Fourier Series & Fourier Transforms

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Synopsis

Lecture 1 :

- Review of trigonometric identities
- Fourier Series
- Analysing the square wave

Lecture 2:

- The Fourier Transform
- Transforms of some common functions

Lecture 3:

Applications in chemistry

- FTIR
- Crystallography

Bibliography

1. The *Chemistry Maths Book* (Chapter 15), Erich Steiner, OUP, 1996.

Introduction

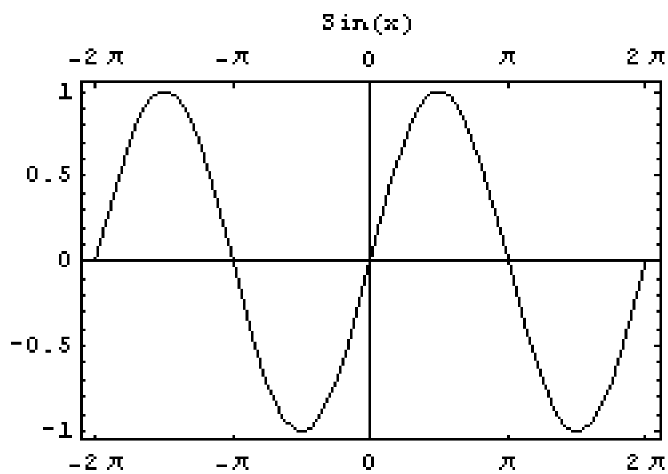
Chemistry often involves the measurement of properties which are the aggregate of many fundamental processes. A variety of techniques have been developed for extracting information about these underlying processes. Fourier analysis is one of the most important and is very widely used - eg: in crystallography, X-ray adsorbtion spectroscopy, NMR, vibrational spectroscopy (FTIR) etc.. As it involves decomposition of functions into partial waves it also appears in many quantum mechanical calculations.

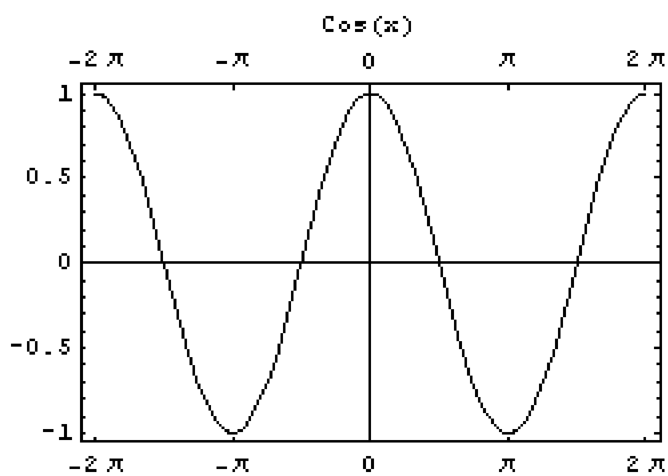
A Little Trigonometry

You will need to be able to manipulate sin() and cos() in order to understand Fourier analysis - a good understanding of the UK's A-level Pure Maths syllabus is sufficient. Here is a brief reminder of some important properties.

Units angles are typically measured in radians: $0 - 360^o$is equivalent to $0 - 2\pi$ radians

Cos and sin curves look like this:





Both sin(x) and cos(x) are periodic on the interval 2π and integrate to 0 over a full period, ie:

$$\int_{-\pi}^{+\pi} \cos{(x)}\, dx = \int_{-\pi}^{+\pi} \sin{(x)}\, dx = 0$$

Wavelength

It should be clear that sin(2x) repeats on the interval $0 \rightarrow \pi$ and sin(3x) on the interval $0 \rightarrow 2\pi/3$ etc. In general sin(nx) and cos(nx) repeat on the interval $0 \rightarrow 2\pi/n$. The repeat distance is the *wavelength* λ and so in general, $\lambda = 2\pi/n$.

The discrete family of functions sin(nx), cos(nx) are all said to be *commensurate* with the period 2π- that is, they all have wavelengths which divide exactly into 2π.

The function sin(kx) for some real number k has an arbitrary wavelength $\lambda = 2\pi/k$.

k is usually referred to as the *wavevector*.

Note: A simple Mathermatica notebook, **trig_1.nb**, is provided with the course and can be used to play with sin and cos functions.

Fourier Series

The idea of a Fourier series is that any (reasonable) function, $f(x)$, that is periodic on the interval 2π (ie: $f(x + 2\pi n) = f(x)$ for all n) can be decomposed into contributions from sin(nx) and cos(nx).

The general Fourier series may be written as:

$$\begin{aligned} f(x) = \frac{a_0}{2} &+ a_1 \cos{(x)} + a_2 \cos{(2x)} + a_3 \cos{(3x)} + \ldots + a_n \cos{(nx)} \\ &+ b_1 \sin{(x)} + b_2 \sin{(2x)} + b_3 \sin{(3x)} + \ldots + b_n \sin{(nx)} \end{aligned} \tag{1}$$

Note:

1. $\cos{(nx)}$ and $\sin{(nx)}$ are periodic on the interval 2π for any integer n.
2. The $a_n$and b_n coefficients measure the strength of contribution from each *"harmonic"*.

Orthogonality

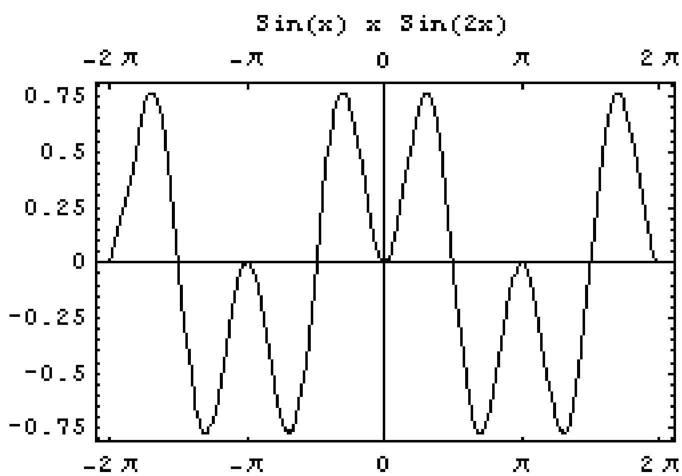
The functions $\cos{(nx)}$ and $\sin{(nx)}$ can be used in this way because they satisfy the following *orthogonality* conditions:

$$
\begin{aligned}
\int_{-\pi}^{+\pi} \cos(mx)\sin(nx)\,dx &= 0 && for\ all\ m,n \\
\int_{-\pi}^{+\pi} \cos(mx)\cos(nx)\,dx &= 0 && m \neq n \\
&= 2\pi && m = n = 0 \\
&= \pi && (m = n) > 0 \\
\int_{-\pi}^{+\pi} \sin(mx)\sin(nx)\,dx &= 0 && m \neq n \\
&= \pi && (m = n) > 0
\end{aligned}
$$

Note that the integrals only need to extend from $-\pi$ to $+\pi$ (or any other period of 2π) as the functions simply repeat outside this range.

These conditions can be proved quite readily but it is relatively easy to see why they are true graphically.

- **cos(mx) sin(nx) ?** This is obvious (!) if you plot cos(x) and sin(x).
- **sin(mx) sin(nx)** $n \neq m$**?** It is easier to see why it is true by picking a special case; say the integral of sin(2x) sin(x) and plotting.



The symmetry of the plot makes it clear that an integral of this function over any period of 2π will yield 0.

- Is it obvious that this will be true for all cases when $n \neq m$?
- Also for the case cos(mx)cos(nx) ?
- Can you prove it in the general case ?

Note: A simple Mathermatica notebook, **trig_1.nb**, is provided with the course and can be used to play with these products and integrals.

- **cos(mx) cos(mx) - ie: the case when** $n = m$

$$
\int_{-\pi}^{+\pi} \cos^2(mx)\,dx = \int_{-\pi}^{+\pi} \frac{1}{2}\left(1 + 2\cos(mx)\right)dx = \frac{1}{2}\left[x + \frac{sin\,(2mx)}{2m}\right]_{-\pi}^{\pi} = \pi
$$

Finding the coefficients

As was shown in the lecture the orthogonality conditions allow us to pick off values for all of the coefficients. Multiplying the whole Fourier series by $1, \cos(nx)$or $\sin(nx)$ and integrating over a complete period leads to terms which are zero apart from one which corresponds to the coefficient a_0, a_n or b_n respectively, that is:

$$\begin{aligned}
a_0 &= \frac{1}{\pi}\int_{-\pi}^{+\pi} f(x)\,dx \\
a_n &= \frac{1}{\pi}\int_{-\pi}^{+\pi} f(x)\cos(nx)\,dx \\
b_n &= \frac{1}{\pi}\int_{-\pi}^{+\pi} f(x)\sin(nx)\,dx
\end{aligned}$$

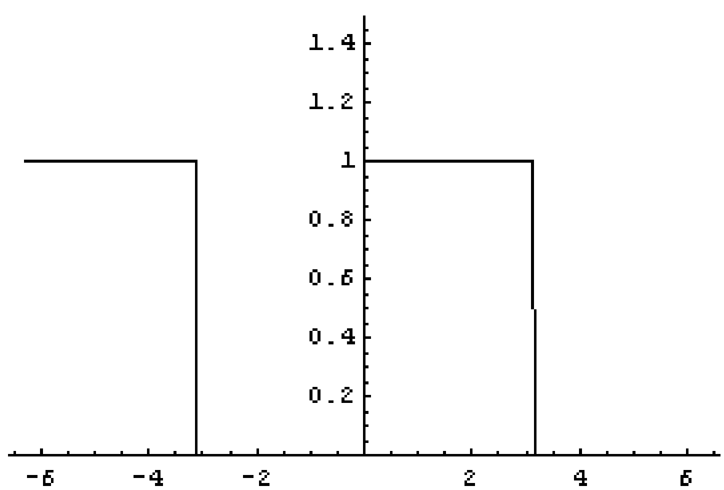
If $f(x)$ is "well behaved" we can perform these integrals and obtain the Fourier *decomposition* of $f(x)$.

Note: Well behaved in this context means that the function obeys the Dirichlet conditions.

An Example

Consider the square wave:

$$\begin{aligned}
f(x) = &\quad 1 &\quad 0 \le x < \pi \\
= &\quad 0 &\quad -\pi \le x < 0 \\
f(x) = &\quad f(x + 2\pi) &
\end{aligned}$$



This appears to be a difficult case - the rather angular square wave does not look as if it will be readily expanded in terms of sine and cosine functions.

The coefficients in the expansion can be determined from the formulae given above.

a_0 is determined by:

$$a_0 = \frac{1}{\pi}\int_{-\pi}^{+\pi} f(x)dx = \frac{1}{\pi}\int_{0}^{+\pi} 1\,dx = \frac{1}{\pi}\times\pi = 1$$

where the restriction of the integral to the region $0 \to \pi$ is simply because $f(x)$ is zero in the region $-\pi \to 0$.

Similarly:

$$a_n = \frac{1}{\pi}\int_{0}^{+\pi} 1\times\cos(nx)\,dx = 0$$

just draw $\cos(x)$to see that its integral from $0 \to \pi$ is zero, so

$$a_n = 0\ for\ all\ n$$

For the b coefficients we have,

$$\begin{aligned} b_n &= \frac{1}{\pi}\int_{0}^{+\pi} 1\times\sin(nx)\,dx \\ &= \frac{1}{\pi}\left[\frac{-\cos(nx)}{n}\right]_0^{\pi} \\ &= \frac{1}{n\pi}\left(1-\cos(n\pi)\right) \end{aligned}$$

but,

$$\begin{aligned} \cos(n\pi) &= &+1 \quad & n-even \\ &= &-1 \quad & n-odd \end{aligned}$$

so,

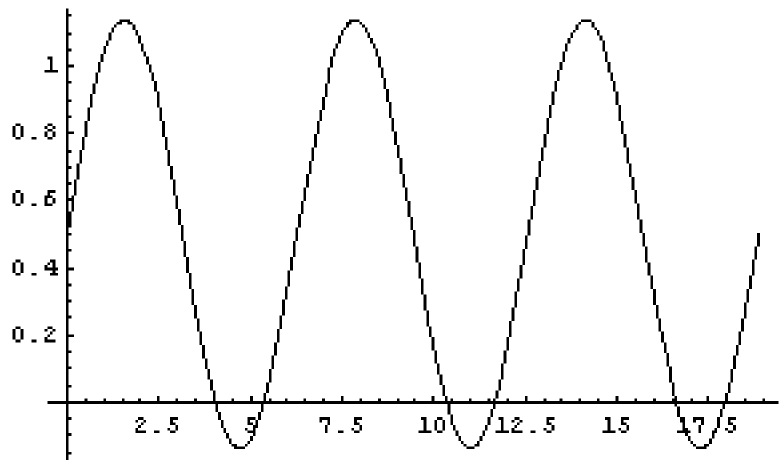
$$\begin{aligned} b_n = \quad & 0 \quad & n-even \\ & \tfrac{2}{n\pi} \quad & n-odd \end{aligned}$$

having determined all of the coefficients we can write the series for $f(x)$ as:

$$f(x) = \frac{1}{2} + \frac{2}{\pi}\left(\sin(x) + \frac{\sin(3x)}{3} + \frac{\sin(5x)}{5} + \ldots\right)$$

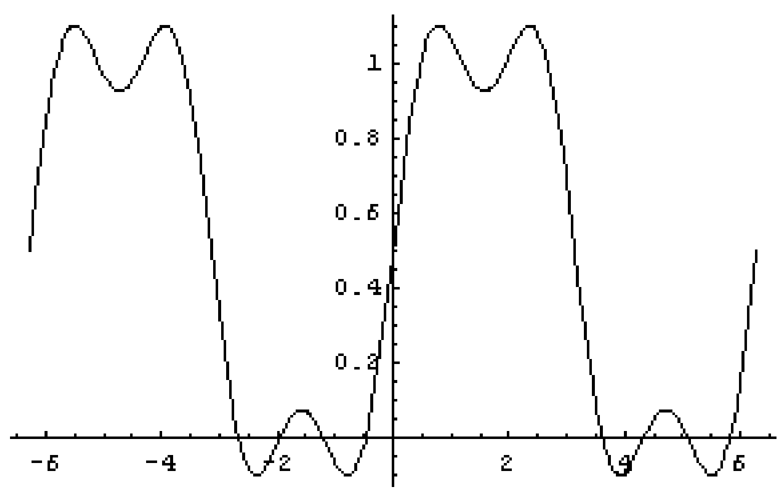
The sum continues to an infinite number of terms. We can see how it converges to the square wave by plotting the truncated sum containing a finite number of terms - lets call the sum containing n-trigonometric terms $f_n(x)$ then $f_0(x) = \frac{1}{2}$is just the average value of the square wave.

$f_1(x) = \frac{1}{2} + \frac{2}{\pi}\sin(x)$ is plotted below



which is the "best" approximation that can be made using just a constant and a sine wave - not great.

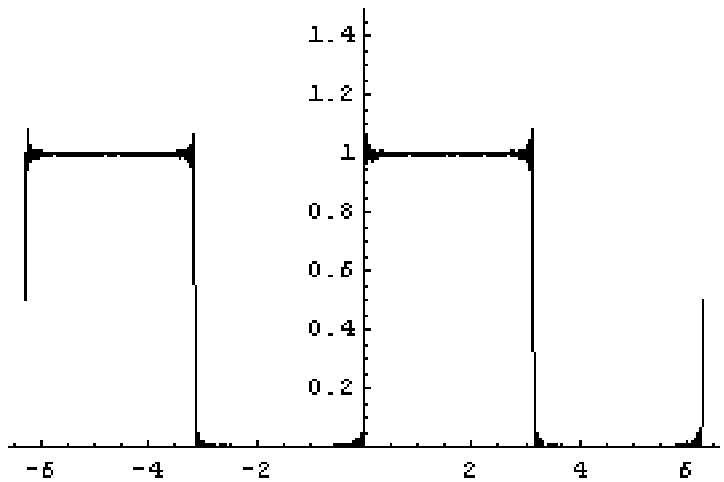
$f_2(x) = \frac{1}{2} + \frac{2}{\pi}\sin(x) + \frac{2}{3\pi}sin(3x)$ looks like this:



which is beginning to look more like a square well.

The weight in each contribution is falling and with each additional term the fine detail of the square wave is being refined.

Including 50 terms, $f_{50}(x)$, we get



which is a pretty decent approximation to the original square wave.

Note that the little spikes at the edge of the square wave are present even after including many hundreds of terms (although they become finer and finer) they are a consequence of trying to describe a discontinuous step function with smooth sine waves – this was noticed and studied by the mathematician JW Gibbs in the late 1890's.

A more compact notation

In many applications you will find that a more compact notation is used for the Fourier series. Using the identity

$$e^{i\theta} = \cos(\theta) + i\sin(\theta)$$

We can write;

$$\cos(\theta) = \frac{1}{2}\left(e^{i\theta} + e^{-i\theta}\right)$$

$$\sin(\theta) = \frac{1}{2i}\left(e^{i\theta} - e^{-i\theta}\right)$$

Using these relations we can rewrite the Fourier series, equation 1, in the more compact exponential notation;

$$f(x) = \frac{a_0}{2} + \frac{1}{2}\sum_{n=1}^{\infty} a_i\left(e^{inx} + e^{-inx}\right) + \frac{1}{2i}\sum_{n=1}^{\infty} b_i\left(e^{inx} + e^{-inx}\right)$$

which can be rearranged as;

$$f(x) = \sum_{n=-\infty}^{\infty} c_n e^{inx}$$

In the exponential notation the orthogonality conditions are;

$$\int_{-\pi}^{+\pi} e^{-imx} e^{inx} dx = 2\pi \qquad if\ m = n$$

and so the coefficients given by

$$c_n = \frac{1}{2\pi} \int_{-\pi}^{+\pi} e^{-inx} f(x) dx$$

The original and compact notations are equivalent and the c_n coefficients are therefore directly related to a_n and b_n

$$\begin{aligned}
c_0 &= \frac{1}{2} a_0 \\
c_n &= \frac{1}{2} (a_n - b_n) \\
c_{-n} &= \frac{1}{2} (a_n + b_n)
\end{aligned}$$

This more compact notation is used in almost all applications.

Fourier Transforms

Functions of arbitrary periodicity

The discussion of Fourier Series above dealt with functions periodic on the interval 2π (ie: $f(x + 2\pi n) = f(x)$ for all n). This can be generalised to functions periodic on any interval.

Functions with a periodicity of 2L (ie: $f(x + 2Ln) = f(x)$ for all n) can be decomposed into contributions from from $\sin\left(n\frac{\pi x}{L}\right)$and $\cos\left(n\frac{\pi x}{L}\right)$which are periodic on the period 2L.

The Fourier series may then be written as:

$$\begin{aligned}
f(x) = \frac{a_0}{2} &+ a_1 \cos\left(\frac{\pi x}{L}\right) + a_2 \cos\left(2\frac{\pi x}{L}\right) + a_3 \cos\left(3\frac{\pi x}{L}\right) + \ldots + a_n \cos\left(n\frac{\pi x}{L}\right) \\
&+ b_1 \sin\left(\frac{\pi x}{L}\right) + b_2 \sin\left(2\frac{\pi x}{L}\right) + b_3 \sin\left(3\frac{\pi x}{L}\right) + \ldots + b_n \sin\left(n\frac{\pi x}{L}\right)
\end{aligned}$$

or

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

or, in the exponential notation,

$$f(x) = \sum_{n=-\infty}^{\infty} c_n e^{in\frac{\pi x}{L}}$$

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

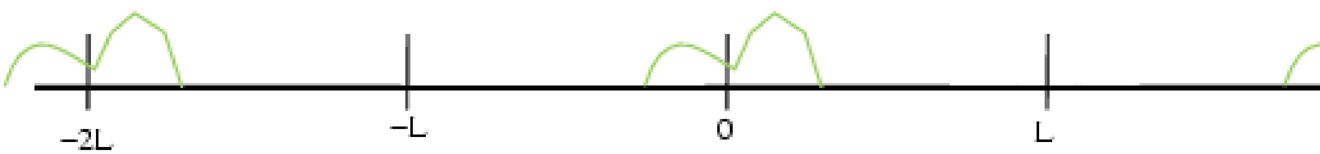
Note: The limits of integration cover a single period of the function which is not 2L rather than 2π.

This allows a function of arbitrary period to be analysed.

Nonperiodic functions

Fourier series are applicable only to periodic functions but non-periodic functions can also be decomposed into Fourier components - this process is called a *Fourier Transform.*

Imagine a function that is of a finite extent that is much less than the periodicity, 2L, as pictured below,



If L becomes very large (tends to infinity) then we will have an isolated, aperiodic, function. We will use this limiting process to develop the equations for the Fourier Transform from the Fourier Series.

Consider the Fourier Series for this function;

$$f(x) = \sum_{n=-\infty}^{\infty} c_n e^{in\frac{\pi x}{L}}$$

Consider the limit in which L becomes very large.

If we define;

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

then

$$f(x) = \sum_{n=-\infty}^{\infty} c_n e^{ik_n x}$$

and it is clear that for very large L the sum contains a very large number of waves with wavevector $k_n$and that each succesive wave differs from the last by a tiny change in wavevector (or if you prefer, wavelength),

$$\Delta k = k_{n+1} - k_n = \frac{\pi}{L}$$

As was shown in the lecture, in the limit of large L k becomes a continuous variable, the discrete coefficients, c_n, become a continuous function of k, $c\,(k)$and the summation can be replaced by an integral and,

$$\begin{aligned} f(x) &= \frac{1}{2\pi}\int_{-\infty}^{+\infty} c(k)e^{ikx}dk \\ c(k) &= \int_{-\infty}^{+\infty} f(x)e^{-ikx}dx \end{aligned}$$

These pair of equations are very often rescaled by substituting $c(k) = \sqrt{2\pi}c(k)$ to obtain;

$$\begin{aligned} f(x) &= \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{+\infty} c(k)e^{ikx}dk \\ c(k) &= \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{+\infty} f(x)e^{-ikx}dx \end{aligned}$$

The functions f and c are called a Fourier transform pair - c is the Fourier transform of f and f is the (inverse) transform of c.