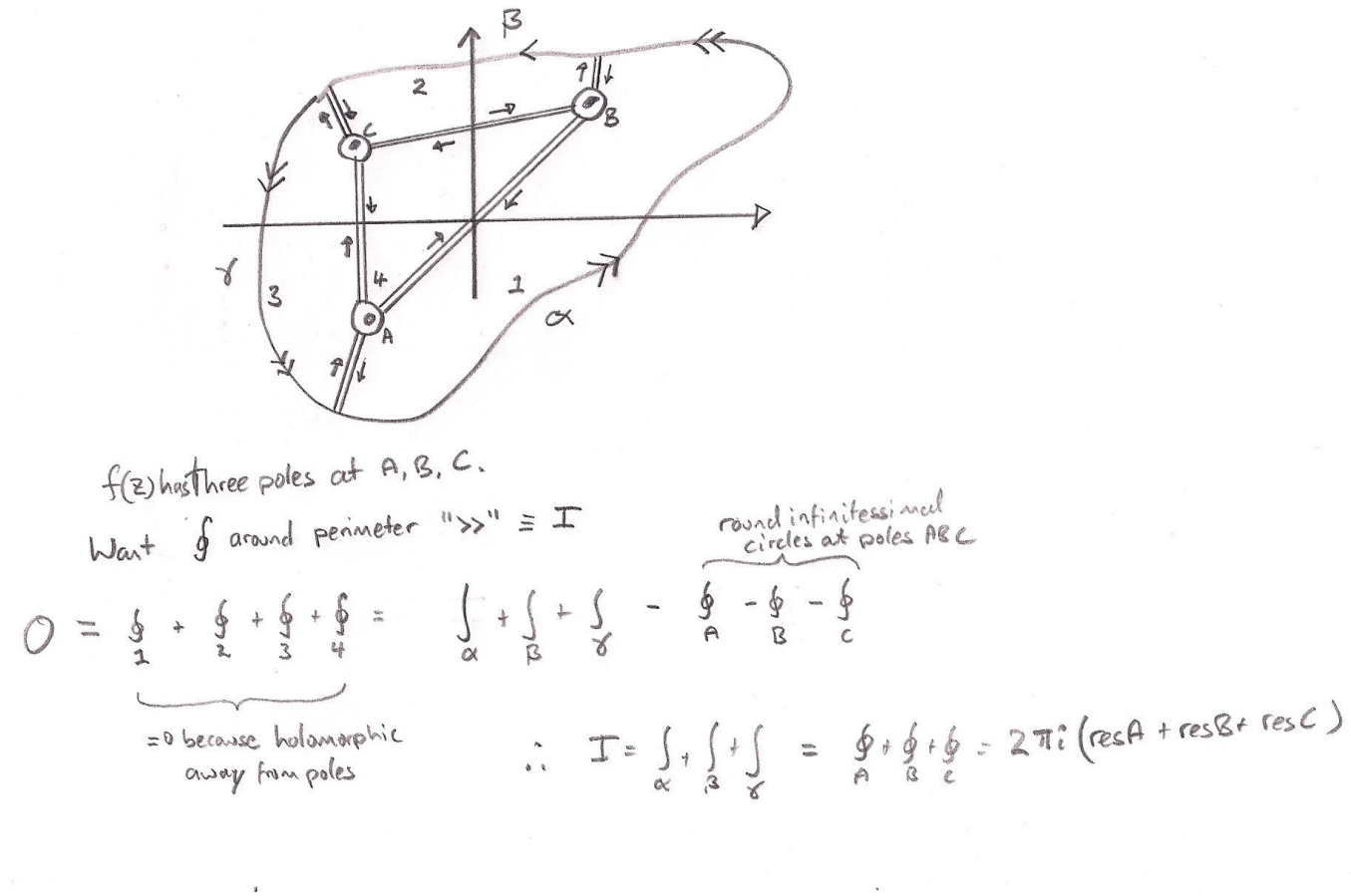
Note, we can always reduce the radius of this circle to lie within the radius of convergence of the series.

12.5 Cauchy's residue theorem

Suppose a function f(z) is holomorphic on a patch except for a finite number of singular points. Then the integral around the patch

$$\oint f(z) dz = 2\pi i \sum_{z_0 \in \text{poles}} \text{res}(f(z), z_0)$$

proof



Since $f(z)$ is holomorphic everywhere except from the poles, we can equate the contour integral to the sum of a set of closed contour integrals containing no poles and a sum of circular integrals lying infinitessimally close to each pole (see above).
Each of the circular integrals can be chosen sufficiently close to lie within the radius of convergence of the Laurent series about its pole z_0, and there contribute $2\pi i \text{res}(f(z), z_0)$ to the latter sum.
The integrals containing no poles are automatically zero, and thus the result is proven.

12.6 Application to difficult integrals

Example: complex integral

Evaluate $\oint \frac{1}{1+z^2}$ around the following circles

- center $z = 0$, radius $r = 2$
- center $z = 0$, radius $r = \frac{1}{2}$
- center $z = i$, radius $r = 1$
- center $z = -i$, radius $r = 1$

Example: real integral with contour closure