Sketch notes for PX276; these are very terse and not a substitute for your own lecture notes.

Fourier Series

Fourier series provide a representation, and analysis, of periodic functions. A function f is periodic with period P if $f(x+P) = f(x)$ for all x. To completely specify a periodic function it is enough to give its value on any interval of length P. In this course we will adopt a standard interval $[-L, L]$, with $P = 2L$. As examples, the functions $\sin(n\pi x/L)$ and $\cos(n\pi x/L)$ for integer n are periodic on $[-L, L]$. Functions on a bounded interval ($[0, L]$, say) that are not periodic can be extended so as to become periodic on $[-L, L]$. As an example, consider the function $\sin(\pi x/L)$ on $[0, L]$. Taking $f(x) = \sin(\pi x/L)$ defines an extension to $[-L, L]$ as an odd function; taking instead $f(x) = |\sin(\pi x/L)|$ defines an even extension; and taking

$$f(x) = \begin{cases} \sin(\pi x/L) & 0 < x < L, \\ 0 & -L < x < 0, \end{cases}$$

gives another choice, with no particular symmetry.

If f is a periodic function then its **Fourier series** is the expression

$$f(x) = \sum_{n=-\infty}^{\infty} c_n \, \mathrm{e}^{in\pi x/L}.$$

The coefficients c_n are called the Fourier coefficients, while the complex exponentials $\mathrm{e}^{in\pi x/L}$ are called Fourier modes (the n^{th} Fourier mode). What is meant by "=" in this equation will not be fully explained. The fourth year module MA433 goes into this. The idea is to study the sequence of functions (Fourier approximants)

$$f_N(x) = \sum_{n=-N}^{N} c_n \, \mathrm{e}^{in\pi x/L},$$

and see whether or not they converge (to the function f) as $N \to \infty$. You are strongly encouraged to experiment with this numerically to develop a feeling for Fourier series.

Examples.

$$f(x) = \cos^3(\pi x/L) = \frac{1}{8}\mathrm{e}^{-i3\pi x/L} + \frac{3}{8}\mathrm{e}^{-i\pi x/L} + \frac{3}{8}\mathrm{e}^{i\pi x/L} + \frac{1}{8}\mathrm{e}^{i3\pi x/L},$$

$$f(x) = x = \frac{L}{\pi}\sum_{n\neq 0} \frac{(-1)^{n+1}}{ni}\mathrm{e}^{in\pi x/L},$$

$$f(x) = \left|\sin(\pi x/L)\right| = \frac{2}{\pi} - \frac{1}{\pi}\sum_{n=2}^{\infty} \frac{1+(-1)^n}{n^2-1}\left(\mathrm{e}^{in\pi x/L} + \mathrm{e}^{-in\pi x/L}\right).$$

Fourier coefficients. Proposition: The Fourier coefficients c_n are given by

$$c_n = \frac{1}{2L}\int_{-L}^{L} \mathrm{e}^{-in\pi x/L} f(x)\, dx.$$

The proof is a direct calculation.

This calculation also establishes the **orthogonality of Fourier modes**. The Fourier modes $\mathrm{e}^{im\pi x/L}$ and $\mathrm{e}^{in\pi x/L}$, for $m \neq n$, are orthogonal on $[-L, L]$

$$\frac{1}{2L}\int_{-L}^{L} \overline{\mathrm{e}^{im\pi x/L}}\,\mathrm{e}^{in\pi x/L}\,dx = \frac{1}{2L}\int_{-L}^{L} \mathrm{e}^{-im\pi x/L}\,\mathrm{e}^{in\pi x/L}\,dx = 0, \qquad m \neq n.$$

It is not hard to see that the same integral is equal to 1 when $m = n$.

Worked example. Consider the function

$$f(x) = \begin{cases} 1 & 0 < x < L, \\ -1 & -L < x < 0. \end{cases}$$

The Fourier coefficients are $c_0 = 0$ and for $n \neq 0$

$$\begin{aligned} c_n = \frac{1}{2L}\int_{-L}^{L} \mathrm{e}^{-in\pi x/L} f(x)\,dx &= \frac{-1}{2L}\int_{-L}^{0} \mathrm{e}^{-in\pi x/L}\,dx + \frac{1}{2L}\int_{0}^{L} \mathrm{e}^{-in\pi x/L}\,dx, \\ &= \frac{1}{2n\pi i}\big(1 - \mathrm{e}^{in\pi}\big) - \frac{1}{2n\pi i}\big(\mathrm{e}^{-in\pi} - 1\big), \\ &= \frac{1 - (-1)^n}{n\pi i}. \end{aligned}$$

This vanishes when n is even and is equal to $2/n\pi i$ when n is odd. Hence the Fourier series is

$$f(x) = \sum_{n\neq 0} \frac{1 - (-1)^n}{n\pi i} \mathrm{e}^{in\pi x/L} = \sum_{n \text{ odd}} \frac{4}{n\pi} \sin(n\pi x/L).$$

Fourier sine and cosine series. In many applications the function f will be real-valued. We can write its Fourier series in a manner where this is explicit using the Euler identity

$$\mathrm{e}^{i\theta} = \cos\theta + i\sin\theta.$$

First, we consider the Fourier coefficients

$$c_n = \frac{1}{2L}\int_{-L}^{L} \left(\cos\frac{n\pi x}{L} - i\sin\frac{n\pi x}{L}\right) f(x)\,dx = \frac{1}{2}\big(a_n - ib_n\big).$$

It is easy to see that $a_{-n} = a_n$ and $b_{-n} = -b_n$. Consequently if f is a real-valued function its Fourier coefficients satisfy $c_{-n} = \overline{c_n}$. Now using the Euler identity again we obtain the Fourier series for a real function in the form

$$f(x) = \frac{a_0}{2} + \sum_{n=1}^{\infty} \left(a_n \cos\frac{n\pi x}{L} + b_n \sin\frac{n\pi x}{L}\right).$$

We deduce from this manipulation the **orthogonality relations** for sine and cosine

$$\begin{aligned} \frac{1}{L}\int_{-L}^{L} \cos(m\pi x/L)\cos(n\pi x/L)\,dx &= \delta_{mn}, \\ \frac{1}{L}\int_{-L}^{L} \sin(m\pi x/L)\sin(n\pi x/L)\,dx &= \delta_{mn}, \\ \frac{1}{L}\int_{-L}^{L} \sin(m\pi x/L)\cos(n\pi x/L)\,dx &= 0. \end{aligned}$$

Worked example: Consider the **step function**

$$f(x) = \begin{cases} 1 & -a < x < a \\ 0 & \text{otherwise} \end{cases},$$

for any $a < L$. The Fourier coefficients are

$$\begin{aligned} c_n = \frac{1}{2L}\int_{-L}^{L} \mathrm{e}^{-in\pi x/L} f(x)\,dx &= \frac{1}{2L}\int_{-a}^{a} \mathrm{e}^{-in\pi x/L}\,dx, \\ &= \frac{-1}{2n\pi i}\Big[\mathrm{e}^{-in\pi a/L} - \mathrm{e}^{in\pi a/L}\Big], \\ &= \frac{\sin(n\pi a/L)}{n\pi}, \end{aligned}$$

for any $n \neq 0$ and $c_0 = a/L$. The Fourier series for the step function is therefore

$$f(x) = \frac{a}{L} + \sum_{n\neq 0} \frac{\sin(n\pi a/L)}{n\pi}\,\mathrm{e}^{in\pi x/L} = \frac{a}{L} + 2\sum_{n=1}^{\infty} \frac{\sin(n\pi a/L)}{n\pi}\cos(n\pi x/L).$$

Some properties of Fourier series. Shift property. Let f, g be functions with Fourier coefficients c_n, d_n and suppose that $g(x) = f(x - x_0)$. Then

$$d_n = \mathrm{e}^{-in\pi x_0/L} c_n.$$

The proof is a direct calculation.

Worked example. Let f be the sum of two step functions from the previous example, both with $a = L/4$, one shifted by $x_0 = L/2$ and the other by $x_0 = -L/2$. The Fourier series is

$$\begin{aligned} f(x) &= \left(\frac{1}{4} + \sum_{n\neq 0} \mathrm{e}^{-in\pi/2}\frac{\sin(n\pi/4)}{n\pi}\mathrm{e}^{in\pi x/L}\right) + \left(\frac{1}{4} + \sum_{n\neq 0} \mathrm{e}^{in\pi/2}\frac{\sin(n\pi/4)}{n\pi}\mathrm{e}^{in\pi x/L}\right), \\ &= \frac{1}{2} + \frac{2}{\pi}\sum_{n\neq 0} \frac{\cos(n\pi/2)\sin(n\pi/4)}{n}\mathrm{e}^{in\pi x/L}, \\ &= \frac{1}{2} + \frac{4}{\pi}\sum_{n=1}^{\infty} \frac{\cos(n\pi/2)\sin(n\pi/4)}{n}\cos(n\pi x/L). \end{aligned}$$

Derivatives. The Fourier coefficients of the derivative of f are $c_n' = \frac{in\pi}{L} c_n$. To see this, consider the Fourier series for f and differentiate term-by-term

$$f(x) = \sum_{n=-\infty}^{\infty} c_n \mathrm{e}^{in\pi x/L}, \qquad \Rightarrow \qquad f'(x) = \sum_{n=-\infty}^{\infty} \frac{in\pi c_n}{L}\mathrm{e}^{in\pi x/L}.$$

Alternatively, we can calculate directly from the definition

$$\begin{aligned} c_n' = \frac{1}{2L}\int_{-L}^{L} \mathrm{e}^{-in\pi x/L} f'(x)\,dx &= \frac{1}{2L}\Big[\mathrm{e}^{-in\pi} f(L) - \mathrm{e}^{in\pi} f(-L)\Big] + \frac{1}{2L}\int_{-L}^{L} \frac{in\pi}{L}\mathrm{e}^{-in\pi x/L} f(x)\,dx, \\ &= \frac{in\pi}{L} c_n. \end{aligned}$$

Here the boundary term vanishes because $\mathrm{e}^{-in\pi} = \mathrm{e}^{in\pi}$ and $f(L) = f(-L)$ by periodicity.

Discontinuities. Suppose f is discontinuous at x_0 but the two one-sided limits $\lim_{\delta\to 0} f(x_0 \pm \delta) = f_\pm(x_0)$ both exist and the Fourier series converges away from x_0. Then at x_0 the Fourier series converges to the midpoint of the jump

$$\sum_{n=-\infty}^{\infty} c_n \mathrm{e}^{in\pi x_0/L} = \lim_{N\to\infty} \sum_{n=-N}^{N} c_n \mathrm{e}^{in\pi x_0/L} \to \frac{1}{2}\Big(f_+(x_0) + f_-(x_0)\Big).$$

Example: Our first worked example had a discontinuity at $x = 0$; the two one-sided limits are $f_\pm(0) = \pm 1$, so the Fourier series should converge to 0. It is easy to see that it does.

Parseval's theorem. Let f, g be functions with Fourier coefficients c_n, d_n. Then

$$\frac{1}{2L}\int_{-L}^{L} \overline{g(x)} f(x)\, dx = \sum_{n=-\infty}^{\infty} \overline{d_n} c_n.$$

The proof is a direct calculation.

Example: Recall our first example

$$f(x) = \begin{cases} 1 & 0 < x < L, \\ -1 & -L < x < 0, \end{cases} \qquad = \sum_{n\neq 0} \frac{1-(-1)^n}{n\pi i} \mathrm{e}^{in\pi x/L}.$$

It is easy to see that $\frac{1}{2L}\int_{-L}^{L} |f(x)|^2\, dx = 1$ so that Parseval's theorem gives

$$1 = \frac{1}{\pi^2}\sum_{n\neq 0} \frac{(1-(-1)^n)^2}{n^2} = \frac{2}{\pi^2}\sum_{n=1}^{\infty} \frac{(1-(-1)^n)^2}{n^2} = \frac{8}{\pi}\sum_{n=1,3,5,\ldots} \frac{1}{n^2},$$

or

$$\sum_{n\geq 1,\ \text{odd}} \frac{1}{n^2} = \frac{\pi}{8}.$$

Riemann-Lebesgue lemma. By way of cursory motivation, we begin with a simple observation. Setting $x = 0$ we have

$$f(0) = \sum_{n=-\infty}^{\infty} c_n.$$

The sum certainly converges if $\sum_n |c_n|$ does, which requires $|c_n| \to 0$ as $n \to \pm\infty$. This property holds generally and is known as the Riemann-Lebesgue lemma. To show it, start with the usual definition of the Fourier coefficients and make the change of variables $y = x + L/n$

$$c_n = \frac{1}{2L}\int_{-L}^{L} \mathrm{e}^{-in\pi x/L} f(x)\, dx = \frac{-1}{2L}\int_{-L+L/n}^{L+L/n} \mathrm{e}^{-in\pi y/L} f(y - L/n)\, dy.$$

Now shift the window of integration from $[-L+L/n, L+L/n]$ back to the usual $[-L, L]$, which does not affect the value of the integral by periodicity. Taking the average of this formula with the usual one then gives

$$\left|\frac{c_n + c_n}{2}\right| = \frac{1}{4L}\left|\int_{-L}^{L} \mathrm{e}^{-in\pi x/L}\big(f(x) - f(x - L/n)\big)\, dx\right| \leq \frac{1}{4L}\int_{-L}^{L} \big|f(x) - f(x - L/n)\big|\, dx \leq \epsilon,$$

for arbitrary ϵ, say with the assumption $f \in C^0([-L, L])$. The same is true when f is simply integrable.

Orthogonal Basis. The orthogonality of Fourier modes can be viewed as exactly analogous to that for the Cartesian basis vectors $\mathbf{e}_i$, namely $\mathbf{e}_i \cdot \mathbf{e}_j = \delta_{ij}$, in a finite-dimensional vector space. The Fourier modes serve as an orthogonal basis for the infinite-dimensional vector space of square-integrable periodic functions, $L^2([-L, L])$. The Fourier coefficients of any function are the 'components' of the vector in the Fourier basis.

This terminology and notation was exploited by Dirac in his presentation of quantum mechanics – the eigenstates of a (free) quantum particle in a (periodic) well are precisely the Fourier modes $\mathrm{e}^{in\pi x/L}$. Writing $\psi_n = \frac{1}{\sqrt{2L}}\mathrm{e}^{in\pi x/L}$ the orthogonality in Dirac's notation becomes

$$\langle \psi_m | \psi_n \rangle = \int_{-L}^{L} \overline{\psi_m} \psi_n \, dx = \frac{1}{2L} \int_{-L}^{L} \mathrm{e}^{-im\pi x/L} \, \mathrm{e}^{in\pi x/L} \, dx = \delta_{mn}.$$

Application: vibrations of a string. Consider a string of length L held under tension T along the x-axis and clamped at both ends. It vibrates in the xy-plane with amplitude $u(x,t)$ that satisfies

$$\rho \frac{\partial^2 u}{\partial t^2} = T \frac{\partial^2 u}{\partial x^2} \qquad \text{or} \qquad \frac{1}{c^2}\frac{\partial^2 u}{\partial t^2} = \frac{\partial^2 u}{\partial x^2},$$

where $c = \sqrt{T/\rho}$ is the speed of sound in the string. It was exactly solving partial differential equations like this that provided the original motivation for the development of Fourier series.

The string occupies the interval $[0, L]$ and is clamped at both ends; we extend the amplitude of vibration $u(x,t)$ as an odd periodic function on $[-L, L]$ and expand it as a Fourier sine series

$$u(x,t) = \sum_{n=1}^{\infty} u_n(t) \sin(n\pi x/L), \qquad \Rightarrow \qquad \frac{1}{c^2}\frac{d^2 u_n}{dt^2} = -\frac{n^2\pi^2}{L^2} u_n.$$

Solving for the Fourier coefficients $u_n(t)$ we find the vibration of the string is

$$u(x,t) = \sum_{n=1}^{\infty} \Big(a_n \cos(n\pi ct/L) + b_n \sin(n\pi ct/L) \Big) \sin(n\pi x/L).$$

The coefficients a_n, b_n are determined from the initial conditions. For instance, the initial displacement of the string is

$$u(x,0) = \sum_{n=1}^{\infty} a_n \sin(n\pi x/L).$$

The energy in the string is

$$E = \int_0^L \left[\frac{1}{2}\rho \left(\frac{\partial u}{\partial t} \right)^2 + \frac{1}{2} T \left(\frac{\partial u}{\partial x} \right)^2 \right] dx = \frac{T}{2} \int_0^L \left[\frac{1}{c^2} \left(\frac{\partial u}{\partial t} \right)^2 + \left(\frac{\partial u}{\partial x} \right)^2 \right] dx.$$

Extending the range of the integral to $[-L, L]$ and multiplying by $\frac{1}{2}$ to compensate, we can compute the energy using Parseval's theorem

$$\begin{aligned} E &= \frac{T}{4} \int_{-L}^{L} \left[\frac{1}{c^2} \left(\frac{\partial u}{\partial t} \right)^2 + \left(\frac{\partial u}{\partial x} \right)^2 \right] dx, \\ &= \frac{T}{4} \sum_{n=1}^{\infty} \frac{n^2\pi^2}{L} \left[\Big(b_n \cos(n\pi ct/L) - a_n \sin(n\pi ct/L) \Big)^2 + \Big(a_n \cos(n\pi ct/L) + b_n \sin(n\pi ct/L) \Big)^2 \right], \\ &= \frac{\pi^2 T}{4L} \sum_{n=1}^{\infty} n^2 (a_n^2 + b_n^2). \end{aligned}$$

The result is independent of time, a reflection of conservation of energy. Moreover, it is a sum of 'energies' $E_n = \frac{\pi^2 n^2 T}{4L}(a_n^2 + b_n^2)$ in each of the independent Fourier modes, which serves to emphasise in physical terms why Fourier analysis is so natural and relevant in physical problems.

Fourier series in more than one dimension. Fourier series extend naturally to higher dimensions where all of the same basic formulae continue to hold. It can be convenient, however, to introduce a more compact notation. Write $f(\mathbf{x})$ for $f(x, y, z)$ and $\mathbf{k}$ for $\frac{\pi}{L}(n_x, n_y, n_z)$. Then the basic formulae are

$$f(\mathbf{x}) = \sum_{\mathbf{k}} c_{\mathbf{k}} \mathrm{e}^{i\mathbf{k}\cdot\mathbf{x}}, \qquad\qquad c_{\mathbf{k}} = \frac{1}{(2L)^3} \int_{[-L,L]^3} \mathrm{e}^{-i\mathbf{k}\cdot\mathbf{x}} f(\mathbf{x})\, d^3x.$$

In these expressions we are thinking of a function that is periodic on the 'cube' $[-L, L]^3$. One further extension is to allow the sides to have different lengths and be non-orthogonal; this finds applications in crystallography, among other areas.

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Fourier Transforms

Fourier transforms extend Fourier series and provide a representation, and analysis, of functions defined on the entire real line. Treatments in physics motivate the definitions by examining the limit $L \to \infty$ of a Fourier series

$$f(x) = \sum_{n=-\infty}^{\infty} c_n \, \mathrm{e}^{in\pi x/L}.$$

In the exponential we write $k \equiv n\pi/L$ and call it the wavevector. The spacing between wavevectors is $\delta k = \pi/L$, so $1 = \frac{L}{\pi}\delta k$. We think of the sum over modes n as a sum over wavevectors k

$$f(x) = \sum_{k} \Big(\frac{L}{\pi}\delta k\Big) c_n \, \mathrm{e}^{ikx}.$$

As $\delta k \to 0$ this has the structure of a Riemann integral. Now also look at the expression for the Fourier coefficients

$$c_n = \frac{1}{2L}\int_{-L}^{L} \mathrm{e}^{-in\pi x/L} f(x)\, dx \qquad \Rightarrow \qquad 2Lc_n = \int_{-L}^{L} \mathrm{e}^{-ikx} f(x)\, dx.$$

We take the limit $L \to \infty$ holding k fixed and write it in the form

$$\tilde{f}(k) = \int_{-\infty}^{\infty} \mathrm{e}^{-ikx} f(x)\, dx, \qquad\qquad f(x) = \frac{1}{2\pi}\int_{-\infty}^{\infty} \mathrm{e}^{ikx} \tilde{f}(k)\, dk.$$

The function $\tilde{f}$ is called the **Fourier transform** of f. The integral expression for f is called its **Fourier representation** or **Fourier decomposition**; it is also termed the **inverse Fourier transform** of $\tilde{f}$.

Conventions. The asymmetry in factors of 2π between these two expressions is considered undesireable by some and there are many alternative definitions designed to 'fix' this, *e.g.*

$$\tilde{f}(k) = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} \mathrm{e}^{-ikx} f(x)\, dx, \qquad f(x) = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} \mathrm{e}^{ikx} \tilde{f}(k)\, dk,$$

$$\tilde{f}(k) = \int_{-\infty}^{\infty} \mathrm{e}^{-i2\pi kx} f(x)\, dx, \qquad f(x) = \int_{-\infty}^{\infty} \mathrm{e}^{i2\pi kx} \tilde{f}(k)\, dk.$$

Example: Consider the step function

$$f(x) = \begin{cases} 1 & -a < x < a, \\ 0 & \text{else.} \end{cases}$$

Its Fourier transform is

$$\tilde{f}(k) = \int_{-\infty}^{\infty} \mathrm{e}^{-ikx} f(x)\, dx = \int_{-a}^{a} \mathrm{e}^{-ikx}\, dx = \frac{\mathrm{e}^{ika} - \mathrm{e}^{-ika}}{ik} = 2a\,\mathrm{sinc}(ka).$$

Suppose instead that the step function is centred on $x = x_0$. Show that the Fourier transform is $2a\mathrm{e}^{-ikx_0}\,\mathrm{sinc}(ka)$.

Example: Consider the exponentially decaying function

$$f(x) = \mathrm{e}^{-|x|/\xi}.$$

Its Fourier transform is

$$\begin{aligned}
\tilde{f}(k) = \int_{-\infty}^{\infty} \mathrm{e}^{-ikx} f(x)\,dx &= \int_{-\infty}^{0} \mathrm{e}^{-ikx}\mathrm{e}^{x/\xi}\,dx + \int_{0}^{\infty} \mathrm{e}^{-ikx}\mathrm{e}^{-x/\xi}\,dx, \\
&= \frac{\mathrm{e}^{-ikx+x/\xi}}{-ik+1/\xi}\bigg|_{x=-\infty}^{0} + \frac{\mathrm{e}^{-ikx-x/\xi}}{-ik-1/\xi}\bigg|_{x=0}^{\infty}, \\
&= \frac{1}{-ik+\xi^{-1}} + \frac{1}{ik+\xi^{-1}}, \\
&= \frac{2\xi^{-1}}{k^2+\xi^{-2}}.
\end{aligned}$$

This is known as a Lorentzian lineshape.

Example: Consider the (normalised) Gaussian function

$$f(x) = \frac{1}{\sqrt{2\pi\sigma^2}}\mathrm{e}^{-x^2/2\sigma^2}.$$

It is normalised and has 'width' (standard deviation) σ. Its Fourier transform is

$$\begin{aligned}
\tilde{f}(k) = \int_{-\infty}^{\infty} \mathrm{e}^{-ikx} f(x)\,dx &= \int_{-\infty}^{\infty} \mathrm{e}^{-ikx}\frac{1}{\sqrt{2\pi\sigma^2}}\mathrm{e}^{-x^2/2\sigma^2}\,dx, \\
&= \frac{1}{\sqrt{2\pi\sigma^2}}\int_{-\infty}^{\infty} \mathrm{e}^{-(x+ik\sigma^2)^2/2\sigma^2+k^2\sigma^2/2}\,dx, \\
&= \frac{1}{\sqrt{2\pi\sigma^2}}\mathrm{e}^{-\sigma^2k^2/2}\int_{-\infty+ik\sigma^2}^{\infty+ik\sigma^2} \mathrm{e}^{-x^2/2\sigma^2}\,dx, \\
&= \mathrm{e}^{-\sigma^2k^2/2}.
\end{aligned}$$

The Fourier transform of a Gaussian is another Gaussian; it is not normalised and has 'width' σ^{-1}. This means we can calculate directly the inverse Fourier transform

$$\begin{aligned}
\frac{1}{2\pi}\int_{-\infty}^{\infty} \mathrm{e}^{ikx}\tilde{f}(k)\,dk &= \frac{1}{2\pi}\int_{-\infty}^{\infty} \mathrm{e}^{ikx-\sigma^2k^2/2}\,dk, \\
&= \frac{1}{2\pi}\mathrm{e}^{-x^2/2\sigma^2}\int_{-\infty}^{\infty} \mathrm{e}^{-\sigma^2(k-ix/\sigma^2)^2/2}\,dk, \\
&= \frac{1}{2\pi}\mathrm{e}^{-x^2/2\sigma^2}\sqrt{\frac{2\pi}{\sigma^2}}, \\
&= f(x).
\end{aligned}$$

This example demonstrates the Fourier inversion theorem explicitly for Gaussian functions. It is established in more general form by adaptation and extension of this result (to the class of 'distributions' dual to 'Schwartz functions').

Real-valued functions. Suppose f is a real-valued function. Then

$$\tilde{f}(-k) = \int_{-\infty}^{\infty} \mathrm{e}^{ikx} f(x)\,dx = \int_{-\infty}^{\infty} \overline{\mathrm{e}^{-ikx}} f(x)\,dx = \overline{\int_{-\infty}^{\infty} \mathrm{e}^{-ikx} f(x)\,dx} = \overline{\tilde{f}(k)}.$$

Shift property. Let f, g be functions with Fourier transforms $\tilde{f}, \tilde{g}$ and suppose that $g(x) = f(x - x_0)$. Then $\tilde{g}(k) = \mathrm{e}^{-ikx_0}\tilde{f}(k)$, as follows from a direct calculation

$$\tilde{g}(k) = \int_{-\infty}^{\infty} \mathrm{e}^{-ikx} g(x)\, dx = \int_{-\infty}^{\infty} \mathrm{e}^{-ikx} f(x - x_0)\, dx = \int_{-\infty}^{\infty} \mathrm{e}^{-ik(y+x_0)} f(y)\, dy = \mathrm{e}^{-ikx_0}\tilde{f}(k).$$

Example: Consider the normalised Gaussian centred on $x = x_0$

$$g(x) = \frac{1}{\sqrt{2\pi\sigma^2}} \mathrm{e}^{-(x-x_0)^2/2\sigma^2}.$$

Appealing to our previous result for the Fourier transform of a Gaussian and the general shift property we see that

$$\tilde{g}(k) = \mathrm{e}^{-ikx_0 - \sigma^2 k^2/2}.$$

We can also verify that $\tilde{g}(-k) = \overline{\tilde{g}(k)}$, as expected since g is a real-valued function.

Derivatives. The Fourier transform of the derivative of f is $\tilde{f}'(k) = ik\tilde{f}(k)$. To show this by direct calculation we have

$$\tilde{f}'(k) = \int_{-\infty}^{\infty} \mathrm{e}^{-ikx} \frac{df}{dx}\, dx = \mathrm{e}^{-ikx} f(x)\Big|_{x=-\infty}^{\infty} + ik \int_{-\infty}^{\infty} \mathrm{e}^{-ikx} f(x)\, dx = ik\tilde{f}(k).$$

Here we used that the function tends to zero as $x \to \pm\infty$ (otherwise it is not integrable). A different demonstration of the same result is to write

$$f'(x) = \frac{d}{dx}\left(\frac{1}{2\pi}\int_{-\infty}^{\infty} \mathrm{e}^{ikx}\tilde{f}(k)\, dk\right) = \frac{1}{2\pi}\int_{-\infty}^{\infty} \frac{d}{dx}\left(\mathrm{e}^{ikx}\tilde{f}(k)\right) dk = \frac{1}{2\pi}\int_{-\infty}^{\infty} \mathrm{e}^{ikx}\left(ik\tilde{f}(k)\right) dk.$$

Here we use that we can differentiate under the integral.

The result evidently generalises. If $f^{(n)}$ denotes the n^{th} derivative of f, *i.e.* $f^{(n)} = d^n f/dx^n$, then $\widetilde{f^{(n)}}(k) = (ik)^n \tilde{f}(k)$.

Example: Consider the wave equation and take its Fourier transform (in x)

$$\frac{1}{c^2}\frac{\partial^2 u}{\partial t^2} = \frac{\partial^2 u}{\partial x^2}, \qquad \Rightarrow \qquad \frac{1}{c^2}\frac{\partial^2 \tilde{u}}{\partial t^2} = (ik)^2\tilde{u} = -k^2\tilde{u}.$$

This is a standard differential equation for $\tilde{u}(k, t)$ whose solution is

$$\tilde{u}(k, t) = \tilde{f}(k)\mathrm{e}^{-ikct} + \tilde{g}(k)\mathrm{e}^{ikct}.$$

Finally, taking the inverse transform we obtain

$$u(x, t) = \frac{1}{2\pi}\int_{-\infty}^{\infty} \mathrm{e}^{ikx}\left(\tilde{f}(k)\mathrm{e}^{-ikct} + \tilde{g}(k)\mathrm{e}^{ikct}\right) dk = f(x - ct) + g(x + ct).$$

Parseval's theorem. Let f, g be functions with Fourier transforms $\tilde{f}, \tilde{g}$. Then

$$\begin{aligned}
\int_{-\infty}^{\infty} \overline{g(x)} f(x)\, dx &= \int_{-\infty}^{\infty} \left(\overline{\frac{1}{2\pi}\int_{-\infty}^{\infty} \mathrm{e}^{ikx}\tilde{g}(k)\, dk}\right) f(x)\, dx, \\
&= \frac{1}{2\pi}\int_{-\infty}^{\infty} \overline{\tilde{g}(k)}\left(\int_{-\infty}^{\infty} \mathrm{e}^{-ikx} f(x)\, dx\right) dk, \\
&= \frac{1}{2\pi}\int_{-\infty}^{\infty} \overline{\tilde{g}(k)}\tilde{f}(k)\, dk.
\end{aligned}$$

In the context of Fourier transforms, Parseval's theorem is also frequently known as Plancherel's theorem.

Example: Consider the decaying exponential function

$$f(x) = \begin{cases} \mathrm{e}^{-x/\xi} & x > 0, \\ 0 & x < 0, \end{cases} \qquad \Rightarrow \qquad \tilde{f}(k) = \frac{1}{ik + \xi^{-1}}.$$

Applying Parseval's theorem with $f = g$ we find

$$\frac{1}{2\pi} \int_{-\infty}^{\infty} \frac{dk}{k^2 + \xi^{-2}} = \int_0^{\infty} \mathrm{e}^{-2x/\xi}\, dx = \frac{\xi}{2},$$

or (provided $\xi^{-1} \neq 0$, $\xi \neq 0$)

$$\int_{-\infty}^{\infty} \frac{\xi^{-1}}{k^2 + \xi^{-2}}\, dk = \pi.$$

Riemann-Lebesgue lemma. By way of partial motivation, setting $x = 0$ we have

$$f(0) = \frac{1}{2\pi} \int_{-\infty}^{\infty} \tilde{f}(k)\, dk.$$

The integral definitely converges if $\int_{-\infty}^{\infty} |\tilde{f}(k)|\, dk$ does, which requires $|\tilde{f}(k)| \to 0$ as $k \to \pm\infty$. This property of Fourier transforms is known as the Riemann-Lebesgue lemma. To establish it, make the change of variables $y = x + \pi/k$ in the formula for $\tilde{f}(k)$

$$\tilde{f}(k) = \int_{-\infty}^{\infty} \mathrm{e}^{-ikx} f(x)\, dx = \int_{-\infty}^{\infty} \mathrm{e}^{-ik(y-\pi/k)} f(y - \pi/k)\, dy = -\int_{-\infty}^{\infty} \mathrm{e}^{-iky} f(y - \pi/k)\, dy.$$

Now form the average with the usual formula

$$\left| \frac{\tilde{f}(k) + \tilde{f}(k)}{2} \right| = \left| \frac{1}{2} \int_{-\infty}^{\infty} \mathrm{e}^{-ikx} \Big(f(x) - f(x - \pi/k) \Big)\, dx \right| \leq \frac{1}{2} \int_{-\infty}^{\infty} \Big| f(x) - f(x - \pi/k) \Big|\, dx,$$

from which we conclude that $|\tilde{f}(k)| \to 0$ as $k \to \pm\infty$.

Convolutions. The convolution of two functions f and g is the function $f * g$ defined by

$$f * g(x) = \int_{-\infty}^{\infty} f(x - y) g(y)\, dy.$$

Proposition: The convolution is symmetric, $f * g = g * f$. The proof is a direct calculation

$$f * g(x) = \int_{-\infty}^{\infty} f(x - y) g(y)\, dy = \int_{\infty}^{-\infty} f(t) g(x - t)\, (-dt) = \int_{-\infty}^{\infty} g(x - t) f(t)\, dt = g * f(x).$$

Example: The convolution of two step functions. Consider the two step functions

$$f(x) = \begin{cases} 1 & -a < x < a, \\ 0 & \text{else}, \end{cases} \qquad g(x) = \begin{cases} 1 & -b < x < b, \\ 0 & \text{else}. \end{cases}$$

Their convolution is

$$f * g(x) = \int_{-\infty}^{\infty} f(x - y) g(y)\, dy = \int_{-b}^{b} f(x - y)\, dy = \int_{x-b}^{x+b} f(t)\, dt.$$

This depends on the overlap of the interval $[x-b, x+b]$ with the interval $[-a, a]$. First, when $x < -(a+b)$ or $x > a+b$ there is no overlap and $f * g(x) = 0$. Show that

$$f * g(x) = \begin{cases} 0 & x < -(a+b), \\ a+b+x & -(a+b) < x < -|a-b|, \\ \min\{2a, 2b\} & -|a-b| < x < |a-b|, \\ a+b-x & |a-b| < x < a+b, \\ 0 & x > a+b. \end{cases}$$

Proposition: The convolution is the inverse Fourier transform of a product. Indeed

$$\begin{aligned} f * g(x) = \int_{-\infty}^{\infty} f(x-y)g(y)\,dy &= \int_{-\infty}^{\infty} \left(\frac{1}{2\pi} \int_{-\infty}^{\infty} \mathrm{e}^{ik(x-y)} \tilde{f}(k)\,dk \right) g(y)\,dy, \\ &= \frac{1}{2\pi} \int_{-\infty}^{\infty} \mathrm{e}^{ikx} \tilde{f}(k) \left(\int_{-\infty}^{\infty} \mathrm{e}^{-iky} g(y)\,dy \right) dk, \\ &= \frac{1}{2\pi} \int_{-\infty}^{\infty} \mathrm{e}^{ikx} \tilde{f}(k)\tilde{g}(k)\,dk. \end{aligned}$$

We may say equivalently, the Fourier transform of a convolution is the product of the Fourier transforms, $\widetilde{f * g}(k) = \tilde{f}(k)\tilde{g}(k)$.

Example: Consider the two Gaussian functions

$$f(x) = \frac{1}{\sqrt{2\pi\sigma_1^2}} \mathrm{e}^{-(x-x_0)^2/2\sigma_1^2}, \qquad\qquad g(x) = \frac{1}{\sqrt{2\pi\sigma_2^2}} \mathrm{e}^{-x^2/2\sigma_2^2}.$$

Using our general results we have

$$\widetilde{f * g}(k) = \tilde{f}(k)\tilde{(g)}(k) = \mathrm{e}^{-ikx_0 - \sigma_1^2 k^2/2} \mathrm{e}^{-\sigma_2^2 k^2/2} = \mathrm{e}^{-ikx_0 - (\sigma_1^2 + \sigma_2^2)k^2/2},$$

and hence the convolution is

$$f * g(x) = \frac{1}{\sqrt{2\pi(\sigma_1^2 + \sigma_2^2)}} \mathrm{e}^{-(x-x_0)^2/2(\sigma_1^2+\sigma_2^2)}.$$

This is a normalised Gaussian centred on x_0 with width $\sqrt{\sigma_1^2 + \sigma_2^2}$.

Sketch notes for PX276; these are very terse and not a substitute for your own lecture notes.

Dirac Delta Function

The Dirac **delta function**, denoted $\delta(x)$, is a sort of 'generalised' function, or 'distribution'.

Consider the Fourier transform pair

$$f(x) = \frac{1}{\sqrt{2\pi\sigma^2}} \mathrm{e}^{-x^2/2\sigma^2}, \qquad \tilde{f}(k) = \mathrm{e}^{-\sigma^2 k^2/2}.$$

Recall that the 'width' of f is σ and that of $\tilde{f}$ is σ^{-1}. Consider the limit as $\sigma \to 0$. $\tilde{f}$ is well-behaved and tends to the constant function 1. What about f? Fix any x different from zero and choose any $\epsilon > 0$. Then we can find a $\sigma > 0$ such that $f(x) < \epsilon$. So for any $x \neq 0$ we have $f(x) \to 0$. On the other hand, $f(x)$ is a properly normalised function for any $\sigma > 0$, *i.e.* its total integral is 1. The limiting construction is a new type of object that the physicists call the **Dirac delta function**, and write $\delta(x)$. The mathematicians incorporated it properly into analysis in 1950 (in the work of Laurent Schwartz) and prefer to use the word distribution, rather than function. (They also refer to it as a Dirac mass, despite the fact that it does not have dimensions of kg; its dimensions are m^{-1}.)

The Dirac delta function is entirely localised (or concentrated) at $x = 0$. Its fundamental property is that integration of any function f against δ simply evaluates the function at the origin

$$\int_{-\infty}^{\infty} \delta(x) f(x)\, dx = f(0).$$

Consistent with this, the Fourier transform of δ is the constant function 1 (as per above). The Fourier representation of δ is the useful formula

$$\delta(x) = \frac{1}{2\pi} \int_{-\infty}^{\infty} \mathrm{e}^{ikx}\, dk.$$

It is easy to see that there is a version of the Dirac delta function localised at any point $x = x_0$ and not only for $x = 0$. We write this as $\delta(x - x_0)$ and the formulae corresponding to the preceding ones are

$$\int_{-\infty}^{\infty} \delta(x - x_0) f(x)\, dx = f(x_0),$$
$$\delta(x - x_0) = \frac{1}{2\pi} \int_{-\infty}^{\infty} \mathrm{e}^{ik(x-x_0)}\, dk.$$

Even function. The delta function behaves as if it is an even function, *i.e.* $\delta(-x) = \delta(x)$. We demonstrate this from its representation as an inverse Fourier transform

$$\begin{aligned}\delta(x_0 - x) &= \frac{1}{2\pi} \int_{-\infty}^{\infty} \mathrm{e}^{ik(x_0-x)}\, dk = \frac{1}{2\pi} \int_{-\infty}^{\infty} \mathrm{e}^{-ik(x-x_0)}\, dk = \frac{1}{2\pi} \int_{\infty}^{-\infty} \mathrm{e}^{ik(x_0-x)}\, (-dk) \\ &= \frac{1}{2\pi} \int_{-\infty}^{\infty} \mathrm{e}^{ik(x-x_0)}\, dk = \delta(x - x_0).\end{aligned}$$

Finite intervals. Sometimes delta functions are not integrated over the entire real line but only a finite interval (a, b). We state the result

$$\int_a^b f(x)\delta(x - x_0)\, dx = \begin{cases} f(x_0) & \text{if } \ x_0 \in (a, b), \\ 0 & \text{otherwise,} \end{cases}$$

which is intuitive given the character of delta as a limit of functions increasingly localised around $x = x_0$.

Example: Three point charges are placed along the x-axis as follows: a charge $-e$ is placed at $x = -4$, a charge $2e$ at $x = 0$, and a charge $-e$ at $x = \pi$. This distribution of charges may be represented as a sum of delta functions as

$$\rho(x) = -e\,\delta(x + 4) + 2e\,\delta(x) - e\,\delta(x - \pi).$$

The total charge is

$$Q = \int_{-\infty}^{\infty} \rho(x)\, dx = \int_{-\infty}^{\infty} \Big[-e\,\delta(x + 4) + 2e\,\delta(x) - e\,\delta(x - \pi)\Big]\, dx = -e + 2e - e = 0,$$

whereas that in the interval $(-3, 3)$ is

$$Q = \int_{-3}^{3} \rho(x)\, dx = \int_{-3}^{3} \Big[-e\,\delta(x + 4) + 2e\,\delta(x) - e\,\delta(x - \pi)\Big]\, dx = 2e.$$

Example: Calculate the Fourier transform of $f(x) = \cos(qx)$. By direct calculation we find

$$\tilde{f}(k) = \int_{-\infty}^{\infty} \mathrm{e}^{-ikx} \cos(qx)\, dx = \frac{1}{2} \int_{-\infty}^{\infty} \Big(\mathrm{e}^{-i(k-q)x} + \mathrm{e}^{-i(k+q)x}\Big)\, dx = \pi\Big(\delta(k - q) + \delta(k + q)\Big).$$

Convolutions. Let f be an ordinary function and consider its convolution with $g(x) = \delta(x - x_0)$. The result is

$$f * g(x) = \int_{-\infty}^{\infty} f(x - y)\delta(y - x_0)\, dy = f(x - x_0).$$

In other words the convolution only shifts (or displaces) the function by an amount x_0, but otherwise preserves its form and all of its properties. This observation provides a means of creating copies of a particular feature, or repeating patterns. The 'feature' can be copied at the locations $x = x_1, x_2, \ldots, x_n$ by convolution of f with the sum of delta functions $g(x) = \sum_{i=1}^{n} \delta(x - x_i)$:

$$f * g(x) = \int_{-\infty}^{\infty} f(x - y)\Big(\sum_{i=1}^{n} \delta(y - x_i)\Big) dy = \sum_{i=1}^{n} \int_{\infty}^{\infty} f(x - y)\delta(y - x_i)\, dy = \sum_{i=1}^{n} f(x - x_i).$$

Of course, everything is consistent with the shift property of Fourier transforms and the convolution theorem. For instance, taking Fourier transforms we have

$$\widetilde{f * g}(k) = \tilde{f}(k)\tilde{g}(k) = \tilde{f}(k)\Big(\sum_{i=1}^{n} \mathrm{e}^{-ikx_i}\Big) = \sum_{i=1}^{n} \mathrm{e}^{-ikx_i}\, \tilde{f}(k),$$

using that the Fourier transform of the delta function $\delta(x - x_i)$ is the plane wave e^{-ikx_i}. By the shift property $\mathrm{e}^{-ikx_i}\tilde{f}(k)$ is the Fourier transform of $f(x - x_i)$.

Dirac comb. The Dirac comb is the infinite set of regularly spaced delta functions localised at the points $x = nP$ for every integer n

$$g(x) = \sum_{n=-\infty}^{\infty} \delta(x - nP).$$

One immediate use of the Dirac comb is in creating a periodic pattern by copying a feature, represented by the function f, at each of the 'points' of the comb; this is done simply by the convolution $f * g$.

Example: A periodic set of rectangular pulses is obtained by convolution of a step function (single pulse) with a Dirac comb. In this example, x may be more naturally thought of as time and so replaced with the symbol t.

Fourier transform: The Fourier transform of a Dirac comb is interesting and has important applications in analysing periodic structures. A direct calculation gives

$$\tilde{g}(k) = \int_{-\infty}^{\infty} \mathrm{e}^{-ikx} \Big(\sum_{n=-\infty}^{\infty} \delta(x - nP) \Big) dx = \sum_{n=-\infty}^{\infty} \int_{-\infty}^{\infty} \mathrm{e}^{-ikx} \delta(x - nP)\, dx = \sum_{n=-\infty}^{\infty} \mathrm{e}^{-iknP}.$$

We recognise this as the Fourier series for a function (of k) that is periodic with period $2L = 2\pi/P$ and where all of the Fourier coefficients are unity, $c_n = 1$. So it is an unusual Fourier series. To see what it is, note that the Dirac comb is itself a periodic function (of x) with period $2L = P$. Therefore, it has a representation as a Fourier series (EXERCISE)

$$g(x) = \sum_{n=-\infty}^{\infty} \frac{1}{P}\, \mathrm{e}^{in\pi x/(P/2)},$$

This leads to the remarkable identity between infinite sums of delta functions and infinite sums of complex exponentials

$$\sum_{n=-\infty}^{\infty} \delta(x - nP) = \frac{1}{P} \sum_{n=-\infty}^{\infty} \mathrm{e}^{i2\pi nx/P}.$$

We now apply this to the Fourier transform of the Dirac comb to get

$$\tilde{g}(k) = \sum_{n=-\infty}^{\infty} \mathrm{e}^{-iknP} = \frac{2\pi}{P} \sum_{n=-\infty}^{\infty} \delta(k - 2\pi n/P).$$

In other words, the Fourier transform of a Dirac comb is another Dirac comb. This result manifests itself in the appearance of (crystal) diffraction patterns.

Delta function with function argument. When the argument of the delta function is itself a function, $\delta(f(x))$, it behaves like a sum of (ordinary) delta functions localised at each of the roots of the function f. Specifically, for a function f with (generic) isolated zeros, we have the following

$$\delta\big(f(x)\big) = \sum_{\text{roots } x_r} \frac{1}{|f'(x_r)|}\, \delta(x - x_r),$$

as an identity of generalised functions (understood as being correct when you integrate against any normal function).

To establish this, let U_r denote an open set containing the root x_r and no others. Since f does not vanish on the complement of all the U_r (*i.e.* $\mathbb{R} \setminus \cup_r U_r$) we have that

$$\int_{-\infty}^{\infty} g(x)\delta\big(f(x)\big)\,dx = \sum_{\text{roots } r} \int_{U_r} g(x)\delta\big(f(x)\big)\,dx.$$

On each U_r the map f restricts to a bijection between U_r and an open set V centred on the origin, so that by the change of variables $y = f(x)$, with inverse $x = \phi(y)$, we get

$$\int_{U_r} g(x)\delta\big(f(x)\big)\,dx = \int_V g\big(\phi(y)\big)\,\delta(y)\,\frac{1}{|f'\big(\phi(y)\big)|}\,dy = \frac{g\big(\phi(0)\big)}{\big|f'\big(\phi(0)\big)\big|} = \frac{g(x_r)}{|f'(x_r)|}.$$

The stated identity follows directly.

Exercise: Calculate the integral $\int_{-\infty}^{\infty} g(x)\,\delta(x^3 + ax)\,dx$, where a is a constant.

The roots of the cubic $x^3 + ax$ are $x = 0$ and $x = \pm\sqrt{-a}$, when a is negative. The derivative is $3x^2 + a$ and takes the values a, $-2a$ and $-2a$ at the three roots (the latter only when $a < 0$). Hence we have

$$\int_{-\infty}^{\infty} g(x)\,\delta(x^3 + ax)\,dx = \begin{cases} \frac{g(0)}{a} & a > 0, \\ \frac{g\left(-\sqrt{-a}\right)}{|2a|} + \frac{g(0)}{|a|} + \frac{g\left(\sqrt{-a}\right)}{|2a|} & a < 0. \end{cases}$$

Note that the integral is undefined when $a = 0$.

Solution of odes and Green functions. Consider the ordinary differential equation

$$\frac{du}{dx} + \gamma u = f(x),$$

where γ is a positive constant. Take its Fourier transform to get

$$\big(ik + \gamma\big)\tilde{u} = \tilde{f}(k) \qquad \Rightarrow \qquad \tilde{u}(k) = \frac{1}{ik + \gamma}\,\tilde{f}(k).$$

As the solution for the Fourier transform is a product, the solution in real space will be convolution

$$u(x) = \int_{-\infty}^{\infty} G(x - y) f(y)\,dy.$$

The function G that appears here is called the **Green function** for the differential equation. In this case, it is the inverse Fourier transform of the function $\frac{1}{ik+\gamma}$, which appeared as one of the problems in week 8: the functions

$$f(x) = \begin{cases} \mathrm{e}^{-\gamma x} & x > 0, \\ 0 & x < 0, \end{cases} \qquad\qquad \tilde{f}(k) = \frac{1}{ik + \gamma},$$

are a Fourier transform pair. So the Green function for our differential equation is $G(x, y) = \mathrm{e}^{-\gamma(x-y)}$ if $x > y$ and zero otherwise. Finally, we may write the general solution of the differential equation as

$$u(x) = \int_{-\infty}^{x} \mathrm{e}^{-\gamma(x-y)} f(y)\,dy.$$

The Green function is the response of the system (described by some differential equation) to a delta function forcing. To see this, simply take $f(x) = \delta(x)$ in the solution

$$u(x) = \int_{-\infty}^{\infty} G(x-y) f(y)\, dy = \int_{-\infty}^{\infty} G(x-y)\delta(y)\, dy = G(x).$$

Example: Determine the response to a periodic forcing $f(x) = \cos(qx)$.

It is convenient to take the forcing to be $f(x) = \mathrm{e}^{iqx}$ and take the real part at the end of our calculation. The response is

$$u(x) = \int_{-\infty}^{x} \mathrm{e}^{-\gamma(x-y)}\, \mathrm{e}^{iqy}\, dy = \mathrm{e}^{-\gamma x} \int_{-\infty}^{x} \mathrm{e}^{(\gamma+iq)y}\, dy = \mathrm{e}^{-\gamma x}\, \frac{1}{\gamma+iq} \mathrm{e}^{(\gamma+iq)x} = \frac{\mathrm{e}^{iqx}}{\gamma+iq},$$

and taking the real part we get

$$u(x) = \frac{\gamma}{\gamma^2+q^2}\cos(qx) + \frac{q}{\gamma^2+q^2}\sin(qx) = \frac{1}{\sqrt{\gamma^2+q^2}}\cos\Big(qx - \arctan\frac{q}{\gamma}\Big).$$

Damped harmonic oscillator: Consider the differential equation for a driven damped harmonic oscillator

$$\frac{d^2u}{dt^2} + 2\gamma\frac{du}{dt} + \omega_0^2 u = f(t),$$

with natural frequency ω_0 and damping coefficient γ. Here we are taking the displacement u to be a function of time t rather than spatial variable x; we will similarly denote the Fourier transform variable by ω rather than k, but take all formulae to be the same.

The Fourier transform of the equation reads

$$\Big[(i\omega)^2 + 2\gamma(i\omega) + \omega_0^2\Big]\tilde{u} = \tilde{f}(\omega), \qquad \Rightarrow \qquad \tilde{u}(\omega) = \frac{1}{(i\omega)^2 + 2\gamma(i\omega) + \omega_0^2}\,\tilde{f}(\omega).$$

Again the solution for $u(t)$ can be written as a convolution

$$u(t) = \int_{-\infty}^{\infty} G(t-s) f(s)\, ds, \qquad \text{where} \quad \tilde{G}(\omega) = \frac{1}{(i\omega)^2 + 2\gamma(i\omega) + \omega_0^2}.$$

To calculate the Green function in real space we use that the roots of $(i\omega)^2 + 2\gamma(i\omega) + \omega_0^2$ are

$$i\omega_\pm = -\gamma \pm i\sqrt{\omega_0^2 - \gamma^2}.$$

Then, expanding in partial fractions we obtain

$$\tilde{G}(\omega) = \frac{1}{2i\sqrt{\omega_0^2-\gamma^2}}\left[\frac{1}{i\omega+\gamma-i\sqrt{\omega_0^2-\gamma^2}} - \frac{1}{i\omega+\gamma+i\sqrt{\omega_0^2-\gamma^2}}\right],$$

which puts it in a form where we can use the same standard Fourier transform results as before. Thus, for $t > 0$ the Green function is

$$G(t) = \frac{1}{2i\sqrt{\omega_0^2-\gamma^2}}\Big[\mathrm{e}^{-\gamma t + i\sqrt{(\omega_0^2-\gamma^2)}\,t} - \mathrm{e}^{-\gamma t - i\sqrt{(\omega_0^2-\gamma^2)}\,t}\Big] = \mathrm{e}^{-\gamma t}\,\frac{\sin\big(\sqrt{\omega_0^2-\gamma^2}\,t\big)}{\sqrt{\omega_0^2-\gamma^2}}.$$

while for $t < 0$ it vanishes.

Finally, the general solution for the amplitude of the harmonic oscillator is

$$u(t) = \int_{-\infty}^{t} \mathrm{e}^{-\gamma(t-s)}\,\frac{\sin\big(\sqrt{\omega_0^2-\gamma^2}\,(t-s)\big)}{\sqrt{\omega_0^2-\gamma^2}}\, f(s)\, ds.$$

Sketch notes for PX276; these are very terse and not a substitute for your own lecture notes.

Fourier Analysis in Multiple Dimensions

The world around us (as we experience it) is three-dimensional. So there is practical need to extend all of our analysis to the case of three spatial dimensions, and perhaps also include time-dependence. Most of this extension is straightforward. The presentation we give will be in dimension n, although of course we have in mind that $n = 3$, or sometimes $n = 2$. We denote the position of a point in $\mathbb{R}^n$ by $\mathbf{x} = (x_1, \ldots, x_n)$ and the corresponding Fourier transform variable (wavevector) by $\mathbf{k} = (k_1, \ldots, k_n)$.

The Fourier transform and inverse Fourier transform are

$$\tilde{f}(\mathbf{k}) = \int_{\mathbb{R}^n} \mathrm{e}^{-i\mathbf{k}\cdot\mathbf{x}} f(\mathbf{x})\, d^n x, \qquad f(\mathbf{x}) = \frac{1}{(2\pi)^n} \int_{\mathbb{R}^n} \mathrm{e}^{i\mathbf{k}\cdot\mathbf{x}} \tilde{f}(\mathbf{k})\, d^n k.$$

Conventions. Different conventions for the normalisation of the Fourier transform and its inverse are widely used in the literature; one which is more symmetric is

$$\tilde{f}(\mathbf{k}) = \frac{1}{(2\pi)^{n/2}} \int_{\mathbb{R}^n} \mathrm{e}^{-i\mathbf{k}\cdot\mathbf{x}} f(\mathbf{x})\, d^n x, \qquad f(\mathbf{x}) = \frac{1}{(2\pi)^{n/2}} \int_{\mathbb{R}^n} \mathrm{e}^{i\mathbf{k}\cdot\mathbf{x}} \tilde{f}(\mathbf{k})\, d^n k.$$

A further convention arises regarding the signs in the complex exponentials when we consider Fourier transforms in both space ($\mathbf{x}$) and time (t). In the physics literature it is common to adopt the following choice of signs

$$\tilde{f}(\mathbf{k}, \omega) = \int_{-\infty}^{\infty} \int_{\mathbb{R}^n} \mathrm{e}^{-i(\mathbf{k}\cdot\mathbf{x} - \omega t)} f(\mathbf{x}, t)\, d^n x\, dt,$$
$$f(\mathbf{x}, t) = \frac{1}{(2\pi)^{n+1}} \int_{-\infty}^{\infty} \int_{\mathbb{R}^n} \mathrm{e}^{i(\mathbf{k}\cdot\mathbf{x} - \omega t)} \tilde{f}(\mathbf{k}, \omega)\, d^n k\, d\omega,$$

with the motivation being that the standard expression for a plane wave is $\mathrm{e}^{i(\mathbf{k}\cdot\mathbf{x} - \omega t)}$ rather than $\mathrm{e}^{i(\mathbf{k}\cdot\mathbf{x} + \omega t)}$. The less applied literature tends not to mix the choice of plus and minus signs in complex exponentials in this way (and also does not use distinct letters as in $(\mathbf{x}, t)$ and $(\mathbf{k}, \omega)$).

Convolutions. The convolution of two functions f and g is the function $f * g$ defined by

$$f * g(\mathbf{x}) = \int_{\mathbb{R}^n} f(\mathbf{x} - \mathbf{y}) g(\mathbf{y})\, d^n y.$$

The convolution is symmetric, $f * g = g * f$, which is proved in the same way as in one dimension.

The convolution theorem holds: if $\tilde{f}$, $\tilde{g}$ are the Fourier transforms of the two functions, then the Fourier transform of the convolution $f * g$ is

$$\widetilde{f * g}(\mathbf{k}) = \tilde{f}(\mathbf{k}) \tilde{g}(\mathbf{k}).$$

This is proved in the same way as in one dimension.

Delta functions. The multi-dimensional delta function behaves like a product of one-dimensional delta functions

$$\delta(\mathbf{x} - \mathbf{y}) = \delta(x_1 - y_1)\, \delta(x_2 - y_2) \cdots \delta(x_n - y_n) = \prod_{i=1}^{n} \delta(x_i - y_i).$$

Its basic property (behaviour with respect to integration) is

$$\int_{\mathbb{R}^n} f(\mathbf{x})\delta(\mathbf{x}-\mathbf{y})\,d^n x = f(\mathbf{y}).$$

The delta function has the representation as an inverse Fourier transform

$$\delta(\mathbf{x}-\mathbf{y}) = \frac{1}{(2\pi)^n}\int_{\mathbb{R}^n} \mathrm{e}^{i\mathbf{k}\cdot(\mathbf{x}-\mathbf{y})}\,d^n k.$$

Parseval's theorem. If f, g are two functions with Fourier transforms $\tilde{f}, \tilde{g}$ then

$$\int_{\mathbb{R}^n} \overline{g(\mathbf{x})} f(\mathbf{x})\,d^n x = \frac{1}{(2\pi)^n}\int_{\mathbb{R}^n} \overline{\tilde{g}(\mathbf{k})}\tilde{f}(\mathbf{k})\,d^n k.$$

Again, the calculation parallels precisely the one given in one dimension. We remark again that in the mathematics literature this result is sometimes referred to as Plancherel's theorem.

Examples.
Gaussians: Determine the inverse Fourier transform of the Gaussian function $\tilde{f}(\mathbf{k}) = \mathrm{e}^{-\frac{1}{2}\mathbf{k}^T\cdot\mathbf{M}\cdot\mathbf{k}}$ where $\mathbf{M}$ is an $n\times n$ matrix.

Assume $\mathbf{M}$ is diagonal with eigenvalues λ_i. Then the inverse Fourier transform is

$$\begin{aligned}
f(\mathbf{x}) &= \frac{1}{(2\pi)^n}\int_{\mathbb{R}^n} \mathrm{e}^{i\mathbf{k}\cdot\mathbf{x}-\frac{1}{2}\mathbf{k}^T\cdot\mathbf{M}\cdot\mathbf{k}}\,d^n k,\\
&= \frac{1}{(2\pi)^n}\int_{\mathbb{R}^n} \mathrm{e}^{i(k_1x_1+k_2x_2+\cdots+k_nx_n)-\frac{1}{2}(\lambda_1k_1^2+\lambda_2k_2^2+\cdots+\lambda_nk_n^2)}\,d^n k,\\
&= \left(\frac{1}{2\pi}\int_{-\infty}^{\infty} \mathrm{e}^{ik_1x_1-\frac{1}{2}\lambda_1k_1^2}\,dk_1\right)\left(\frac{1}{2\pi}\int_{-\infty}^{\infty} \mathrm{e}^{ik_2x_2-\frac{1}{2}\lambda_2k_2^2}\,dk_2\right)\cdots\left(\frac{1}{2\pi}\int_{-\infty}^{\infty} \mathrm{e}^{ik_nx_n-\frac{1}{2}\lambda_nk_n^2}\,dk_n\right),\\
&= \left(\frac{1}{\sqrt{2\pi\lambda_1}}\mathrm{e}^{-\frac{1}{2}\lambda_1^{-1}x_1^2}\right)\left(\frac{1}{\sqrt{2\pi\lambda_2}}\mathrm{e}^{-\frac{1}{2}\lambda_2^{-1}x_2^2}\right)\cdots\left(\frac{1}{\sqrt{2\pi\lambda_n}}\mathrm{e}^{-\frac{1}{2}\lambda_n^{-1}x_n^2}\right),\\
&= \frac{1}{(2\pi)^{n/2}\sqrt{\det\mathbf{M}}}\,\mathrm{e}^{-\frac{1}{2}\mathbf{x}^T\cdot\mathbf{M}^{-1}\cdot\mathbf{x}}.
\end{aligned}$$

This calculation is extended to the case where $\mathbf{M}$ is diagonalisable, but not already diagonal, by writing the decomposition $\mathbf{M} = \mathbf{BDB}^{-1}$. The change of variables $\mathbf{q} = \mathbf{B}^{-1}\mathbf{k}$ then reduces this more general case to the diagonal one we have just considered.

Box function: Let $f(\mathbf{x})$ be the 'box' function

$$f(\mathbf{x}) = \begin{cases} 1 & \mathbf{x}\in(-a_1,a_1)\times(-a_2,a_2)\times\cdots\times(-a_n,a_n),\\ 0 & \text{otherwise.}\end{cases}$$

Then its Fourier transform is

$$\tilde{f}(\mathbf{k}) = \left(2a_1\frac{\sin(k_1a_1)}{k_1a_1}\right)\left(2a_1\frac{\sin(k_2a_2)}{k_2a_2}\right)\cdots\left(2a_1\frac{\sin(k_na_n)}{k_na_n}\right) = V\prod_{i=1}^{n}\frac{\sin(k_ia_i)}{k_ia_i},$$

where V is the volume of the box. This follows from a direct calculation.

Coulomb potential: The functions $f(\mathbf{x}) = \frac{1}{4\pi r}$ and $\tilde{f}(\mathbf{k}) = \frac{1}{k^2}$, where $r = |\mathbf{x}|$ and $k = |\mathbf{k}|$, are a Fourier transform pair.

We calculate the Fourier transform of the Yukawa potential, $Y(\mathbf{x}) = \frac{1}{4\pi r}\mathrm{e}^{-r/\xi}$, and at the end take a limit $\xi \to \infty$. By direct calculation we have

$$\begin{aligned}
\tilde{Y}(\mathbf{k}) &= \int_{\mathbb{R}^3} \mathrm{e}^{-i\mathbf{k}\cdot\mathbf{x}} \frac{1}{4\pi r}\mathrm{e}^{-r/\xi}\, d^3x, \\
&= \int_{\phi=0}^{2\pi}\int_{\theta=0}^{\pi}\int_{r=0}^{\infty} \frac{\mathrm{e}^{-ikr\cos\theta - r/\xi}}{4\pi r}\, r^2 \sin\theta\, dr d\theta d\phi, \\
&= \frac{1}{2}\int_0^{\infty}\left[\frac{1}{ik}\mathrm{e}^{-ikr\cos\theta}\right]_{\theta=0}^{\pi} \mathrm{e}^{-r/\xi}\, dr, \\
&= \frac{1}{2ik}\int_0^{\infty}\left[\mathrm{e}^{(ik-\xi^{-1})r} - \mathrm{e}^{-(ik+\xi^{-1})r}\right] dr, \\
&= \frac{1}{2ik}\left[\frac{1}{-ik+\xi^{-1}} - \frac{1}{ik+\xi^{-1}}\right], \\
&= \frac{1}{k^2+\xi^{-2}}.
\end{aligned}$$

Finally, taking the limit $\xi \to \infty$ we obtain the stated result.

Derivatives. For a smooth function f its gradient is the vector field

$$\nabla f = \mathbf{e}_1 \frac{\partial f}{\partial x_1} + \mathbf{e}_2 \frac{\partial f}{\partial x_2} + \cdots + \mathbf{e}_n \frac{\partial f}{\partial x_n},$$

where the $\mathbf{e}_i$ are the usual Cartesian basis vectors. Provided f vanishes at infinity ($f(\mathbf{x}) \to 0$ as $|\mathbf{x}| \to \infty$) the Fourier transform of its gradient is

$$\widetilde{\nabla f}(\mathbf{k}) = i\mathbf{k}\,\tilde{f}(\mathbf{k}).$$

This is proved in exactly the same way as in one dimension, using also the linearity of the integral

$$\begin{aligned}
\widetilde{\nabla f}(\mathbf{k}) &= \int_{\mathbb{R}^n} \mathrm{e}^{-i\mathbf{k}\cdot\mathbf{x}}\left(\mathbf{e}_1 \frac{\partial f}{\partial x_1} + \mathbf{e}_2 \frac{\partial f}{\partial x_2} + \cdots + \mathbf{e}_n \frac{\partial f}{\partial x_n}\right) d^n x, \\
&= \mathbf{e}_1 \int_{\mathbb{R}^n} \mathrm{e}^{-i\mathbf{k}\cdot\mathbf{x}} \frac{\partial f}{\partial x_1}\, d^n x + \mathbf{e}_2 \int_{\mathbb{R}^n} \mathrm{e}^{-i\mathbf{k}\cdot\mathbf{x}} \frac{\partial f}{\partial x_2}\, d^n x + \cdots + \mathbf{e}_n \int_{\mathbb{R}^n} \mathrm{e}^{-i\mathbf{k}\cdot\mathbf{x}} \frac{\partial f}{\partial x_n}\, d^n x, \\
&= \mathbf{e}_1\, ik_1\, \tilde{f}(\mathbf{k}) + \mathbf{e}_2\, ik_2\, \tilde{f}(\mathbf{k}) + \cdots + \mathbf{e}_n\, ik_n\, \tilde{f}(\mathbf{k}), \\
&= i\mathbf{k}\,\tilde{f}(\mathbf{k}).
\end{aligned}$$

A further result that arises in many applications is the Fourier transform of the Laplacian

$$\nabla^2 f = \frac{\partial^2 f}{\partial x_1^2} + \frac{\partial^2 f}{\partial x_2^2} + \cdots + \frac{\partial^2 f}{\partial x_n^2}, \qquad \Rightarrow \qquad \widetilde{\nabla^2 f} = -k^2\,\tilde{f}(\mathbf{k}).$$

This may be proved by an analogous calculation utilising the linearity of the integral.

Solution of pdes and Green functions.

Wave equation: The wave equation in three dimensions is

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

where c is the wave speed (speed of light). It can be solved by Fourier transform. Indeed the Fourier transform of the equation gives

$$\frac{1}{c^2}\frac{\partial^2 \tilde{u}}{\partial t^2} = -k^2 \tilde{u}, \qquad \Rightarrow \quad \tilde{u}(\mathbf{k},t) = \tilde{f}(\mathbf{k})\mathrm{e}^{-ikct} + \tilde{g}(\mathbf{k})\mathrm{e}^{ikct}.$$

Let us take the initial value problem $u(\mathbf{x},0) = u_0(\mathbf{x})$, $\frac{\partial u}{\partial t}(\mathbf{x},0) = v_0(\mathbf{x})$. Then we can solve for $\tilde{f}, \tilde{g}$ in terms of the initial data, obtaining

$$\tilde{u}(\mathbf{k},t) = \frac{1}{2}\Big[\mathrm{e}^{-ikct} + \mathrm{e}^{ikct}\Big]\tilde{u}_0(\mathbf{k}) + \frac{1}{2cik}\Big[\mathrm{e}^{ikct} - \mathrm{e}^{-ikct}\Big]\tilde{v}_0(\mathbf{k}).$$

The final part depends on whether or not we can do the inverse Fourier transform. We leave the details of the three-dimensional calculation to an extended problem.

Diffusion equation: The diffusion equation in three dimensions is

$$\frac{\partial u}{\partial t} - D\nabla^2 u = f(\mathbf{x},t),$$

where $f(\mathbf{x},t)$ acts as a 'source' for the 'solute' u. Taking the Fourier transform in space we find

$$\frac{\partial \tilde{u}}{\partial t} + Dk^2\tilde{u} = \tilde{f}(\mathbf{k},t).$$

This is a one-dimensional ordinary differential equation in t, which can be solved by integrating factor (say). A different strategy is to also take the Fourier transform with respect to time to get

$$\Big(-i\omega + Dk^2\Big)\tilde{u}(\mathbf{k},\omega) = \tilde{f}(\mathbf{k},\omega), \qquad \Rightarrow \qquad \tilde{u}(\mathbf{k},\omega) = \frac{1}{-i\omega + Dk^2}\,\tilde{f}(\mathbf{k},\omega).$$

The solution, upon taking the inverse Fourier transform, is therefore a convolution

$$u(\mathbf{x},t) = \int_{-\infty}^{\infty}\int_{\mathbb{R}^n} G(\mathbf{x}-\mathbf{y}, t-s) f(\mathbf{y},s)\, d^n y\, ds,$$

where G is the **Green function** for the pde, in this case the diffusion equation. It is the inverse Fourier transform of the function $\frac{1}{-i\omega+Dk^2}$. As in one dimension, the Green function is the response of the differential equation to a delta function source, $f(\mathbf{x},t) = \delta(\mathbf{x})\delta(t)$ – delta function localised in both space and time. We can obtain it explicitly using standard results for Fourier transforms we have encountered already. First, taking the inverse transform with respect to frequency ω we get

$$\tilde{G}(\mathbf{k},\omega) = \frac{1}{-i\omega + Dk^2}, \qquad \Rightarrow \qquad \tilde{G}(\mathbf{k},t) = \begin{cases} \mathrm{e}^{-Dk^2 t} & t > 0, \\ 0 & t < 0. \end{cases}$$

We see that the Green function vanishes for $t < 0$. This makes sense since the response should be to the release of the source at $t = 0$ and so be confined to later times, without any premonition. For $t > 0$, the inverse Fourier transform with respect to $\mathbf{k}$ then gives

$$G(\mathbf{x},t) = \frac{1}{(2\pi)^n}\int_{\mathbb{R}^n} \mathrm{e}^{i\mathbf{k}\cdot\mathbf{x} - Dk^2 t}\, d^n k = \frac{1}{(2\pi)^{n/2}(2Dt)^{n/2}}\,\mathrm{e}^{-\frac{|\mathbf{x}|^2}{4Dt}},$$

using the result we found for Gaussians. This is frequently called the **heat kernel**.

The Green function method is applied here to the diffusion equation, but applies generally to linear pdes in $\mathbb{R}^n$ with constant coefficients.

These notes are designed to be very terse and are not a substitute for your own lecture notes.

Fraunhofer Diffraction

Diffraction is the spreading out of waves after they have passed through a small opening. Small here means compared to the wavelength of the waves; the opening should be of a 'similar' size to the wavelength for the effects of diffraction to be noticeable. For us, small will also mean compared to the distance from the opening at which we subsequently observe the wave pattern. This is referred to as **Fraunhofer diffraction**.

Most waves exhibit the phenomenon of diffraction; sound, surface water waves, and light are perhaps the most immediate to come to mind. For our applications we will focus on the diffraction of light (*diffraction optics*). Light is an electromagnetic wave, but we will not make use of this full character; it is enough that it is a wave. Indeed, the analysis we give will be for the scalar wave equation

$$\frac{-1}{c^2}\frac{\partial^2 U}{\partial t^2} + \nabla^2 U = 0,$$

and therefore apply to any physical quantity which satisfies this equation. (We leave it to courses on Electricity & Magnetism to demonstrate that electromagnetic waves satisfy the wave equation.)

Spherical Waves. Our presentation of diffraction optics will be based on the fundamental solution of the wave equation, corresponding to a point source. The waves emitted by a point source spread out equally in all directions; they are **spherical waves**. We simplify the analysis by considering only waves of a single frequency, $\omega = ck$. Such waves are called monochromatic and can be represented by a wave amplitude $U(\mathbf{x}, t) = \mathrm{e}^{-ickt}u(\mathbf{x})$. For these waves the wave equation reduces to the **Helmholtz equation**

$$\big(\nabla^2 + k^2\big)u = 0.$$

The spherical wave solution we seek is spherically symmetric and depends only on the radial distance r from the origin (source). Hence we can write the Helmholtz equation as

$$\frac{1}{r^2}\frac{d}{dr}\left(r^2\frac{du}{dr}\right) + k^2 u = 0.$$

(In this course you are not expected to know the form of the Laplace operator in any coordinate system other than Cartesians, but you are expected to work with it when it is given to you.) The fundamental solution of this equation follows from the identity

$$\frac{1}{r^2}\frac{d}{dr}\left(r^2\frac{du}{dr}\right) = \frac{1}{r}\frac{d^2}{dr^2}\big(ru\big),$$

which we leave as an exercise. We then find $ru \propto \mathrm{e}^{\pm ikr}$ and in fact the fundamental solution we want is

$$u = \frac{-1}{4\pi r}\mathrm{e}^{ikr} =: G(\mathbf{x}).$$

Two choices have been made in writing this. First, we chose the solution $\sim \mathrm{e}^{ikr}$ rather than $\sim \mathrm{e}^{-ikr}$; this is because the full waveform has the dependence $\sim \mathrm{e}^{ik(r-ct)}$ and the wavefronts propagate radially outwards as time increases, *i.e.* they are **outgoing spherical waves**. This is what we expect for a source. The other choice gives ingoing waves and is appropriate for something that is receiving signals rather than emitting them.

Second, the constant of proportionality has been taken as $\frac{-1}{4\pi}$. To see why, integrate the Helmholtz equation over a ball of radius R centred on the origin and apply the divergence theorem to the Laplacian term

$$\int_{B(\mathbf{0},R)} \big(\nabla^2 + k^2\big) G \, dV = \int_{\partial B(\mathbf{0},R)} \mathbf{n} \cdot \nabla G \, dA + \int_{B(\mathbf{0},R)} k^2 G \, dV,$$

where $\mathbf{n}$ is the unit outward normal to $\partial B(\mathbf{0}, R)$. Now we do each of the integrals in turn:

$$\begin{aligned}
\int_{B(\mathbf{0},R)} k^2 G \, dV &= \int_{\phi=0}^{2\pi} \int_{\theta=0}^{\pi} \int_{r=0}^{R} \frac{-k^2}{4\pi r} \mathrm{e}^{ikr} \, r^2 \sin\theta \, dr d\theta d\phi, \\
&= -k^2 \int_0^R r \mathrm{e}^{ikr} \, dr, \\
&= ikR \, \mathrm{e}^{ikR} - \mathrm{e}^{ikR} + 1. \\
\int_{\partial B(\mathbf{0},R)} \mathbf{n} \cdot \nabla G \, dA &= \int_{\phi=0}^{2\pi} \int_{\theta=0}^{\pi} \frac{\partial}{\partial r} \left(\frac{-1}{4\pi r} \mathrm{e}^{ikr} \right) \Big|_{r=R} R^2 \sin\theta \, d\theta d\phi, \\
&= \mathrm{e}^{ikR} - ikR \, \mathrm{e}^{ikR}.
\end{aligned}$$

Putting our calculations together we find the result

$$\int_{B(\mathbf{0},R)} \big(\nabla^2 + k^2\big) G \, dV = 1,$$

independent of the value of R. The correct interpretation of this is that $\big(\nabla^2 + k^2\big) G = \delta(\mathbf{x})$, *i.e.* our fundamental solution is the (outgoing) Green function for the Helmholtz equation. This makes sense: we put a source at the origin.

The Fraunhofer Diffraction Integral. We first state in words the basic result encoded in the Fraunhofer diffraction integral:

The diffracted wave amplitude observed on a screen a large distance from an aperture is proportional to the Fourier transform of the aperture.

To derive the result, we introduce some notation. We will consider an **aperture** (screen with some holes in it) lying in the plane $z \equiv x_3 = 0$ and observe the diffraction pattern on a screen a distance D beyond it, *i.e.* the plane $z \equiv x_3 = D$. We parameterise the aperture plane by coordinates (y_1, y_2), *i.e.* the points of the aperture plane are the points $(y_1, y_2, 0) = \mathbf{y}$. Similarly, we parameterise the observation plane by coordinates (x_1, x_2), *i.e.* the points of the aperture plane are the points $(x_1, x_2, D) = \mathbf{x}$. The aperture itself will be given by a function $A(y_1, y_2)$ that takes the value 1 at points where light can get through the screen and 0 at points where it cannot.

Imagine each point of the aperture acts as a simple source, generating a spherical outgoing wave $\frac{-1}{4\pi|\mathbf{x}-\mathbf{y}|}\exp\{ik|\mathbf{x}-\mathbf{y}|\}$. The total diffracted wave amplitude is then given by adding up these sources from each point of the aperture

$$u(\mathbf{x}) = \int_{\mathbb{R}^2} \frac{-1}{4\pi|\mathbf{x}-\mathbf{y}|} \mathrm{e}^{ik|\mathbf{x}-\mathbf{y}|} \, A(y_1, y_2) \, dy_1 dy_2.$$

Frequently, this is referred to as **Huygen's principle** or the method of secondary sources.

Now we make use of the Fraunhofer limit: we observe the diffraction pattern at large distances from the aperture. In symbols this means D is large compared to any of x_1, x_2, y_1, y_2. More

directly (although not exactly the same) $|\mathbf{x}| \gg |\mathbf{y}|$. At the crudest level of approximation $|\mathbf{x}-\mathbf{y}| \approx D$; this will be sufficient for the amplitude prefactor, $\frac{-1}{4\pi|\mathbf{x}-\mathbf{y}|}$, but not for the phase part. For the phase we compute more carefully

$$|\mathbf{x}-\mathbf{y}| = \big[(\mathbf{x}-\mathbf{y})\cdot(\mathbf{x}-\mathbf{y})\big]^{1/2} = \Big[|\mathbf{x}|^2 - 2\mathbf{x}\cdot\mathbf{y} + |\mathbf{y}|^2\Big]^{1/2} = |\mathbf{x}| - \frac{\mathbf{x}\cdot\mathbf{y}}{|\mathbf{x}|} + \cdots,$$
$$\approx D - \frac{x_1y_1 + x_2y_2}{D},$$

using a first order Taylor expansion. Using this approximate expression for the phase in the diffracted wave amplitude we arrive at the **Fraunhofer diffraction integral**

$$u(\mathbf{x}) = \frac{-\mathrm{e}^{ikD}}{4\pi D}\int_{\mathbb{R}^2} \mathrm{e}^{-ik(x_1y_1+x_2y_2)/D} A(y_1,y_2)\,dy_1dy_2.$$

Rectangular Slit. For the basic example consider a rectangular slit of width $2w$ and height $2h$, for which the aperture function is

$$A(y_1,y_2) = \begin{cases} 1 & (y_1,y_2)\in[-w,w]\times[-h,h], \\ 0 & \text{otherwise.}\end{cases}$$

The Fourier transform is one we have seen previously and evaluates to

$$\tilde{A}(x_1,x_2) := \int_{\mathbb{R}^2} \mathrm{e}^{-ik(x_1y_1+x_2y_2)/D} A(y_1,y_2)\,dy_1dy_2 = \left(2w\frac{\sin(kwx_1/D)}{kwx_1/D}\right)\left(2h\frac{\sin(khx_2/D)}{khx_2/D}\right).$$

The intensity of the observed diffraction pattern is

$$I(x_1,x_2) \propto \big|\tilde{A}(x_1,x_2)\big|^2 = I_0\left(\frac{\sin(kwx_1/D)}{kwx_1/D}\right)^2\left(\frac{\sin(khx_2/D)}{khx_2/D}\right)^2,$$

where $I_0 := I(0,0)$ is the intensity at the centre of the observation screen. This normalisation follows from the well-known limit $\lim_{x\to 0}\frac{\sin x}{x} = 1$.

The intensity is maximal at the centre of the observation screen. It vanishes along the lines $x_1 = n\pi D/kw = n\lambda D/2w$, $n\in\mathbb{Z}^*$, and $x_2 = n\pi D/kh = n\lambda D/2h$, $n\in\mathbb{Z}^*$. The distance of the zero in intensity scales **inversely** with the physical size of the aperture, *i.e.* as $2w$ and $2h$, respectively. This inverse relationship between features in the diffraction pattern and the linear dimensions of the aperture is a general characteristic of diffraction. The *angular* spread in the diffracted light is approximately $x_1/D = \lambda/2w$ horizontally and $x_2/D = \lambda/2h$ vertically. Thus to see any appreciable spread in a beam the linear dimensions of the aperture should be comparable to the wavelength of the light.

Non-Normal Incidence. Suppose the incident light makes an anlge θ to the normal direction of the aperture, *i.e.* its wavevector is $(k\sin\theta, 0, k\cos\theta)$. This modulates the light at the aperture ($z = x_3 = 0$) by a phase factor $\mathrm{e}^{ik\sin\theta y_1}$ such that the aperture function for non-normal incidence is

$$A_\theta(y_1,y_2) = \mathrm{e}^{ik\sin\theta y_1} A_0(y_1,y_2),$$

where $A_0(y_1,y_2)$ is the aperture function for normally incident light. By the shift property of Fourier transforms, or the convolution theorem, the diffracted wave amplitude is therefore proportional to

$$\widetilde{A_\theta}(x_1,x_2) = \widetilde{A_0}\big(x_1 - D\sin\theta, x_2\big).$$

In other words, the diffraction pattern is the same but its position is shifted from the centre of the screen to a point corresponding to the straight line between the source and the screen (making angle θ with the normal direction), the geometrical optics expectation.

Young's Double Slits. The foundation of interference phenomena is Thomas Young's famous 'double slit' experiment (1803). Consider two identical rectangular slits of width $2w$ and height $2h$, with centres separated by a distance 2ℓ along the horizontal direction (y_1). The aperture function may be written in terms of that of a single rectangular slit as

$$A(y_1, y_2) = A_{\text{slit}}(y_1 + \ell, y_2) + A_{\text{slit}}(y_1 - \ell, y_2).$$

The diffracted wave amplitude then follows from the shift property of Fourier transforms

$$\tilde{A}(x_1, x_2) = \mathrm{e}^{ik\ell x_1/D}\widetilde{A_{\text{slit}}}(x_1, x_2) + \mathrm{e}^{-ik\ell x_1/D}\widetilde{A_{\text{slit}}}(x_1, x_2) = 2\cos\big(k\ell x_1/D\big)\widetilde{A_{\text{slit}}}(x_1, x_2).$$

Using $I \propto |\tilde{A}|^2$, it then follows that the intensity observed on a distant screen is

$$I(x_1, x_2) = I_0 \cos^2\big(k\ell x_1/D\big)\left(\frac{\sin(kwx_1/D)}{kwx_1/D}\right)^2\left(\frac{\sin(khx_2/D)}{khx_2/D}\right)^2.$$

Exercise: Sketch this pattern, marking the three length scales $D(\lambda/2w)$, $D(\lambda/2h)$ and $D(\lambda/2\ell)$.

The Airy Pattern. The ubiquity of circular apertures is hard to overstate. You'll find them in every sort of camera, microscope, telescope and eye, whether human, animal, bird, insect or fish. We can take it as self-evident that a course dealing with applications should want to cover this problem.

The diffraction pattern created by a circular aperture is rightly celebrated: it is known as the **Airy pattern**, after George Biddell Airy (1801-1892). It consists of a bright central spot surrounded by a set of rings of lower and diminishing intensity.

We consider a circular aperture of diameter $2a$ so that the aperture function is

$$A(y_1, y_2) = \begin{cases} 1 & \sqrt{y_1^2 + y_2^2} < a, \\ 0 & \text{otherwise.} \end{cases}$$

It will be convenient to work in polar coordinates, writing $r = \sqrt{x_1^2 + x_2^2}$, $\rho = \sqrt{y_1^2 + y_2^2}$ for the radial distances and ϕ for the angle in the aperture plane. Then

$$\tilde{A}(r) = \int_{\phi=-\pi}^{\pi}\int_{\rho=0}^{a} \mathrm{e}^{-ikr\rho\cos\phi/D}\,\rho\,d\rho d\phi = \int_{\rho=0}^{a}\left(\int_{\phi=-\pi}^{\pi} \mathrm{e}^{-ikr\rho\cos\phi/D} d\phi\right)\rho\,d\rho.$$

The integral is the definition of a special function – the **Bessel function** of the first kind and order zero

$$\frac{1}{2\pi}\int_{-\pi}^{\pi} \mathrm{e}^{-ikr\rho\cos\phi/D} d\phi = J_0\big(kr\rho/D\big).$$

Thus we have

$$\tilde{A}(r) = \int_0^a 2\pi J_0\big(kr\rho/D\big)\,\rho\,d\rho = \frac{2\pi}{(kr/D)^2}\int_0^{kra/D} xJ_0(x)\,dx.$$

To complete the integral we need to know some of the properties of Bessel functions and specifically that

$$xJ_0(x) = \frac{d}{dx}\Big[xJ_1(x)\Big].$$

The integral can then be done immediately and gives

$$\tilde{A}(r) = \pi a^2 \, \frac{2J_1(kra/D)}{kra/D}.$$

Finally, the intensity of the diffraction pattern is

$$I(r) = I_0 \left(\frac{2J_1(kra/D)}{kra/D} \right)^2.$$

The intensity at the centre of the bright Airy disc ($r = 0$) is I_0 and it first vanishes when $J_1(kra/D) = 0$ for $r \neq 0$. The zeros of Bessel functions are not given in simple form the way that they are for sine and cosine, but they have been extensively studied and many properties determined. The first non-trivial zero of $J_1(x)$ occurs when $x \approx 1.22\pi$, which gives the angular size (r/D) of the Airy disc as

$$\text{angular size} \;\approx 1.22 \frac{\lambda}{2a}.$$

Bessel Functions. Bessel functions are properly defined using contour integrals and complex analysis. However, we can develop a less rigorous approach to them using Fourier methods. The basic idea is to recognise that the function

$$f(\phi) = \mathrm{e}^{ix\sin\phi},$$

is periodic with period 2π and hence can be expressed as a Fourier series

$$\mathrm{e}^{ix\sin\phi} = \sum_n J_n(x)\,\mathrm{e}^{in\phi}, \qquad\qquad J_n(x) = \frac{1}{2\pi}\int_{-\pi}^{\pi} \mathrm{e}^{-in\phi + ix\sin\phi}\, d\phi.$$

The index n is called the **order** of the Bessel function. We work with $\mathrm{e}^{ix\sin\phi}$ rather than $\mathrm{e}^{-ix\cos\phi}$ to match standard treatments of Bessel functions. The two may be related by noting $\sin(\phi - \pi/2) = -\cos\phi$, leading to

$$\mathrm{e}^{-ix\cos\phi} = \sum_n (-i)^n J_n(x)\,\mathrm{e}^{in\phi}, \qquad\qquad J_n(x) = \frac{i^n}{2\pi}\int_{-\pi}^{\pi} \mathrm{e}^{-in\phi - ix\cos\phi}\, d\phi.$$

There exist a large number of identities relating the Bessel functions of different orders, which typically go under the name of **recurrence relations**. For example, differentiating the defining Fourier expansion with respect to x we find

$$\sum_n \frac{dJ_n}{dx}\,\mathrm{e}^{in\phi} = i\sin\phi\,\mathrm{e}^{ix\sin\phi} = \sum_n iJ_n(x)\frac{\mathrm{e}^{i\phi} - \mathrm{e}^{-i\phi}}{2i}\mathrm{e}^{in\phi} = \frac{1}{2}\sum_n \big(J_{n-1}(x) - J_{n+1}(x)\big)\mathrm{e}^{in\phi},$$

$$\Rightarrow \qquad \frac{dJ_n}{dx} = \frac{1}{2}\big(J_{n-1}(x) - J_{n+1}(x)\big).$$

Differentiating the defining Fourier expansion with respect to ϕ we find

$$\sum_n inJ_n(x)\,\mathrm{e}^{in\phi} = ix\cos\phi\,\mathrm{e}^{ix\sin\phi} = \sum_n ixJ_n(x)\frac{\mathrm{e}^{i\phi} + \mathrm{e}^{-i\phi}}{2}\mathrm{e}^{in\phi} = \frac{ix}{2}\sum_n \big(J_{n-1}(x) + J_{n+1}(x)\big)\mathrm{e}^{in\phi},$$

$$\Rightarrow \qquad J_{n-1}(x) - \frac{2n}{x}J_n(x) + J_{n+1}(x) = 0.$$

Combining these two recurrence relations we obtain

$$\frac{dJ_n}{dx} = J_{n-1}(x) - \frac{n}{x}J_n(x), \qquad \Rightarrow \qquad \frac{d}{dx}\Big[x^n J_n(x)\Big] = x^n J_{n-1}(x),$$

which we use, in the case $n = 1$, in our derivation of the Airy diffraction pattern.

To correctly normalise the intensity in the Airy pattern we need to know the (first term in the) Taylor series for the Bessel functions. This follows from the Taylor series for the exponential function and orthogonality of Fourier modes

$$J_n(x) = \frac{1}{2\pi}\int_{-\pi}^{\pi} \mathrm{e}^{-in\phi} \sum_{k=0}^{\infty} \frac{1}{k!}\left(\frac{x}{2}\big(\mathrm{e}^{i\phi} - \mathrm{e}^{-i\phi}\big)\right)^k d\phi = \sum_{k=0}^{\infty} \frac{(-1)^k}{k!(n+k)!}\left(\frac{x}{2}\right)^{n+2k}.$$

In particular, for the case $n = 1$ we deduce

$$\lim_{x\to 0} \frac{2J_1(x)}{x} = 1,$$

which enables us to correctly normalise the Airy pattern.

Bessel functions arose historically because they satisfy a particular differential equation that comes up in numerous applications where there is cylindrical symmetry (or geometry). **Bessel's equation** is

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

We leave it as an exercise to show that Bessel functions, as we have defined them, satisfy this differential equation.

Resolution: The Rayleigh Criterion. The Airy pattern provides a means for quantifying an optical instrument's ability to resolve or distinguish two sources. Consider two (point) sources with angular separation θ (or a single source of angular size θ). Suppose the light from one of them is incident normally on the aperture, then the light from the other will be incident at an angle θ to the normal direction and its image Airy disc will be displaced from the centre of the observation screen by an amount $r = D\sin\theta \approx D\theta$. Now the size of each Airy disc is $1.22D\lambda/2a$ and whether we can resolve the two images or not clearly depends on whether the Airy discs are well separated or closely overlapping, *i.e.* which of these two distances is bigger. Lord Rayleigh suggested the criterion that the two images are just resolved when they are equal

$$\theta = 1.22\,\frac{\lambda}{2a} = 1.22\,\frac{\text{wavelength}}{\text{diameter of aperture}}.$$

Example: We use Rayleigh's criterion to determine the diameter of a telescope needed to resolve the four Galilean moons of Jupiter.

The four Galilean moons of Jupiter – Io, Europa, Ganymede and Callisto – have distances from Jupiter and angular separations (as perceived at the Earth) as given in the table below.

	semi-major axis (km)	angular separation (radians)
Io	4.22×10^5	6.7×10^{-4}
Europa	6.71×10^5	1.1×10^{-3}
Ganymede	1.07×10^6	1.7×10^{-3}
Callisto	1.88×10^6	3.0×10^{-3}

The angular separations have been calculated using the difference between the semi-major axis of Jupiter (7.79×10^8 km) and of the Earth (1.50×10^8 km). The smallest separation is for the moon Io. Using it in Rayleigh's criterion, we estimate that the diameter of our telescope must be at least

$$\text{diameter} > 1.22\,\frac{\lambda}{6.7\times10^{-4}},$$

and taking an average value of 550 nm for the wavelength of light we obtain a minimum diameter of ~ 1 mm.

Diffraction Gratings. A diffraction grating is an optical element (aperture) consisting of a large number of identical, equally spaced, narrow slits. We will suppose as usual that the slits are rectangular of width $2w$ and height $2h$, and that the spacing between them is 2ℓ. Let there be N slits in total. It can be convenient to treat separately the cases of even and odd N; for definitiveness we suppose N is even. Then we may take the positions of the (centres of the) slits to be

$$y_1 = -(N-1)\ell + n\,2\ell, \qquad n = 0, 1, \ldots, N-1,$$

and $y_2 = 0$. The aperture function is

$$A(y_1, y_2) = \sum_{n=0}^{N-1} A_{\text{slit}}(y_1 + (N-1)\ell - 2n\ell, y_2),$$

and hence the diffracted wave amplitude is

$$\begin{aligned}
\tilde{A}(x_1, x_2) &= \sum_{n=0}^{N-1} \mathrm{e}^{ik(N-1)\ell x_1/D - i2nk\ell x_1/D}\,\widetilde{A_{\text{slit}}}(x_1, x_2),\\
&= \mathrm{e}^{ik(N-1)\ell x_1/D}\left(\sum_{n=0}^{N-1} \mathrm{e}^{-i2nk\ell x_1/D}\right)\widetilde{A_{\text{slit}}}(x_1, x_2),\\
&= \mathrm{e}^{ik(N-1)\ell x_1/D}\left(\frac{1-\mathrm{e}^{-i2Nk\ell x_1/D}}{1-\mathrm{e}^{-i2k\ell x_1/D}}\right)\widetilde{A_{\text{slit}}}(x_1, x_2),\\
&= \frac{\sin\bigl(Nk\ell x_1/D\bigr)}{\sin\bigl(k\ell x_1/D\bigr)}\;\widetilde{A_{\text{slit}}}(x_1, x_2).
\end{aligned}$$

So finally we can write the intensity of the diffraction pattern as

$$I(x_1, x_2) = I_0\left(\frac{\sin\bigl(Nk\ell x_1/D\bigr)}{N\sin\bigl(k\ell x_1/D\bigr)}\right)^2\left(\frac{\sin\bigl(kwx_1/D\bigr)}{kwx_1/D}\right)^2\left(\frac{\sin\bigl(khx_2/D\bigr)}{khx_2/D}\right)^2,$$

where, as usual, I_0 is the intensity at the centre of the pattern.

The main feature of the result is the location of the 'interference' peaks and zeros, which are determined (largely) by the first factor. The intensity is zero at

$$\frac{x_1}{D} = n\,\frac{\lambda}{2N\ell}, \qquad n \in \mathbb{Z}\setminus N\mathbb{Z},$$

while the principal maxima are at

$$\frac{x_1}{D} = n\,\frac{\lambda}{2\ell}, \qquad n \in \mathbb{Z}^*.$$

(The secondary maxima between the principal peaks are dimmer by a factor of order $1/N^2$.) So the diffraction peaks are bright and very narrow, becoming more so as the number of slits N increases.

Diffraction gratings are used to separate spectral lines. To see how this works, suppose we have two wavelengths, $\lambda_1 < \lambda_2$, and consider the positions of the first diffraction peak (*i.e.* not the central peak); these are

$$\frac{x_1}{D} = \frac{\lambda_1}{2\ell}, \qquad \text{and} \qquad \frac{x_1}{D} = \frac{\lambda_2}{2\ell},$$

so that the distance between them is therefore

$$\frac{\Delta x_1}{D} = \frac{\lambda_2 - \lambda_1}{2\ell}.$$

If this is larger than the width of each peak we will be able to tell that there are two peaks and not just one, which yields the criterion for resolving the two wavelengths of

$$\frac{\lambda_2 - \lambda_1}{2\ell} \gtrsim \frac{(\lambda_1 + \lambda_2)/2}{2N\ell}, \qquad \text{or} \qquad N \gtrsim \frac{(\lambda_1 + \lambda_2)/2}{\lambda_2 - \lambda_1} = \frac{\lambda}{\Delta\lambda}.$$

Example: The two sodium D lines have wavelength 589 nm and 589.6 nm. It follows that a diffraction grating will resolve them so long as the number of slits is at least

$$N > \frac{589.3 \text{ nm}}{0.6 \text{ nm}} = 982.2\,.$$

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Lagrange Multipliers

The method of Lagrange multipliers is used to find critical points of functions subject to some constraint. We begin with the unconstrained situation.

A **critical point** of a function $f : \mathbb{R}^n \to \mathbb{R}$ is a point $\mathbf{x} \in \mathbb{R}^n$ at which the gradient of f vanishes identically; equivalently all of the partial derivatives $\partial f/\partial x_i$ vanish. The value of f at the critical point is called a **critical value**. As basic examples for $n = 3$, each of the functions

$$x^2 + y^2 + z^2, \qquad x^2 + y^2 - z^2, \qquad x^2 - y^2 - z^2, \qquad -x^2 - y^2 - z^2,$$

has an isolated critical point at the origin with critical value 0. A critical point is called **non-degenerate** (or **Morse**) if the matrix of second derivatives

$$\frac{\partial^2 f}{\partial x_i \partial x_j},$$

is non-singular at the critical point. This matrix of second derivative is called the **Hessian** matrix of the function. The functions in our basic example are all non-degenerate. The number of minus signs appearing in each function ($0, 1, 2$ or 3) is the dimension of the negative eigenspace of the Hessian at the critical point, which is known as the **Morse index**. The Morse lemma establishes that all non-degenerate critical points are equivalent to one of these canonical forms. As an example of a degenerate critical point one may take the function $f = x^3 + y^2 + z^2$, known as the A_2 singularity, or **fold catastrophe**.

By a **constraint** we will mean a function $c : \mathbb{R}^n \to \mathbb{R}$ whose value we are required to make vanish. This restricts the domain of f from all of $\mathbb{R}^n$ to $c^{-1}(0)$. A basic example in $\mathbb{R}^3$ is given by the constraint function $c(x, y, z) = z$. The preimage of zero is the set of points in $\mathbb{R}^3$ of the form $(x, y, 0)$. In this case we can parameterise the inverse image set $c^{-1}(0)$ explicity and so impose the constraint on f directly, obtaining a new function depending on fewer variables, whose critical points can be obtained in the normal way. However, in general we will not be able to do this (at least as easily as here) and so we seek an alternative approach.

Method of Lagrange Multipliers. Let $f : \mathbb{R}^n \to \mathbb{R}$ be a function and $c_i : \mathbb{R}^n \to \mathbb{R}$, $i = 1, \ldots, k$, a collection of k constraint functions. Then the critical points of f subject to the constraints $c_i = 0$ are given by the *unconstrained* critical points of the function

$$F = f - \sum_{i=1}^{k} \lambda_i c_i,$$

together with the k constraint equations $c_i = 0$. Equivalently, all of the partial derivatives

$$\frac{\partial F}{\partial x_j} = \frac{\partial f}{\partial x_j} - \sum_{i=1}^{k} \lambda_i \frac{\partial c_i}{\partial x_j} = 0,$$

must vanish. The parameters λ_i are called **Lagrange multipliers**.

Here, we are thinking of F as a function of $\mathbf{x}$ with the Lagrange multipliers as additional parameters. We can also view the Lagrange multipliers as variables and F as a function

$\mathbb{R}^n \times \mathbb{R}^k \to \mathbb{R}$. In this case, the constrained critical points of f are given by the unconstrained critical points of F and we do not need to separately impose the constraint equations as they are contained in the conditions $\partial F/\partial \lambda_i = 0$.

Example: Find the critical points of $f = x^2+y^2+z^2$ subject to the constraint $c = x+y+z-1$.

By the method of Lagrange multipliers these are given by the set of four equations

$$\frac{\partial F}{\partial x} = 2x - \lambda = 0, \qquad \frac{\partial F}{\partial y} = 2y - \lambda = 0, \qquad \frac{\partial F}{\partial z} = 2z - \lambda = 0,$$
$$c = x + y + z - 1 = 0.$$

It follows that x, y and z are all equal – each is equal to $\frac{1}{2}\lambda$ – and then by the constraint they must all take the value $\frac{1}{3}$. So we have found a single constrained critical point $(\frac{1}{3}, \frac{1}{3}, \frac{1}{3})$.

Exercise: Find the critical points of $f = x^2 + y^2 - z^2$ for the same constraint.

Example: Find the critical points of $f = x + y$ subject to the constraint $c = xy - 1 = 0$.

By the method of Lagrange multipliers we obtain the conditions

$$\frac{\partial(f - \lambda c)}{\partial x} = 1 - \lambda y = 0, \qquad \frac{\partial(f - \lambda c)}{\partial y} = 1 - \lambda x = 0,$$

together with the constraint equation. It follows that $x = y$ and then from the constraint we find two constrained critical points at $(-1, -1)$ and $(1, 1)$.

A Geometrical View. The method of Lagrange multipliers has its origins in a geometric understanding of the gradient of a function and its differential df. The gradient measures both the rate at which a function changes and the direction in which it is increasing. This direction is normal to the level sets of f.

Now, given a small displacement $d\mathbf{x}$, the change in the value of the function is (to linear order)

$$df = d\mathbf{x} \cdot \nabla f.$$

At a critical point $df = 0$ for all choices of $d\mathbf{x}$. In the constrained case, we are not free to choose $d\mathbf{x}$ arbitrarily, since we must preserve the constraint; that is, the only displacements we may consider are those for which $dc_i = d\mathbf{x} \cdot \nabla c_i = 0$. Thus $d\mathbf{x}$ is orthogonal to each of the gradient vectors ∇c_i. A constrained critical point of f is a point $\mathbf{x}$ where $df = d\mathbf{x} \cdot \nabla f = 0$ for all admissable displacements $d\mathbf{x}$. It follows that

$$\nabla f \in \text{span}\langle \nabla c_1, \ldots, \nabla c_k \rangle,$$

or ∇f is a linear combination of the gradients ∇c_i. Any such linear relation can be written

$$\nabla f = \sum_{i=1}^{k} \lambda_i \nabla c_i \qquad \text{or} \qquad \nabla f - \sum_{i=1}^{k} \lambda_i \nabla c_i = 0,$$

which is the content of the 'method of Lagrange multipliers'.

Height Functions. We consider now some examples involving critical points of the 'height function', *i.e.* the function $f = z$ (in $\mathbb{R}^3$).

Example: Find the critical points of the height over the surface of the unit sphere. Clearly these are the points $(0, 0, \pm 1)$. We verify this using the method of Lagrange multipliers, taking

for the constraint the function $c = x^2 + y^2 + z^2 - 1 = 0$. The method gives the critical points as the solutions of

$$0 - \lambda\, 2x = 0, \qquad 0 - \lambda\, 2y = 0, \qquad 1 - \lambda\, 2z = 0,$$

together with the constraint $x^2 + y^2 + z^2 = 1$. The first two equations give $x = y = 0$ as the possible solution $\lambda = 0$ is ruled out by the third equation. The constraint then determines $z = \pm 1$.

Example: Thus time we take the surface to be a torus. This is captured by the constraint function

$$c = \Big(x^2 + y^2 + z^2 + R^2 - \rho^2\Big)^2 - 4R^2\big(y^2 + z^2\big) = 0,$$

for constants R and ρ, with $0 < \rho < R$. The method of Lagrange multipliers gives the constrained critical points as solutions of

$$\begin{aligned} 0 - \lambda\, 4x\Big(x^2 + y^2 + z^2 + R^2 - \rho^2\Big) &= 0, \\ 0 - \lambda\Big[4y\Big(x^2 + y^2 + z^2 + R^2 - \rho^2\Big) - 8R^2 y\Big] &= 0, \\ 1 - \lambda\Big[4z\Big(x^2 + y^2 + z^2 + R^2 - \rho^2\Big) - 8R^2 z\Big] &= 0, \end{aligned}$$

together with the constraint equation. Again, we see $x = y = 0$; other conceivable solutions (*e.g.* $\lambda = 0$) leading to inconsistency, much as before. The constraint equation then gives

$$z^2 + R^2 - \rho^2 = \pm 2Rz,$$

from which we deduce that there are four critical points

$$\big(0, 0, -R - \rho\big), \qquad \big(0, 0, -R + \rho\big), \qquad \big(0, 0, R - \rho\big), \qquad \big(0, 0, R + \rho\big).$$

Exercise: Verify that these are, respectively, a minimum, a saddle, a saddle and a maximum.

Distance Functions. A second class of examples are provided by the constrained critical points of the (squared) distance function $f = x^2 + y^2 + z^2$. It can be convenient to consider the (squared) distance from a general point $\mathbf{a} = (a_x, a_y, a_z)$ and not just the origin; in that case the relevant function is $f_{\mathbf{a}} = (x - a_x)^2 + (y - a_y)^2 + (z - a_z)^2$.

Example: Find the critical points of $f_{\mathbf{a}}$ subject to the constraint $c = z = 0$. The method of Lagrange multipliers gives

$$2(x - a_x) - \lambda\, 0 = 0, \qquad 2(y - a_y) - \lambda\, 0 = 0, \qquad 2(z - a_z) - \lambda\, 1 = 0,$$

together with the constraint, $z = 0$. It follows that there is a single constrained critical point at $(a_x, a_y, 0)$.

Example: Find the constrained critical points of $f_{\mathbf{a}}$ subject to the constraint $c = x^2 + y^2 + z^2 - 1 = 0$. Applying the method of Lagrange multipliers leads to the system of equations

$$2(x - a_x) - \lambda\, 2x = 0, \qquad 2(y - a_y) - \lambda\, 2y = 0, \qquad 2(z - a_z) - \lambda\, 2z = 0,$$

together with the constraint. These have the geometrical interpretation that the critical points lie on the straight line connecting the origin to the point $\mathbf{a} = (a_x, a_y, a_z)$. Thus they are given by $\pm\mathbf{a}/|\mathbf{a}|$.

Stationary Phase. Wave disturbances in a field $u(x,t)$ can be written as a Fourier decomposition

$$u(x,t) = \frac{1}{(2\pi)^2} \int \mathrm{e}^{i(kx-\omega t)}\, \tilde{u}(k,\omega)\, dk d\omega,$$

where the integral is taken over all (k,ω) that satisfy the **dispersion relation** $D(k,\omega) = 0$. In such an integral, the oscillations in the complex exponential interfere destructively except near those points (k,ω) where the phase is stationary, subject to the constraint that the dispersion relation is satisfied. Thus the wave disturbance can be approximated by the condition of **stationary phase**, a heuristic that captures a key method in mathematical physics.

Applying the method of Lagrange multipliers gives the constrained critical points of the phase as

$$x - \lambda \frac{\partial D}{\partial k} = 0, \qquad\qquad -t - \lambda \frac{\partial D}{\partial \omega} = 0,$$

or

$$\frac{x}{t} = \frac{-\partial D/\partial k}{\partial D/\partial \omega}.$$

Thinking of ω as a function of k this is the same as $x/t = \partial\omega/\partial k$. The physical interpretation is that the wave disturbance propagates through space ($x = (\partial\omega/\partial k)t$) at the **group velocity** $v_g = \partial\omega/\partial k$.

Example: For sound waves the dispersion relation is $\omega^2 = c^2k^2$ and we have $v_g = ck$.

Example: For linear surface water waves on deep water the dispersion relation is $\omega^2 = gk$, where g is the acceleration due to gravity. It follows that the group velocity is $v_g = \frac{1}{2}\sqrt{g/k}$.

Multiple Constraints. We give some examples of applying the method of Lagrange multipliers to problems with multiple constraints.

Example: Find the critical points of the height function $f = z$ subject to the constraints

$$c_1 = x^2 + y^2 + z^2 - 1 = 0, \qquad\qquad c_2 = hx + ky + lz = 0.$$

Applying the method of Lagrange multipliers we find

$$\lambda_1\, 2x - \lambda_2\, h = 0, \qquad \lambda_1\, 2y - \lambda_2\, k = 0, \qquad 1 - \lambda_1\, 2z - \lambda_2\, l = 0,$$

together with the two constraint equations. Suppose the two Lagrange multipliers are both non-zero. Then the first two equations yield $kx = hy$. Eliminating x from the two constraints gives

$$(h^2 + k^2)y^2 + k^2\big(z^2 - 1\big) = 0, \qquad\qquad (h^2 + k^2)y + klz = 0,$$

and then eliminating y we arrive at $(h^2 + k^2 + l^2)z^2 = h^2 + k^2$. It follows that the constrained critical points are

$$x = \frac{\mp hl}{\sqrt{h^2 + k^2}\sqrt{h^2 + k^2 + l^2}}, \qquad y = \frac{\mp kl}{\sqrt{h^2 + k^2}\sqrt{h^2 + k^2 + l^2}}, \qquad z = \frac{\pm\sqrt{h^2 + k^2}}{\sqrt{h^2 + k^2 + l^2}}.$$

We note that the form of the solution is valid provided h and k are not both zero.

Exercise: We assumed that neither of the Lagrange multipliers vanished. Show that there are no solutions if $\lambda_2 = 0$. Are there any solutions when $\lambda_1 = 0$?

Example: Maximise the area enclosed by a simple polygon in the plane with N vertices all constrained to lie on the unit circle.

Denote the positions of the vertices by (x_i, y_i), $i = 1, \ldots, N$. That these lie on the unit circle gives N constraints $c_i = x_i^2 + y_i^2 - 1 = 0$. The area enclosed by the polygon is

$$A = \frac{1}{2}\sum_{i=1}^{N}\big(x_i y_{i+1} - x_{i+1} y_i\big),$$

where it is understood that $(x_{N+1}, y_{N+1}) \equiv (x_1, y_1)$, and may be thought of as a function $A : \mathbb{R}^{2N} \to \mathbb{R}$. The method of Lagrange multpliers gives the $2N$ equations

$$\frac{\partial(A - \sum_j \lambda_j c_j)}{\partial x_i} = \frac{1}{2}\big(y_{i+1} - y_{i-1}\big) - \lambda_i\, 2x_i = 0,$$
$$\frac{\partial(A - \sum_j \lambda_j c_j)}{\partial y_i} = \frac{1}{2}\big(x_{i-1} - x_{i+1}\big) - \lambda_i\, 2y_i = 0,$$

together with the constraint equations. Eliminating λ_i we find

$$x_i\big(x_{i-1} - x_{i+1}\big) = y_i\big(y_{i+1} - y_{i-1}\big) \qquad \text{or} \qquad x_{i-1}x_i + y_{i-1}y_i = x_i x_{i+1} + y_i y_{i+1}.$$

The combination (dot product) $x_i x_{i+1} + y_i y_{i+1}$ is simply the angle between successive vertices, so this says that the area is maximised when all the angles are equal, *i.e.* for a regular N-gon.

Shannon Entropy. In 1948 Claude Shannon introduced a method for choosing probabilities based on only partial information. Suppose X is a random variable taking one of N values x_i, $i = 1, \ldots, N$, with probabilities p_i. If all we are told is that the average value (expectation value) of X is $\langle X \rangle$, then what values should we take for the probabilities? Is there a choice that is 'optimal' in any sense? Shannon's solution is that we should choose the probabilities to maximise the **entropy**

$$S = -\sum_{i=1}^{N} p_i \ln p_i,$$

subject to the given constraints.

We can do this using the method of Lagrange multipliers. There are two constraints

$$c_1 = \sum_{i=1}^{N} p_i - 1 = 0, \qquad\qquad c_2 = \sum_{i=1}^{N} p_i x_i - \langle X \rangle = 0,$$

and the method of Lagrange multipliers yields the equations

$$\frac{\partial(S - \lambda_1 c_1 - \lambda_2 c_2)}{\partial p_i} = -\big(\ln p_i + 1\big) - \lambda_1 - \lambda_2 x_i = 0, \qquad \text{for each } i,$$

together with the two constraint equations. Rearranging, this gives the probabilities as

$$p_i = \mathrm{e}^{-(1+\lambda_1)-\lambda_2 x_i},$$

and the constraint c_1 identifies $\mathrm{e}^{1+\lambda_1} = \sum_{i=1}^{N} \mathrm{e}^{-\lambda_2 x_i} =: Z$, which is called (in statistical mechanics) the **partition function**. The Lagrange multiplier λ_2 is determined from the constraint c_2 through the relation

$$\langle X \rangle = \frac{1}{Z}\sum_{i=1}^{N} x_i\, \mathrm{e}^{-\lambda_2 x_i} = -\frac{\partial \ln Z}{\partial \lambda_2}.$$

Exactly this formalism arises in statistical mechanics, where we take for X the energy and interpret λ_2 as the inverse temperature, $\lambda_2 = (k_{\mathrm{B}} T)^{-1}$.

These notes are designed to be very terse and are not a substitute for your own lecture notes.

Index Notation

Good notation helps to keep working tidy, formulae neat and concise, and can clarify ideas and make insights easier to spot. The **index notation** is used universally throughout theoretical physics and (much of) applied mathematics. The basic idea is to use subscripts to denote the coordinates of points, components of a vector, entries in a matrix, components of a general tensor *etc.* We begin with a few elementary examples you have already seen.

The coordinates of a point of $\mathbb{R}^n$ are written $(x_1, x_2, \ldots, x_n)$ and the i^{th} coordinate denoted x_i.

The Cartesian basis vectors in (the vector space) $\mathbb{R}^n$ are written $\mathbf{e}_1, \mathbf{e}_2, \ldots, \mathbf{e}_n$ and the i^{th} basis vector denoted $\mathbf{e}_i$. A general vector is then written

$$\mathbf{v} = \sum_{i=1}^{n} v_i \, \mathbf{e}_i,$$

with the number v_i giving the i^{th} component of the vector (in the given basis).

The entry in the i^{th} row and j^{th} column of the matrix $\mathbf{M}$ is denoted M_{ij}.

Einstein's Summation Convention. Einstein's **summation convention** can be stated succinctly:

Do not write summation signs; they are implied by repeated (twice only) indices.

For instance, for the dot product of two vectors $\mathbf{u}$ and $\mathbf{v}$ we write

$$\mathbf{u} \cdot \mathbf{v} = \sum_{i=1}^{n} u_i v_i \equiv u_i v_i.$$

As a second example, for the product of two matrices $\mathbf{A}$ and $\mathbf{B}$ we write

$$\big[\mathbf{AB}\big]_{ij} = \sum_{k=1}^{n} A_{ik} B_{kj} \equiv A_{ik} B_{kj}.$$

Good practice must be maintained in using the index notation, otherwise you can write expressions that others will not be able to interpret, or worse are plain nonsense. One such is to use different letters: compare the following two expressions purporting to represent the ij^{th} element of the matrix product $\mathbf{ABC}$

$$\big[\mathbf{ABC}\big]_{ij} = A_{ik} B_{kk} C_{kj}, \qquad\qquad \big[\mathbf{ABC}\big]_{ij} = A_{ik} B_{kl} C_{lj}.$$

The rule of thumb to follow is that an index should only ever appear either exactly once, in which case you do not sum it, or exactly twice, in which case you do sum it. If an index appears more than twice you should presume that you have made a mistake.

Indices that are summed over – k and l above – are called **dummy** indices; those that are not – i and j above – are called **free** indices. The latter must never change during your

calculations; the former you can change at will, *i.e.*

$$A_{ik}B_{kl}C_{lj} = A_{im}B_{ml}C_{lj} = A_{ia}B_{ab}C_{bj} = A_{il}B_{lk}C_{kj}, \qquad \textbf{correct},$$
$$A_{ik}B_{kl}C_{lj} = A_{jm}B_{ml}C_{li} = A_{ia}B_{ab}C_{bk} = A_{kl}B_{lk}C_{kl}, \qquad \textbf{very bad}.$$

Special Symbols. We will make frequent use of the following two symbols:

$$\delta_{ij} = \begin{cases} 1 & i = j, \\ 0 & \text{otherwise}, \end{cases} \qquad \epsilon_{ijk} = \begin{cases} +1 & i,j,k \text{ an even permutation of } 1,2,3, \\ -1 & i,j,k \text{ an odd permutation of } 1,2,3, \\ 0 & \text{otherwise}. \end{cases}$$

δ_{ij} is called the **Kronecker delta**. There is a version of it in every spatial dimension but it is always written the same way. It is the same as the components of the $n\times n$ identity matrix, $[\mathbf{I}]_{ij} = \delta_{ij}$.

ϵ_{ijk} is called the **Levi-Civita symbol**, or fully antisymmetric symbol. Strictly, ϵ_{ijk} is the fully antisymmetric symbol in three dimensions, but there are versions of it in all dimensions. In particular, in two dimensions we write ϵ_{ij}, whose components are $\epsilon_{12} = +1$, $\epsilon_{21} = -1$, and $\epsilon_{11} = \epsilon_{22} = 0$.

Vectors and Matrices. The components of the matrix $\mathbf{A}$ are A_{ij} and of the vector $\mathbf{b}$ are b_i. The famous equation $\mathbf{Ax} = \mathbf{b}$ reads

$$A_{ij}x_j = b_i.$$

Example: We might write the defining equation for the eigenvalues and eigenvectors of a matrix $\mathbf{A}$ in the form

$$A_{ij}v_j^{(\alpha)} = \lambda_{(\alpha)}v_i^{(\alpha)}, \qquad \alpha = 1,\ldots,n.$$

Note that in writing this the Greek index α is **not** being summed over – it is not participating in the 'index notation' at all.

A matrix $\mathbf{R}$ is orthogonal if $\mathbf{R}^T\mathbf{R} = \mathbf{I}$, where $\mathbf{R}^T$ denotes the transpose of $\mathbf{R}$. The components of $\mathbf{R}^T$ are $[\mathbf{R}^T]_{ij} = R_{ji}$. So in index notation the statement that $\mathbf{R}$ is orthogonal reads

$$R_{ki}R_{kj} = \delta_{ij}.$$

A matrix is symmetric if $\mathbf{R} = \mathbf{R}^T$, or $R_{ij} = R_{ji}$. The Kronecker delta, δ_{ij}, is symmetric.

Example: The rotation matrices are orthogonal. The rotation matrices in two dimensions are $\mathbf{R} = \left[\begin{smallmatrix} \cos\theta & -\sin\theta \\ \sin\theta & \cos\theta \end{smallmatrix}\right]$. We verify

$$R_{k1}R_{k1} = \big(\cos\theta\big)\big(\cos\theta\big) + \big(\sin\theta\big)\big(\sin\theta\big) = 1,$$
$$R_{k1}R_{k2} = \big(\cos\theta\big)\big(-\sin\theta\big) + \big(\sin\theta\big)\big(\cos\theta\big) = 0,$$

and leave the other two cases for you to do yourselves.

A matrix is antisymmetric if $\mathbf{A} = -\mathbf{A}^T$, or $A_{ij} = -A_{ji}$. The two-dimensional rotation matrices can be written as $\exp\left\{\left[\begin{smallmatrix} 0 & -\theta \\ \theta & 0 \end{smallmatrix}\right]\right\}$. The matrix $\left[\begin{smallmatrix} 0 & -\theta \\ \theta & 0 \end{smallmatrix}\right]$ is antisymmetric.

The trace of a matrix is $\operatorname{tr}\mathbf{A} = A_{ii}$.

Example: The trace of the Kronecker delta is $\delta_{ii} = n$.

Example: $\operatorname{tr}\mathbf{AB} = \operatorname{tr}\mathbf{BA}$. We write this in index notation

$$\operatorname{tr}\mathbf{AB} \overset{1}{=} A_{ij}B_{ji} \overset{2}{=} B_{ji}A_{ij} \overset{3}{=} \operatorname{tr}\mathbf{BA}.$$

Step 1 is the definition. Step 2 uses that A_{ij} and B_{ji} are ordinary numbers and so commute. Step 3 is again the definition.

Excercise: Show that $\operatorname{tr}\mathbf{ABC} = \operatorname{tr}\mathbf{CAB}$.

A decomposition of matrices. For an $n\times n$ matrix we write

$$M_{ij} = \frac{1}{n}M_{kk}\,\delta_{ij} + \frac{1}{2}\big(M_{ij} - M_{ji}\big) + \left(\frac{1}{2}\big(M_{ij} + M_{ji}\big) - \frac{1}{n}M_{kk}\,\delta_{ij}\right).$$

The utility of this decomposition is that the three pieces transform separately (do not mix) under the action of the rotation group. In fancier language one says that they each belong to different irreducible representations of the rotation group.

The determinant of a 3×3 matrix is $\det\mathbf{M} = \epsilon_{ijk}M_{1i}M_{2j}M_{3k}$. The corresponding formula in two dimensions is $\det\mathbf{M} = \epsilon_{ij}M_{1i}M_{2j}$ and in n dimensions is

$$\det\mathbf{M} = \epsilon_{i_1i_2\cdots i_n}M_{1i_1}M_{2i_2}\cdots M_{ni_n}.$$

Example: The rotation matrices in two dimensions, $\mathbf{R} = \left[\begin{smallmatrix}\cos\theta & -\sin\theta\\ \sin\theta & \cos\theta\end{smallmatrix}\right]$, have determinant $+1$. We write

$$\det\mathbf{R} = \epsilon_{ij}R_{1i}R_{2j} = \epsilon_{12}R_{11}R_{22} + \epsilon_{21}R_{12}R_{21} = (+1)\big(\cos\theta\big)\big(\cos\theta\big) + (-1)\big(-\sin\theta\big)\big(\sin\theta\big) = 1.$$

Scalar and Vector Products. Let $\mathbf{u}$ and $\mathbf{v}$ be two vectors with components u_i and v_i. Their scalar product is the number

$$\mathbf{u}\cdot\mathbf{v} = u_1v_1 + u_2v_2 + u_3v_3 = u_iv_i.$$

Exercise: Verify that this can also be written as $\delta_{ij}u_iv_j$.

Their cross product is the vector

$$\mathbf{u}\times\mathbf{v} = \big(u_2v_3 - u_3v_2\big)\,\mathbf{e}_1 + \big(u_3v_1 - u_1v_3\big)\,\mathbf{e}_2 + \big(u_1v_2 - u_2v_1\big)\,\mathbf{e}_3.$$

In the index notation, the components of this vector are written in compact form as $\big(\mathbf{u}\times\mathbf{v}\big)_i = \epsilon_{ijk}u_jv_k$.

Exercise: Verify this.

Example: We use the index notation to show that $\mathbf{u}\times\mathbf{u} = 0$ for any vector $\mathbf{u}$. This is not because it is hard, but because the calculational method is one that is used often. The calculation goes as follows:

$$\big(\mathbf{u}\times\mathbf{u}\big)_i \overset{1}{=} \epsilon_{ijk}u_ju_k \overset{2}{=} \epsilon_{ijk}u_ku_j \overset{3}{=} \epsilon_{ikj}u_ju_k \overset{4}{=} -\epsilon_{ijk}u_ju_k.$$

The first step converts to index notation. The second uses that $u_ju_k = u_ku_j$ – we say that u_ju_k is **symmetric** in j and k. The third is a relabelling of dummy indices. The fourth uses that $\epsilon_{ikj} = -\epsilon_{ijk}$, *i.e.* Levi-Civita is **antisymmetric** under interchange of any two indices. The conclusion is that $\mathbf{u}\times\mathbf{u}$ is equal to $-\mathbf{u}\times\mathbf{u}$ and hence must be zero.

Triple Products. Let $\mathbf{u}, \mathbf{v}, \mathbf{w}$ be three vectors with components u_i, v_i, w_i. Their triple scalar product is

$$\mathbf{u} \cdot (\mathbf{v} \times \mathbf{w}) = \epsilon_{ijk} u_i v_j w_k.$$

The proof is nothing more than a writing out of definitions.

Exercise: Use the index notation to show that $\mathbf{v} \cdot (\mathbf{u} \times \mathbf{w}) = -\mathbf{u} \cdot (\mathbf{v} \times \mathbf{w})$ and $\mathbf{w} \cdot (\mathbf{u} \times \mathbf{v}) = \mathbf{u} \cdot (\mathbf{v} \times \mathbf{w})$.

The vector triple product is $\mathbf{u} \times (\mathbf{v} \times \mathbf{w}) = (\mathbf{u} \cdot \mathbf{w})\mathbf{v} - (\mathbf{u} \cdot \mathbf{v})\mathbf{w}$. Writing this in index notation we obtain

$$\epsilon_{ijk} u_j \big(\epsilon_{klm} v_l w_m\big) = \big(u_j w_j\big) v_i - \big(u_j v_j\big) w_i = \Big(\delta_{il}\delta_{jm} - \delta_{im}\delta_{jl}\Big) u_j v_l w_m.$$

Since this holds for any three vectors $\mathbf{u}, \mathbf{v}, \mathbf{w}$ we have established the useful identity

$$\epsilon_{ijk}\epsilon_{klm} = \delta_{il}\delta_{jm} - \delta_{im}\delta_{jl}.$$

Exercise: Show that $\epsilon_{ijk}\epsilon_{ljk} = 2\delta_{il}$.

Derivatives and Differential Equations. For writing partial derivatives we adopt the notation

$$\frac{\partial}{\partial x_i} \quad \longrightarrow \quad \partial_i.$$

Example: Maxwell's equations in free space are

$$\begin{aligned}
\nabla \cdot \mathbf{E} = 0 \qquad &\longrightarrow \qquad \partial_i E_i = 0, \\
\nabla \cdot \mathbf{B} = 0 \qquad &\longrightarrow \qquad \partial_i B_i = 0, \\
\nabla \times \mathbf{E} + \frac{\partial \mathbf{B}}{\partial t} = 0 \qquad &\longrightarrow \qquad \epsilon_{ijk}\partial_j E_k + \partial_t B_i = 0, \\
\nabla \times \mathbf{B} - \mu_0\epsilon_0 \frac{\partial \mathbf{E}}{\partial t} = 0 \qquad &\longrightarrow \qquad \epsilon_{ijk}\partial_j B_k - \mu_0\epsilon_0\, \partial_t E_i = 0.
\end{aligned}$$

Example: We calculate $\nabla \times \nabla\phi$ using index notation

$$\big(\nabla \times \nabla\phi\big)_i \stackrel{1}{=} \epsilon_{ijk}\partial_j\partial_k\phi \stackrel{2}{=} \epsilon_{ijk}\partial_k\partial_j\phi \stackrel{3}{=} -\epsilon_{ikj}\partial_k\partial_j\phi \stackrel{4}{=} -\big(\nabla \times \nabla\phi\big)_i.$$

The first step converts to index notation. The second uses symmetry of mixed partial derivatives $\partial_j\partial_k\phi = \partial_k\partial_j\phi$. The third uses antisymmetry of the Levi-Civita symbol, $\epsilon_{ijk} = \epsilon_{ikj}$. The fourth converts back from index notation; the conclusion is clearly that $\nabla \times \nabla\phi = 0$.

Example: We establish the identity $\nabla \times (\nabla \times \mathbf{E}) = \nabla(\nabla \cdot \mathbf{E}) - \nabla^2\mathbf{E}$. The left-hand-side is

$$\big[\nabla \times \big(\nabla \times \mathbf{E}\big)\big]_i \stackrel{1}{=} \epsilon_{ijk}\partial_j\big(\epsilon_{klm}\partial_l E_m\big) \stackrel{2}{=} \big(\delta_{il}\delta_{jm} - \delta_{im}\delta_{jl}\big)\partial_j\partial_l E_m \stackrel{3}{=} \partial_i\partial_j E_j - \partial_j\partial_j E_i.$$

The first step is conversion to index notation. The second applies the identity for contracted Levi-Civita symbols. The third simplifies the Kronecker deltas and tidies up.

Tensors

A vector is a physical quantity with magnitude and direction. Examples include velocity, force, displacement, electric and magnetic fields. A tensor is a physical quantity that generalises this notion in depending (in general) on more than one direction. Examples include stress, strain, conductivity, the dielectric tensor, piezoelectricity, elasticity and the Riemann curvature tensor.

Stress is force per unit area. It characterises the exertion needed to sustain relative motion, or relative displacement, between adjacent material elements. It depends on two directions: the direction of the force f_i; and the direction of the area element dA_j. We write the relation between force, area and stress as

$$f_i = \sigma_{ij} dA_j,$$

where σ_{ij} is the stress tensor. It is easy to see that linearity of the vectors f_i and dA_j implies **bilinearity** of the stress. We say that the stress is a **rank two tensor**.

Closely similar things can be said about conductivity, which describes the physical relationship between an applied electric field E_i and a current flow J_i

$$J_i = \sigma_{ij} E_j.$$

Again, linearity of the two vectors J_i and E_j imply bilinearity for the conductivity σ_{ij}; it is also a rank two tensor. (It is purely coincidental that the conventional symbols for stress and conductivity are the same.)

The degree of linearity of a tensor is called its **rank**. If a tensor is k-linear then we say it is a rank k tensor. Rank 1 tensors are simply vectors[1]. There are plenty of examples of higher rank tensors. For example, the elasticity tensor relating material stress and strain has rank 4, as does the Riemann curvature tensor. We describe briefly one other. We are all familiar with the notion that an elastic material will extend (or compress) under the action of a mechanical force (*i.e.* pulling on it). In some materials the same response can be generated by applying an electric field; this behaviour is called **piezoelectricity**. The electric field E_i induces a material stress σ_{ij}, which the system relaxes by deforming elastically. The relationship between the stress and electric field is linear

$$\sigma_{ij} = \gamma_{ijk} E_k,$$

where γ_{ijk} is the piezoelectric tensor. It is a rank three tensor.

Finally, we wish to emphasise that not all things are tensors and in particular not all things that are written with indices. An important example of a quantity that is not a tensor is a coordinate transformation, for instance rotation matrix R_{ij}. Another example is provided by electrons; they have half-integer spin which turns out not to be a tensor – we call them **spinors**.

Coordinate Transformations. Under a general change of coordinates, the new coordinates x'_i will be related to the old ones by a transformation

$$x'_i = R_{ij} x_j + t_i,$$

where t_i is a translation and R_{ij} an orthogonal transformation – rotation or reflection. In this course we will restrict to transformations that preserve the origin and have $t_i = 0$. These are known as **homogeneous** transformations; they form a group, called the orthogonal group

[1] Rank 0 tensors are scalars, like temperature and density.

$O(n)$. Indeed, any such transformation does not change the length of the vector $\mathbf{x}$, which implies

$$x_i x_i = x'_i x'_i = R_{ij} x_j R_{ik} x_k, \qquad \Rightarrow \quad R_{ij} R_{ik} = \delta_{jk}.$$

The orthogonal group consists of two disconnected components, the transformations that preserve orientation (*i.e.* the rotations) and those that reverse it (*i.e.* the reflections). The rotations form the subgroup of proper coordinate transformations, called the special orthogonal group $SO(n)$.

Since the coordinates x_i are equally the components of the position vector $\mathbf{x}$, the relationship $x'_i = R_{ij} x_j$ also describes how the components of a vector change under the coordinate transformation. Thus, for any other vector like the force f_i or electric field E_i we have the same relationship

$$f'_i = R_{ij} f_j, \qquad\qquad E'_i = R_{ij} E_j.$$

Let us see what this implies for other tensors. We use as an example the conductivity, $J_i = \sigma_{ij} E_j$. We have, trivially, that $J'_i = \sigma'_{ij} E'_j$ and then by the transformation for vector components

$$R_{ik} J_k = \sigma'_{ij} R_{jl} E_l, \qquad \Rightarrow \quad R_{ik} \sigma_{kl} = R_{jl} \sigma'_{ij}.$$

Finally, using that R_{ij} is an orthogonal transformation we can write this as

$$\sigma'_{ij} = R_{ik} R_{jl} \sigma_{kl}.$$

For a tensor of rank n, one finds the natural extension of this relationship: the components transform according to

$$T'_{i_1 i_2 \cdots i_n} = R_{i_1 j_1} R_{i_2 j_2} \cdots R_{i_n j_n} T_{j_1 j_2 \cdots j_n}.$$

In some presentations this transformation law is upgraded to the definition of a rank n tensor.

Isotropic Tensors. The term **isotropic** is used to convey that some property or quantity has no intrinsic directionality, or 'looks the same from all directions'. For a tensor to be isotropic its components must be the same for all choices of coordinates, *i.e.*

$$T'_{i_1 i_2 \cdots i_n} = T_{i_1 i_2 \cdots i_n}, \qquad \Rightarrow \quad T_{i_1 i_2 \cdots i_n} = R_{i_1 j_1} R_{i_2 j_2} \cdots R_{i_n j_n} T_{j_1 j_2 \cdots j_n},$$

for all R_{ij}. This places strong constraints on the form any such **isotropic tensor** can take.

Exercise: Show that $\mathbf{0}$ is the only isotropic vector.

Example: The Kronecker delta is isotropic. Indeed,

$$R_{ik} R_{jl} \delta_{kl} = \delta_{ij},$$

since R_{ij} is orthogonal.

In fact, the only (independent) isotropic rank 2 tensors in two dimensions are δ_{ij} and ϵ_{ij}, while in three dimensions the only isotropic rank 2 tensor is δ_{ij}. We prove the former. The idea is to choose particular transformations R_{ij} that restrict the possible values the components T_{ij} can take. For instance, a rotation by 90°, which is represented by the transformation $\left[\begin{smallmatrix} 0 & 1 \\ -1 & 0 \end{smallmatrix}\right]$ gives the relations

$$T_{11} = R_{1k} R_{1l} T_{kl} = T_{22},$$
$$T_{12} = R_{1k} R_{2l} T_{kl} = -T_{21},$$

and this already reduces things to the form

$$T_{ij} = \begin{bmatrix} A & B \\ -B & A \end{bmatrix}_{ij} = A\delta_{ij} + B\epsilon_{ij}.$$

We have already seen that δ_{ij} is isotropic, so to verfiy that we cannot reduce any further we need only check that ϵ_{ij} is also isotropic.

Exercise: Check that ϵ_{ij} is isotropic.

We state without proof that in three dimensions there is only one (linearly independent) rank 3 isotropic tensor — namely the Levi-Civita tensor ϵ_{ijk} — however there are three linearly independent rank 4 isotropic tensors

$$\delta_{ij}\delta_{kl}, \qquad \delta_{ik}\delta_{jl}, \qquad \text{and} \qquad \delta_{il}\delta_{jk}.$$

Elasticity. The elastic distortion of a material is described in terms of the **Eulerian displacement field**, u_i, which specifies the displacement of each material point from its 'rest' location. Evidently, uniform displacements do not distort the material, so the elasticity is really sensitive to the gradients in the displacement field $\partial_i u_j$, which are called material **strains**. How the material responds is contained in a relationship between the stress σ_{ij} it experiences in response to a given strain

$$\sigma_{ij} = C_{ijkl}\partial_k u_l.$$

Here, C_{ijkl} is a rank 4 tensor characteristic of the material – the **elasticity tensor**. If the material is isotropic then this must be an isotropic tensor and hence of the form (in three dimensions)

$$C_{ijkl} = C^{(1)}\delta_{ij}\delta_{kl} + C^{(2)}\delta_{ik}\delta_{jl} + C^{(3)}\delta_{il}\delta_{jk}.$$

However, general arguments involving conservation of angular momentum establish that the stress tensor is symmetric $\sigma_{ij} = \sigma_{ji}$, which requires that $C^{(2)} = C^{(3)}$. In other words, the elastic response of an isotropic material depends on just two material dependent parameters. In standard form the stress-strain relation is written

$$\sigma_{ij} = B\left(\partial_k u_k\right)\delta_{ij} + G\left(\partial_i u_j + \partial_j u_i - \left(\partial_k u_k\right)\frac{2}{3}\delta_{ij}\right),$$

where B is the **bulk modulus** and G the **shear modulus**.