F32CO5 Wave phenomena (F32FOU Fourier methods)
4. Fourier methods summary

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Contents

1 Introduction to Fourier analysis

Fourier analysis involves writing a function as a superposition of waves of different frequencies. We will first look at Fourier series (writing periodic functions as a sum of waves) before moving on to Fourier transforms (writing functions as an integral of waves).

1.1 Applications

Fourier analysis has applications in many areas of science (including physics, engineering, chemistry and materials science) and also everyday life (digital phones, DVDs, JPEGs...).

The physics related applications include

- **Optics**
  Light can be decomposed into spectral components and certain colours filtered out. We will also see in Sec. 6 that Fraunhofer diffraction calculations are easier using Fourier techniques.
- **Acoustics**
  Notes played on different instruments are made up of different frequency components (not just a pure sine wave with a single frequency), see e.g. http://www.phy.mtu.edu/~suits/sax_sounds/index.html for a comparison of saxophone sounds. If you know what frequencies a particular real instrument produces you can electronically reproduce its sound. You can also design speakers or auditoria suited to the music played through or in them. We saw in *Fourier 1* how Fourier analysis allows you to filter out unwanted noises (i.e. a vuvuzuela) and is behind the operation of touch-tone phones.
- **Electronics**
  Any desired signal (e.g. square wave, sawtooth) can be generated from a sum of harmonic (sin and cos) waves. Filters can be used to modify signals. For instance a low pass filter removes high frequency components (i.e. it lets low frequencies pass, hence the name). The web-site http://www.falstad.com/dfilter/ lets you see (and hear) the effect of various filters on different signals.
- **Image processing**
  Images can be enhanced by manipulating their frequency components. For instance a low pass filter reduces noise (which tends to occur on small scales, and hence has a high frequency). A high pass filter enhances edges (which are also a small scale feature and hence correspond to high frequencies). This has many applications, in areas ranging from the real world (removing noise from images of bar codes) to astronomy (deblurring images of galaxies). We'll see how this works in *Fourier 8*.

1.2 Textbooks

The lectures are mainly based on chapters 12 and 13 of the recommended 2nd year maths textbook: 'Mathematical methods for physics and engineering', K. F. Riley, M. P. Hobson and

S. J. Bence (available from the library as an e-book).

There are many other relevant textbooks:

- ‘Mathematical methods in the physical sciences’, M. L. Boas
- ‘Lectures on Fourier series’, L. Solymar
- ‘Fourier analysis’, H. P. Hsu
- ‘Fourier analysis’, M. R. Spiegel
- ‘A student’s guide to Fourier transforms’, J. F. James

which you might find useful for alternative/additional explanations and problems. However beware that different books sometimes have different conventions/definitions (e.g. for the normalization of the Fourier transform).

The optics textbooks (‘Introduction to optics’, Pedrotti, Pedrotti and Pedrotti and ‘Optics’, Hecht) will be useful for the optics applications towards the end of the module.

1.3 Problems

The only way to learn how to solve physics problems is to practise (this is especially true of more mathematical topics, like Fourier analysis). There are plenty of practice problems available: ‘homework’ problems in lectures, problem sheets, textbooks and past exam papers (available from Moodle). Fourier analysis was previously covered in F32AM4: Elements of mathematical physics. See Moodle for a list of recommended problems from textbooks.

Answers to the workshop questions and examples sheets will be available from Moodle. You’ll get far more benefit from the questions if you try them yourself first before looking at the answers.

1.4 Some useful maths

Fourier analysis will use maths techniques and results which you covered in first year. You will need to be familiar with using them to be able to do Fourier analysis calculations. WolframAlpha (http://www.wolframalpha.com/) is useful for checking integrals (and other calculations). However you need to be able to do the calculations on your own: you won’t have access to WolframAlpha in the exam!

1.4.1 Trigonometric functions

Cosine is an even function, $\cos(-\theta) = \cos(\theta)$, while sine is odd, $\sin(-\theta) = -\sin(\theta)$. The values of $\sin\theta$ and $\cos\theta$ at integer multiples of π are given by

$$\sin(n\pi) = 0\,, \tag{1}$$
$$\cos(n\pi) = (-1)^n\,. \tag{2}$$

Products of trigonometric functions can be expressed in terms of sums of trigonometric functions (and vice versa) using:

$$\sin(A \pm B) = \sin A \cos B \pm \cos A \sin B\,, \tag{3}$$
$$\cos(A \pm B) = \cos A \cos B \mp \sin A \sin B\,. \tag{4}$$

The integral of sine or cos over a period is zero i.e.:

$$\int_0^L \sin\left(\frac{2\pi x}{L}\right) \mathrm{d}x = 0\,. \tag{5}$$

1.4.2 $\exp(i\theta)$

Euler's equation tells us that

$$\exp(i\theta) = \cos\theta + i\sin\theta\,, \tag{6}$$

and $\cos\theta$ and $\sin\theta$ can be written in terms of exponentials:

$$\cos\theta = \frac{\exp(i\theta) + \exp(-i\theta)}{2}\,, \tag{7}$$
$$\sin\theta = \frac{\exp(i\theta) - \exp(-i\theta)}{2i}\,. \tag{8}$$

You should memorize these expressions (as they come up repeatedly in Fourier analysis calculations), however if you forget them you can derive them quickly (see week 19 coursework).

The value of $\exp(i\theta)$ at integer multiples of π is given by

$$\exp(i\pi n) = (-1)^n\,. \tag{9}$$

1.4.3 Powers

Products of power can be combined into a single power e.g.

$$x^a x^b = x^{(a+b)}\,, \quad \exp(a)\exp(b) = \exp(a+b)\,. \tag{10}$$

This is useful in particular when integrating. It's also sometime useful to split a power up (we'll do this when we study the orthogonality of exponentials in *Fourier 4*).

1.4.4 Integration

Fourier analysis involves a lot of integration (in particular of functions multiplied by an exponential or cos or sine).
The integral of the exponential function is the exponential function:

$$\int_{x_1}^{x_2} \exp x \,\mathrm{d}x = [\exp x]_{x_1}^{x_2} = \exp x_2 - \exp x_1\,. \tag{11}$$

The definite integral of zero is zero:

$$\int_{x_1}^{x_2} 0 \,\mathrm{d}x = [\mathrm{c}]_{x_1}^{x_2} = (c - c) = 0\,, \tag{12}$$

(c is a constant). You will sometimes need to use integration by parts:

$$\int u \frac{\mathrm{d}v}{\mathrm{d}x}\,\mathrm{d}x = uv - \int \frac{\mathrm{d}u}{\mathrm{d}x} v\,\mathrm{d}x\,. \tag{13}$$

When you integrate a function of the integration variable times a constant, the result is the integral of the function, divided by the constant:

$$\int f'(ax)\,\mathrm{d}x = \frac{1}{a} f(ax)\,, \tag{14}$$

where a is a constant and $f' \equiv \mathrm{d}f/\mathrm{d}x$. You can show this by making the substitution $y = ax$, so that $\mathrm{d}y = a\mathrm{d}x$ and

$$\int f'(ax)\,\mathrm{d}x = \frac{1}{a}\int f'(y)\,\mathrm{d}y = \frac{1}{a} f(y) = \frac{1}{a} f(ax)\,. \tag{15}$$

An example of this sort of integral, which we'll encounter in Fourier analysis, is $f = \sin(ax)$ and $a = 2\pi/L$:

$$\int_{x_1}^{x_2} \sin\left(\frac{2\pi x}{L}\right)\mathrm{d}x = \frac{L}{2\pi}\left[-\cos\left(\frac{2\pi x}{L}\right)\right]_{x_1}^{x_2}\,. \tag{16}$$

When doing calculations yourself you can use as many steps and substitutions as you like, but in lectures we will use these results without going through all the steps. A way of checking that you've got an integral right is to differentiate your result (and check that you get the function you were originally trying to integrate).

1.5 Appendices

The appendices of these notes contain additional derivations or calculations, which are outside the syllabus (and hence non-examinable), but may be of interest.

2 Fourier series (RHB 12)

2.1 Periodicity and harmonics

A spatial function is periodic if $f(x) = f(x+L)$ for all x, where L is the period of the function. A function of time is periodic if $f(t) = f(t+T)$ for all t, where T is the time period of the function. For instance $\sin\theta$ is periodic with period 2π since $\sin\theta = \sin(\theta + 2\pi)$ for all θ.

Consider the function $f(x) = \sin(2\pi r x/L)$ where r is a integer. We showed in *Fourier 1* that this has period L/r. It's sometimes useful to define a fundamental wavenumber

$$k_0 = \frac{2\pi}{L}\,, \tag{17}$$

or, for a function of time, a fundamental frequency

$$\omega_0 = \frac{2\pi}{T}\,. \tag{18}$$

The function $f(x)$ above can then be rewritten as $f(x) = \sin(k_r x)$ where $k_r = r k_0$. These waves with wavenumbers that are an integer multiple of the fundamental wavenumber are called harmonics. The function $f(x)$ and its first two harmonics ($r = 2$ and 3) are shown in Fig. 1.

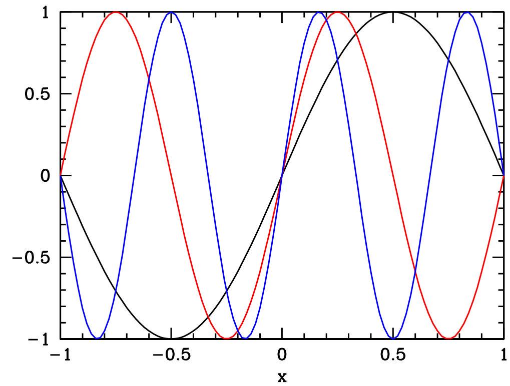

Figure 1: $f(x) = \sin(\pi x)$ and its first two harmonics ($\sin(r\pi x)$ with $r = 2$ in red and $r = 3$ in blue).

2.2 Trigonometric form (RHB 12.2)

Most [1] periodic functions can be written as a sum of harmonic waves (i.e. sine and cos) with different frequencies:

$$f(x) = \frac{a_0}{2} + \sum_{r=1}^{\infty} \left[a_r \cos\left(\frac{2\pi r x}{L}\right) + b_r \sin\left(\frac{2\pi r x}{L}\right) \right] , \tag{19}$$

or equivalently

$$f(x) = \frac{a_0}{2} + \sum_{r=1}^{\infty} \left[a_r \cos(r k_0 x) + b_r \sin(r k_0 x) \right] , \tag{20}$$

with the fundamental wavenumber k_0 defined in eq. (17) above. This is known as the trigonometric form of the Fourier series. The waves making up the Fourier series are harmonics of the fundamental wavenumber; they have wavenumbers that are integer multiples of the fundamental wavenumber: $k_r = r k_0$. Exactly the same thing can be done for functions of time, rather than space, with $x \to t$, $k \to \omega$ and $L \to T$.

The coefficients of the Fourier series are calculated using

$$a_r = \frac{2}{L} \int_{x_0}^{x_0+L} f(x) \cos\left(\frac{2\pi r x}{L}\right) \mathrm{d}x \, , \tag{21}$$

$$b_r = \frac{2}{L} \int_{x_0}^{x_0+L} f(x) \sin\left(\frac{2\pi r x}{L}\right) \mathrm{d}x \, , \tag{22}$$

[1] There are some conditions which the function has to be satisfy, we'll look at these in Sec. 2.3.

or equivalently

$$
\begin{aligned}
a_r &= \frac{2}{L}\int_{x_0}^{x_0+L} f(x)\cos\left(rk_0x\right)\mathrm{d}x\,, &(23)\\
b_r &= \frac{2}{L}\int_{x_0}^{x_0+L} f(x)\sin\left(rk_0x\right)\mathrm{d}x\,. &(24)
\end{aligned}
$$

x_0 is arbitrary (the integration just has to be done over a period). You can chose x_0 to be whatever you like, however it often makes the calculations easier to chose $x_0 = 0$ or $-L/2$. The expression for a_0 can be found by setting $r = 0$ in the equation for a_r:

$$
a_0 = \frac{2}{L}\int_{x_0}^{x_0+L} f(x)\,\mathrm{d}x\,. \tag{25}
$$

The first term in the Fourier series, $a_0/2$, is the average value of the function over a period.

We derived the expression for a_r in *Fourier 2* by multiplying the Fourier series for $f(x)$, eq. (19), by $\cos\left(2\pi px/L\right)$, integrating over a period and using the orthogonality of sine and cos:

$$
\int_{x_0}^{x_0+L} \sin\left(\frac{2\pi rx}{L}\right)\sin\left(\frac{2\pi px}{L}\right)\mathrm{d}x = \begin{cases} 0 & \text{if } r=p=0\,, \\ \frac{L}{2} & \text{if } r=p>0\,, \\ 0 & \text{if } r\neq p\,, \end{cases} \tag{26}
$$

$$
\int_{x_0}^{x_0+L} \cos\left(\frac{2\pi rx}{L}\right)\cos\left(\frac{2\pi px}{L}\right)\mathrm{d}x = \begin{cases} L & \text{if } r=p=0\,, \\ \frac{L}{2} & \text{if } r=p>0\,, \\ 0 & \text{if } r\neq p\,, \end{cases} \tag{27}
$$

$$
\int_{x_0}^{x_0+L} \sin\left(\frac{2\pi rx}{L}\right)\cos\left(\frac{2\pi px}{L}\right)\mathrm{d}x = 0\,. \tag{28}
$$

These formulae can themselves be derived using the trigonometric identities in eqs. (3) and (4). We derived eq. (26) in *Fourier 2*.

As an example we looked at a square wave

$$
f(x) = \begin{cases} 0 & \text{if } -1<x<0\,, \\ 1 & \text{if } 0<x<1\,. \end{cases} \tag{29}
$$

In *Fourier 3* we found that its Fourier coefficients are $a_0 = 1$, $a_r = 0$ for $r \neq 0$ and

$$
b_r = \begin{cases} 0 & r \text{ even}\,, \\ \frac{2}{\pi r} & r \text{ odd}\,, \end{cases} \tag{30}
$$

i.e. $b_1 = 2/\pi$, $b_2 = 0$, $b_3 = 2/(3\pi)$ and so on. In other words it can be built up from a constant plus a sum of sine waves:

$$
f(x) = \frac{1}{2} + \left(\frac{2}{\pi}\right)\left[\sin\left(\pi x\right) + \frac{\sin\left(3\pi x\right)}{3\pi x} + ...\right], \tag{31}
$$

which can be written more compactly as a sum:

$$f(x) = \frac{1}{2} + \left(\frac{2}{\pi}\right) \sum_{j=0}^{\infty} \frac{\sin[(2j+1)\pi x]}{(2j+1)} \; . \tag{32}$$

If $j = 0, 1, 2, ...$, then $(2j + 1) = 1, 3, 5, ...$ so that we get odd multiples of πx in the sum, as required. We could have used $(2j - 1)$ instead. In that case the sum would start at $j = 1$, so that $(2j-1) = 1, 3, 5, ...$ still. In Sec. 2.4 we'll see why only sine waves are needed in this case.

The web-site http://www.falstad.com/dfilter/ allows you to experiment and see how different functions can be made from sine and cosine waves (and you will do (or did) this yourself using Matlab in the first Waves/Fourier workshop this semester).

2.3 Dirichlet conditions (RHB 12.1 & 12.4)

If a function $f(x)$

1. is periodic,
2. is single valued and continuous (except possibly at a finite number of finite discontinuities per period),
3. has only a finite number of maxima and minima within one period,
4. the integral over one period of $|f(x)|$ converges,

then it can be expanded as a Fourier series which converges to $f(x)$ at all points where $f(x)$ is continuous.

At discontinuities the value of the Fourier series converges to the mean of the values of the function either side of the discontinuity i.e. if a discontinuity occurs at $x = x_{\rm d}$ then

$$f(x_{\rm d}) \rightarrow \frac{1}{2}\lim_{\epsilon\rightarrow 0}\left[f(x_{\rm d} + \epsilon) + f(x_{\rm d} - \epsilon)\right] \; . \tag{33}$$

Close to the discontinuity the series overshoots the value of the function. This is known as Gibbs' phenomenon. As the number of terms included in the Fourier series is increased the position of the overshoot moves closer to the discontinuity, but it never disappears, even in the limit of an infinite number of terms. Fig. 2 shows the sum of the first 20 terms of the Fourier series of our square wave. The Gibbs' phenomenon is visible at $x = \pm n$.

2.4 Odd and even functions (RHB 12.3)

Even functions: A function is even if $f(x) = f(-x)$. Examples of even functions include $f(x) = x^2$ and $\cos x$ (we can show that x^2 is even easily: $f(-x) = (-x)^2 = x^2 = f(x)$). For an even function the graph for negative x is the graph for positive x reflected in the y-axis.

Odd functions: A function is odd if $f(x) = -f(-x)$. Examples of odd functions include $f(x) = x$ and $\sin x$ (we can show that x is odd easily: $f(-x) = (-x) = -x = -f(x)$). For

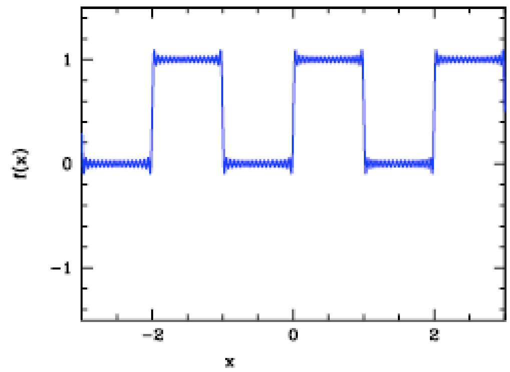

Figure 2: Sum of the first 20 terms of the Fourier series of our square wave.

an odd function the graph for negative x is the graph for positive x reflected in the x and the y-axes (one after the other).

Some functions are neither odd nor even. In other words they satisfy neither $f(x) = f(-x)$ nor $f(x) = -f(-x)$. Fig. 3 shows examples of functions that are odd, even and neither odd nor even.

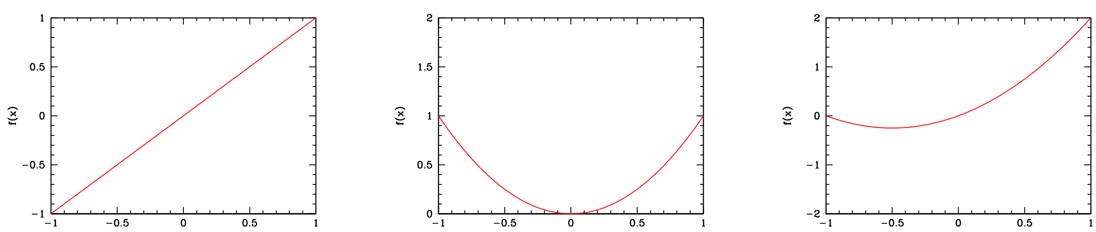

Figure 3: An example of an odd function, $f(x) = x$, (left) and an even function, $f(x) = x^2$ (middle). The function in the right hand panel, $f(x) = x + x^2$, is neither odd nor even.

Since cos is even and sine is odd, the Fourier series of an even function only contains cosine terms, while the Fourier series of an odd function only contains sine terms. The properties of the products of odd and even functions and their integrals (see Appendix A) also allow us to simplify the calculation of the non-zero coefficients:

Even function

$$
\begin{aligned}
a_r &= \frac{4}{L}\int_0^{L/2} f(x)\,\cos\left(\frac{2\pi r x}{L}\right)\mathrm{d}x\,, && (34)\\
b_r &= 0\,. && (35)
\end{aligned}
$$

Odd function

$$
\begin{aligned}
a_r &= 0\,, && (36)\\
b_r &= \frac{4}{L}\int_0^{L/2} f(x)\,\sin\left(\frac{2\pi r x}{L}\right)\mathrm{d}x\,. && (37)
\end{aligned}
$$

Thinking about whether a function is odd or even before calculating the Fourier series will save you doing unnecessary calculations (i.e. calculating coefficients which must be zero).

2.5 Analytic continuation (RHB 12.5)

If a function is only specified over a finite range we need to extend it outside the specified range to make it periodic. This is known as analytic continuation. The Fourier series then correctly represents the original function over the originally specified range. In some cases we can choose to make the extended function odd or even (which reduces the number of calculations required). The period of the function (e.g. L or $2L$) depends on how it's extended. The extension should ideally be continuous at the end-points (otherwise the Fourier series won't converge to the required values at these points).

2.6 Complex form (RHB 12.7)

Since sine and cos can be expressed in terms of exponentials, eqs. (7) and (8), the Fourier series can also be written as a sum of exponential waves:

$$
f(x) = \sum_{r=-\infty}^{\infty} c_r \exp\left(\frac{2\pi i r x}{L}\right), \tag{38}
$$

or equivalently

$$
f(x) = \sum_{r=-\infty}^{\infty} c_r \exp\left(i k_0 r x\right), \tag{39}
$$

where the fundamental wavenumber k_0 is defined in eq. (17) as before. This is known as the complex form, as the coefficients of the series, c_r, are in general complex. Calculations are typically easier using the complex form, however it is easier to visualise the trigonometric Fourier series. Note that the sum over r runs from $-\infty$ to ∞ (rather than 0 to ∞ as in the case of the trigonometric Fourier series).

The coefficients of the complex Fourier series are calculated using

$$
c_r = \frac{1}{L}\int_{x_0}^{x_0+L} f(x)\exp\left(-\frac{2\pi i r x}{L}\right)\mathrm{d}x\,. \tag{40}
$$

We derived this expression in *Fourier 4* by multiplying the Fourier series for $f(x)$, eq. (38), by $\exp(2\pi ipx/L)$, integrating over a period and using the orthogonality of exponentials (homework from *Fourier 4*):

$$\int_{x_0}^{x_0+L} \exp\left(-\frac{2\pi ipx}{L}\right)\exp\left(\frac{2\pi irx}{L}\right) \mathrm{d}x \;=\; \begin{cases} L & \text{if } r = p\,, \\ 0 & \text{if } r \neq p\,. \end{cases} \tag{41}$$

It can be shown (see Appendix B) using eqs. (7) and (8), that the complex form of the Fourier series is equivalent to the trigonometric form with:

$$c_0 \;=\; \frac{a_0}{2}\,, \tag{42}$$

$$c_r \;=\; \frac{1}{2}(a_r - ib_r)\,, \tag{43}$$

$$c_{-r} \;=\; \frac{1}{2}(a_r + ib_r)\,. \tag{44}$$

If

- $f(x)$ is even then the c_r are real ($b_r = 0$).
- $f(x)$ is odd then the c_r are imaginary ($a_r = 0$).
- $f(x)$ is neither even nor odd then the c_r are complex.
- $f(x)$ is real then $c_{-r} = c_r^\star$, where $\star$ denotes the complex conjugate.

In *Fourier 4* we found the co-efficients of the complex Fourier series of our square wave, eq. (29): $c_0 = 1/2$ and

$$c_r = \frac{i}{2\pi r}[(-1)^r - 1] = \begin{cases} 0 & \text{if } r \text{ is even}\,, \\ -\frac{i}{\pi r} & \text{if } r \text{ is odd}\,, \end{cases} \tag{45}$$

so the complex Fourier series can be written as

$$f(x) \;=\; \frac{1}{2} - \frac{i}{\pi}\left[(\exp(i\pi x) - \exp(-i\pi x)) + \frac{1}{3}(\exp(3i\pi x) - \exp(-3i\pi x)) + ...\right], \tag{46}$$

$$\;=\; \frac{1}{2} + \frac{i}{\pi}\left[\sum_{j=0}^{\infty} \frac{\exp(-(2j+1)i\pi x) - \exp((2j+1)i\pi x)}{2j+1}\right]. \tag{47}$$

Using eq. (7) we can rewrite this as

$$f(x) = \frac{1}{2} + \left(\frac{2}{\pi}\right)\sum_{j=0}^{\infty} \frac{\sin((2j+1)\pi x)}{(2j+1)}\,, \tag{48}$$

recovering the trigonometric Fourier series, eq. (32).

2.7 Parseval's theorem (RHB 12.8)

Parseval's theorem relates the mean, over a period, of the modulus squared of the function to the sum of the squares of the moduli of the Fourier co-efficients:

$$\frac{1}{L}\int_{x_0}^{x_0+L} |f(x)|^2\,\mathrm{d}x = \sum_{r=-\infty}^{\infty} |c_r|^2 = \left(\frac{a_0}{2}\right)^2 + \frac{1}{2}\sum_{r=1}^{\infty}\left(a_r^2+b_r^2\right)\ . \tag{49}$$

This is useful for finding the intensity of a sound wave or the energy dissipated in an electrical circuit (both of which are proportional to the square of the amplitude of the wave/signal). Instead of integrating the expression for the square of the pressure or current directly you can use Parseval's theorem and a known expression for the sum of the squares of the Fourier co-efficients.

It can also be used (in the opposite direction) to find the sum of a series. If you know the function whose Fourier co-efficients squared are the series you want to sum, then you can integrate the square of the function directly and use Parseval's theorem to evaluate the sum of the series (see e.g. Fourier series problem sheet q10c).

The derivation of Parseval's theorem for the complex form, which we went through in *Fourier 4*, involves taking the complex conjugate of the expression for the Fourier series of $f(x)$, multiplying this by the Fourier series of $f(x)$ and integrating over a period.

2.8 Graphical representation

This involves simply plotting the coefficients of the Fourier series as a function of r. Since the coefficients of the complex Fourier series are complex the real and imaginary parts have to be plotted separately. The coefficients of the trigonometric Fourier series of our square wave, eq. (30), are plotted in Fig. 4 and the coefficients of the complex Fourier series, eq. (45), are plotted in Fig. 5. The dotted line shows the envelope of the coefficients. Don't forget that the coefficients are discrete (i.e. r only takes integer values).

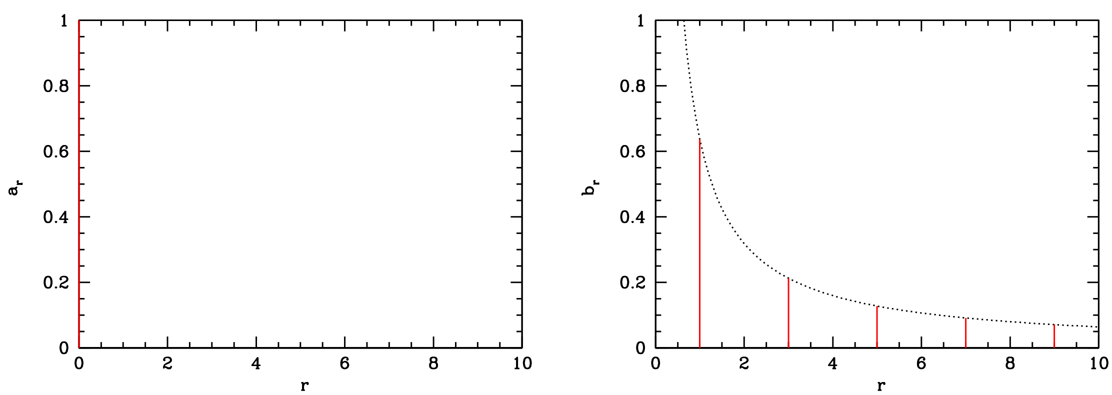

Figure 4: Coefficients of the trigonometric Fourier series, a_r left and b_r right, of our square wave, eq. (30). The dotted blue line shows the envelope of the coefficients.

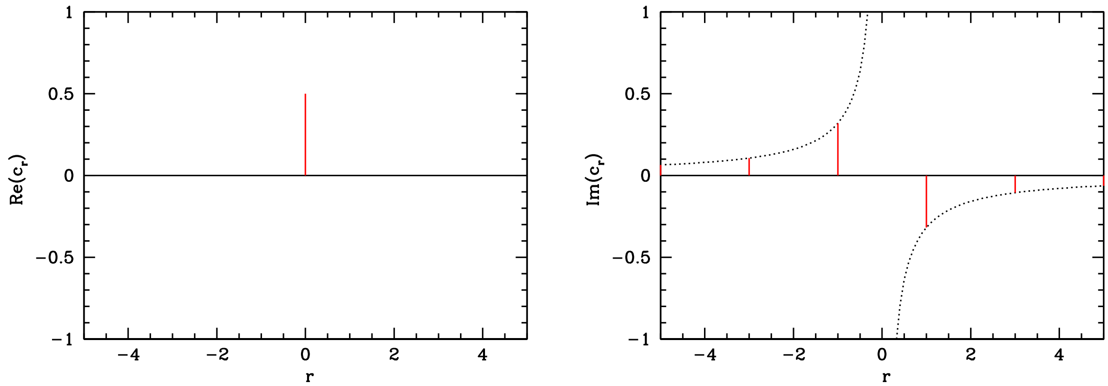

Figure 5: Real (left) and imaginary (right) parts of the coefficients of the complex Fourier series of our square wave, eq. (45).

3 Fourier transforms (RHB 13.1)

3.1 Introduction and definitions

We saw in the previous section that periodic functions can be written as a Fourier series, a sum of waves with frequencies that are integer multiples of the fundamental frequency. However most functions that appear in nature are non-periodic (for instance a voltage pulse in a circuit, wave trains in optics and wave functions in quantum mechanics). We'll now see that for non-periodic functions we can generalise the Fourier series to the Fourier transform.

First let's consider a rectangular wave with unequal peaks and troughs:

$$f(t) = \begin{cases} 1 & \text{if } nT - \Delta/2 \leq t \leq nT + \Delta/2\,, \\ 0 & \text{otherwise}\,, \end{cases} \tag{50}$$

where n is an integer, T is the period of the rectangular wave and Δ is the width of the peaks. We found in *Fourier 5* that the coefficients of the complex Fourier series of this function are

$$c_r = \frac{\Delta}{T} \text{sinc} \left(\frac{\omega_r \Delta}{2} \right) , \tag{51}$$

where $\omega_r = r\omega_0 = 2\pi r/T$ and

$$\text{sinc}(x) \equiv \frac{\sin x}{x} \,. \tag{52}$$

At this point we'll take a slight diversion and study the properties of the sinc function. As $x \rightarrow 0$

$$\lim_{x\rightarrow 0}(\text{sinc}(x)) = \lim_{x\rightarrow 0} \left(\frac{x - \frac{x^3}{3} + ...}{x} \right) = \lim_{x\rightarrow 0} \left(1 - \frac{x^2}{2} + ... \right) = 1\,. \tag{53}$$

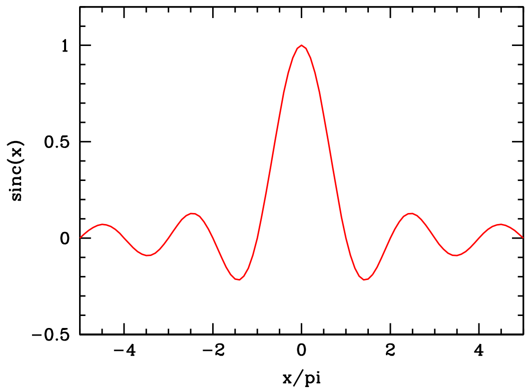

Figure 6: The sinc function.

Alternatively this can be seen using l'Hopitals rule: if $f(x) = g(x)/h(x)$ and $\lim_{x\to x_0}(g(x)) \to 0$ and $\lim_{x\to x_0}(h(x)) \to 0$ then

$$\lim_{x\to x_0}(f(x)) = \frac{\lim_{x\to x_0}\left(\frac{\mathrm{d}g(x)}{\mathrm{d}x}\right)}{\lim_{x\to x_0}\left(\frac{\mathrm{d}h(x)}{\mathrm{d}x}\right)} . \tag{54}$$

In this case we have

$$\lim_{x\to 0}(\mathrm{sinc}(x)) = \frac{\lim_{x\to 0}\left(\frac{\mathrm{d}\sin x}{\mathrm{d}x}\right)}{\lim_{x\to 0}\left(\frac{\mathrm{d}x}{\mathrm{d}x}\right)} = \frac{\lim_{x\to 0}(\cos x)}{\lim_{x\to 0}(1)} = 1 . \tag{55}$$

For $x \neq 0$, $\mathrm{sinc}(x) = 0$ when $\sin x = 0$ i.e. when $x = n\pi$ with $n = \pm 1, \pm 2, ...$ (but not $n = 0$). The sinc function is plotted in Fig. 6. The width of the sinc function (i.e. the gap between the first zeros) is $\Delta x = 2\pi$.

Returning to the square wave with uneven peaks and troughs, if we increase T the gaps between the peaks get larger. What happens to the coefficients of the Fourier series? The pre-factor in the expression for c_r, (Δ/T), will get smaller, and the gap between the frequencies $\omega_{r+1} - \omega_r = (r+1)\omega_0 - r\omega_0 = \omega_0 = 2\pi/T$ will get smaller (see plots in Fig. 7).

If we take $T \to \infty$ the square wave will become a single pulse of width Δ (i.e. a non-periodic top-hat function). What happens to the coefficients of the Fourier series? The shape of the envelope of c_r stays the same but its amplitude tends to zero. The envelope of the coefficients multiplied by T remains constant

$$c_r T = \mathrm{sinc}\left(\frac{\omega_r \Delta}{2}\right) , \tag{56}$$

as it is independent of T [2]. The gap between the frequencies $\omega_{r+1} - \omega_r = 2\pi/T$ tends to zero. Therefore in the limit $T \to \infty$ instead of a series of discrete values of ω_r we get a continuous function of ω.

[2]If our initial function had had a different shape, then the shape of the envelope would have been different. The general behaviour, in particular the fact that $c_r T$ is independent of T, would have been the same however.

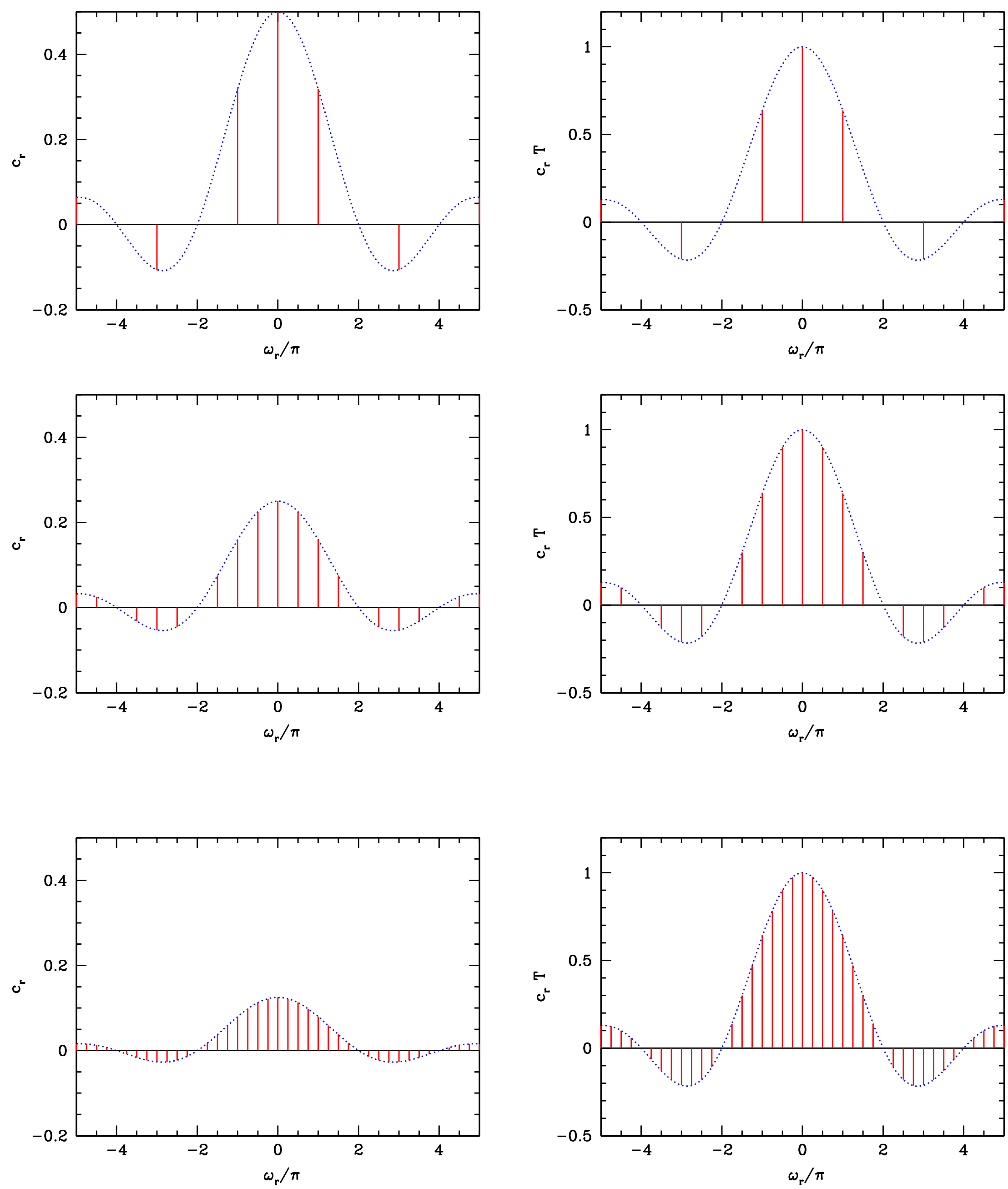

Figure 7: The coefficients, c_r, (left) and products $c_r T$ (right) of the complex Fourier series of the square wave with unequal peaks and troughs, eq. (50), for $\Delta = 1$ and (from top to bottom) $T = 2, 4$ and 8.

If we take the expression for the coefficients of the Fourier series and multiply it by T:

$$c_r T = \int_{t_0}^{t_0+T} f(t) \exp\left(-i\omega_0 r t\right) \mathrm{d}t \,, \tag{57}$$

and make the substitutions $\omega_r = r\omega_0 \to \omega$ and $c_r T \to \sqrt{2\pi} F(\omega)$ [3] we get the definition of the Fourier transform:

$$F(\omega) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} f(t) \exp\left(-i\omega t\right) \mathrm{d}t \,. \tag{58}$$

Similarly from the definition of the Fourier series

$$f(t) = \sum_{r=-\infty}^{\infty} c_r \exp\left(i\omega_0 r t\right) , \tag{59}$$

we get the definition of the inverse Fourier transform:

$$f(t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} F(\omega) \exp\left(i\omega t\right) \mathrm{d}\omega \,. \tag{60}$$

Note that there are different conventions for the pre-factors in the definitions of the Fourier transform and its inverse. In general

$$F(\omega) = A \int_{-\infty}^{\infty} f(t) \exp\left(-i\omega t\right) \mathrm{d}t \,, \tag{61}$$

$$f(t) = B \int_{-\infty}^{\infty} F(\omega) \exp\left(i\omega t\right) \mathrm{d}\omega \,, \tag{62}$$

where we must have $AB = 1/(2\pi)$ if the original function $f(t)$ is to be recovered when $F(\omega)$ calculated using eq. (61) is inserted in eq. (62) (see Appendix D for a derivation which uses some of the properties of the Dirac delta-function which we derive in *Fourier 6*). We have followed Riley, Hobson and Bence and 'divided' the (2π) symmetrically between the Fourier transform and its inverse. Some other textbooks use $A = 1, B = 2\pi$ or $A = 2\pi, B = 1$ (so take care if using results or equations from different sources). As with the Fourier series, the same relations hold for spatial functions with $t \to x$ and $\omega \to k$.

Our original rectangular wave with unequal peaks and troughs could be written as a complex Fourier series with coefficients

$$c_r = \frac{\Delta}{T} \mathrm{sinc}\left(\frac{\omega_r \Delta}{2}\right) . \tag{63}$$

As $T \to \infty$ we get a single 'top-hat' pulse of width Δ:

$$f(t) = \begin{cases} 1 & \text{if } -\Delta/2 \le t \le \Delta/2 \,, \\ 0 & \text{otherwise} \,, \end{cases} \tag{64}$$

which has Fourier transform

$$F(\omega) = \frac{\tau}{\sqrt{2\pi}} \mathrm{sinc}\left(\frac{\omega \Delta}{2}\right) . \tag{65}$$

[3] See the paragraph beneath eq. (62) for the explanation of where the $\sqrt{2\pi}$ comes from.

n.b. to illustrate how the Fourier transform arises from for the Fourier series we've calculated the Fourier transform of the top-hat function by taking the $T \to \infty$ limit of the Fourier series of a rectangular wave with unequal peaks and troughs. However this is not how you calculate Fourier transforms in general. You take whatever function you're interested it and insert it in the definition of the Fourier transform, eq. (58).

To summarise, a Fourier series expresses a periodic function as a sum of exponential waves, weighted by discrete coefficients, c_r. A Fourier transform expresses a function as an integral of exponentials, weighted by a continuous function $F(\omega)$. Both c_r and $F(\omega)$ are, in general, complex.

3.2 Dirac delta-function (RHB 13.1.3)

If we normalise the single 'top-hat' pulse of width Δ so that its integral equals one:

$$f(t) = \begin{cases} \frac{1}{\Delta} & \text{if } -\Delta/2 \le t \le \Delta/2\,, \\ 0 & \text{otherwise}\,, \end{cases} \tag{66}$$

then its Fourier transform is given by

$$F(\omega) = \frac{1}{\sqrt{2\pi}} \text{sinc}\left(\frac{\omega\Delta}{2}\right)\,. \tag{67}$$

What happens to $f(t)$ and $F(\omega)$ as Δ is decreased? The width of $f(t)$ decreases and its amplitude increases. $F(0)$ remains constant ($F(0) = 1/\sqrt{2\pi}$ independent of Δ) and the peaks in the sinc function spread out (the first zeros are at $\omega = \pm 2\pi/\Delta$).

In the limit that $\Delta \to 0$ the single top-hat pulse tends to something called the Dirac delta-function:

$$f(t) \to \delta(t) = \begin{cases} \infty & \text{if } t = 0\,, \\ 0 & \text{otherwise}\,, \end{cases} \tag{68}$$

and its Fourier transform tends towards a constant

$$F(\omega) \to \frac{1}{\sqrt{2\pi}}\,. \tag{69}$$

In general a Dirac delta-function centered at $t = t_0$ is written as

$$\delta(t - t_0) = \begin{cases} \infty & \text{if } t = t_0\,, \\ 0 & \text{otherwise}\,, \end{cases} \tag{70}$$

subject to the normalisation condition

$$\int_{-\infty}^{\infty} \delta(t - t_0)\, \mathrm{d}t = 1\,. \tag{71}$$

Note that $\delta(t - t_0) = \delta(t_0 - t)$ (a delta-function is only non-zero when its argument is zero and $t - t_0 = 0$ and $t_0 - t = 0$ are equivalent).

A useful alternative definition of the Dirac delta-function can be found by inserting its Fourier transform, $F(\omega) = 1/\sqrt{2\pi}$, into the definition of the inverse Fourier transform, eq. (60), which gives:

$$\delta(t) = \frac{1}{2\pi} \int_{-\infty}^{\infty} \exp(i\omega t)\, \mathrm{d}\omega\,. \tag{72}$$

Integrating the product of a function with a Dirac delta-function centered at x_0 gives us the function evaluated at x_0

$$\int_{-\infty}^{\infty} \delta(x - x_0) g(x)\, \mathrm{d}x = g(x_0)\,. \tag{73}$$

This is sometimes known as the 'sifting' property of the Dirac delta-function (and we derived it in *Fourier 6* by considering the delta-function as the limit of the normalised top-hat function as its width tends to zero).

The Heaviside step function is defined as

$$h(t) = \begin{cases} 1 & \text{if } t > 0\,, \\ 0 & \text{it } t < 0\,. \end{cases} \tag{74}$$

As $h(t)$ is discontinuous at $t = 0$, it's conventional to take $h(0) = 1/2$. The differential of the Heaviside step function is the Dirac delta-function

$$\frac{\mathrm{d}h(t)}{\mathrm{d}t} = \delta(t)\,. \tag{75}$$

Intuitively this makes sense since for $t = 0$, $h(t)$ is discontinuous and hence its derivative is infinite, while for $t \neq 0$, $h(t)$ is constant and hence its derivative is zero. See RHB 13.1.3 and Appendix E for a mathematical proof of this relationship.

3.3 Fourier transform of an infinite monochromatic wave

We showed in *Fourier 7* that the Fourier transform of an infinite monochromatic wave with frequency ω_0

$$f(t) = \exp(i\omega_0 t)\,, \tag{76}$$

is a delta-function centered at $\omega = \omega_0$:

$$F(\omega) = \sqrt{2\pi}\delta(\omega - \omega_0)\,, \tag{77}$$

since the wave is composed of a single frequency ω_0.

3.4 Some properties of Fourier transforms (RHB 13.1.5)

Notation: 'FT' is short-hand for Fourier Transform, and we will use small letters to denote functions, and the corresponding capital letter to denote their Fourier transform. i.e. $FT[f(x)] = F(k)$.

The Fourier transform of a sum is the sum of the individual Fourier transforms:

$$FT[f_1(t) + f_2(t)] = F_1(\omega) + F_2(\omega)\,. \tag{78}$$

The Fourier transform of a constant times a function is the constant times the Fourier transform of the function:

$$FT[af(t)] = aF(\omega)\,. \tag{79}$$

The Fourier transform has some other properties which can be used to simplify calculations:

- **Differentiation**

$$FT\left[\frac{\mathrm{d}f(t)}{\mathrm{d}t}\right] = i\omega F(\omega)\,, \tag{80}$$

$$FT\left[\frac{\mathrm{d}^n f(t)}{\mathrm{d}t^n}\right] = (i\omega)^n F(\omega)\,, \tag{81}$$

  where n is an integer.

- **Translation**

$$FT\left[f(t-t_0)\right] = \exp\left(-i\omega t_0\right) F(\omega)\,. \tag{82}$$

- **Multiplication by an exponential**

$$FT\left[\exp\left(i\omega_0 t\right) f(t)\right] = F(\omega - \omega_0)\,, \tag{83}$$

where ω_0 and t_0 are constants. We derived these relations in *Fourier 6 and 7*. They also hold for functions of position with $t \to x$ and $\omega \to k$.

3.5 Fourier transform of a finite wave train

A finite wave

$$\tilde{f}(t) = \begin{cases} \exp\left(i\omega_0 t\right) & \text{for } -\Delta/2 \le t \le \Delta/2\,, \\ 0 & \text{otherwise}\,, \end{cases} \tag{84}$$

can be written as an infinite monochromatic wave, eq. (76), multiplied by a top-hat function, eq. (64). In *Fourier 7* we used the 'multiplication by an exponential' relation, eq. (83), to calculate the Fourier transform of the finite wave

$$F(\omega) = \frac{\Delta}{\sqrt{2\pi}} \mathrm{sinc}\left(\frac{(\omega - \omega_0)\Delta}{2}\right)\,, \tag{85}$$

i.e. a sinc function centered at $\omega = \omega_0$. A range of frequencies, centered on ω_0, contribute to the Fourier transform. Contrast this with the Fourier transform of the infinite wave, where $F(\omega) = 0$ for $\omega \neq \omega_0$. The first zeros of the FT of the finite wave occur at $\omega = \omega_0 \pm (2\pi/\Delta)$, so that its width is proportional to $1/\Delta$ i.e. inversely proportional to the width of the original finite wave, $\tilde{f}(t)$. Fig 8 shows the Fourier transform of a finite wave with $\omega_0 = 2\,\mathrm{s}^{-1}$ and $\Delta = 5$ s.

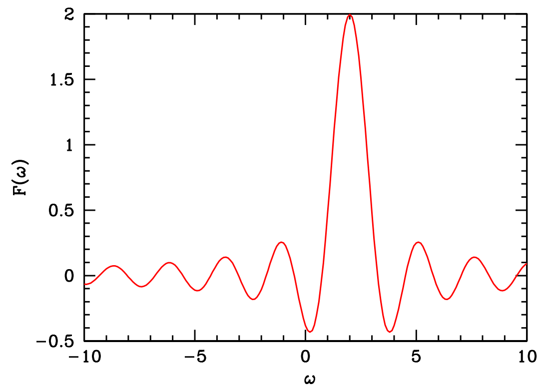

Figure 8: The Fourier transform of a finite wave with $\omega_0 = 2\,\mathrm{s}^{-1}$ and $\Delta = 5$ s, eq. (85).

3.6 Fourier transform of a gaussian (RHB 13.1.1)

Gaussian distributions are very common in physics. The Fourier transform of a gaussian [4] with width Δ,

$$f(t) = \frac{1}{\sqrt{2\pi}\Delta} \exp\left(-\frac{t^2}{2\Delta^2}\right), \tag{86}$$

is another gaussian[5]:

$$F(\omega) = \frac{1}{\sqrt{2\pi}} \exp\left(-\frac{\Delta^2\omega^2}{2}\right) = \frac{1}{\sqrt{2\pi}} \exp\left(-\frac{\omega^2}{2(\Delta_\omega)^2}\right), \tag{87}$$

with width $\Delta_\omega = 1/\Delta$ i.e. their widths are inversely proportional to each other. The derivation of this result (which uses a cunning technique, 'completing the square') is in Appendix F. Fig. 9 shows gaussians of varying widths and their Fourier transforms.

3.7 Fourier transform of an exponential

We showed in *Fourier 7* that the Fourier transform of an exponential function

$$f(t) = \begin{cases} \exp(-\alpha t) & \text{if } t \geq 0\,, \\ 0 & \text{otherwise}\,, \end{cases} \tag{88}$$

is

$$F(\omega) = \frac{1}{\sqrt{2\pi}} \frac{1}{\alpha + i\omega}\,. \tag{89}$$

This will be useful later on.

[4] This gaussian is normalized to unity...

[5] ... but this gaussian isn't.

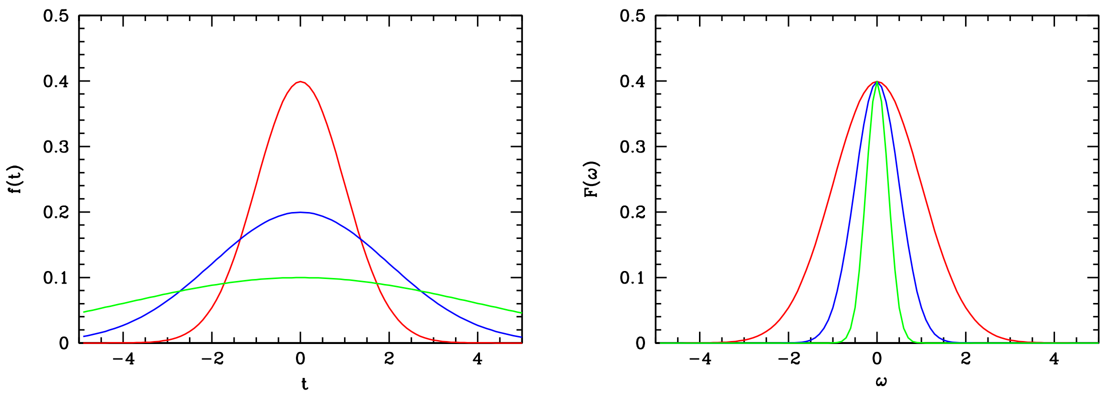

Figure 9: A gaussian, eq. (86), with width $\Delta = 1$ (red), 2 (blue) and 4 (green) (left) and its Fourier transform, eq. (87) (right).

Table 1: A list of Fourier transform pairs.

top hat	sinc
$\frac{1}{\tau}$ for $\frac{\tau}{2} < t < \frac{\tau}{2}$	$\frac{1}{\sqrt{2\pi}}\mathrm{sinc}\left(\frac{\omega\tau}{2}\right)$
Dirac delta-function	constant
$\delta(t)$	$\frac{1}{\sqrt{2\pi}}$
gaussian	gaussian
$\frac{1}{\sqrt{2\pi}\Delta}\exp\left(-\frac{t^2}{2\Delta^2}\right)$	$\frac{1}{\sqrt{2\pi}}\exp\left(-\frac{\Delta^2\omega^2}{2}\right)$
exponential	
$\exp(-\alpha t)$ for $t > 0$	$\frac{1}{\sqrt{2\pi}}\frac{1}{\alpha+i\omega}$

3.8 Fourier transform pairs

A function, $f(t)$, and its Fourier transform $FT[f(t)] = F(\omega)$, form a Fourier transform pair.

For some Fourier transform pairs, it's easier to calculate the Fourier transform than the Inverse Fourier Transform. An example of this is the exponential in Sec. 3.7. It's far, far easier to calculate the FT of the exponential than the Inverse FT of $1/(\alpha + i\omega)$. Therefore lists of Fourier transform pairs are useful. Table 1 contains a list of the Fourier transform pairs that we've encountered so far.

The narrower the function, the wider its Fourier transform and vice versa. Physically, to make a narrow function you need to add up waves with a wide range of frequencies (and to make a broad function you need a narrow range of frequencies).

3.9 Parseval's theorem (RHB 13.1.9)

The equivalent of eq. (49) for the Fourier transform is

$$\int_{-\infty}^{\infty} |f(x)|^2 \, \mathrm{d}x = \int_{-\infty}^{\infty} |F(k)|^2 \, \mathrm{d}k \,. \tag{90}$$

$|F(k)|^2$ is often referred to as the power spectrum. Physically it is the energy per unit wavenumber (or for a function of time, frequency). As well as being useful for calculating the total energy of a signal it can be used to calculate mathematical results, such as

$$\int_{-\infty}^{\infty} \frac{\sin^2(\omega)}{\omega^2} \, \mathrm{d}\omega = \pi \,, \tag{91}$$

(see *Fourier 7*).

4 Convolution (RHB 13.1.7)

4.1 Introduction

Finite experimental resolution make it impossible to measure things perfectly. For instance in astronomy the point spread function of the telescope blurs the image. How can we recover the underlying distribution of a quantity from the measured distribution? For instance how can we deblur images from telescopes?

4.2 Definition

The convolution (from the latin 'to roll together') of two functions, $f(x)$ and $g(x)$, is defined as [6]

$$h(x') = f \star g = \int_{-\infty}^{\infty} f(x) g(x' - x) \, \mathrm{d}x \,. \tag{93}$$

The physical interpretation of convolution is that the measured distribution of a quantity $h(x)$ is the convolution of the underlying distribution of the quantity, $f(x)$, with the resolution (or response function) of the instrument being used to make the measurement, $g(x)$ [7]. This happens frequently in physics and reality e.g. electronics (amplifier), optics (spectrograph, telescope), mechanical systems, acoustics.

[6] This definition could also be written, by swapping x and x', as

$$h(x) = f \star g = \int_{-\infty}^{\infty} f(x') g(x - x') \, \mathrm{d}x' \,. \tag{92}$$

[7] For an unrealistic perfect measuring instrument with perfect resolution, $g(x)$ would be a delta-function and $h(x) = f(x)$ i.e. the measured distribution is identical to the underlying distribution.

You can visualize convolution by plotting $f(x)$ and $g(-x)$ on separate pieces of paper. Then move $g(-x)$ incrementally across $f(x)$ (i.e. vary x'). The convolution is the area under the product of the two functions at each point.

Figs. 10 and 11 show this process for the convolution of a top-hat

$$f(x) = \begin{cases} 1 & \text{if } |x| \leq 4\,, \\ 0 & \text{otherwise}\,, \end{cases} \tag{94}$$

with a triangular function

$$g(x) = \begin{cases} x & \text{if } 0 \leq x \leq 4\,, \\ 0 & \text{otherwise}\,. \end{cases} \tag{95}$$

The resulting convolution, $h(x')$, is plotted in fig, 12. The website http://www.jhu.edu/˜signals/convolve/ allows you to try this yourself. See also http://mathworld.wolfram.com/Convolution.html.

A special case is convolution with a delta-function:

$$h(x') = \delta(x - x_0) \star g = \int_{-\infty}^{\infty} \delta(x - x_0) g(x' - x)\,\mathrm{d}x\,. \tag{96}$$

Using the sifting property of the delta-function, eq. (73), $\int_{-\infty}^{\infty} \delta(x - x_0) g(x)\,\mathrm{d}x = g(x_0)$, this becomes

$$h(x') = g(x' - x_0) \tag{97}$$

i.e. convolving a function with a delta-function centered at x_0 produces the function centered at x_0.

4.3 Convolution theorem (RHB 13.1.8)

Is it possible to 'undo' the experimental response and recover the underlying distribution $f(x)$ from the measured distribution $h(x)$? In *Fourier 8* we derived the convolution theorem, which relates the Fourier transforms of $f(x), g(x)$ and $h(x)$:

$$H(k) = \sqrt{2\pi} F(k) G(k)\,. \tag{98}$$

Therefore *if* we know what the experimental response, $g(x)$, is we can recover the original distribution. The procedure is:

- calculate $G(k)$ and $H(k)$ (the Fourier transforms of the experimental response and the measured distribution respectively),
- use eq. (98) to calculate $F(k)$: $F(k) = H(k)/(\sqrt{2\pi} G(k))$,
- recover the underlying distribution, $f(x)$, by calculating the inverse Fourier transform of $F(k)$: $f(x) = IFT[F(k)]$.

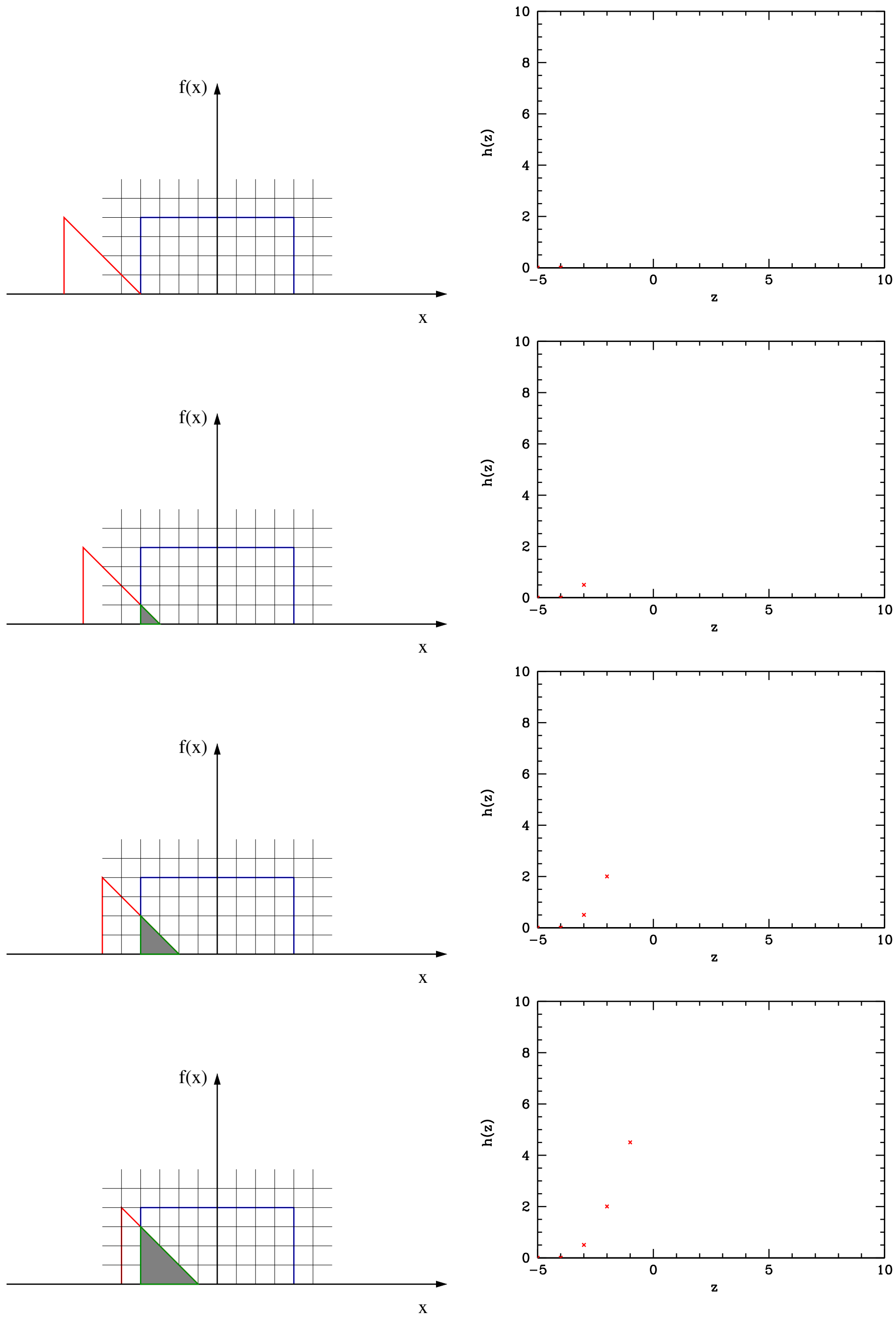

Figure 10: Part one of calculating the convolution of a top-hat, eq. (94), and a triangular function, eq. (95), graphically.

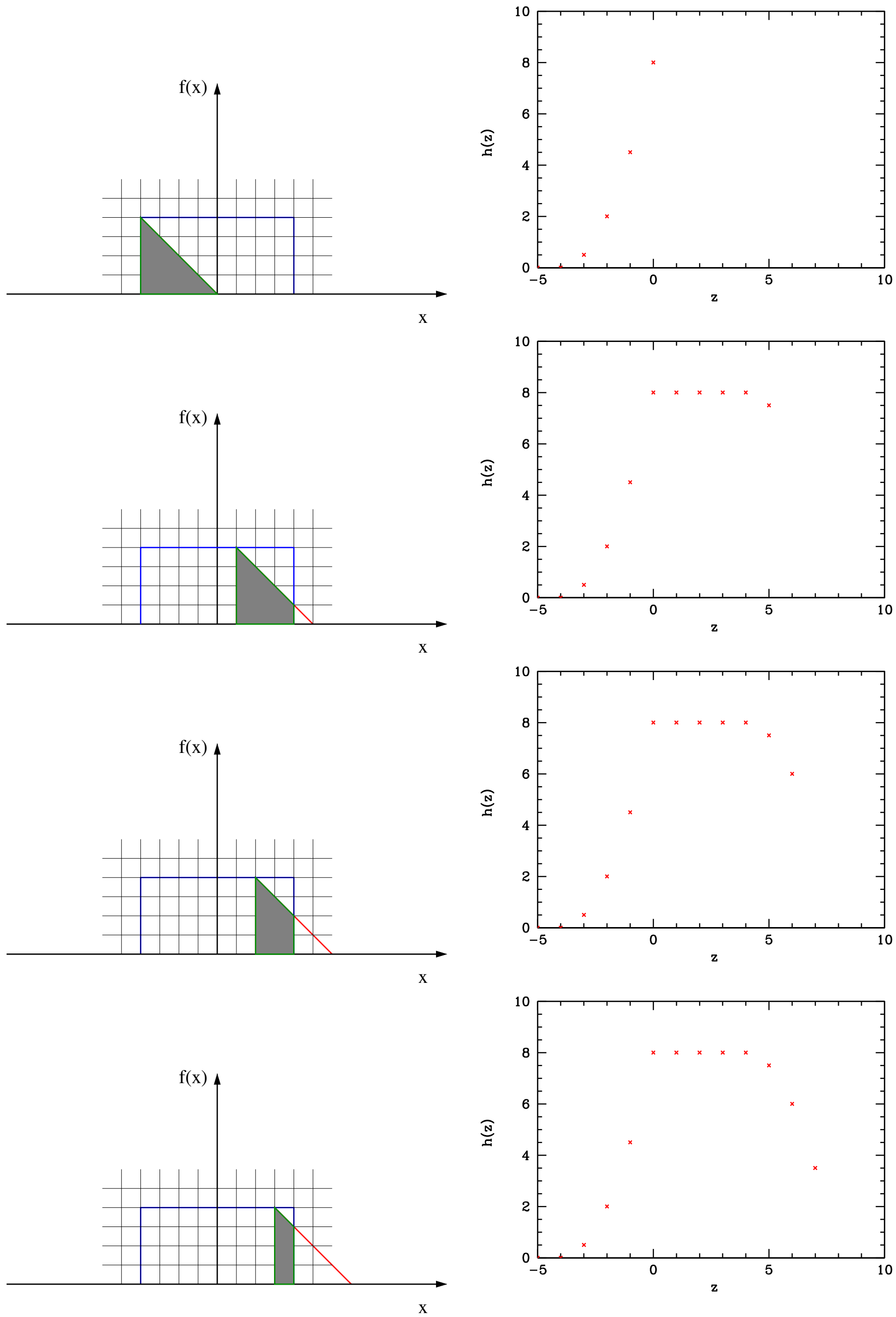

Figure 11: Part two of calculating the convolution of a top-hat, eq. (94), and a triangular function, eq. (95), graphically.

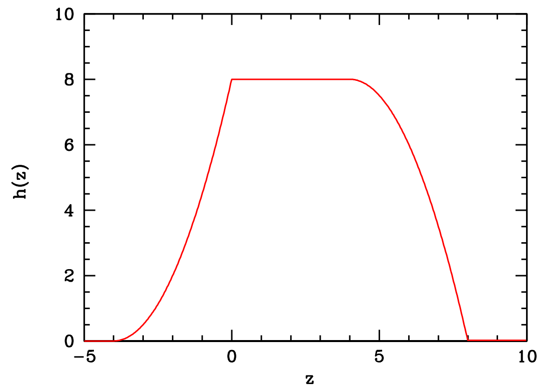

Figure 12: The convolution of a top-hat, eq. (94), and a triangular function, eq. (95).

The convolution theorem also has several other useful applications:
i) As we'll see in the final Waves/Fourier workshop, when doing numerical calculations it's quicker to do convolutions in Fourier space (i.e. take the Fourier transforms of the 2 functions you want to convolve, multiply the Fourier transforms together and then take the inverse Fourier transform).
ii) A signal can be improved by manipulating its frequency components e.g. you can remove noise (which corresponds to high spatial frequencies) from an image by multiplying its Fourier transform with a low-pass filter and then taking the inverse Fourier transform.

There's another useful equation, sometimes referred to as the Frequency convolution theorem, which relates the Fourier transform of the product of two functions to the convolution of their Fourier transforms:

$$FT[f(x)g(x)] = \frac{1}{\sqrt{2\pi}} F(k) \star G(k) \,. \tag{99}$$

5 Discrete Fourier transforms

5.1 Introduction

Fourier analysis is a powerful technique for finding out what frequencies a signal is made up of. However even if an underlying quantity is continuous, data is in reality discrete i.e. measurements are made at regular intervals in time or space, see Fig. 13.

We showed in *Fourier 9* that if data is sampled at time intervals $t = n\Delta t$ then the Fourier transform is periodic with period $\omega_{\rm p} = 2\pi/\Delta t$. As illustrated in Fig. 14, frequencies greater than $\omega_{\rm p}$ are indistinguishable from lower frequencies when discretely sampled. This is an example of aliasing. **Aliasing** refers to signals being indistinguishable after sampling and also to the distortions which occur when a signal is reconstructed from samples. Other examples of aliasing include the wave like features which appear in low resolution images of objects with a

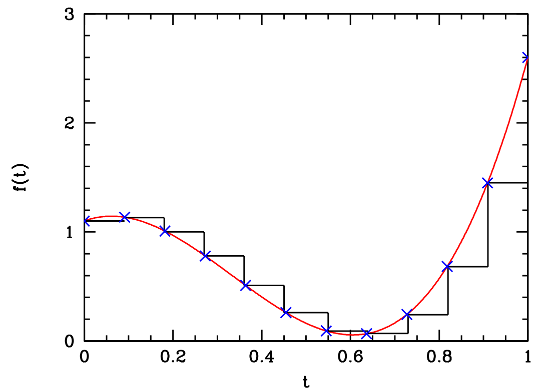

Figure 13: A function $f(t)$ sampled at regular intervals in time $t = n\Delta t$, with $n = 0, 1, 2, ...$

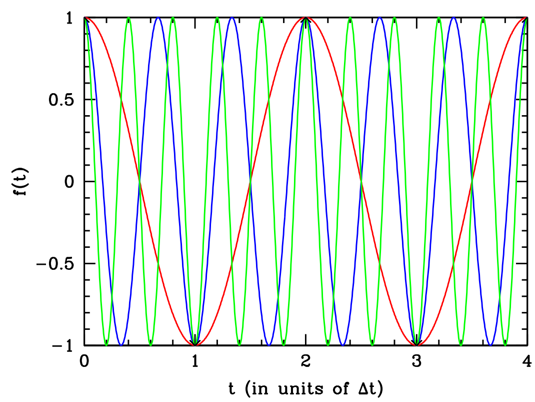

Figure 14: Waves with frequencies greater than $\omega_{\rm p} = 2\pi/\Delta t$ are indistinguishable when sampled at discrete intervals $t = n\Delta t$, with $n = 0, 1, 2, ...$

regular pattern (e.g. a brick wall) or the wagon wheel effect.

The **Nyquist frequency**, $\omega_{\rm c}$

$$\omega_{\rm c} = \frac{\omega_p}{2} = \frac{2\pi}{2\Delta t}\,, \tag{100}$$

is the maximum frequency which can be detected in sampled data. As shown in Fig. 15, signals with frequency above the Nyquist frequency can not be distinguished from signals with frequency below the Nyquist frequency.

A function is referred to as being bandwidth limited if its Fourier transform is zero for all frequencies greater than some value $\omega_{\rm max}$: $F(\omega) = 0$ for $\omega > \omega_{\rm max}$. In this case no information is lost (i.e. the function is completely specified by discrete samples) provided the data is sampled at a appropriate frequency. If the function is not bandwidth limited then aliasing is

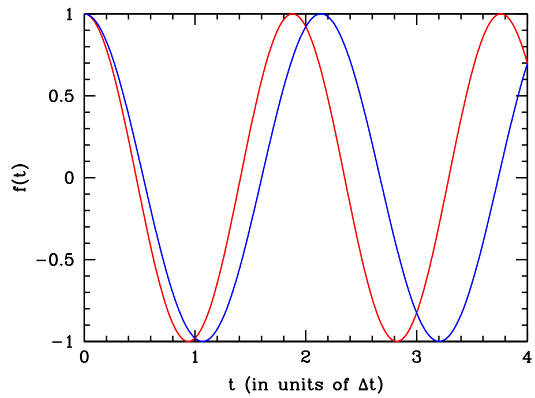

Figure 15: Waves with frequencies above ($\omega_2 = \omega_c + a$, where a is a constant, in red) and below ($\omega_1 = \omega_c - a$, in blue) the Nyquist frequency, ω_c, by the same amount are identical when sampled at times which are integer multiples of Δt.

inevitable. In practice this problem is solved by passing the signal through a low-pass filter before sampling.

5.2 Definitions

The expressions for the Fourier transform and inverse Fourier transform involve integrals from $-\infty$ to ∞. In reality we typically have N measurements taken at intervals Δt between $t = 0$ and some final time $t = (N-1)\Delta t$. Since the data is discrete (and to do numerical calculations) we'd like the Fourier transform to be discrete too. We showed in *Fourier 9* that the discrete Fourier transform and discrete inverse Fourier transform can be defined as

$$F_k = \sum_{n=0}^{N-1} f_n \exp\left(-\frac{2\pi ikn}{N}\right), \tag{101}$$

$$f_n = \frac{1}{N}\sum_{k=0}^{N-1} F_k \exp\left(\frac{2\pi ikn}{N}\right). \tag{102}$$

There are N data points, f_n, separated by Δt between $t = 0$ and $(N-1)\Delta t$ i.e. $f_n = f(n\Delta t)$ with $n = 0, ..., N-1$. The Fourier transform, F_k, has N frequencies separated by $\Delta\omega$ between $\omega = 0$ and $(N-1)\Delta\omega = (N-1)2\pi/(N\Delta t)$ i.e. $F_k = F(k\Delta\omega)$ with $k = 0, ..., N-1$. n.b. Here k is just a label for an integer, and not wavenumber.

Writing out (some of) the terms explicitly

$$\begin{aligned}
F_0 &= f_0 + f_1 + f_2 + ... + f_{N-1}\,, \\
F_1 &= f_0 + f_1 \exp\left(-\frac{2\pi i}{N}\right) + f_2 \exp\left(-\frac{4\pi i}{N}\right) + ... + f_{N-1} \exp\left(-\frac{2(N-1)\pi i}{N}\right), \\
. &\quad ... \\
F_{N-1} &= f_0 + f_1 \exp\left(-\frac{2(N-1)\pi i}{N}\right) + f_2 \exp\left(-\frac{4(N-1)\pi i}{N}\right) + ... + f_{N-1} \exp\left(-\frac{2(N-1)^2\pi i}{N}\right).
\end{aligned} \tag{103}$$

The convolution of discrete data is given by

$$h_n = \sum_m f_m g_{(n-m)}\,, \tag{104}$$

while the convolution theorem becomes

$$H_k = F_k G_k\,. \tag{105}$$

5.3 Fast Fourier transform

Calculating the discrete Fourier transform of a data set consisting of N points requires of order N^2 calculations. If N is very large this is very slow. The Fast Fourier transform (FFT) is a clever algorithm for calculating the discrete Fourier transform quickly.

FFTs are frequently used in lots of areas of physics. Matlab has a FFT and IFFT command, and we will use these in the final workshop of the module. If you'd like to find out more about FFTs, then I'd suggest looking at Appendix G for a little bit more detail or the chapter on FFTs in one of the 'Numerical methods in....', series of books by Press et al. for a lot more detail.

6 Optics (and other) applications

6.1 Recap of plane and spherical waves (H 2.5 and 2.7)

For a plane wave the surfaces of constant phase, $\phi = kx - \omega t + \phi_0$, are planes which are perpendicular to the direction of travel of the wave. Plane waves occur frequently in optics; optical devices often produce plane waves and a long way from its source a spherical wave resembles a plane wave. See animations at: http://www.falstad.com/ripple/index.html.

A harmonic plane wave propagating in the $+\mathbf{r}$ direction has the form

$$\psi(\mathbf{r}, t) \propto \exp\left[i(\mathbf{k}.\mathbf{r} - \omega t)\right]. \tag{106}$$

A spherically symmetric harmonic wave has the form

$$\psi(r, t) = \frac{a}{r} \exp\left[ik(r \mp vt)\right]. \tag{107}$$

The $-$ sign corresponds to a wave travelling radially outwards (and the $+$ sign radially inwards).

6.2 Fraunhofer diffraction (PPP 16 & 25.1, RHB 13.1.2, H 11)

Fraunhofer (or far-field) diffraction occurs when a plane wave passes through an aperture, and the diffraction pattern is (effectively) observed far enough away that the diffracted light also has planar wavefronts. This is usually achieved by either
i) placing the source at the focal point of a lens and the observation screen in the focal plane of another lens (see fig. 16)
or ii) using a parallel light source (e.g. a laser) and placing the screen at a large distance from the aperture.

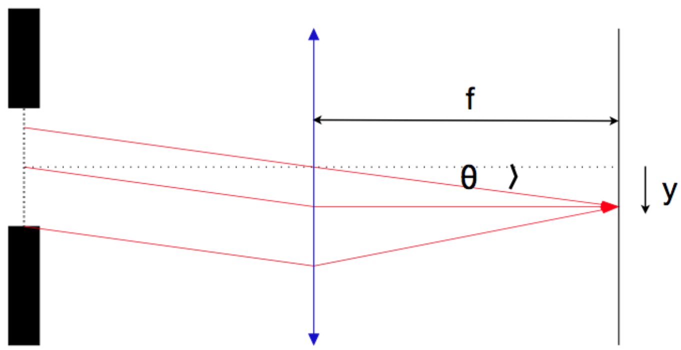

Figure 16: The Fraunhofer diffraction pattern can be viewed by placing the observations screen in the focal plane of a lens. Positions on the screen are related to angles by $y = f \tan\theta$ and since θ is small $y \approx f\theta$.

Consider a plane wave which has passed through a 1d aperture. According to the Hugyens-Fresnel principle each element $\mathrm{d}s$ of the aperture acts as a source of spherical wavelets with amplitude, at a distance r away,

$$\mathrm{d}E_{\mathrm{P}} = \left(\frac{E_{\mathrm{L}}\mathrm{d}s}{r}\right)\exp\left[i(kr - \omega t)\right], \tag{108}$$

where E_{L} is the amplitude per unit width of the slit. If we set $r = r_0$ for the middle of the aperture then for other points $r = r_0 - \Delta = r_0 - s\sin\theta$ (see Fig. 17) and in the far field limit (r much bigger than aperture width):

$$\mathrm{d}E_{\mathrm{P}} \approx \left(\frac{E_{\mathrm{L}}}{r_0}\right)\exp\left[i(kr_0 - ks\sin\theta - \omega t)\right]\mathrm{d}s, \tag{109}$$

and integrating over the entire aperture the total amplitude is

$$E_{\mathrm{P}} \approx \left(\frac{E_{\mathrm{L}}}{r_0}\int_{\mathrm{aperture}} \exp\left(-iks\sin\theta\right)\mathrm{d}s\right)\exp\left[i(kr_0 - \omega t)\right]. \tag{110}$$

If we define the aperture (or transmission) function, $\mathcal{A}(s)$, as [8]

$$\mathcal{A}(s) = E_{\mathrm{L}}, \tag{111}$$

[8] There are different definitions, some textbooks use $\mathcal{A}(s) = E_{\mathrm{L}}/r_0$.

within the aperture, and zero elsewhere, then

$$E_{\mathrm{P}} \approx \frac{\exp\left[i(kr_0 - \omega t)\right]}{r_0} \int \mathcal{A}(s) \exp\left(-i\tilde{k}s\right) \mathrm{d}s\,, \tag{112}$$

where $\tilde{k} = k \sin\theta$ (k is the wavenumber and θ is the viewing angle) i.e. the total amplitude can be written in terms of the Fourier transform of the aperture function:

$$E_{\mathrm{P}} \approx \sqrt{2\pi}\, \frac{\exp\left[i(kr_0 - \omega t)\right]}{r_0} FT[\mathcal{A}(s)]\,, \tag{113}$$

since by definition

$$FT[\mathcal{A}(s)] = \frac{1}{\sqrt{2\pi}} \int \mathcal{A}(s) \exp\left(-i\tilde{k}s\right) \mathrm{d}s\,. \tag{114}$$

The irradiance (flux density incident on a surface) is given by

$$I = \left(\frac{\epsilon_0 c}{2}\right) E_{\mathrm{R}}^2\,, \tag{115}$$

where E_{R} is the amplitude of the radiation (i.e. $E_{\mathrm{P}} = E_{\mathrm{R}} \exp\left[i(kr_0 - \omega t)\right]$), and it can therefore be written in terms of the Fourier transform of the aperture function:

$$I(\theta) = \left(\frac{\epsilon_0 c}{2}\right) \left(\frac{2\pi}{r_0^2}\right) |FT[\mathcal{A}(s)]|^2\,. \tag{116}$$

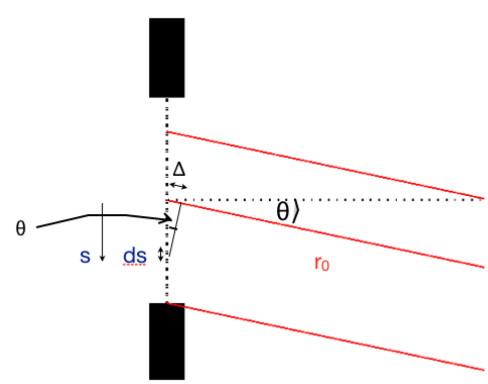

Figure 17: Zoom in to aperture.

Therefore to calculate a Fraunhofer diffraction pattern you 'just' need to calculate the Fourier transform of the aperture. Often we can do this fairly easily using standard Fourier transforms which we've already calculated (e.g. the Fourier transform of a top-hat function) combined, in some cases, with the relations in Sec 3.4 and/or the convolution theorem.

6.3 Single slit

A single slit with width b centered at $x = 0$ has aperture function:

$$\mathcal{A}(s) = \begin{cases} E_{\rm L} & \text{if } -\frac{b}{2} \le x \le \frac{b}{2}\,, \\ 0 & \text{otherwise}\,, \end{cases} \tag{117}$$

i.e. a top-hat function with width b and amplitude $E_{\rm L}$, which has Fourier transform

$$FT[\mathcal{A}(s)] = \frac{bE_{\rm L}}{\sqrt{2\pi}}\text{sinc}\left(\frac{\tilde{k}b}{2}\right)\,, \tag{118}$$

and hence, using eq. (116), the irradiance is

$$I = I_0\text{sinc}^2\left(\frac{\tilde{k}b}{2}\right) = I_0\text{sinc}^2\left(\frac{kb\sin\theta}{2}\right) = I_0\text{sinc}^2\beta\,, \tag{119}$$

with

$$\beta = \frac{kb\sin\theta}{2}\,, \tag{120}$$

and

$$I_0 = \left(\frac{\epsilon_0 c}{2}\right)\left(\frac{E_{\rm L}b}{r_0}\right)^2\,. \tag{121}$$

The resulting Fraunhofer diffraction pattern is shown in Fig. 18 as a function of $\tilde{k}$ for $b = 1$. [9]

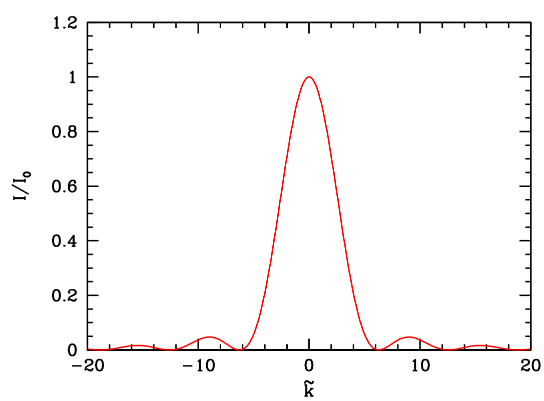

Figure 18: The Fraunhofer diffraction pattern from a single slit with width $b = 1$, eq. (119).

[9]Strictly speaking we should specify what units b is measured in. In fact the diffraction pattern will look the same, provided $\tilde{k}$ is measured in the same units, i.e. if b is in μm then k is in $(\mu\text{m})^{-1}$ as β must be dimensionless.

6.4 Double slit

Consider a double slit, where each slit has width b and the slit separation is a. To calculate the diffraction pattern we need to calculate the Fourier transform of the double slit. We can make the calculation easier by realising that the double slit is the convolution of a top-hat function with two Dirac delta-functions, i.e. $h = g * f$ where h is the double slit, g a top-hat function of width b and f a pair of delta-functions centered at $x = x_0 = \pm a/2$. Using the definition of a convolution, eq. (92), and the delta-function sift property, eq. (73),

$$h(x') = \int_{-\infty}^{\infty} f(x)g(x'-x)\,\mathrm{d}x = \int_{-\infty}^{\infty} [\delta(x+a/2)+\delta(x-a/2)]g(x'-x)\,\mathrm{d}x = g(x'+a/2)+g(x'-a/2)\,. \tag{122}$$

The convolution theorem, eq. (98), tells us that the Fourier transform of the convolution is given by $H(k) = \sqrt{2\pi}F(k)G(k)$. The Fourier transform of the top-hat function is

$$G(\tilde{k}) = \frac{b}{\sqrt{2\pi}}\mathrm{sinc}\left(\frac{\tilde{k}b}{2}\right)\,, \tag{123}$$

where $\tilde{k} = k\sin\theta$. The Fourier transform of a delta-function centered at $x = 0$ is

$$FT[\delta(x)] = \frac{1}{\sqrt{2\pi}}\,, \tag{124}$$

and the 'translation' relation tells us that $FT[f(x-x_0)] = \exp(-ikx_0)F(k)$ so that the Fourier transform of the pair of delta-functions centered at $\pm a/2$ is

$$F(k) = \frac{1}{\sqrt{2\pi}}\left[\exp\left(-\frac{i\tilde{k}a}{2}\right) + \exp\left(\frac{i\tilde{k}a}{2}\right)\right] = \frac{2}{\sqrt{2\pi}}\cos\left(\frac{\tilde{k}a}{2}\right). \tag{125}$$

Putting this together we get:

$$\begin{aligned} I &= \left(\frac{\epsilon_0 c}{2}\right)\left(\frac{2\pi}{r_0^2}\right)|H(\tilde{k})|^2 = \left(\frac{\epsilon_0 c}{2}\right)\left(\frac{2\pi}{r_0}\right)^2 F^2(\tilde{k})G^2(\tilde{k})\,, \\ &= 4I_0\mathrm{sinc}^2(\beta)\cos^2(\gamma)\,, \end{aligned} \tag{126}$$

where

$$\beta = \frac{\tilde{k}b}{2} = \frac{kb\sin\theta}{2}\,, \tag{127}$$

$$\gamma = \frac{\tilde{k}a}{2} = \frac{ka\sin\theta}{2}\,. \tag{128}$$

Interference between the two slits gives the $\cos^2(\gamma)$ term, and the overall intensity is modulated by the $\mathrm{sinc}^2(\beta)$ diffraction term. Missing orders occur when an interference maximum coincides with a diffraction minimum (and also us to deduce the ratio of the slit width and separation). The resulting irradiance distribution is shown in Fig. 19 as a function of $\tilde{k} = k\sin\theta$ for $a = 5b$ and $b = 1$, in which case the central diffraction maximum contains nine bright fringes.

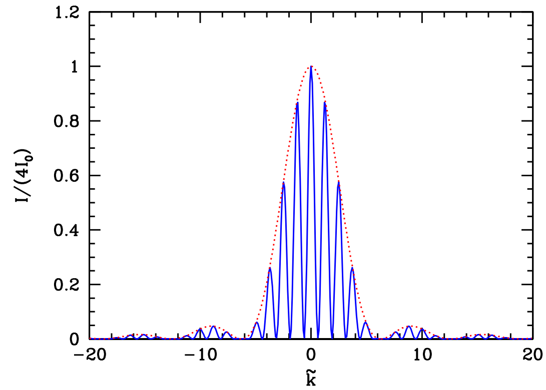

Figure 19: The Fraunhofer diffraction pattern from a double slit with separation $a = 5b$ and width $b = 1$, eq. (126). The dotted (red) line shows the diffraction envelope from a single slit.

6.5 Multiple slits

Multiple slits are the generalisation of a double slit to N slits. Just like the double slit could be written as the convolution of a top-hat with a pair of Dirac delta-functions, multiple slits can be written as the convolution of a top-hat with a row of Dirac delta-functions (known as a Dirac comb [10]) i.e. $h = g * f$ where h is the multiple slits, g a top-hat function of width b and f a row of delta-functions centered at $x_0 = ja$ with $j = 0, ..., N-1$ (i.e. $x_0 = 0, a, 2a, ...$):

$$f(x) = \sum_{j=0}^{N-1} \delta(x - ja) . \tag{129}$$

In this case, using the translation rule, $FT[f(x - x_0)] = \exp(-ikx_0)F(k)$, once more, the Fourier transform of our row of Delta-functions is

$$\begin{aligned} F(\tilde{k}) &= FT\left[\sum_{j=0}^{N-1} \delta(x - ja)\right] = \sum_{j=0}^{N-1} \left(FT\left[\delta(x - ja)\right]\right) , \\ &= \sum_{j=0}^{N-1} \left[\exp(-i\tilde{k}ja) FT[\delta(x)]\right] = \sum_{j=0}^{N-1} \left[\exp(-i\tilde{k}ja)\frac{1}{\sqrt{2\pi}}\right] , \\ &= \frac{1}{\sqrt{2\pi}} \sum_{j=0}^{N-1} \exp(-i\tilde{k}ja) = \frac{1}{\sqrt{2\pi}} \sum_{j=0}^{N-1} \left[\exp(-i\tilde{k}a)\right]^j . \end{aligned} \tag{130}$$

since $\exp(-i\tilde{k}ja) = [\exp(-i\tilde{k}a)]^j$. The sum in the final expression is a geometric progression $(a + ar + ar^2 + ...)$ with $a = 1$ and $r = \exp(-i\tilde{k}a)$. The sum of the first N terms of a geometric progression is

$$S_N = a\left(\frac{1 - r^N}{1 - r}\right) , \tag{131}$$

[10] Technically a Dirac comb consists of an infinite number of delta-functions.

and hence

$$F(\tilde{k}) = \frac{1}{\sqrt{2\pi}} \frac{1-\exp(-i\tilde{k}aN)}{1-\exp(-i\tilde{k}a)} = \frac{1}{\sqrt{2\pi}} \exp(-i\tilde{k}a(N-1)/2) \left[\frac{\sin(\tilde{k}aN/2)}{\sin(\tilde{k}a/2)} \right] . \tag{132}$$

The irradiance is proportion to the square of the Fourier transform of the aperture function and using the convolution theorem, $H(k) = \sqrt{2\pi}F(k)G(k)$, we get:

$$\begin{aligned} I &= \left(\frac{\epsilon_0 c}{2}\right)\left(\frac{2\pi}{r_0^2}\right)|H(\tilde{k})|^2 = \left(\frac{\epsilon_0 c}{2}\right)\left(\frac{2\pi}{r_0}\right)^2 F^2(\tilde{k})G^2(\tilde{k}) \,, \\ &= I_0 \mathrm{sinc}^2(\beta) \frac{\sin^2(\gamma N)}{\sin^2(\gamma)} \,, \end{aligned} \tag{133}$$

with β and γ defined as before in eqs. (127) and (128). The first term is the diffraction envelope from a single slit and the second term is due to the intereference between the multiple slits. The numerator and denominator of the intereference term both tend to zero as $\gamma \to n\pi$, therefore we need to use l'Hopital's rule, eq. (54) to study its behaviour in this limit:

$$\lim_{\gamma\to n\pi} \frac{\sin(\gamma N)}{\sin(\gamma)} = \frac{\lim_{\gamma\to n\pi}[N\cos(\gamma N)]}{\lim_{\gamma\to n\pi}[\cos(\gamma)]} = \pm N \,. \tag{134}$$

The left panel of Fig. 20 shows the diffraction and interference terms separately, the right panel the resulting irradiance distribution.

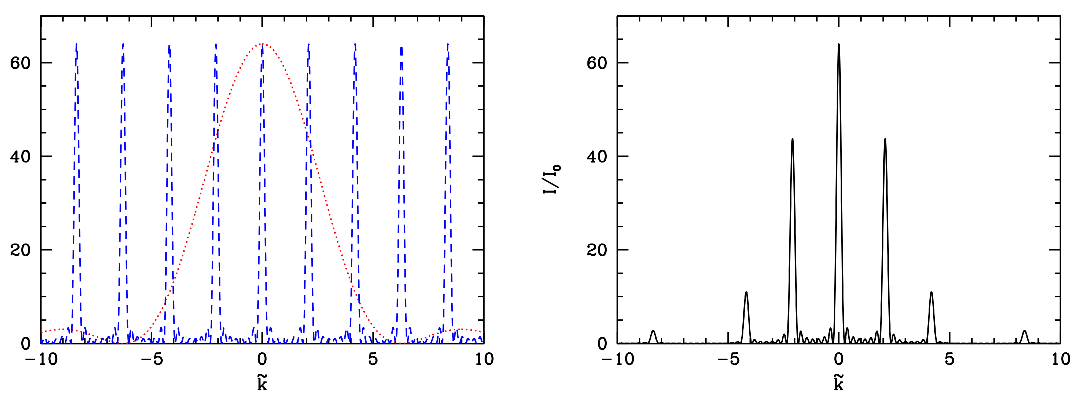

Figure 20: The Fraunhofer diffraction pattern from $N = 8$ multiple slits with separation $a = 3b$, and width $b = 1$ eq. (133). In the left hand panel the dotted (red) line shows the diffraction envelope from a single slit and the dashed (blue) line the intereference term. The right panel shows the resulting irradiance distribution.

Sometimes a diffraction grating is covered with an apodizing mask (from the Greek 'without feet'). In this case the aperture function is no longer constant. This is done in order to reduce the intensity of side lobes so faint satellite lines don't get swamped by side lobes of the main line and can be identified. For instance in astronomy this allows a faint binary companion to be observed.

6.6 3d Fourier transform (RHB 13.1.10)

The Fourier transform can easily be generalised to 3d ($x \to \mathbf{r} = (x, y, z)$ and wave-number $k \to$ wave-vector $\mathbf{k} = (k_x, k_y, k_z)$)

$$
\begin{aligned}
F(\mathbf{k}) &= \frac{1}{(2\pi)^{3/2}} \int f(x, y, z)\, \exp(-ik_x x) \exp(-ik_y y) \exp(-ik_z z)\, \mathrm{d}x\, \mathrm{d}y\, \mathrm{d}z\,, && (135)\\
f(\mathbf{r}) &= \frac{1}{(2\pi)^{3/2}} \int F(k_x, k_y, k_z)\, \exp(ik_x x) \exp(ik_y y) \exp(ik_z z) \mathrm{d}k_x\, \mathrm{d}k_y\, \mathrm{d}k_z\,, && (136)
\end{aligned}
$$

or equivalently, but more compactly,

$$
\begin{aligned}
F(\mathbf{k}) &= \frac{1}{(2\pi)^{3/2}} \int f(\mathbf{r})\, \exp(-i\mathbf{k}.\mathbf{r})\, \mathrm{d}^3\mathbf{r}\,, && (137)\\
f(\mathbf{r}) &= \frac{1}{(2\pi)^{3/2}} \int F(\mathbf{k})\, \exp(i\mathbf{k}.\mathbf{r})\, \mathrm{d}^3\mathbf{k}\,. && (138)
\end{aligned}
$$

For a spherically symmetric function, $f(r)$, using spherical polar coordinates $\mathrm{d}^3\mathbf{r} = r^2 \sin\theta \mathrm{d}r\, \mathrm{d}\theta\, \mathrm{d}\phi$ and $\mathbf{k}.\mathbf{r} = \cos\theta$, eq. (137) becomes

$$
F(k) = \frac{1}{(2\pi)^{3/2}} \int_0^\infty \mathrm{d}r \int_0^\pi \mathrm{d}\theta \int_0^{2\pi} \mathrm{d}\phi f(r) r^2 \sin\theta \exp(-ikr\cos\theta)\,, \tag{139}
$$

and after carrying out the θ and ϕ integrals (see Appendix H)

$$
F(k) = \frac{1}{(2\pi)^{3/2}} \int_0^\infty \mathrm{d}r 4\pi r^2 f(r) \left[\frac{\sin(kr)}{kr}\right]\,. \tag{140}
$$

6.7 Rectangular aperture (PPP 25.1)

In 2d each element $\mathrm{d}x\, \mathrm{d}y$ of the aperture acts as a source of spherical wavelets with amplitude, at a distance r away,

$$
\mathrm{d}E = \left(\frac{E_{\mathrm{s}} \mathrm{d}x\, \mathrm{d}y}{r}\right) \exp\left[i(kr - \omega t)\right]\,, \tag{141}
$$

where E_{s} is the amplitude per unit area. In 2d the difference in path length between a general point in the aperture and the centre of the aperture becomes

$$
r - r_0 \approx x \sin\theta + y \sin\phi\,, \tag{142}
$$

and hence the diffraction amplitude is

$$
E_{\mathrm{P}} \approx \left(\frac{E_{\mathrm{s}}}{r_0} \int_{\mathrm{aperture}} \exp\left[-i(\tilde{k}_x x + \tilde{k}_y y)\right] \mathrm{d}x\, \mathrm{d}y\right) \exp\left[i(kr_0 - \omega t)\right]. \tag{143}
$$

where $\tilde{k}_x = k \sin\theta$ and $\tilde{k}_y = k \sin\phi$. This can be written in terms of the 2d aperture function, defined as

$$
\mathcal{A}(x, y) = E_{\mathrm{s}}\,, \tag{144}
$$

within the aperture and zero elsewhere, as

$$\begin{aligned} E_{\rm P} &\approx \frac{\exp\left[i(kr_0 - \omega t)\right]}{r_0} \int \mathcal{A}(x,y) \exp\left(-i(\tilde{k}_x x + \tilde{k}_y y)\right) {\rm d}x\, {\rm d}y\,, \\ &\approx (2\pi)\frac{\exp\left[i(kr_0 - \omega t)\right]}{r_0} FT[\mathcal{A}(x,y)]\,, \end{aligned} \tag{145}$$

where

$$FT[\mathcal{A}(x,y)] = \frac{1}{2\pi} \int \mathcal{A}(x,y) \exp\left(-i(\tilde{k}_x x + \tilde{k}_y y)\right) {\rm d}x\, {\rm d}y\,. \tag{146}$$

The irradiance is then proportional to the square of the 2d Fourier transform:

$$I(\theta,\phi) = \left(\frac{\epsilon_0 c}{2}\right) \left(\frac{2\pi}{r_0}\right)^2 |FT[\mathcal{A}(x,y)]|^2\,. \tag{147}$$

The aperture function of a rectangular (a by b) aperture can be written as:

$$\mathcal{A}(x,y) = \begin{cases} E_{\rm s} & \text{if } -b/2 \leq x \leq b/2 \text{ and } -a/2 \leq y \leq a/2\,, \\ 0 & \text{otherwise}\,, \end{cases} \tag{148}$$

i.e. the aperture is proportional to the product of a top-hat of width b in the x direction with a top-hat of width a in the y direction. Therefore the Fourier transform of the aperture function is $E_{\rm s}$ times the product of the FTs of two top-hat functions with unit amplitude and hence the irradiance is:

$$I = I_0 {\rm sinc}^2(\beta)\, {\rm sinc}^2(\alpha)\,, \tag{149}$$

where

$$\beta = \frac{\tilde{k}_x b}{2} = \frac{kb \sin\theta}{2}\,, \tag{150}$$

$$\alpha = \frac{\tilde{k}_y a}{2} = \frac{ka \sin\phi}{2}\,, \tag{151}$$

and in this case

$$I_0 = \left(\frac{\epsilon_0 c}{2}\right) \left(\frac{E_{\rm s} ab}{r_0}\right)^2\,. \tag{152}$$

The diffraction patterns from a square aperture (a special case of a rectangular aperture with $a = b$) and a hexagonal aperture are shown in Fig. 21. This demonstrates that by looking at the properties of the diffraction pattern we could deduce the shape of the aperture. As you'll see in solid state physics in 3rd year something similar happens with X-ray diffraction: the diffraction pattern is proportional to the Fourier transform of the crystal (and hence you can deduce the crystal structure from the diffraction pattern).

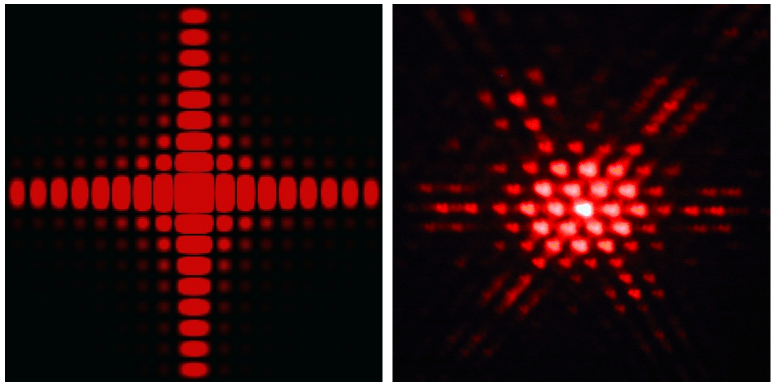

Figure 21: The diffraction pattern a square aperture (left) and a hexagonal aperture (right), courtesy of http://en.wikipedia.org/wiki/File:Square diffraction.jpg and http://www1.union.edu/newmanj/lasers/Light as a Wave/light as a wave.htm

6.8 Fourier transform of the charge distribution of the hydrogen atom

You'll see in solid state physics that the X-ray diffraction pattern is proportional to the structure function, which in turn is proportional to the Fourier transform of the charge distribution. The hydrogen atom has electron number density

$$f(r) = \frac{1}{\pi a_0^3} \exp\left(-2r/a_0\right) . \tag{153}$$

Inserting this into the definition of the 3d spherically symmetric Fourier transform gives

$$F(k) \propto \frac{1}{\left[1 + \left(\frac{ka_0}{2}\right)^2\right]^2} . \tag{154}$$

7 Solving differential equations

Differential equations are ubiquitous in physics.

Ordinary differential equations (ODEs) contain functions of only one independent variable and one or more of their derivatives with respect to that variable (in other words they only contain ordinary, total derivatives). For example the equation of simple harmonic motion:

$$\frac{\mathrm{d}^2 x}{\mathrm{d}t^2} = -\omega^2 x \, , \tag{155}$$

is an ODE.

Partial differential equations contain functions of more than one independent variable and one or more of their partial derivatives with respect to these variables (in other words they contain partial derivatives). For example the wave equation:

$$\frac{\partial^2 \psi}{\partial t^2} = v^2 \frac{\partial^2 \psi}{\partial x^2}\,, \tag{156}$$

and the heat flow equation

$$\frac{\partial u}{\partial t} = \alpha \frac{\partial^2 u}{\partial x^2}\,, \tag{157}$$

are PDEs.

7.1 Ordinary differential equations

Fourier transforms can be used to solve some ODEs. Consider, for instance, the current flow, $i(t)$ in a RL circuit with voltage source $v(t)$. Using Kirchoff's 2nd law (around a closed loop voltages sum to zero) we find

$$v(t) = i(t)R + L\frac{\mathrm{d}i(t)}{\mathrm{d}t}\,. \tag{158}$$

We showed in *Fourier 12* that by taking the Fourier transform of both sides of this equation and using the differentiation relation, eq. (80), we get

$$I(\omega) = \frac{V(\omega)}{R + i\omega L}\,. \tag{159}$$

So if we can calculate the Fourier transform of the voltage source, $V(\omega) = FT[v(t)]$, we can use this equation to calculate the Fourier transform of the current, $I(\omega)$, and then calculate the current itself by taking the inverse Fourier transform, $i(t) = IFT[I(\omega)]$.
If $v(t)$ is a voltage spike at $t = 0$: $v(t) = V_0\delta(t)$ then

$$V(\omega) = V_0 FT[\delta(t)] = \frac{V_0}{\sqrt{2\pi}}\,, \tag{160}$$

and therefore

$$I(\omega) = \frac{V_0}{\sqrt{2\pi}}\frac{1}{R + i\omega L} = \frac{V_0}{\sqrt{2\pi}L}\frac{1}{(R/L) + i\omega}\,. \tag{161}$$

Taking the IFT of this directly (by substituting it into the definition of the IFT) would be tricky, however remember that in *Fourier 7* we showed that if

$$f(t) = \begin{cases} \exp\left(-\alpha t\right) & \text{if } t > 0\,, \\ 0 & \text{otherwise}\,, \end{cases} \tag{162}$$

then

$$F(\omega) = \frac{1}{\sqrt{2\pi}}\frac{1}{\alpha + i\omega}\,. \tag{163}$$

Here we have

$$I(\omega) = \frac{V_0}{L}F(\omega)\,, \tag{164}$$

with $\alpha = R/L$ and therefore

$$i(t) = \begin{cases} \frac{V_0}{L} \exp\left(-\frac{Rt}{L}\right) & \text{if } t \geq 0\,, \\ 0 & \text{otherwise}\,, \end{cases} \tag{165}$$

i.e. a delta-function voltage spike in this circuit produces an exponentially decaying current.

To summarise, to find the current flowing in a RL circuit, $i(t)$, due to a voltage input $v(t)$ we

- Took the FT of the ODE relating $i(t)$ and $v(t)$.
- Calculated $V(\omega) = FT[v(t)]$.
- Used the FT of the ODE to calculate $I(\omega)$.
- Calculated $i(t) = IFT[I(\omega)]$.

The success of this approach depends on whether it is possible to calculate the IFT of the FT of the solution. In this case the FT was part of a common FT pair, so we didn't need to do the calculation explicitly.

7.2 Partial differential equations: general solution (RHB 20.3.3)

In *Intro 1* we stated than the general solution of the 1d wave equation

$$\frac{\partial^2 \psi}{\partial x^2} = \frac{1}{v^2} \frac{\partial^2 \psi}{\partial t^2}\,, \tag{166}$$

has the form

$$\psi(x,t) = a_1 f(x - vt) + a_2 g(x + vt)\,, \tag{167}$$

where a_1 and a_2 are constants, and f and g are any function of $(x - vt)$ and $(x + vt)$ respectively.

We can in fact **show** that this is the general solution. The strategy to do this is to write $\psi(x,t) = f(p)$ where p is some function of x and t. The idea is that when we substitute this into the wave equation and then deduce the form p has to take in order for the terms containing $f(p)$ to cancel. Differentiating twice with respect to x and t respectively we find

$$\begin{aligned} \frac{\partial^2 \psi}{\partial x^2} &= \frac{\mathrm{d}f}{\mathrm{d}p} \frac{\partial^2 p}{\partial x^2} + \frac{\mathrm{d}^2 f}{\mathrm{d}p^2} \left(\frac{\partial p}{\partial x}\right)^2\,, \\ \frac{\partial^2 \psi}{\partial t^2} &= \frac{\mathrm{d}f}{\mathrm{d}p} \frac{\partial^2 p}{\partial t^2} + \frac{\mathrm{d}^2 f}{\mathrm{d}p^2} \left(\frac{\partial p}{\partial t}\right)^2\,, \end{aligned} \tag{168}$$

and substituting these expressions into the wave-equation we get

$$\frac{\mathrm{d}f}{\mathrm{d}p} \frac{\partial^2 p}{\partial x^2} + \frac{\mathrm{d}^2 f}{\mathrm{d}p^2} \left(\frac{\partial p}{\partial x}\right)^2 = \frac{1}{v^2} \left[\frac{\mathrm{d}f}{\mathrm{d}p} \frac{\partial^2 p}{\partial t^2} + \frac{\mathrm{d}^2 f}{\mathrm{d}p^2} \left(\frac{\partial p}{\partial t}\right)^2\right]\,. \tag{169}$$

In order for the $f(p)$ dependent terms to cancel we need either the derivatives multiplying $\mathrm{d}f/\mathrm{d}p$ or $\mathrm{d}^2f/\mathrm{d}p^2$ to be zero. If we had $\frac{\partial p}{\partial x}=0$ and $\frac{\partial p}{\partial t}=0$, then $\frac{\partial^2 p}{\partial x^2}$ and $\frac{\partial^2 p}{\partial t^2}$ would be zero too, and we'd be left with $0=0$ (which is a solution, but not a particularly interesting one). So what we want is $\frac{\partial^2 p}{\partial x^2}=0$ and $\frac{\partial^2 p}{\partial t^2}=0$. This tells us p must have the form $p=ax+bt$ where a and b are constants. Then $\frac{\partial p}{\partial x}=a$ and $\frac{\partial p}{\partial t}=b$ so that eq. (169) reduces to

$$a^2\frac{\mathrm{d}^2 f}{\mathrm{d}p^2}=\frac{b^2}{v^2}\frac{\mathrm{d}^2 f}{\mathrm{d}p^2}\,, \tag{170}$$

which gives us $a=\pm b/v$. We can take $a=1$, hence $b=\pm v$ and therefore $p=x\pm vt$ so that the general solution is indeed given by eq. (167).

7.3 Partial differential equations: separation of variables (RHB 21.1 & 22.2)

A function is separable if it can be written as the product of functions of a single variable e.g. $f(x,t)=x^2t$ is separable as it can be written as $f(x,t)=X(x)T(t)$ with $X(x)=x^2$ and $T(t)=t$, while $f(x,t)=x^2t+xt^2$ is not separable as it can't be written in this form.

The separation of variables method of solving pdes involves looking for solutions which are separable. For the 1d wave equation, we look for solutions with the form $\psi(x,t)=X(x)T(t)$. This gives

$$\begin{aligned}\frac{\partial^2\psi}{\partial x^2} &= \frac{\mathrm{d}^2X}{\mathrm{d}x^2}T\,,\\ \frac{\partial^2\psi}{\partial t^2} &= \frac{\mathrm{d}^2T}{\mathrm{d}t^2}X\,.\end{aligned} \tag{171}$$

Substituting into the wave equation and dividing by XT gives

$$\frac{1}{X}\frac{\mathrm{d}^2X}{\mathrm{d}x^2}=\frac{1}{v^2T}\frac{\mathrm{d}^2T}{\mathrm{d}t^2}\,. \tag{172}$$

This can only be true for all x and t if both sides of the equation are equal to a constant. It's useful to write this constant as $-m^2$, so that

$$\begin{aligned}\frac{\mathrm{d}^2X}{\mathrm{d}x^2} &= -m^2X\,,\\ \frac{\mathrm{d}^2T}{\mathrm{d}t^2} &= -m^2v^2T\,.\end{aligned} \tag{173}$$

These equations have solutions $X(x)=a\cos(mx)+b\sin(mx)$ and $T(t)=c\cos(mvt)+d\sin(mvt)$ (where a,b,c,d are constants). Therefore the general separable solution to the 1d wave equation has the form

$$\psi(x,t)=A\sin(mx)\sin(mvt)+B\sin(mx)\cos(mvt)+C\cos(mx)\sin(mvt)+D\cos(mx)\cos(mvt)\,. \tag{174}$$

The values of the constants A,B,C,D depend on the boundary conditions. If we'd taken the separation constant to be $+m^2$ (instead of $-m^2$) we would have got a solution composed of exponentials instead of sine and cos. Which you should choose to use depends on the physical system you're considering. For waves on a string, where the amplitude is zero at either end, it's easier to apply the boundary conditions if you use sine and cos. For a system which extends to infinity exponentials may be more appropriate, see Differential equations problem sheet q5.

Consider a string which is fixed at $x = 0$ and $x = l$. In this case $\psi(0,t) = \psi(l,t) = 0$. Applying the first of these boundary conditions we have

$$\psi(0,t) = C\sin(mvt) + D\cos(mvt) = 0\,. \tag{175}$$

This expression can only be zero for all t if $C = D = 0$. The second boundary condition gives us

$$\psi(l,t) = A\sin(ml)\sin(mvt) + B\sin(ml)\cos(mvt) = 0\,. \tag{176}$$

This expression only be zero for all t if $\sin(ml) = 0$ i.e. $m = n\pi/l$ where n is an integer. The string is initially stationary so we must also have $\left(\frac{\partial\psi}{\partial t}\right)_{t=0} = 0$ for all x

$$\begin{aligned}
\left(\frac{\partial\psi}{\partial t}\right) &= \left(\frac{n\pi v}{L}\right)\left[A\sin\left(\frac{n\pi x}{l}\right)\cos\left(\frac{n\pi vt}{l}\right) - B\sin\left(\frac{n\pi x}{l}\right)\sin\left(\frac{n\pi vt}{l}\right)\right], \\
\left(\frac{\partial\psi}{\partial t}\right)_{t=0} &= \left(\frac{n\pi v}{L}\right)A\sin\left(\frac{n\pi x}{l}\right),
\end{aligned} \tag{177}$$

so we need $A = 0$.
The general solution is the superposition of the solutions for all possible values of n:

$$\psi(x,t) = \sum_{n=1}^{\infty} B_n \sin\left(\frac{n\pi x}{l}\right)\cos\left(\frac{n\pi vt}{l}\right). \tag{178}$$

To determine B_n we need to know the shape of the string at $t = 0$, $\psi(x,0) = f(x)$. We then need to find the values of the coefficients B_n such that

$$\psi(x,0) = \sum_{n=1}^{\infty} B_n \sin\left(\frac{n\pi x}{l}\right) = f(x)\,. \tag{179}$$

This is the Fourier series of an odd function. Our initial condition $f(x)$ must be analytically continued outside of the region $0 < x < l$, so that it is odd (and has period $L = 2l$). The coefficients of the (odd) Fourier series are then given by

$$B_n = \frac{4}{L}\int_0^{L/2} f(x)\sin\left(\frac{2\pi nx}{L}\right)\mathrm{d}x = \frac{2}{l}\int_0^{l} f(x)\sin\left(\frac{\pi nx}{l}\right)\mathrm{d}x\,. \tag{180}$$

The shape of a string plucked in the middle (with maximum height h) can be approximated by a triangle:

$$f(x) = \begin{cases} \frac{2h}{l}x & \text{if } 0 < x \le l/2\,, \\ \frac{2h}{l}(l-x) & \text{if } l/2 < x \le l\,, \end{cases} \tag{181}$$

We showed in q5 of the Fourier series problem sheet that the coefficients of the Fourier series of the odd analytic continuation of this function are

$$B_1 = \left(\frac{8h}{\pi^2}\right) , \quad B_2 = 0 , \quad B_3 = -\left(\frac{8h}{\pi^2}\right)\frac{1}{9} \quad B_4 = 0 , \dots . \tag{182}$$

(this calculation isn't difficult, but you need to be very careful with signs etc. to get the right answer). Inserting these coefficients into eq. (178), which we found by applying the other boundary conditions (ends are fixed so that $\psi(0,t) = \psi(l,t) = 0$ and string is initially stationary so that $(\partial\psi/\partial t)_{t=0} = 0$), we find the final solution

$$\psi(x,t) = \frac{8h}{\pi^2}\left[\sin\left(\frac{\pi x}{l}\right)\cos\left(\frac{\pi v t}{l}\right) - \frac{1}{9}\sin\left(\frac{3\pi x}{l}\right)\cos\left(\frac{3\pi v t}{l}\right) + \dots\right] . \tag{183}$$

If we'd hit the string rather than plucking it, the initial conditions would have been $\psi(x,0) = 0$ and $\left(\frac{\partial\psi}{\partial t}\right)_{t=0} = g(x)$ where $g(x)$ is the initial velocity.

We've focused on the wave equation, but these techniques can be used to solve other partial differential equations, e.g. Laplace's equation in 2d

$$\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} = 0 , \tag{184}$$

which arises in various branches of physics (gravity, electrostatics, fluid dynamics). See the differential equations problem sheet and questions from past exam papers.

7.4 Partial differential equations: using Fourier transforms (RHB 21.4)

FTs can be used to turn a PDE in real space into an ODE in Fourier space (which is easier to solve). Consider the heat flow equation:

$$\frac{\partial u(x,t)}{\partial t} = \alpha\frac{\partial^2 u(x,t)}{\partial x^2} , \tag{185}$$

where $u(x,t)$ is the temperature at position x at time t and α is the thermal diffusivity [11]. If an infinitely long bar is touched in the middle with a heat source, what is the subsequent temperature distribution?

Taking the FT of both sides of eq. (185) with respect to x [12]

$$U(k,t) = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} u(x,t)\exp(-ikx)\,\mathrm{d}x , \tag{186}$$

[11] In thermal physics the thermal diffusivity is often called λ, but we've called it α here to avoid confusion with wavelength.

[12] The FT involves integrating with respect to x from $-\infty$ to $+\infty$, so this method is only strictly valid if the bar is infinite.

and applying the differentiation property

$$FT\left[\frac{\partial^n u}{\partial x^n}\right] = (ik)^n FT[u]\,, \tag{187}$$

we get

$$\frac{\partial U(k,t)}{\partial t} = -\alpha k^2 U(k,t)\,, \tag{188}$$

which has solution

$$U(k,t) = U(k,0)\exp\left(-\alpha k^2 t\right), \tag{189}$$

where $U(k,0)$ is the FT of the initial temperature distribution

$$U(k,0) = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} u(x,0)\exp\left(-ikx\right)\mathrm{d}x\,. \tag{190}$$

Finally to find the solution in real space we would take the IFT of $U(k,t)$:

$$u(x,t) = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} U(k,t)\exp\left(ikx\right)\mathrm{d}k = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} U(k,0)\exp\left(-\alpha k^2 t\right)\exp\left(ikx\right)\mathrm{d}k\,. \tag{191}$$

This is easier than solving the initial PDE, but (in general) still not straightforward.

In this case (for the heat flow equation) we can however use the convolution theorem to find the solution, $u(x,t)$. $\exp\left(-\alpha k^2 t\right)$ is a gaussian and we saw in Sec. 3.6 that the Fourier transform of a gaussian is another gaussian (with width inversely proportional to that of the original gaussian) i.e. if

$$f(x) = \frac{1}{\sqrt{2\pi}\Delta}\exp\left(-\frac{x^2}{2\Delta^2}\right), \tag{192}$$

then

$$F(k) = \frac{1}{\sqrt{2\pi}}\exp\left(-\frac{k^2\Delta^2}{2}\right). \tag{193}$$

We have $\Delta^2 = 2\alpha t$, and so

$$\exp\left(-\alpha k^2 t\right) = FT\left[\frac{1}{\sqrt{2\alpha t}}\exp\left(-\frac{x^2}{4\alpha t}\right)\right]. \tag{194}$$

Remember that $U(k,0) = FT[u(x,0)]$. Therefore the FT of our solution, $U(k,t) = FT[u(x,t)]$, is the product of two Fourier transforms:

$$U(k,t) = (\sqrt{2\pi})FT[u(x,0)]FT\left[\frac{1}{\sqrt{2\pi}}\frac{1}{\sqrt{2\alpha t}}\exp\left(-\frac{x^2}{4\alpha t}\right)\right]. \tag{195}$$

From Sec. 4, if h is the convolution of f and g

$$h(x') = f \star g = \int_{-\infty}^{\infty} f(x)g(x'-x)\,\mathrm{d}x\,, \tag{196}$$

then the convolution theorem tells us that

$$H(k) = \sqrt{2\pi} F(k) G(k) \,. \tag{197}$$

Comparing this with eq. (195) we have

$$\begin{aligned} F(k) &\equiv FT[u(x,0)] \,, &(198)\\ G(k) &\equiv FT\left[\frac{1}{\sqrt{2\pi}}\frac{1}{\sqrt{2\alpha t}}\exp\left(-\frac{x^2}{4\alpha t}\right)\right] \,. &(199)\end{aligned}$$

Therefore our solution, $h(x') = u(x', t)$, is the convolution of $f(x) = u(x, 0)$ and

$$g(x) = \frac{1}{\sqrt{2\pi}}\frac{1}{\sqrt{2\alpha t}}\exp\left(-\frac{x^2}{4\alpha t}\right) \,. \tag{200}$$

So using the convolution definition

$$u(x', t) = \frac{1}{\sqrt{2\pi}}\frac{1}{\sqrt{2\alpha t}}\int_{-\infty}^{\infty} u(x, 0)\exp\left(-\frac{(x'-x)^2}{4\alpha t}\right)\mathrm{d}x \,. \tag{201}$$

If our initial heat source is a delta-function centered at $x = 0$: $u(x, 0) = \delta(x)$ then

$$u(x', t) = \frac{1}{\sqrt{2\pi}}\frac{1}{\sqrt{2\alpha t}}\int_{-\infty}^{\infty} \delta(x)\exp\left(-\frac{(x'-x)^2}{4\alpha t}\right)\mathrm{d}x' \,. \tag{202}$$

Remembering the sifting property of the delta-function

$$\int_{-\infty}^{\infty} \delta(x - x_0) g(x)\mathrm{d}x = g(x_0) \,, \tag{203}$$

(here we have $x_0 = 0$). Therefore

$$u(x', t) = \frac{1}{\sqrt{2\pi}}\frac{1}{\sqrt{2\alpha t}}\exp\left(-\frac{(x')^2}{4\alpha t}\right) \,, \tag{204}$$

and the final step is to change our label for the x co-ordinate back to x:

$$u(x, t) = \frac{1}{\sqrt{2\pi}}\frac{1}{\sqrt{2\alpha t}}\exp\left(-\frac{x^2}{4\alpha t}\right) \,. \tag{205}$$

Therefore for $t > 0$ the temperature distribution is a gaussian with width which increases with time (see Fig. 22). It is sometimes referred to as the point spread function (it tells us how a point source of heat spreads out) or Green's function.

To summarise, to find the temperature distribution, $u(x, t)$ in an infinitely long metal bar we

- Took the FT of the PDE which $u(x, t)$ obeys.
- Solved the resulting ODE.

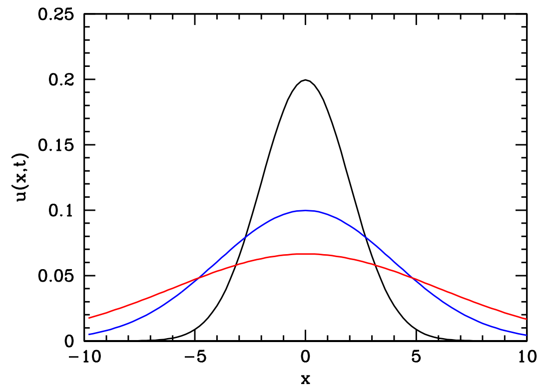

Figure 22: The temperature function in an infinitely long metal bar with thermal diffusivity $\alpha = 1\,\mathrm{m}^2\mathrm{s}^{-1}$ at $t = 1, 2, 3\,\mathrm{s}$ after it has been touched instantaneously with a heat source at $x = 0$ m at $t = 0$ s.

- Took the FT of the initial conditions $U(k, 0) = FT[u(x, t)]$.
- Calculated $u(t) = IFT[U(k, t)]$.

This process is shown in Fig. 23. For the heat flow equation the solution in the Fourier domain (or in Fourier space) is a gaussian, therefore the solution $u(x, t)$ is a convolution of a gaussian and the initial condition. If the initial condition is a delta-function, the solution is a gaussian with width that increases with time.

8 Summary

Fourier analysis involves writing a function as a superposition of waves of different frequencies. Periodic functions can be written as a sum of waves (a Fourier series).

The Fourier series comes in two, equivalent, forms; trigonometric with real coefficients a_r and b_r

$$f(x) = \frac{a_0}{2} + \sum_{r=1}^{\infty} \left[a_r \cos\left(rk_0x\right) + b_r \sin\left(rk_0x\right)\right] \,, \tag{206}$$

and complex, with complex coefficients c_r,

$$f(x) = \sum_{r=-\infty}^{\infty} c_r \exp\left(irk_0x\right) , \tag{207}$$

where, in both cases $k_0 = 2\pi/L$ is the fundamental wavenumber.

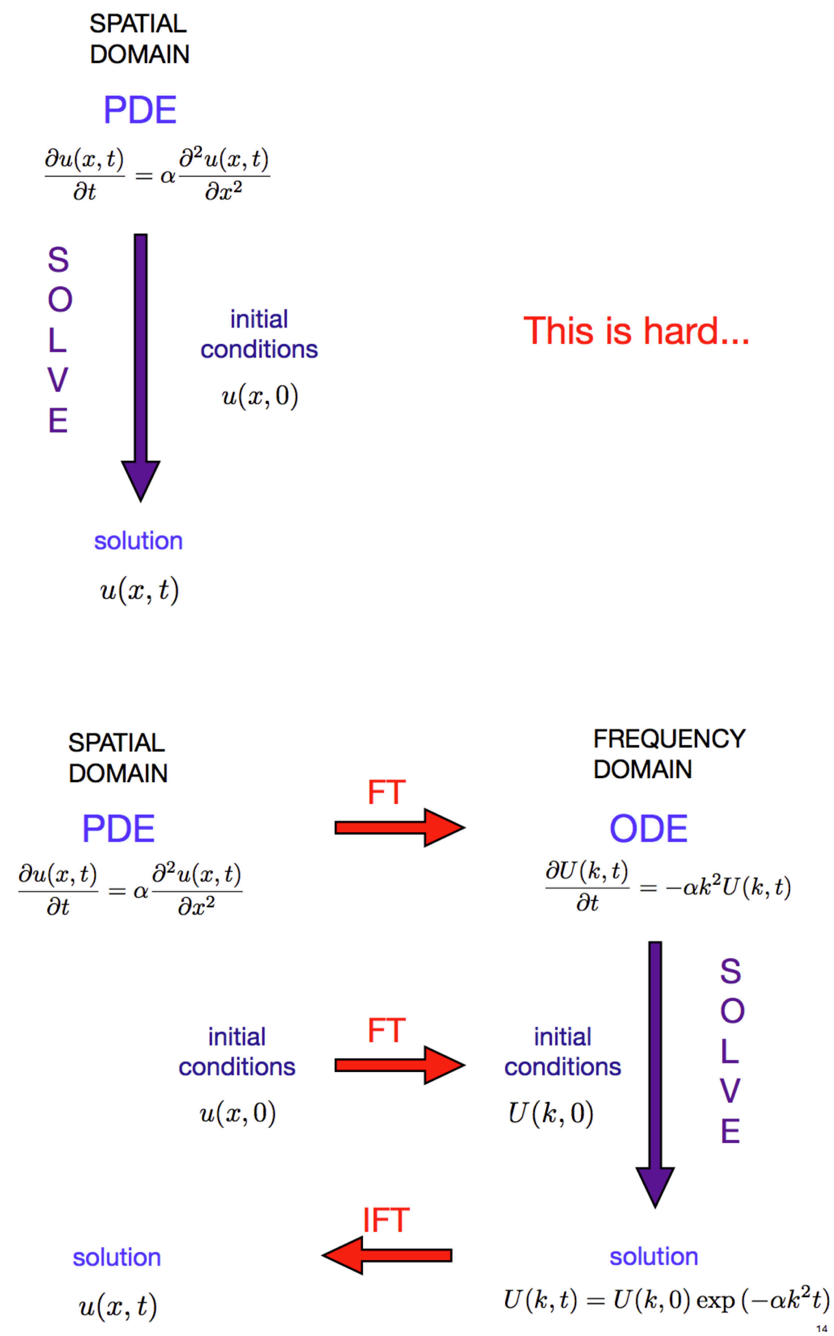

Figure 23: A graphical illustration of how using FTs turns solving a PDE from a hard calculation (top) into a series of less difficult calculations (bottom).

Non-periodic functions can be written as an integral of waves (a Fourier transform) weighted by a (in general complex) function $F(k)$

$$f(x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} F(k) \exp(ikx)\, \mathrm{d}k\,. \tag{208}$$

For functions of time $x \to t$, $k \to \omega$ and $T \to L$.

Fourier analysis has applications in many areas of science including physics, engineering and chemistry. For instance it allows us to generate signals in electronics, remove the experimental response from data (e.g. blurring of an astronomical image), calculate Fraunhofer diffraction patterns in optics and solve differential equations.

A Products of odd and even functions and their integrals

The product of two even functions is even: $f(x) = f_{e1}(x) f_{e2}(x)$. $f_{e1}(-x) = f_{e1}(x)$ and $f_{e2}(-x) = f_{e2}(x)$. Therefore $f(-x) = f_{e1}(-x) f_{e2}(-x) = f_{e1}(x) f_{e2}(x) = f(x)$.

The product of two odd functions is also even: $f(x) = f_{o1}(x) f_{o2}(x)$. $f_{o1}(-x) = -f_{o1}(x)$ and $f_{o2}(-x) = -f_{o2}(x)$. Therefore $f(-x) = f_{o1}(-x) f_{o2}(-x) = (-f_{o1}(x))(-f_{o2}(x)) = f(x)$.

The integral of an even function from $-A$ to $+A$ is twice the integral from 0 to A: $\int_{-A}^{A} f_e(x)\,\mathrm{d}x = \int_{-A}^{0} f_e(x)\,\mathrm{d}x + \int_0^A f_e(x)\,\mathrm{d}x$ and
$\int_{-A}^{0} f_e(x)\,\mathrm{d}x = -\int_0^{-A} f_e(x)\,\mathrm{d}x = -\int_0^A f_e(-\tilde{x})\,\mathrm{d}(-\tilde{x}) = \int_0^A f_e(\tilde{x})\,\mathrm{d}\tilde{x} = \int_0^A f_e(x)\,\mathrm{d}x$. Therefore $\int_{-A}^{A} f_e(x)\,\mathrm{d}x = 2\int_0^A f_e(x)\,\mathrm{d}x$.

This allows us to simply the calculation of the trigonometric Fourier coefficients of odd and even functions (see Sec. 2.4).

B Relationship between coefficients of complex and trigonometric Fourier series

Inserting eqs. (7) and (8) into eq. (19) we get

$$\begin{aligned}
f(x) &= \frac{a_0}{2} + \frac{1}{2}\left[\sum_{r=1}^{\infty} a_r \left(\exp\left(\frac{2\pi r x}{L}\right) + \exp\left(-\frac{2\pi r x}{L}\right)\right) + b_r \left(\frac{1}{i}\right)\left(\exp\left(\frac{2\pi r x}{L}\right) - \exp\left(-\frac{2\pi r x}{L}\right)\right)\right], \\
&= \frac{a_0}{2} + \frac{1}{2}\left[\sum_{r=1}^{\infty} (a_r - ib_r)\exp\left(\frac{2\pi r x}{L}\right) + (a_r + ib_r)\exp\left(-\frac{2\pi r x}{L}\right)\right], \\
&= \frac{a_0}{2} + \frac{1}{2}\sum_{r=1}^{\infty} (a_r - ib_r)\exp\left(\frac{2\pi r x}{L}\right) + \frac{1}{2}\sum_{r=-1}^{-\infty} (a_r + ib_r)\exp\left(\frac{2\pi r x}{L}\right), \\
&= \sum_{r=-\infty}^{\infty} c_r \exp\left(\frac{2\pi r x}{L}\right), \qquad (209)
\end{aligned}$$

with

$$
\begin{aligned}
c_0 &= \frac{a_0}{2}\,, && (210)\\
c_r &= \frac{1}{2}(a_r - ib_r)\,, && (211)\\
c_{-r} &= \frac{1}{2}(a_r + ib_r)\,. && (212)
\end{aligned}
$$

C Derivation of Parseval's theorem for complex Fourier series

$$
\frac{1}{L}\int_{x_0}^{x_0+L} |f(x)|^2\,\mathrm{d}x = \frac{1}{L}\int_{x_0}^{x_0+L} f(x)f^\star(x)\,\mathrm{d}x\,, \tag{213}
$$

where * denotes the complex conjugate. Using the definition of the complex Fourier series, eq. (38), and its complex conjugate:

$$
\begin{aligned}
\frac{1}{L}\int_{x_0}^{x_0+L} |f(x)|^2\,\mathrm{d}x &= \frac{1}{L}\int_{x_0}^{x_0+L}\left[\sum_{r=-\infty}^{\infty} c_r \exp\left(\frac{2\pi r x}{L}\right)\right]\left[\sum_{p=-\infty}^{\infty} c_p^\star \exp\left(-\frac{2\pi p x}{L}\right)\right]\mathrm{d}x\,,\\
&= \frac{1}{L}\left[\sum_{r=-\infty}^{\infty}\left[\sum_{p=-\infty}^{\infty} c_r c_p^\star \int_{x_0}^{x_0+L} \exp\left(\frac{2\pi r x}{L}\right)\exp\left(-\frac{2\pi p x}{L}\right)\mathrm{d}x\right]\right] \qquad (214)
\end{aligned}
$$

and using eq. (41) we get

$$
\frac{1}{L}\int_{x_0}^{x_0+L} |f(x)|^2\,\mathrm{d}x = \frac{1}{L}\sum_{r=-\infty}^{\infty} L c_r c_r^\star = \sum_{r=-\infty}^{\infty} |c_r|^2\,, \tag{215}
$$

as required.

D The pre-factors in the definition of Fourier transform and the inverse Fourier transform

The definitions of the Fourier transform and its inverse both contain constant pre-factors, A and B:

$$
\begin{aligned}
F(\omega) &= A\int_{-\infty}^{\infty} f(t)\exp(-i\omega t)\,\mathrm{d}t\,, && (216)\\
f(t) &= B\int_{-\infty}^{\infty} F(\omega)\exp(i\omega t)\,\mathrm{d}\omega\,. && (217)
\end{aligned}
$$

We will now show that if the original function $f(t)$ is to be recovered when $F(\omega)$ calculated using eq. (216) is inserted in eq. (217), we must have $AB = 1/(2\pi)$.

Inserting eq. (216) into eq. (217) we get

$$
f(t) = A\int_{-\infty}^{\infty}\left[B\int_{-\infty}^{\infty} f(\tilde{t})\exp(-i\omega\tilde{t})\,\mathrm{d}\tilde{t}\right]\exp(i\omega t)\,\mathrm{d}\omega\,. \tag{218}
$$

Rearranging the order of the integrals (and taking the constant B outside) we get

$$f(t) = AB \int_{-\infty}^{\infty} f(\tilde{t}) \left[\int_{-\infty}^{\infty} \exp\left(i\omega(t-\tilde{t})\right) \mathrm{d}\omega \right] \mathrm{d}\tilde{t} \,. \tag{219}$$

In Sec. 3.2 we met an alternative definition of the Dirac delta-function:

$$\delta(t) = \frac{1}{2\pi} \int_{-\infty}^{\infty} \exp\left(i\omega t\right) \mathrm{d}\omega \,, \tag{220}$$

or equivalently, with $t \to t - \tilde{t}$,

$$\delta(t-\tilde{t}) = \frac{1}{2\pi} \int_{-\infty}^{\infty} \exp\left(i\omega(t-\tilde{t})\right) \mathrm{d}\omega \,. \tag{221}$$

Inserting this in eq. (219) we get

$$f(t) = AB \int_{-\infty}^{\infty} f(\tilde{t}) 2\pi \delta(t-\tilde{t}) \, \mathrm{d}\tilde{t} \,, \tag{222}$$

and using the sifting property of the Dirac delta-function

$$\int_{-\infty}^{\infty} \delta(x-x_0) g(x) \, \mathrm{d}x = g(x_0) \,, \tag{223}$$

with $x \to \tilde{t}$, $x_0 \to t$ and $g \to f$ (and remembering that $\delta(t) = \delta(-t)$) we get

$$f(t) = AB 2\pi f(t) \,, \tag{224}$$

so that $AB = 1/(2\pi)$.

E Relationship between the Heaviside step function and the Dirac delta-function

If $h(t)$ is the Heaviside step function (as defined in Eq. (74)) then comparing the integral:

$$\begin{aligned}
\int_{-\infty}^{\infty} f(t) \left(\frac{\mathrm{d}h(t)}{\mathrm{d}t} \right) \mathrm{d}t &= [f(t)h(t)]_{-\infty}^{\infty} - \int_{-\infty}^{\infty} \left(\frac{\mathrm{d}f(t)}{\mathrm{d}t} \right) h(t) \, \mathrm{d}t \,, \\
&= f(\infty) - \int_{0}^{\infty} \left(\frac{\mathrm{d}f(t)}{\mathrm{d}t} \right) \mathrm{d}t \,, \\
&= f(\infty) - [f(t)]_0^{\infty} = f(0) \,,
\end{aligned} \tag{225}$$

with the Dirac delta-function sifting property, eq. (73), with $t_0 = 0$

$$\int_{-\infty}^{\infty} \delta(t) f(t) \, \mathrm{d}t = f(0) \,, \tag{226}$$

gives us

$$\frac{\mathrm{d}h(t)}{\mathrm{d}t} = \delta(t) \,, \tag{227}$$

i.e. the differential of the Heaviside step function is equal to the Dirac delta-function.

F Calculation of the Fourier transform of a gaussian

Inserting the gaussian, eq. (86), into the definition of the Fourier transform, eq. (58), we get

$$\begin{aligned} F(\omega) &= \frac{1}{\sqrt{2\pi}}\left[\frac{1}{\sqrt{2\pi}\Delta}\int_{-\infty}^{\infty}\exp\left(-\frac{t^2}{2\Delta^2}\right)\exp\left(-i\omega t\right)\mathrm{d}t\right], \\ &= \frac{1}{\sqrt{2\pi}}\left[\frac{1}{\sqrt{2\pi}\Delta}\int_{-\infty}^{\infty}\exp\left(-\left(\frac{t^2}{2\Delta^2}+i\omega t\right)\right)\right]\mathrm{d}t\,. \end{aligned} \tag{228}$$

To solve this we 'complete the square'. Multiplying by $\exp\left(-A^2\omega^2\right)\exp\left(A^2\omega^2\right)$ we get

$$F(\omega) = \frac{1}{\sqrt{2\pi}}\exp\left(-A^2\omega^2\right)\left[\frac{1}{\sqrt{2\pi}\Delta}\int_{-\infty}^{\infty}\exp\left(-\left(\frac{t^2}{2\Delta^2}+i\omega t - A^2\omega^2\right)\right)\mathrm{d}t\right]. \tag{229}$$

We want to choose A so that

$$\left(\frac{t}{\sqrt{2}\Delta}+iA\omega\right)^2 = \frac{t^2}{2\Delta^2}+i\omega t - A^2\omega^2\,, \tag{230}$$

i.e.

$$\begin{aligned} \frac{t^2}{2\Delta^2}+\frac{\sqrt{2}iA\omega t}{\Delta}-A^2\omega^2 &= \frac{t^2}{2\Delta^2}+i\omega t - A^2\omega^2\,, \\ \frac{\sqrt{2}iA\omega t}{\Delta} &= i\omega t\,, \\ A &= \frac{\Delta}{\sqrt{2}}\,, \end{aligned} \tag{231}$$

and then

$$\left(\frac{t}{\sqrt{2}\Delta}+iA\omega\right)^2 = \left(\frac{t}{\sqrt{2}\Delta}+\frac{i\Delta\omega}{\sqrt{2}}\right)^2 = \frac{\left(t+i\Delta^2\omega\right)^2}{2\Delta^2}\,, \tag{232}$$

so that the Fourier transform becomes

$$\begin{aligned} F(\omega) &= \frac{1}{\sqrt{2\pi}}\exp\left(-\frac{\Delta^2\omega^2}{2}\right)\left[\frac{1}{\sqrt{2\pi}\Delta}\int_{-\infty}^{\infty}\exp\left(-\frac{(t+i\Delta^2\omega)^2}{2\Delta^2}\right)\mathrm{d}t\right], \\ &= \frac{1}{\sqrt{2\pi}}\exp\left(-\frac{\Delta^2\omega^2}{2}\right), \end{aligned} \tag{233}$$

since

$$\frac{1}{\sqrt{2\pi}\Delta}\int_{-\infty}^{\infty}\exp\left(-\frac{(t+i\Delta^2\omega)^2}{2\Delta^2}\right)\mathrm{d}t \equiv \frac{1}{\sqrt{2\pi}\sigma}\int_{-\infty}^{\infty}\exp\left(-\frac{y^2}{2\sigma^2}\right)\mathrm{d}y\,, \tag{234}$$

[13] with $\sigma=\Delta$ and $y = t+i\Delta^2\omega$ and

$$\frac{1}{\sqrt{2\pi}\sigma}\int_{-\infty}^{\infty}\exp\left(-\frac{y^2}{2\sigma^2}\right)\mathrm{d}y = 1\,. \tag{235}$$

[13] To show this properly requires results from complex variable theory (see RHB 24).

G More on the Fast Fourier Transform

The discrete Fourier transform is defined as

$$F_k = \sum_{n=0}^{N-1} f_n \exp\left(-\frac{2\pi ikn}{N}\right). \tag{236}$$

If we define a complex number

$$W \equiv \exp\left(-\frac{2\pi i}{N}\right), \tag{237}$$

so that

$$W^{kn} = \exp\left(-\frac{2\pi ikn}{N}\right), \tag{238}$$

then the DFT can be written as

$$F_k = \sum_{n=0}^{N-1} W^{kn} f_n\,, \tag{239}$$

i.e. a vector f_n multiplied by a matrix whose (k, n)th element is W to the power of $k \times n$. To calculate one of the components of F_k takes N (complex) multiplications and N (complex) additions:

$$F_i = W^{i0} f_0 + ... + W^{i(N-1)} f_{N-1}\,. \tag{240}$$

In total N^2 operations are required and if N is large this is very slow.

The FFT is a clever algorithm for calculating the DFT quickly. The traditional (Cooley-Tookey) algorithm involves dividing a Fourier transform of length 2^n into sums of odd and even terms repeatedly until it is written in terms of N Fourier transforms of the individual data points:

$$\begin{aligned} F_k &= \sum_{j=0}^{(N/2)-1} \exp\left(-\frac{2\pi ik(2j)}{N}\right) f_{2j} + \sum_{j=0}^{(N/2)-1} \exp\left(-\frac{2\pi ik(2j+1)}{N}\right) f_{2j+1}\,, \\ &= \sum_{j=0}^{(N/2)-1} \exp\left(-\frac{2\pi ik(j)}{(N/2)}\right) f_{2j} + \exp\left(-\frac{2\pi ik}{N}\right) \sum_{j=0}^{(N/2)-1} \exp\left(-\frac{2\pi ikj}{(N/2)}\right) f_{2j+1}\,, \\ &= \sum_{j=0}^{(N/2)-1} \exp\left(-\frac{2\pi ik(j)}{(N/2)}\right) f_{2j} + W^k \sum_{j=0}^{(N/2)-1} \exp\left(-\frac{2\pi ikj}{(N/2)}\right) f_{2j+1}\,, \\ &= F_k^e + W^k F_k^0\,. \end{aligned} \tag{241}$$

If $N = 2^n$ this process can be repeated until the data is divided into N DFTs of length 1. And the DFT of a number is just the number. So the elements of the original data need to be combined into 2-point FTs, and then 4-point FTs and so on to calculate the full DFT (the elements then need to be rearranged to get them in the right order. This reduces the number of calculations required to $\sim N\log_2 N$, which is much smaller (and therefore faster) than the original $\sim N^2$. This algorithm only works if the number of data points is an integer power of 2, $N = 2^n$. There are now other algorithms which work for $N = 3^n, 5^n$, and 7^n.

H 3d spherically symmetric Fourier transform

For a spherically symmetric function, $f(r)$, using spherical polar coordinates $\mathrm{d}^3\mathbf{r} = r^2 \sin\theta \mathrm{d}r\,\mathrm{d}\theta\,\mathrm{d}\phi$ and $\mathbf{k}.\mathbf{r} = \cos\theta$ and eq. (137) becomes

$$
\begin{aligned}
F(k) &= \frac{1}{(2\pi)^{3/2}} \int_0^\infty \mathrm{d}r \int_0^\pi \mathrm{d}\theta \int_0^{2\pi} \mathrm{d}\phi f(r) r^2 \sin\theta \exp\left(-ikr\cos\theta\right), \\
&= \frac{1}{(2\pi)^{3/2}} \int_0^\infty \mathrm{d}r \int_0^\pi \mathrm{d}\theta f(r) r^2 \sin\theta \exp\left(-ikr\cos\theta\right) [\phi]_0^{2\pi}, \\
&= \frac{1}{(2\pi)^{3/2}} \int_0^\infty \mathrm{d}r 2\pi r^2 f(r) \int_0^\pi \mathrm{d}\theta \sin\theta \exp\left(-ikr\cos\theta\right), \\
&= \frac{1}{(2\pi)^{3/2}} \int_0^\infty \mathrm{d}r 2\pi r^2 f(r) \left[\frac{\exp\left(-ikr\cos\theta\right)}{ikr}\right]_{\theta=0}^{\pi}, \\
&= \frac{1}{(2\pi)^{3/2}} \int_0^\infty \mathrm{d}r 2\pi r^2 f(r) \left[\frac{\exp\left(ikr\right) - \exp\left(-ikr\right)}{ikr}\right], \\
&= \frac{1}{(2\pi)^{3/2}} \int_0^\infty \mathrm{d}r 4\pi r^2 f(r) \left[\frac{\sin\left(kr\right)}{kr}\right]. \qquad (242)
\end{aligned}
$$