FOURIER SERIES

A Fourier series is a series of sine and cosine functions, or else exponential functions, used to represent a function of interest. For any of the functions we consider in our applications, the appropriate series converges to the function. Such series are used extensively in solid state physics to represent electron wave functions and atomic displacement.

Let $f(x)$ be a periodic function of one variable with period a: $f(x) = f(x + na)$ for all values of x and for all integers n. If $f(x)$ is single valued, if it has a finite number of maxima and minima in any range of width a, if it is continuous or has a finite number of finite discontinuities in any range of width a, and if the integral $\int |f(x)|^2\, dx$ over an interval of width a is finite, then $f(x)$ can be represented by a convergent Fourier series:

$$f(x) = \tfrac{1}{2}A_0 + \sum_{k=0}^{\infty} A_k \cos\left(\frac{2\pi k x}{a}\right) + \sum_{k=0}^{\infty} B_k \sin\left(\frac{2\pi k x}{a}\right), \qquad \text{(F-1)}$$

where the sums are over all positive integers. The Fourier coefficients are given by

$$A_k = \frac{2}{a}\int_{-a/2}^{+a/2} f(x)\cos\left(\frac{2\pi k x}{a}\right) dx \qquad \text{(F-2)}$$

and

$$B_k = \frac{2}{a}\int_{-a/2}^{+a/2} f(x)\sin\left(\frac{2\pi k x}{a}\right) dx\,. \qquad \text{(F-3)}$$

If the function is known, Eqs. F-2 and F-3 can be used to find the coefficients. In most practical applications the function is not known, but we nevertheless assume it can be expanded as a Fourier series and, for example, substitute the series into an appropriate differential equation. The differential equation is then used to determine the Fourier coefficients. In some cases, only a few terms in the series are needed to reproduce the function with sufficient accuracy. In many solid state applications, however, several thousand terms might be required and a high-speed computer is used to evaluate the sums.

If $f(x)$ is continuous at some point x_0, then the series converges to $f(x_0)$. If $f(x)$ is discontinuous at x_0, then the limiting value of $f(x)$ as x approaches x_0 from above is different from the limiting value as it approaches from below. For $x = x_0$, the series converges to the average of the two limiting values.

Notice that the series consists of sinusoidal functions with periods that are submultiples of the period of $f(x)$. No sinusoidal function with a period greater than that of $f(x)$ enters the sum. Short period sinusoidal functions are needed to reproduce details of $f(x)$, all of which must, of necessity, occur in ranges smaller than a. Qualitatively, the more rapidly $f(x)$ varies, the larger the coefficients associated with high k terms.

Since $\cos(2\pi n x/a) = \frac{1}{2}[e^{i2\pi kx/a} + e^{-i2\pi kx/a}]$ and $\sin(2\pi kx/a) = \frac{1}{2}i[e^{i2\pi kx/a} - e^{-i2\pi kx/a}]$, a Fourier series can also be written in terms of exponential functions:

$$f(x) = \sum_{k=-\infty}^{+\infty} C_k e^{i2\pi kx/a}, \qquad \text{(F-4)}$$

where

$$C_k = \frac{1}{a}\int_{-a/2}^{+a/2} f(x) e^{-i2\pi kx/a}\, dx\,. \qquad \text{(F-5)}$$

Both positive and negative exponents must be included, so k takes on both positive and negative integer values. A series of exponentials is often more convenient than a series of sine and cosine functions.

The expression for C_k clearly follows from Eq. F-4. We first note that

$$\int_{-a/2}^{+a/2} e^{i2\pi(k-k')/a}\, dx = a\delta_{kk'}, \qquad \text{(F-6)}$$

where $\delta_{kk'}$ is the Kronecker delta, a quantity that is 1 if $k = k'$ and 0 if $k \neq k'$. Multiply Eq. F-4 by $e^{-i2\pi k'x/a}$ and integrate the result from $-a/2$ to $+a/2$ to obtain

$$\int_{-a/2}^{+a/2} f(x) e^{-i2\pi k'x/a}\, dx = \sum_k c_k a\delta_{kk'}\,. \qquad \text{(F-7)}$$

Every term in the sum vanishes except the $k = k'$ term, so the sum is equal to $aC_{k'}$. Equation F-5 follows immediately when k' is replaced by k.

The statements made above are easily generalized to three dimensions. Suppose $f(\mathbf{r})$ is periodic and its periodicity is described by a lattice with primitive vectors $\mathbf{a}$, $\mathbf{b}$, and $\mathbf{c}$. That is, $f(\mathbf{r} + n_1\mathbf{a} + n_2\mathbf{b} + n_3\mathbf{c}) = f(\mathbf{r})$ for any $\mathbf{r}$ and any three integers n_1, n_2, and n_3.

Write $\mathbf{r} = u\mathbf{a} + v\mathbf{b} + w\mathbf{c}$ and consider u, v, and w to be the independent variables instead of the components of $\mathbf{r}$. The function $f(\mathbf{r})$ is periodic in each of the variables and, for each, its period is 1. First consider $f(\mathbf{r})$ to be a function of u and expand it as a one-dimensional Fourier series. The coefficients depend on v and w. Each coefficient may now be expanded as a series in v, with coefficients that depend on w. Finally each of these coefficients may be written as a series in w. The end result is

$$f(\mathbf{r}) = \sum_{k=-\infty}^{+\infty}\sum_{\ell=-\infty}^{+\infty}\sum_{l=-\infty}^{+\infty} C_{k\ell l}\, e^{i2\pi(ku+\ell v+lw)}, \qquad \text{(F-8)}$$

See back →.

where

$$C_{hk\ell} = \int_{-1/2}^{+1/2}\int_{-1/2}^{+1/2}\int_{-1/2}^{+1/2} f(\mathbf{r})e^{-i2\pi(hu+kv+\ell w)}\,du\,dv\,dw\,. \qquad \text{(F-9)}$$

Now $2\pi(hu + kv + \ell w) = \mathbf{G}\cdot\mathbf{r}$, where $\mathbf{G}$ is the reciprocal lattice vector $h\mathbf{A} + k\mathbf{B} + \ell\mathbf{C}$. The volume of a unit cell is $\tau = |\mathbf{a}\cdot\mathbf{b}\times\mathbf{c}|$ and an infinitesimal volume element is $d\tau = |\mathbf{a}\cdot\mathbf{b}\times\mathbf{c}|\,du\,dv\,dw = \tau\,du\,dv\,dw$. Equations F-8 and F-9 can therefore be written

$$f(\mathbf{r}) = \sum_{\mathbf{G}} C(\mathbf{G})e^{i\mathbf{G}\cdot\mathbf{r}} \qquad \text{(F-10)}$$

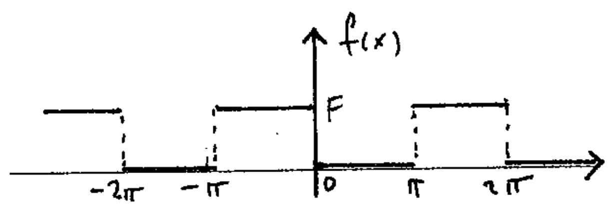
and

$$C(\mathbf{G}) = \frac{1}{\tau}\int_{\substack{\text{unit}\\ \text{cell}}} f(\mathbf{r})e^{-i\mathbf{G}\cdot\mathbf{r}}\,d\tau\,, \qquad \text{(F-11)}$$

respectively. We have written $C_{hk\ell}$ as $C(\mathbf{G})$. The sum in Eq. F-10 is over all reciprocal lattice vectors.

* * *

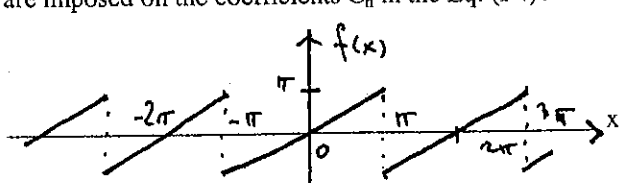
Now turn $90^\circ = \frac{\pi}{2}$ and exercise!



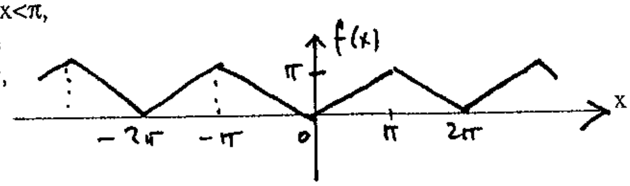
F1 Take a <u>step-wave</u> function (see fig.), $f(x) = 0$ at $-\pi<x<0$, and $f(x) = F$ at $0<x<\pi$ calculate the Fourier coefficients A_h, B_h, and write down the resulting series. Plot (use Mathematica, or Maple, or MatLab) the series <u>truncated</u> up to h=1, 3, 5, 7, watch for the Gibbs phenomenon, i.e. a "splash" near the discontinuity point.

F2 For a "phase-shifted" form, $f(x) = A_0/2 + \sum_{1}^{\infty} \alpha_h \cos(hx-\theta_h)$ show that $A_h = \alpha_h \cos\theta_h$ and $B_h = \alpha_h \sin\theta_h$. Or vice versa, $\alpha_h^2 = A_h^2 + B_h^2$, and $\tan\theta_h = B_h/A_h$

F3 If a function is real, $f^*(x) = f(x)$, what restrictions are imposed on the coefficients C_h in the Eq. (F4)?



F4 A <u>sawtooth-wave</u> (see fig.), $f(x) = x$, $-\pi<x<\pi$. Find the Fourier series.



F5 A <u>triangular wave</u> is represented by $f(x) = x$ at $0<x<\pi$, and $f(x) = -x$ at $-\pi<x<0$. Find Fourier series. Do the coefficients A_h, B_h (and C_h) decrease faster or slower, with the number h, than in the Problems F1 or F4?

F6 If the coefficients A_h, B_h are known for a function $f(x)$, find the coefficients in the Fourier series for df/dx and for d^2f/dx^2. Try the higher derivatives, and exercise with the exponential representation Eq. (F4), that is the C_h.