2.1 Complex Fourier Series

The phases $\exp(inx)/\sqrt{2\pi}$, one for each integer n, are orthonormal on an interval of length 2π

$$\int_{0}^{2\pi} \left(\frac{e^{imx}}{\sqrt{2\pi}}\right)^{*} \frac{e^{inx}}{\sqrt{2\pi}} dx = \int_{0}^{2\pi} \frac{e^{i(n-m)x}}{2\pi} dx = \delta_{m,n}$$
(2.1)

where $\delta_{n,m} = 1$ if n = m, and $\delta_{n,m} = 0$ if $n \neq m$. So if a function f(x) is a sum of these phases

$$f(x) = \sum_{n=-\infty}^{\infty} f_n \, \frac{e^{inx}}{\sqrt{2\pi}} \tag{2.2}$$

then their orthonormality (2.1) gives the *n*th coefficient f_n as the integral

$$\int_{0}^{2\pi} \frac{e^{-inx}}{\sqrt{2\pi}} f(x) \, dx = \int_{0}^{2\pi} \frac{e^{-inx}}{\sqrt{2\pi}} \sum_{m=-\infty}^{\infty} f_m \, \frac{e^{imx}}{\sqrt{2\pi}} \, dx = \sum_{m=-\infty}^{\infty} \delta_{n,m} f_m = f_n \quad (2.3)$$

(Joseph Fourier 1768–1830).

The Fourier series (2.2) is periodic with period 2π because the phases are periodic with period 2π , $\exp(in(x + 2\pi)) = \exp(inx)$. Thus even if the function f(x) which we use in (2.3) to make the Fourier coefficients f_n is not periodic, its Fourier series (2.2) will nevertheless be strictly periodic, as illustrated by Figs. 2.2 & 2.4.

If the Fourier series (2.2) converges uniformly (section 2.7), then the termby-term integration implicit in the formula (2.3) for f_n is permitted.

How is the Fourier series for the complex-conjugate function $f^*(x)$ related

to the series for f(x)? The complex conjugate of the Fourier series (2.2) is

$$f^*(x) = \sum_{n = -\infty}^{\infty} f_n^* \frac{e^{-inx}}{\sqrt{2\pi}} = \sum_{n = -\infty}^{\infty} f_{-n}^* \frac{e^{inx}}{\sqrt{2\pi}}$$
(2.4)

so the coefficients $f_n(f^*)$ for $f^*(x)$ are related to those $f_n(f)$ for f(x) by

$$f_n(f^*) = f^*_{-n}(f).$$
(2.5)

Thus if the function f(x) is real, then

$$f_n(f) = f_n(f^*) = f_{-n}^*(f).$$
 (2.6)

Thus the Fourier coefficients f_n for a real function f(x) satisfy

$$f_n = f_{-n}^*. (2.7)$$

Example 2.1 (Fourier Series by Inspection). The doubly exponential function $\exp(\exp(ix))$ has the Fourier series

$$\exp\left(e^{ix}\right) = \sum_{n=0}^{\infty} \frac{1}{n!} e^{inx}$$
(2.8)

in which $n! = n(n-1) \dots 1$ is *n*-factorial with $0! \equiv 1$.

Example 2.2 (Beats). The sum of two sines $f(x) = \sin \omega_1 x + \sin \omega_2 x$ of similar frequencies $\omega_1 \approx \omega_2$ is the product (exercise 2.1)

$$f(x) = 2\cos\frac{1}{2}(\omega_1 - \omega_2)x \sin\frac{1}{2}(\omega_1 + \omega_2)x.$$
 (2.9)

The first factor $\cos \frac{1}{2}(\omega_1 - \omega_2)x$ is the **beat**; it modulates the second factor $\sin \frac{1}{2}(\omega_1 + \omega_2)x$ as illustrated by Fig. 2.1.

2.2 The Interval

In equations (2.1–2.3), we singled out the interval $[0, 2\pi]$, but to represent a periodic function f(x) of period 2π , we could have used any interval of length 2π , such as the interval $[-\pi, \pi]$ or $[r, r + 2\pi]$

$$f_n = \int_r^{r+2\pi} e^{-inx} f(x) \frac{dx}{\sqrt{2\pi}}.$$
 (2.10)

This integral is independent of its lower limit r when the function f(x) is periodic with period 2π . The choice $r = -\pi$ often is convenient. With this



Figure 2.1 The curve $\sin \omega_1 x + \sin \omega_2 x$ for $\omega_1 = 30$ and $\omega_2 = 32$.

choice of interval, the coefficient f_n is the integral (2.3) shifted by $-\pi$

$$f_n = \int_{-\pi}^{\pi} e^{-inx} f(x) \frac{dx}{\sqrt{2\pi}}.$$
 (2.11)

But if the function f(x) is not periodic with period 2π , then the Fourier coefficients (2.10) do depend upon the choice r of interval.

2.3 Where to put the 2π 's

In Eqs.(2.2 & 2.3), we used the orthonormal functions $\exp(inx)/\sqrt{2\pi}$, and so we had factors of $1/\sqrt{2\pi}$ in both equations. One can avoid having two square roots by setting $d_n = f_n/\sqrt{2\pi}$ and writing the Fourier series (2.2) and the orthonormality relation (2.3) as

$$f(x) = \sum_{n = -\infty}^{\infty} d_n e^{inx} \text{ and } d_n = \frac{1}{2\pi} \int_0^{2\pi} dx \, e^{-inx} \, f(x).$$
 (2.12)





Figure 2.2 The 10-term (dashes) Fourier series (2.16) for the function $\exp(-2|x|)$ on the interval $(-\pi,\pi)$ is plotted from -2π to 2π . All Fourier series are periodic, but the function $\exp(-2|x|)$ (solid) is not.

Alternatevely one set $c_n = \sqrt{2\pi} f_n$ and may use the rules

$$f(x) = \frac{1}{2\pi} \sum_{n=-\infty}^{\infty} c_n e^{inx}$$
 and $c_n = \int_{-\pi}^{\pi} f(x) e^{-inx} dx.$ (2.13)

Example 2.3 (Fourier Series for $\exp(-m|x|)$). Let's compute the Fourier series for the real function $f(x) = \exp(-m|x|)$ on the interval $(-\pi, \pi)$. Using Eq.(2.10) for the shifted interval and the 2π -placement convention (2.12), we find that the coefficient d_n is the integral

$$d_n = \int_{-\pi}^{\pi} \frac{dx}{2\pi} e^{-inx} e^{-m|x|}$$
(2.14)

which we may split into the two pieces

$$d_n = \int_{-\pi}^0 \frac{dx}{2\pi} e^{(m-in)x} + \int_0^{\pi} \frac{dx}{2\pi} e^{-(m+in)x}$$

= $\frac{1}{\pi} \frac{m}{m^2 + n^2} \left[1 - (-1)^n e^{-\pi m} \right]$ (2.15)

which shows that $d_n = d_{-n}$. Since *m* is real, the coefficients d_n also are real, $d_n = d_n^*$. They therefore satisfy the condition (2.7) that holds for real functions, $d_n = d_{-n}^*$, and give the Fourier series for $\exp(-m|x|)$ as

$$e^{-m|x|} = \sum_{n=-\infty}^{\infty} d_n e^{inx} = \sum_{n=-\infty}^{\infty} \frac{1}{\pi} \frac{m}{m^2 + n^2} \left[1 - (-1)^n e^{-\pi m} \right] e^{inx}$$

$$= \frac{(1 - e^{-\pi m})}{m\pi} + \sum_{n=1}^{\infty} \frac{2}{\pi} \frac{m}{m^2 + n^2} \left[1 - (-1)^n e^{-\pi m} \right] \cos(nx).$$
(2.16)

In Fig. 2.2, the 10-term (dashes) Fourier series for m = 2 is plotted from $x = -2\pi$ to $x = 2\pi$. The function $\exp(-2|x|)$ itself is represented by a solid line. Although $\exp(-2|x|)$ is not periodic, its Fourier series is periodic with period 2π . The 10-term Fourier series represents the function $\exp(-2|x|)$ quite well within the interval $[-\pi, \pi]$.

In what follows, we usually won't bother to use different letters to distinguish between the symmetric (2.2 & 2.3) and asymmetric (2.13) conventions on the placement of the 2π 's.

2.4 Real Fourier Series for Real Functions

The rules (2.1–2.3 and 2.10–2.13) for Fourier series are simple and apply to functions that are continuous and periodic whether complex or real. If a function f(x) is real, then its Fourier coefficients obey the rule (2.7) that holds for real functions, $d_{-n} = d_n^*$. Thus d_0 is real, $d_0 = d_0^*$, and we may write the Fourier series (2.12) for a real function f(x) as

$$f(x) = d_0 + \sum_{n=1}^{\infty} d_n e^{inx} + \sum_{n=-\infty}^{-1} d_n e^{inx}$$

= $d_0 + \sum_{n=1}^{\infty} \left[d_n e^{inx} + d_{-n} e^{-inx} \right] = d_0 + \sum_{n=1}^{\infty} \left[d_n e^{inx} + d_n^* e^{-inx} \right]$
= $d_0 + \sum_{n=1}^{\infty} d_n \left(\cos nx + i \sin nx \right) + d_n^* \left(\cos nx - i \sin nx \right)$
= $d_0 + \sum_{n=1}^{\infty} \left(d_n + d_n^* \right) \cos nx + i (d_n - d_n^*) \sin nx.$ (2.17)

In terms of the real coefficients

$$a_n = d_n + d_n^*$$
 and $b_n = i(d_n - d_n^*),$ (2.18)

the Fourier series (2.17) of a real function f(x) is

$$f(x) = \frac{a_0}{2} + \sum_{n=1}^{\infty} a_n \cos nx + b_n \sin nx.$$
 (2.19)

What are the formulas for a_n and b_n ? By (2.18 & 2.12), the coefficient a_n is

$$a_n = \int_0^{2\pi} \left[e^{-inx} f(x) + e^{inx} f^*(x) \right] \frac{dx}{2\pi} = \int_0^{2\pi} \frac{\left(e^{-inx} + e^{inx} \right)}{2} f(x) \frac{dx}{\pi}$$
(2.20)

since the function f(x) is real. So the coefficient a_n of $\cos nx$ in (2.19) is the cosine integral of f(x)

$$a_n = \int_0^{2\pi} \cos nx \, f(x) \, \frac{dx}{\pi}.$$
 (2.21)

Similarly, equations (2.18 & 2.12) and the reality of f(x) imply that the coefficient b_n is the sine integral of f(x)

$$b_n = \int_0^{2\pi} i \frac{\left(e^{-inx} - e^{inx}\right)}{2} f(x) \frac{dx}{\pi} = \int_0^{2\pi} \sin nx \, f(x) \frac{dx}{\pi} \tag{2.22}$$

The real Fourier series (2.19) and the cosine (2.21) and sine (2.22) integrals

for the coefficients a_n and b_n also follow from the orthogonality relations

$$\int_{0}^{2\pi} \sin mx \, \sin nx \, dx = \begin{cases} \pi & \text{if } n = m \neq 0\\ 0 & \text{otherwise,} \end{cases}$$
(2.23)

$$\int_{0}^{2\pi} \cos mx \, \cos nx \, dx = \begin{cases} \pi & \text{if } n = m \neq 0\\ 2\pi & \text{if } n = m = 0\\ 0 & \text{otherwise, and} \end{cases}$$
(2.24)

$$\int_{0}^{2\pi} \sin mx \, \cos nx \, dx = 0, \tag{2.25}$$

which hold for integer values of n and m.

If the function f(x) is periodic with period 2π , then instead of the interval $[0, 2\pi]$, one may choose any interval of length 2π such as $[-\pi, \pi]$.

What if a function f(x) is not periodic? The Fourier series for an aperiodic function is itself strictly periodic, is sensitive to its interval $(r, r + 2\pi)$ of definition, may differ somewhat from the function near the ends of the interval, and usually differs markedly from it outside the interval.

Example 2.4 (The Fourier Series for x^2). The function x^2 is even and so the integrals (2.22) for its sine Fourier coefficients b_n all vanish. Its cosine coefficients a_n are given by (2.21)

$$a_n = \int_{-\pi}^{\pi} \cos nx \, f(x) \, \frac{dx}{\pi} = \int_{-\pi}^{\pi} \cos nx \, x^2 \, \frac{dx}{\pi}.$$
 (2.26)

Integrating twice by parts, we find for $n \neq 0$

$$a_n = -\frac{2}{n} \int_{-\pi}^{\pi} x \sin nx \, \frac{dx}{\pi} = \left[\frac{2x \cos nx}{\pi n^2}\right]_{-\pi}^{\pi} = (-1)^n \frac{4}{n^2} \tag{2.27}$$

and

$$a_0 = \int_{-\pi}^{\pi} x^2 \, \frac{dx}{\pi} = \frac{2\pi^2}{3}.$$
 (2.28)

Equation (2.19) now gives for x^2 the cosine Fourier series

$$x^{2} = \frac{a_{0}}{2} + \sum_{n=1}^{\infty} a_{n} \cos nx = \frac{\pi^{2}}{3} + 4 \sum_{n=1}^{\infty} (-1)^{n} \frac{\cos nx}{n^{2}}.$$
 (2.29)

This series rapidly converges within the interval [-1, 1] as shown in Fig. 2.3, but not near the endpoints $\pm \pi$.

Example 2.5 (The Gibbs overshoot). The function f(x) = x on the interval $[-\pi, \pi]$ is not periodic. So we expect trouble if we represent it as a Fourier





Figure 2.3 The function x^2 (solid) and its Fourier series of 7 terms (dot dash) and 20 terms (dashes). The Fourier series (2.29) for x^2 quickly converges well inside the interval $(-\pi, \pi)$.

series. Since x is an odd function, equation (2.21) tells us that the coefficients a_n all vanish. By (2.22), the b_n 's are

$$b_n = \int_{-\pi}^{\pi} \frac{dx}{\pi} x \sin nx = 2 \, (-1)^{n+1} \, \frac{1}{n}.$$
 (2.30)

As shown in Fig. 2.4, the series

$$\sum_{n=1}^{\infty} 2 \, (-1)^{n+1} \, \frac{1}{n} \, \sin nx \tag{2.31}$$

differs by about 2π from the function f(x) = x for $-3\pi < x < -\pi$ and for $\pi < x < 3\pi$ because the series is periodic while the function x isn't.

Within the interval $(-\pi, \pi)$, the series with 100 terms is very accurate except for $x \gtrsim -\pi$ and $x \lesssim \pi$, where it overshoots by about 9% of the 2π discontinuity, a defect called a **Gibbs overshoot** (J. Willard Gibbs 1839–1903. Incidentally, Gibbs's father helped defend the Africans of the schooner



Figure 2.4 (top) The Fourier series (2.31) for the function x (solid line) with 10 terms (...) and 100 terms (solid curve) for $-2\pi < x < 2\pi$. The Fourier series is periodic, but the function x is not. (bottom) The differences between x and the 10-term (...) and the 100-term (solid curve) on $(-\pi,\pi)$ exhibit a Gibbs overshoot of about 9% at $x \gtrsim -\pi$ and at $x \lesssim \pi$.

Amistad). Any time we use a Fourier series to represent an aperiodic function, a Gibbs overshoot will occur near the endpoints of the interval. \Box

2.5 Stretched Intervals

If the interval of periodicity is of length L instead of 2π , then we may use the phases $\exp(i2\pi nx/\sqrt{L})$ which are orthonormal on the interval [0, L]

$$\int_{0}^{L} dx \, \left(\frac{e^{i2\pi nx/L}}{\sqrt{L}}\right)^{*} \frac{e^{i2\pi mx/L}}{\sqrt{L}} = \delta_{nm}.$$
(2.32)

The Fourier series

$$f(x) = \sum_{n=-\infty}^{\infty} f_n \frac{e^{i2\pi nx/L}}{\sqrt{L}}$$
(2.33)

is periodic with period L. The coefficient f_n is the integral

$$f_n = \int_0^L \frac{e^{-i2\pi nx/L}}{\sqrt{L}} f(x) \, dx.$$
 (2.34)

These relations (2.32-2.34) generalize to the interval [0, L] our earlier formulas (2.1-2.3) for the interval $[0, 2\pi]$.

If the function f(x) is periodic $f(x \pm L) = f(x)$ with period L, then we may shift the domain of integration by any real number r

$$f_n = \int_r^{L+r} \frac{e^{-i2\pi nx/L}}{\sqrt{L}} f(x) \, dx$$
 (2.35)

without changing the coefficients f_n . An obvious choice is r = -L/2 for which (2.33) and (2.34) give

$$f(x) = \sum_{n=-\infty}^{\infty} f_n \frac{e^{i2\pi nx/L}}{\sqrt{L}} \quad \text{and} \quad f_n = \int_{-L/2}^{L/2} \frac{e^{-i2\pi nx/L}}{\sqrt{L}} f(x) \, dx. \quad (2.36)$$

If the function f(x) is real, then on the interval [0, L] in place of Eqs.(2.19), (2.21), & (2.22), one has

$$f(x) = \frac{a_0}{2} + \sum_{n=1}^{\infty} a_n \cos\left(\frac{2\pi nx}{L}\right) + b_n \sin\left(\frac{2\pi nx}{L}\right), \qquad (2.37)$$

$$a_n = \frac{2}{L} \int_0^L dx \, \cos\left(\frac{2\pi nx}{L}\right) f(x), \qquad (2.38)$$

and

$$b_n = \frac{2}{L} \int_0^L dx \, \sin\left(\frac{2\pi nx}{L}\right) \, f(x). \tag{2.39}$$

The corresponding orthogonality relations, which follow from Eqs.(2.23),

(2.24), & (2.25), are:

$$\int_{0}^{L} dx \sin\left(\frac{2\pi mx}{L}\right) \sin\left(\frac{2\pi nx}{L}\right) = \begin{cases} L/2 & \text{if } n = m \neq 0\\ 0 & \text{otherwise,} \end{cases}$$
(2.40)

$$\int_{0}^{L} dx \cos\left(\frac{2\pi mx}{L}\right) \cos\left(\frac{2\pi nx}{L}\right) = \begin{cases} L/2 & \text{if } n = m \neq 0\\ L & \text{if } n = m = 0\\ 0 & \text{otherwise, and} \end{cases}$$
(2.41)

$$\int_{0}^{L} dx \, \sin\left(\frac{2\pi mx}{L}\right) \, \cos\left(\frac{2\pi nx}{L}\right) = 0. \tag{2.42}$$

They hold for integer values of n and m, and they imply Eqs.(2.37)-2.39).

2.6 Fourier Series in Several Variables

On the interval [-L, L], the Fourier-series formulas (2.33 & 2.34) are

$$f(x) = \sum_{n=-\infty}^{\infty} f_n \frac{e^{i\pi nx/L}}{\sqrt{2L}}$$
(2.43)

$$f_n = \int_{-L}^{L} \frac{e^{-i\pi nx/L}}{\sqrt{2L}} f(x) \, dx.$$
 (2.44)

We may generalize these equations from a single variable to N variables $x = (x_1, \ldots, x_N)$ with $n \cdot x = n_1 x_1 + \ldots + n_N x_N$

$$f(x) = \sum_{n_1 = -\infty}^{\infty} \dots \sum_{n_N = -\infty}^{\infty} f_n \, \frac{e^{i\pi n \cdot x/L}}{(2L)^{N/2}}$$
(2.45)

$$f_n = \int_{-L}^{L} dx_1 \dots \int_{-L}^{L} dx_N \, \frac{e^{-i\pi n \cdot x/L}}{(2L)^{N/2}} f(x).$$
(2.46)

2.7 How Fourier Series Converge

A Fourier series represents a function f(x) as the limit of a sequence of functions $f_N(x)$ given by

$$f_N(x) = \sum_{k=-N}^{N} f_k \frac{e^{i2\pi kx/L}}{\sqrt{L}} \quad \text{in which} \quad f_k = \int_0^L f(x) e^{-i2\pi kx/L} \frac{dx}{\sqrt{L}}.$$
 (2.47)

Since the exponentials are periodic with period L, a Fourier series always is periodic. So if the function f(x) is not periodic, then its Fourier series will

represent the periodic extension f_p of f defined by $f_p(x+nL) = f(x)$ for all integers n and for $0 \le x \le L$.

A sequence of functions $f_N(x)$ converges to a function f(x) on a (closed) interval [a, b] if for every $\epsilon > 0$ and each point $a \le x \le b$, there exists an integer $N(\epsilon, x)$ such that

$$|f(x) - f_N(x)| < \epsilon \quad \text{for all} \quad N > N(\epsilon, x).$$
(2.48)

If this holds for an $N(\epsilon, x) = N(\epsilon)$ that is independent of $x \in [a, b]$, then the sequence of functions $f_N(x)$ converges uniformly to f(x) on the interval [a, b].

A function f(x) is **continuous** on an *open* interval (a, b) if for every point a < x < b the two limits

$$f(x-0) \equiv \lim_{0 < \epsilon \to 0} f(x-\epsilon)$$
 and $f(x+0) \equiv \lim_{0 < \epsilon \to 0} f(x+\epsilon)$ (2.49)

agree; it also is continuous on the closed interval [a, b] if f(a+0) = f(a) and f(b-0) = f(b). A function continuous on [a, b] is bounded and integrable on that interval.

If a sequence of continuous functions $f_N(x)$ converges uniformly to a function f(x) on a closed interval $a \le x \le b$, then we know that $|f_N(x) - f(x)| < \epsilon$ for $N > N(\epsilon)$, and so

$$\left| \int_{a}^{b} f_{N}(x) \, dx - \int_{a}^{b} f(x) \, dx \right| \leq \int_{a}^{b} |f_{N}(x) - f(x)| \, dx < (b-a)\epsilon.$$
(2.50)

Thus one may integrate a uniformly convergent sequence of continuous functions on a closed interval [a, b] term by term

$$\lim_{N \to \infty} \int_{a}^{b} f_{N}(x) \, dx = \int_{a}^{b} \lim_{N \to \infty} f_{N}(x) \, dx = \int_{a}^{b} f(x) \, dx.$$
(2.51)

A function is **piecewise continuous** on [a, b] if it is continuous there except for finite jumps from f(x-0) to f(x+0) at a finite number of points x. At such jumps, we *define* the periodically extended function f_p to be the mean $f_p(x) = [f(x-0) + f(x+0)]/2$.

Fourier's convergence theorem (Courant, 1937, p. 439): The Fourier series of a function f(x) that is piecewise continuous with a piecewise continuous first derivative converges to its periodic extension $f_p(x)$. This convergence is uniform on every closed interval on which the function f(x) is continuous (and absolute if the function f(x) has no discontinuities). Examples 2.11 and 2.12 illustrate this result.

A function whose kth derivative is continuous is in class C^k . On the interval $[-\pi, \pi]$, its Fourier coefficients (2.13) are

$$f_n = \int_{-\pi}^{\pi} f(x) \, e^{-inx} \, dx. \tag{2.52}$$

If f is both periodic and in C^k , then one integration by parts gives

$$f_n = \int_{-\pi}^{\pi} \left\{ \frac{d}{dx} \left[f(x) \frac{e^{-inx}}{-in} \right] - f'(x) \frac{e^{-inx}}{-in} \right\} \, dx = \int_{-\pi}^{\pi} f'(x) \frac{e^{-inx}}{in} \, dx$$

and k integrations by parts give

$$f_n = \int_{-\pi}^{\pi} f^{(k)}(x) \,\frac{e^{-inx}}{(in)^k} \,dx \tag{2.53}$$

since the derivatives $f^{(\ell)}(x)$ of a C^k periodic function also are periodic. Moreover if $f^{(k+1)}$ is piecewise continuous, then

$$f_n = \int_{-\pi}^{\pi} \left\{ \frac{d}{dx} \left[f^{(k)}(x) \frac{e^{-inx}}{-(in)^{k+1}} \right] - f^{(k+1)}(x) \frac{e^{-inx}}{-(in)^{k+1}} \right\} dx$$

= $\int_{-\pi}^{\pi} f^{(k+1)}(x) \frac{e^{-inx}}{(in)^{k+1}} dx.$ (2.54)

Since $f^{(k+1)}(x)$ is piecewise continuous on the closed interval $[-\pi, \pi]$, it is bounded there in absolute value by, let us say, M. So the Fourier coefficients of a C^k periodic function with $f^{(k+1)}$ piecewise continuous are bounded by

$$|f_n| \le \frac{1}{n^{k+1}} \int_{-\pi}^{\pi} |f^{(k+1)}(x)| \ dx \le \frac{2\pi M}{n^{k+1}}.$$
(2.55)

We often can carry this derivation one step further. In most simple examples, the piecewise continuous periodic function $f^{(k+1)}(x)$ actually is piecewise continuously differentiable between its successive jumps at x_j . In this case, the derivative $f^{(k+2)}(x)$ is a piecewise continuous function plus a sum of a finite number of delta functions with finite coefficients. Thus we can integrate once more by parts. If for instance the function $f^{(k+1)}(x)$ jumps J times between $-\pi$ and π by $\Delta f_j^{(k+1)}$, then its Fourier coefficients are

$$f_n = \int_{-\pi}^{\pi} f^{(k+2)}(x) \frac{e^{-inx}}{(in)^{k+2}} dx$$

= $\sum_{j=1}^{J} \int_{x_j}^{x_{j+1}} f_s^{(k+2)}(x) \frac{e^{-inx}}{(in)^{k+2}} dx + \sum_{j=1}^{J} \Delta f_j^{(k+2)} \frac{e^{-inx_j}}{(in)^{k+2}}$ (2.56)

in which the subscript s means that we've separated out the delta functions. The Fourier coefficients then are bounded by

$$|f_n| \le \frac{2\pi M}{n^{k+2}} \tag{2.57}$$

in which M is related to the maximum absolute values of $f_s^{(k+2)}(x)$ and of the $\Delta f_j^{(k+1)}$. The Fourier series of periodic C^k functions converge very rapidly if k is big.

Example 2.6 (Fourier Series of a C^0 Function). The function defined by

$$f(x) = \begin{cases} 0 & -\pi \le x < 0\\ x & 0 \le x < \pi/2\\ \pi - x & \pi/2 \le x \le \pi \end{cases}$$
(2.58)

is continuous on the interval $[-\pi, \pi]$ and its first derivative is piecewise continuous on that interval. By (2.55), its Fourier coefficients f_n should be bounded by M/n. In fact they are (exercise 2.8)

$$f_n = \int_{-\pi}^{\pi} f(x) e^{-inx} \frac{dx}{\sqrt{2\pi}} = \frac{(-1)^{n+1}}{\sqrt{2\pi}} \frac{(i^n - 1)^2}{n^2}$$
(2.59)

bounded by $2\sqrt{2/\pi}/n^2$ in agreement with the stronger inequality (2.57). \Box

Example 2.7 (Fourier Series for a C^1 Function). The function defined by $f(x) = 1 + \cos 2x$ for $|x| \le \pi/2$ and f(x) = 0 for $|x| \ge \pi/2$ has a periodic extension f_p that is continuous with a continuous first derivative and a piecewise continuous second derivative. Its Fourier coefficients (2.52)

$$f_n = \int_{-\pi/2}^{\pi/2} (1 + \cos 2x) \, e^{-inx} \, \frac{dx}{\sqrt{2\pi}} = \frac{8 \sin n\pi/2}{\sqrt{2\pi}(4n - n^3)}$$

satisfy the inequalities (2.55) and (2.57) for k = 1.

Example 2.8 (The Fourier Series for $\cos \mu x$). The Fourier series for the even function $f(x) = \cos \mu x$ has only cosines with coefficients (2.21)

$$a_n = \int_{-\pi}^{\pi} \cos nx \, \cos \mu x \, \frac{dx}{\pi} = \int_0^{\pi} [\cos(\mu + n)x + \cos(\mu - n)x] \frac{dx}{\pi}$$

= $\frac{1}{\pi} \left[\frac{\sin(\mu + n)\pi}{\mu + n} + \frac{\sin(\mu - n)\pi}{\mu - n} \right] = \frac{2}{\pi} \frac{\mu(-1)^n}{\mu^2 - n^2} \sin \mu \pi.$ (2.60)

Thus whether or not μ is an integer, the series (2.19) gives us

$$\cos \mu x = \frac{2\mu \sin \mu \pi}{\pi} \left(\frac{1}{2\mu^2} - \frac{\cos x}{\mu^2 - 1^2} + \frac{\cos 2x}{\mu^2 - 2^2} - \frac{\cos 3x}{\mu^2 - 3^2} + \dots \right) \quad (2.61)$$

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which is continuous at $x = \pm \pi$ (Courant, 1937, chap. IX).

Example 2.9 (The Sine as an Infinite Product). In our series (2.61) for $\cos \mu x$, we set $x = \pi$, divide by $\sin \mu \pi$, replace μ with x, and so find for the cotangent the expansion

$$\cot \pi x = \frac{2x}{\pi} \left(\frac{1}{2x^2} + \frac{1}{x^2 - 1^2} + \frac{1}{x^2 - 2^2} + \frac{1}{x^2 - 3^2} + \dots \right)$$
(2.62)

or equivalently

$$\cot \pi x - \frac{1}{\pi x} = -\frac{2x}{\pi} \left(\frac{1}{1^2 - x^2} + \frac{1}{2^2 - x^2} + \frac{1}{3^2 - x^2} + \dots \right).$$
(2.63)

For $0 \le x \le q < 1$, the absolute value of the *n*th term on the right is less than $2q/(\pi(n^2 - q^2))$. Thus this series converges uniformly on [0, x], and so we may integrate it term by term. We find (exercise 2.11)

$$\pi \int_0^x \left(\cot \pi t - \frac{1}{\pi t} \right) dt = \ln \frac{\sin \pi x}{\pi x} = \sum_{n=1}^\infty \int_0^x \frac{-2t \, dt}{n^2 - t^2} = \sum_{n=1}^\infty \ln \left[1 - \frac{x^2}{n^2} \right].$$
(2.64)

Exponentiating, we get the infinite-product formula

$$\frac{\sin \pi x}{\pi x} = \exp\left[\sum_{n=1}^{\infty} \ln\left(1 - \frac{x^2}{n^2}\right)\right] = \prod_{n=1}^{\infty} \left(1 - \frac{x^2}{n^2}\right) \tag{2.65}$$

for the sine from which one can derive the infinite product (exercise 2.12)

$$\cos \pi x = \prod_{n=1}^{\infty} \left(1 - \frac{x^2}{(n - \frac{1}{2})^2} \right)$$
(2.66)

for the cosine (Courant, 1937, chap. IX).

Fourier series can represent a much wider class of functions than those that are continuous. If a function f(x) is square integrable on an interval [a, b], then its N-term Fourier series $f_N(x)$ will converge to f(x) in the mean, that is

$$\lim_{N \to \infty} \int_{a}^{b} dx \, |f(x) - f_N(x)|^2 = 0.$$
(2.67)

What happens to the convergence of a Fourier series if we integrate or differentiate term by term? If we integrate the series

$$f(x) = \sum_{n=-\infty}^{\infty} f_n \frac{e^{i2\pi nx/L}}{\sqrt{L}}$$
(2.68)

then we get a series

$$F(x) = \int_{a}^{x} dx' f(x') = \frac{f_{0}}{\sqrt{L}} (x-a) - i \frac{\sqrt{L}}{2\pi} \sum_{n=-\infty}^{\infty} \frac{f_{n}}{n} \left(e^{i2\pi nx/L} - e^{i2\pi na/L} \right)$$
(2.69)

that converges **better** because of the extra factor of 1/n. An integrated function f(x) is smoother, and so its Fourier series converges better.

But if we differentiate the same series, then we get a series

$$f'(x) = i \frac{2\pi}{L^{3/2}} \sum_{n = -\infty}^{\infty} n f_n e^{i2\pi n x/L}$$
(2.70)

that converges **less well** because of the extra factor of n. A differentiated function is rougher, and so its Fourier series converges less well.

2.8 Quantum-Mechanical Examples

Suppose a particle of mass m is trapped in an infinitely deep one-dimensional square well of potential energy

$$V(x) = \begin{cases} 0 & \text{if } 0 < x < L \\ \infty & \text{otherwise.} \end{cases}$$
(2.71)

The hamiltonian operator is

$$H = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + V(x), \qquad (2.72)$$

in which \hbar is Planck's constant divided by 2π . This tiny bit of action, $\hbar = 1.055 \times 10^{-34}$ J s, sets the scale at which quantum mechanics becomes important. Quantum-mechanical corrections to classical predictions can be big in processes whose action is less than \hbar .

An eigenfunction $\psi(x)$ of the hamiltonian H with energy E satisfies the equation $H\psi(x) = E\psi(x)$ which breaks into two simple equations:

$$-\frac{\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2} = E\psi(x) \quad \text{for} \quad 0 < x < L$$
 (2.73)

and

$$-\frac{\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2} + \infty\psi(x) = E\psi(x) \quad \text{for} \quad x < 0 \quad \text{and for} \quad x > L. \quad (2.74)$$

Every solution of these equations with finite energy E must vanish outside the interval 0 < x < L. So we must find solutions of the first equation (2.73) that satisfy the boundary conditions

$$\psi(x) = 0 \quad \text{for} \quad x \le 0 \text{ and } x \ge L.$$
 (2.75)

For any integer $n \neq 0$, the function

$$\psi_n(x) = \sqrt{\frac{2}{L}} \sin\left(\frac{\pi nx}{L}\right) \quad \text{for} \quad x \in [0, L]$$
 (2.76)

and $\psi_n(x) = 0$ for $x \notin (0, L)$ satisfies the boundary conditions (2.75). When inserted into equation (2.73)

$$-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\psi_n(x) = \frac{\hbar^2}{2m}\left(\frac{n\pi}{L}\right)^2\psi_n(x) = E_n\psi_n(x)$$
(2.77)

it reveals its energy to be $E_n = (n\pi\hbar/L)^2/2m$.

These eigenfunctions $\psi_n(x)$ are complete in the sense that they span the space of all functions f(x) that are square-integrable on the interval (0, L) and vanish at its end points. They provide for such functions the **sine** Fourier series

$$f(x) = \sum_{n=1}^{\infty} f_n \sqrt{\frac{2}{L}} \sin\left(\frac{\pi nx}{L}\right)$$
(2.78)

which is periodic with period 2L and is the Fourier series for a function that is odd f(-x) = -f(x) on the interval (-L, L) and zero at both ends.

Example 2.10 (Time Evolution of an Initially Piecewise Continuous Wave Function). Suppose now that at time t = 0 the particle is confined to the middle half of the well with the square-wave wave function

$$\psi(x,0) = \sqrt{\frac{2}{L}} \quad \text{for} \quad \frac{L}{4} < x < \frac{3L}{4}$$
 (2.79)

and zero otherwise. This piecewise continuous C^{-1} wave function is discontinuous at x = L/4 and at x = 3L/4. Since the functions $\langle x|n \rangle = \psi_n(x)$ are orthonormal on [0, L]

$$\int_{0}^{L} dx \sqrt{\frac{2}{L}} \sin\left(\frac{\pi nx}{L}\right) \sqrt{\frac{2}{L}} \sin\left(\frac{\pi mx}{L}\right) = \delta_{nm}$$
(2.80)

the coefficients f_n in the Fourier series

$$\psi(x,0) = \sum_{n=1}^{\infty} f_n \sqrt{\frac{2}{L}} \sin\left(\frac{\pi nx}{L}\right)$$
(2.81)

are the inner products

$$f_n = \langle n | \psi, 0 \rangle = \int_0^L dx \sqrt{\frac{2}{L}} \sin\left(\frac{\pi nx}{L}\right) \psi(x, 0).$$
 (2.82)



Figure 2.5 The piecewise continuous wave function $\psi(x, 0)$ for L = 2 (2.79, straight solid lines) and its Fourier series (2.81) with 10 terms (solid curve) and 100 terms (dashes). Gibbs overshoots occur near the discontinuities at x = 1/2 and x = 3/2.

They are proportional to 1/n in accord with (2.57)

$$f_n = \frac{2}{L} \int_{L/4}^{3L/4} dx \, \sin\left(\frac{\pi nx}{L}\right) = \frac{2}{\pi n} \left[\cos\left(\frac{\pi n}{4}\right) - \cos\left(\frac{3\pi n}{4}\right)\right]. \quad (2.83)$$

Figure 2.5 plots the square wave function $\psi(x, 0)$ (2.79, straight solid lines) and its 10-term (solid curve) and 100-term (dashes) Fourier series (2.81) for an interval of length L = 2. Gibbs's overshoot reaches 1.093 at x = 0.52 for 100 terms and 1.0898 at x = 0.502 for 1000 terms (not shown), amounting to about 9% of the unit discontinuity at x = 1/2. A similar overshoot occurs at x = 3/2.

How does $\psi(x, 0)$ evolve with time? Since $\psi_n(x)$, the Fourier component (2.76), is an eigenfunction of H with energy E_n , the time-evolution operator



Figure 2.6 For an interval of length L = 2, the probability distributions $P(x,t) = |\psi(x,t)|^2$ of the 1000-term Fourier series (2.85) for the wave function $\psi(x,t)$ at t = 0 (thick curve), $t = 10^{-3} \tau$ (medium curve), and $\tau = 2mL^2/\hbar$ (thin curve). The jaggedness of P(x,t) arises from the two discontinuities in the initial wave function $\psi(x,0)$ (2.86) at x = L/4 and x = 3L/4.

 $U(t) = \exp(-iHt/\hbar)$ takes $\psi(x,0)$ into

$$\psi(x,t) = e^{-iHt/\hbar} \psi(x,0) = \sum_{n=1}^{\infty} f_n \sqrt{\frac{2}{L}} \sin\left(\frac{\pi nx}{L}\right) e^{-iE_n t/\hbar}.$$
 (2.84)

Because $E_n = (n\pi\hbar/L)^2/2m$, the wave function at time t is

$$\psi(x,t) = \sum_{n=1}^{\infty} f_n \sqrt{\frac{2}{L}} \sin\left(\frac{\pi nx}{L}\right) e^{-i\hbar(n\pi)^2 t/(2mL^2)}.$$
 (2.85)

It is awkward to plot complex functions, so Fig. 2.6 displays the probability distributions $P(x,t) = |\psi(x,t)|^2$ of the 1000-term Fourier series (2.85) for the wave function $\psi(x,t)$ at t = 0 (thick curve), $t = 10^{-3} \tau$ (medium curve), and



Figure 2.7 The continuous wave function $\psi(x,0)$ (2.86, solid) and its 10-term Fourier series (2.89–2.90, dashes) are plotted for the interval [0, 2].

 $\tau = 2mL^2/\hbar$ (thin curve). The discontinuities in the initial wave function $\psi(x,0)$ cause both the Gibbs overshoots at x = 1/2 and x = 3/2 seen in the series for $\psi(x,0)$ plotted in Fig. 2.5 and the choppiness of the probability distribution P(x,t) exhibited in Fig.(2.6).

Example 2.11 (Time Evolution of a Continuous Function). What does the Fourier series of a continuous function look like? How does it evolve with time? Let us take as the wave function at t = 0 the C^0 function

$$\psi(x,0) = \frac{2}{\sqrt{L}} \sin\left(\frac{2\pi(x-L/4)}{L}\right) \quad \text{for} \quad \frac{L}{4} < x < \frac{3L}{4}$$
 (2.86)

and zero otherwise. This initial wave function is a continuous function with a piecewise continuous first derivative on the interval [0, L], and it satisfies the periodic boundary condition $\psi(0, 0) = \psi(L, 0)$. It therefore satisfies the conditions of Fourier's convergence theorem (Courant, 1937, p. 439), and so its Fourier series converges uniformly (and absolutely) to $\psi(x, 0)$ on [0, L].



Figure 2.8 For the interval [0,2], the probability distributions $P(x,t) = |\psi(x,t)|^2$ of the 1000-term Fourier series (2.92) for the wave function $\psi(x,t)$ at t = 0, $10^{-2} \tau$, $10^{-1} \tau$, $\tau = 2mL^2/\hbar$, 10τ , and 100τ are plotted as successively thinner curves.

As in Eq.(2.82), the Fourier coefficients f_n are given by the integrals

$$f_n = \int_0^L dx \sqrt{\frac{2}{L}} \sin\left(\frac{\pi nx}{L}\right) \psi(x,0), \qquad (2.87)$$

which now take the form

$$f_n = \frac{2\sqrt{2}}{L} \int_{L/4}^{3L/4} dx \, \sin\left(\frac{\pi nx}{L}\right) \, \sin\left(\frac{2\pi(x-L/4)}{L}\right).$$
(2.88)

Doing the integral, one finds for f_n that for $n \neq 2$

$$f_n = -\frac{\sqrt{2}}{\pi} \frac{4}{n^2 - 4} \left[\sin(3n\pi/4) + \sin(n\pi/4) \right]$$
(2.89)

while $c_2 = 0$. These Fourier coefficients satisfy the inequalities (2.55) and (2.57) for k = 0. The factor of $1/n^2$ in f_n guarantees the absolute convergence

of the series

$$\psi(x,0) = \sum_{n=1}^{\infty} f_n \sqrt{\frac{2}{L}} \sin\left(\frac{\pi nx}{L}\right)$$
(2.90)

because asymptotically the coefficient f_n is bounded by $|f_n| \leq A/n^2$ where A is a constant $(A = 144/(5\pi\sqrt{L})$ will do) and the sum of $1/n^2$ converges to the Riemann zeta function (4.99)

$$\sum_{n=1}^{\infty} \frac{1}{n^2} = \zeta(2) = \frac{\pi^2}{6}.$$
(2.91)

Figure 2.7 plots the 10-term Fourier series (2.90) for $\psi(x, 0)$ for L = 2. Because this series converges absolutely and uniformly on [0,2], the 100-term and 1000-term series were too close to $\psi(x, 0)$ to be seen clearly in the figure and so were omitted.

As time goes by, the wave function $\psi(x,t)$ evolves from $\psi(x,0)$ to

$$\psi(x,t) = \sum_{n=1}^{\infty} f_n \sqrt{\frac{2}{L}} \sin\left(\frac{\pi nx}{L}\right) e^{-i\hbar(n\pi)^2 t/(2mL^2)}.$$
 (2.92)

in which the Fourier coefficients are given by (2.89). Because $\psi(x, 0)$ is continuous and periodic with a piecewise continuous first derivative, its evolution in time is much calmer than that of the piecewise continuous square wave (2.79). Figure 2.8 shows this evolution in successively thinner curves at times t = 0, $10^{-2} \tau$, $10^{-1} \tau$, $\tau = 2mL^2/\hbar$, 10τ , and 100τ . The curves at t = 0 and $t = 10^{-2} \tau$ are smooth, but some wobbles appear at $t = 10^{-1} \tau$ and at $t = \tau$ due to the discontinuities in the first derivative of $\psi(x, 0)$ at x = 0.5 and at x = 1.5.

Example 2.12 (Time Evolution of a Smooth Wave Function). Finally, let's try a wave function $\psi(x, 0)$ that is periodic and infinitely differentiable on [0, L]. An infinitely differentiable function is said to be **smooth** or C^{∞} . The infinite square-well potential V(x) of equation (2.71) imposes the periodic boundary conditions $\psi(0, 0) = \psi(L, 0) = 0$, so we try

$$\psi(x,0) = \sqrt{\frac{2}{3L}} \left[1 - \cos\left(\frac{2\pi x}{L}\right) \right].$$
(2.93)

Its Fourier series

$$\psi(x,0) = \sqrt{\frac{1}{6L}} \left(2 - e^{2\pi i x/L} - e^{-2\pi i x/L} \right)$$
(2.94)

has coefficients that satisfy the upper bounds (2.55) by vanishing for |n| > 1.



Figure 2.9 The wave function $\psi(x,0)$ (2.93) is infinitely differentiable, and so the first 10 terms of its uniformly convergent Fourier series (2.96) offer a very good approximation to it.

The coefficients of the Fourier sine series for the wave function $\psi(x, 0)$ are given by the integrals (2.82)

$$f_n = \int_0^L dx \sqrt{\frac{2}{L}} \sin\left(\frac{\pi nx}{L}\right) \psi(x,0)$$

$$= \frac{2}{\sqrt{3}L} \int_0^L dx \sin\left(\frac{\pi nx}{L}\right) \left[1 - \cos\left(\frac{2\pi x}{L}\right)\right]$$

$$= \frac{8\left[(-1)^n - 1\right]}{\pi\sqrt{3}n(n^2 - 4)}$$
(2.95)

with all the even coefficients zero, $c_{2n} = 0$. The f_n 's are proportional to $1/n^3$ which is more than enough to ensure the absolute and uniform convergence



Figure 2.10 The probability distributions $P(x,t) = |\psi(x,t)|^2$ of the 1000term Fourier series (2.97) for the wave function $\psi(x,t)$ at t = 0, $10^{-2}\tau$, $10^{-1}\tau$, $\tau = 2mL^2/\hbar$, 10τ , and 100τ are plotted as successively thinner curves. The time evolution is calm because the wave function $\psi(x,0)$ is smooth.

of its Fourier sine series

$$\psi(x,0) = \sum_{n=1}^{\infty} f_n \sqrt{\frac{2}{L}} \sin\left(\frac{\pi nx}{L}\right).$$
(2.96)

As time goes by, it evolves to

$$\psi(x,t) = \sum_{n=1}^{\infty} f_n \sqrt{\frac{2}{L}} \sin\left(\frac{\pi nx}{L}\right) e^{-i\hbar(n\pi)^2 t/(2mL^2)}$$
(2.97)

and remains absolutely convergent for all times t.

The effects of the absolute and uniform convergence with $f_n \propto 1/n^3$ are obvious in the graphs. Figure 2.9 shows (for L = 2) that only 10 terms are required to nearly overlap the initial wave function $\psi(x, 0)$. Figure 2.10 shows that the evolution of the probability distribution $|\psi(x, t)|^2$ with time is

smooth, with no sign of the jaggedness of Fig. 2.6 or the wobbles of Fig. 2.8. Because $\psi(x, 0)$ is smooth and periodic, it evolves calmly as time passes. \Box

2.9 Dirac Notation

Vectors $|j\rangle$ that are orthonormal $\langle k|j\rangle = \delta_{k,j}$ span a vector space and express the identity operator I of the space as (1.141)

$$I = \sum_{j=1}^{N} |j\rangle\langle j|.$$
(2.98)

Multiplying from the right by any vector $|g\rangle$ in the space, we get

$$|g\rangle = I|g\rangle = \sum_{j=1}^{N} |j\rangle\langle j|g\rangle$$
(2.99)

which says that every vector $|g\rangle$ in the space has an expansion (1.142) in terms of the N orthonormal basis vectors $|j\rangle$. The coefficients $\langle j|g\rangle$ of the expansion are inner products of the vector $|g\rangle$ with the basis vectors $|j\rangle$.

These properties of finite-dimensional vector spaces also are true of infinitedimensional vector spaces of functions. We may use as basis vectors the phases $\exp(inx)/\sqrt{2\pi}$. They are orthonormal with inner product (2.1)

$$(m,n) = \int_0^{2\pi} \left(\frac{e^{imx}}{\sqrt{2\pi}}\right)^* \frac{e^{inx}}{\sqrt{2\pi}} dx = \int_0^{2\pi} \frac{e^{i(n-m)x}}{2\pi} dx = \delta_{m,n} \qquad (2.100)$$

which in Dirac notation with $\langle x|n\rangle = \exp(inx)/\sqrt{2\pi}$ and $\langle m|x\rangle = \langle x|m\rangle^*$ is

$$\langle m|n\rangle = \int_0^{2\pi} \langle m|x\rangle \langle x|n\rangle \, dx = \int_0^{2\pi} \frac{e^{i(n-m)x}}{2\pi} \, dx = \delta_{m,n}.$$
 (2.101)

The identity operator for Fourier's space of functions is

$$I = \sum_{n = -\infty}^{\infty} |n\rangle \langle n|.$$
 (2.102)

So we have

$$|f\rangle = I|f\rangle = \sum_{n=-\infty}^{\infty} |n\rangle \langle n|f\rangle$$
 (2.103)

and

$$\langle x|f\rangle = \langle x|I|f\rangle = \sum_{n=-\infty}^{\infty} \langle x|n\rangle \langle n|f\rangle = \sum_{n=-\infty}^{\infty} \frac{e^{inx}}{\sqrt{2\pi}} \langle n|f\rangle$$
(2.104)

which with $\langle n|f\rangle = f_n$ is the Fourier series (2.2). The coefficients $\langle n|f\rangle = f_n$ are the inner products (2.3)

$$\langle n|f\rangle = \int_0^{2\pi} \langle n|x\rangle \langle x|f\rangle \, dx = \int_0^{2\pi} \frac{e^{-inx}}{\sqrt{2\pi}} \, \langle x|f\rangle \, dx = \int_0^{2\pi} \frac{e^{-inx}}{\sqrt{2\pi}} \, f(x) \, dx.$$
(2.105)

2.10 Dirac's Delta Function

A Dirac delta function is a (continuous, linear) map from a space of suitably well-behaved functions into the real or complex numbers. It is a **functional** that associates a number with each function in the function space. Thus $\delta(x - y)$ associates the number f(y) with the function f(x). We may write this association as

$$f(y) = \int f(x) \,\delta(x - y) \,dx.$$
 (2.106)

Delta functions pop up all over physics. The inner product of two of the kets $|x\rangle$ that appear in the Fourier-series formulas (2.104) and (2.105) is a delta function, $\langle x|y\rangle = \delta(x-y)$. The formula (2.105) for the coefficient $\langle n|f\rangle$ becomes obvious if we write the identity operator for functions defined on the interval $[0, 2\pi]$ as

$$I = \int_0^{2\pi} |x\rangle \langle x| \, dx \tag{2.107}$$

for then

$$\langle n|f\rangle = \langle n|I|f\rangle = \int_0^{2\pi} \langle n|x\rangle \langle x|f\rangle \, dx = \int_0^{2\pi} \frac{e^{-inx}}{\sqrt{2\pi}} \langle x|f\rangle \, dx.$$
(2.108)

The equation $|y\rangle = I|y\rangle$ with the identity operator (2.107) gives

$$|y\rangle = I|y\rangle = \int_0^{2\pi} |x\rangle \langle x|y\rangle \, dx. \tag{2.109}$$

Multiplying (2.107) from the right by $|f\rangle$ and from the left by $\langle y|$, we get

$$f(y) = \langle y|I|f \rangle = \int_0^{2\pi} \langle y|x \rangle \langle x|f \rangle \, dx = \int_0^{2\pi} \langle y|x \rangle f(x) \, dx.$$
 (2.110)

These relations (2.109 & 2.110) say that the inner product $\langle y|x\rangle$ is a **delta function**, $\langle y|x\rangle = \langle x|y\rangle = \delta(x-y)$.

The Fourier-series formulas (2.104) and (2.105) lead to a statement about

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the completeness of the phases $\exp(inx)/\sqrt{2\pi}$

$$f(x) = \sum_{n = -\infty}^{\infty} f_n \frac{e^{inx}}{\sqrt{2\pi}} = \sum_{n = -\infty}^{\infty} \int_0^{2\pi} \frac{e^{-iny}}{\sqrt{2\pi}} f(y) \frac{e^{inx}}{\sqrt{2\pi}} dy.$$
(2.111)

Interchanging and rearranging, we have

$$f(x) = \int_0^{2\pi} \left(\sum_{n = -\infty}^{\infty} \frac{e^{in(x-y)}}{2\pi} \right) f(y) \, dy.$$
 (2.112)

But f(x) and the phases e^{inx} are **periodic** with period 2π , so we also have

$$f(x+2\pi\ell) = \int_0^{2\pi} \left(\sum_{n=-\infty}^\infty \frac{e^{in(x-y)}}{2\pi}\right) f(y) \, dy.$$
(2.113)

Thus we arrive at the **Dirac comb**

$$\sum_{n=-\infty}^{\infty} \frac{e^{in(x-y)}}{2\pi} = \sum_{\ell=-\infty}^{\infty} \delta(x-y-2\pi\ell)$$
(2.114)

or more simply

$$\sum_{n=-\infty}^{\infty} \frac{e^{inx}}{2\pi} = \frac{1}{2\pi} \left[1 + 2\sum_{n=1}^{\infty} \cos(nx) \right] = \sum_{\ell=-\infty}^{\infty} \delta(x - 2\pi\ell).$$
(2.115)

Example 2.13 (Dirac's Comb). The sum of the first 100,000 terms of this cosine series (2.115) for the Dirac comb is plotted for the interval (-15, 15) in Fig. 2.11. Gibbs overshoots appear at the discontinuities. The integral of the first 100,000 terms from -15 to 15 is 5.0000.

The stretched Dirac comb is

$$\sum_{n=-\infty}^{\infty} \frac{e^{2\pi i n(x-y)/L}}{L} = \sum_{\ell=-\infty}^{\infty} \delta(x-y-\ell L).$$
 (2.116)

Example 2.14 (Parseval's Identity). Using our formula (2.34) for the Fourier coefficients of a stretched interval, we can relate a sum of products $f_n^* g_n$ of the Fourier coefficients of the functions f(x) and g(x) to an integral of the product $f^*(x) g(x)$

$$\sum_{n=-\infty}^{\infty} f_n^* g_n = \sum_{n=-\infty}^{\infty} \int_0^L dx \, \frac{e^{i2\pi nx/L}}{\sqrt{L}} f^*(x) \, \int_0^L dy \, \frac{e^{-i2\pi ny/L}}{\sqrt{L}} g(y). \quad (2.117)$$



Figure 2.11 The sum of the first 100,000 terms of the series (2.115) for the Dirac comb is plotted for $-15 \le x \le 15$. Both Dirac spikes and Gibbs overshoots are visible.

This sum contains Dirac's comb (2.116) and so

$$\sum_{n=-\infty}^{\infty} f_n^* g_n = \int_0^L dx \, \int_0^L dy \, f^*(x) \, g(y) \, \frac{1}{L} \, \sum_{n=-\infty}^{\infty} e^{i2\pi n(x-y)/L} \\ = \int_0^L dx \, \int_0^L dy \, f^*(x) \, g(y) \, \sum_{\ell=-\infty}^{\infty} \delta(x-y-\ell L).$$
(2.118)

But because only the $\ell = 0$ tooth of the comb lies in the interval [0, L], we have more simply

$$\sum_{n=-\infty}^{\infty} f_n^* g_n = \int_0^L dx \, \int_0^L dy \, f^*(x) \, g(y) \, \delta(x-y) = \int_0^L dx \, f^*(x) \, g(x). \tag{2.119}$$

In particular, if the two functions are the same, then

$$\sum_{n=-\infty}^{\infty} |f_n|^2 = \int_0^L dx \, |f(x)|^2 \tag{2.120}$$

which is **Parseval's identity**. Thus if a function is **square integrable** on an interval, then the sum of the squares of the absolute values of its Fourier coefficients is the integral of the square of its absolute value.

Example 2.15 (Derivatives of Delta Functions). Delta functions and other generalized functions or distributions map smooth functions that vanish at infinity into numbers in ways that are linear and continuous. Derivatives of delta functions are defined so as to allow integrations by parts. Thus the nth derivative of the delta function $\delta^{(n)}(x-y)$ maps the function f(x) to $(-1)^n$ times its *n*th derivative $f^{(n)}(y)$ at y

$$\int \delta^{(n)}(x-y) f(x) dx = \int \delta(x-y) (-1)^n f^{(n)}(x) dx = (-1)^n f^{(n)}(y) \quad (2.121)$$
with no surface term.

with no surface term.

Example 2.16 (The Equation xf(x) = a). Dirac's delta function sometimes appears unexpectedly. For instance, the general solution to the equation x f(x) = a is $f(x) = a/x + b \delta(x)$ where b is an arbitrary constant (Dirac, 1967, sec. 15), (Waxman and Peck, 1998). Similarly, the general solution to the equation $x^2 f(x) = a$ is $f(x) = a/x^2 + b \delta(x)/x + c \delta(x) + d \delta'(x)$ in which $\delta'(x)$ is the derivative of the delta function, and b, c, and d are arbitrary constants.

2.11 The Harmonic Oscillator

The hamiltonian for the harmonic oscillator is

$$H = \frac{p^2}{2m} + \frac{1}{2}m\omega^2 q^2.$$
 (2.122)

The commutation relation $[q, p] \equiv qp - pq = i\hbar$ implies that the **lowering** and **raising** operators

$$a = \sqrt{\frac{m\omega}{2\hbar}} \left(q + \frac{ip}{m\omega} \right) \quad \text{and} \quad a^{\dagger} = \sqrt{\frac{m\omega}{2\hbar}} \left(q - \frac{ip}{m\omega} \right)$$
 (2.123)

obey the commutation relation $[a, a^{\dagger}] = 1$. In terms of a and a^{\dagger} , which also are called the **annihilation** and **creation** operators, the hamiltonian H has

the simple form

$$H = \hbar \omega \left(a^{\dagger} a + \frac{1}{2} \right). \tag{2.124}$$

There is a unique state $|0\rangle$ that is annihilated by the operator a, as may be seen by solving the differential equation

$$\langle q'|a|0\rangle = \sqrt{\frac{m\omega}{2\hbar}} \langle q'|\left(q + \frac{ip}{m\omega}\right)|0\rangle = 0.$$
 (2.125)

Since $\langle q'|q = q'\langle q'|$ and

$$\langle q'|p|0\rangle = \frac{\hbar}{i} \frac{d\langle q'|0\rangle}{dq'} \tag{2.126}$$

the resulting differential equation is

$$\frac{d\langle q'|0\rangle}{dq'} = -\frac{m\omega}{\hbar}q'\langle q'|0\rangle.$$
(2.127)

Its suitably normalized solution is the wave function for the ground state of the harmonic oscillator

$$\langle q'|0\rangle = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} \exp\left(-\frac{m\omega q'^2}{2\hbar}\right).$$
 (2.128)

For n = 0, 1, 2, ..., the *n*th eigenstate of the hamiltonian *H* is

$$|n\rangle = \frac{1}{\sqrt{n!}} \left(a^{\dagger}\right)^{n} |0\rangle \qquad (2.129)$$

where $n! \equiv n(n-1) \dots 1$ is *n*-factorial and 0! = 1. Its energy is

$$H|n\rangle = \hbar\omega \left(n + \frac{1}{2}\right)|n\rangle.$$
(2.130)

The identity operator is

$$I = \sum_{n=0}^{\infty} |n\rangle \langle n|.$$
 (2.131)

An arbitrary state $|\psi\rangle$ has an expansion in terms of the eigenstates $|n\rangle$

$$|\psi\rangle = I|\psi\rangle = \sum_{n=0}^{\infty} |n\rangle\langle n|\psi\rangle$$
 (2.132)

and evolves in time like a Fourier series

$$|\psi,t\rangle = e^{-iHt/\hbar}|\psi\rangle = e^{-iHt/\hbar}\sum_{n=0}^{\infty}|n\rangle\langle n|\psi\rangle = e^{-i\omega t/2}\sum_{n=0}^{\infty}e^{-in\omega t}|n\rangle\langle n|\psi\rangle$$
(2.133)

with wave function

$$\psi(q,t) = \langle q|\psi,t\rangle = e^{-i\omega t/2} \sum_{n=0}^{\infty} e^{-in\omega t} \langle q|n\rangle \langle n|\psi\rangle.$$
(2.134)

The wave functions $\langle q|n \rangle$ of the energy eigenstates are related to the Hermite polynomials (example 8.6)

$$H_n(x) = (-1)^n e^{x^2} \frac{d^n}{dx^n} e^{-x^2}$$
(2.135)

by a change of variables $x = \sqrt{m\omega/\hbar} q \equiv sq$ and a normalization factor

$$\langle q|n\rangle = \frac{\sqrt{s}\,e^{-(sq)^2/2}}{\sqrt{2^n n!}\sqrt{\pi}}\,H_n(sq) = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4}\frac{e^{-m\omega q^2/2\hbar}}{\sqrt{2^n n!}}\,H_n\left(\left(\frac{m\omega}{\hbar}\right)^{1/2}q\right).$$
(2.136)

The coherent state $|\alpha\rangle$

$$|\alpha\rangle = e^{-|\alpha|^2/2} e^{\alpha a^{\dagger}} |0\rangle = e^{-|\alpha|^2/2} \sum_{n=0}^{\infty} \frac{\alpha^n}{\sqrt{n!}} |n\rangle$$
(2.137)

is an eigenstate $a|\alpha\rangle = \alpha |\alpha\rangle$ of the lowering (or annihilation) operator a with eigenvalue α . Its time evolution is simply

$$|\alpha,t\rangle = e^{-i\omega t/2} e^{-|\alpha|^2/2} \sum_{n=0}^{\infty} \frac{\left(\alpha e^{-i\omega t}\right)^n}{\sqrt{n!}} |n\rangle = e^{-i\omega t/2} |\alpha e^{-i\omega t}\rangle.$$
(2.138)

2.12 Nonrelativistic Strings

If we clamp the ends of a nonrelativistic string at x = 0 and x = L, then the amplitude y(x, t) will obey the boundary conditions

$$y(0,t) = y(L,t) = 0 (2.139)$$

and the wave equation

$$v^2 \frac{\partial^2 y}{\partial x^2} = \frac{\partial^2 y}{\partial t^2} \tag{2.140}$$

as long as y(x,t) remains small. The functions

$$y_n(x,t) = \sin \frac{n\pi x}{L} \left(f_n \sin \frac{n\pi vt}{L} + d_n \cos \frac{n\pi vt}{L} \right)$$
(2.141)

satisfy this wave equation (2.140) and the boundary conditions (2.139). They represent waves traveling along the x-axis with speed v.

The space S_L of functions f(x) that satisfy the boundary condition (2.139) is spanned by the functions $\sin(n\pi x/L)$. One may use the integral formula

$$\int_0^L \sin \frac{n\pi x}{L} \sin \frac{m\pi x}{L} \, dx = \frac{L}{2} \,\delta_{nm} \tag{2.142}$$

to derive for any function $f \in S_L$ the Fourier series

$$f(x) = \sum_{n=1}^{\infty} f_n \sin \frac{n\pi x}{L}$$
(2.143)

with coefficients

$$f_n = \frac{2}{L} \int_0^L \sin \frac{n\pi x}{L} f(x) dx \qquad (2.144)$$

and the representation

$$\sum_{m=-\infty}^{\infty} \delta(x-z-2mL) = \frac{2}{L} \sum_{n=1}^{\infty} \sin\frac{n\pi x}{L} \sin\frac{n\pi z}{L}$$
(2.145)

for the Dirac comb on S_L .

2.13 Periodic Boundary Conditions

Periodic boundary conditions often are convenient. For instance, rather than study an infinitely long one-dimensional system, we might study the same system, but of length L. The ends cause effects not present in the infinite system. To avoid them, we imagine that the system forms a circle and impose the periodic boundary condition

$$\psi(x \pm L, t) = \psi(x, t).$$
 (2.146)

In three dimensions, the analogous conditions are

$$\psi(\mathbf{x} \pm \mathbf{L}, y, z, t) = \psi(\mathbf{x}, y, z, t)$$

$$\psi(\mathbf{x}, \mathbf{y} \pm \mathbf{L}, z, t) = \psi(\mathbf{x}, \mathbf{y}, z, t)$$

$$\psi(\mathbf{x}, y, \mathbf{z} \pm \mathbf{L}, t) = \psi(\mathbf{x}, y, z, t).$$

(2.147)

The eigenstates $|\mathbf{p}\rangle$ of the free hamiltonian $H = \mathbf{p}^2/2m$ have wave functions

$$\psi_{\mathbf{p}}(\mathbf{x}) = \langle \mathbf{x} | \mathbf{p} \rangle = e^{i\mathbf{x} \cdot \mathbf{p}/\hbar} / (2\pi\hbar)^{3/2}.$$
 (2.148)

The periodic boundary conditions (2.147) require that each component p_i of momentum satisfy $Lp_i/\hbar = 2\pi n_i$ or

$$\boldsymbol{p} = \frac{2\pi\hbar\boldsymbol{n}}{L} = \frac{\hbar\boldsymbol{n}}{L} \tag{2.149}$$

where n is a vector of integers, which may be positive or negative or zero.

Periodic boundary conditions naturally arise in the study of solids. The atoms of a perfect crystal are at the vertices of a **Bravais** lattice

$$\boldsymbol{x}_i = \boldsymbol{x}_0 + \sum_{i=1}^3 n_i \boldsymbol{a}_i$$
 (2.150)

in which the three vectors a_i are the **primitive vectors** of the lattice and the n_i are three integers. The hamiltonian of such an infinite crystal is invariant under translations in space by

$$\sum_{i=1}^{3} n_i a_i.$$
 (2.151)

To keep the notation simple, let's restrict ourselves to a cubic lattice with lattice spacing a. Then since the momentum operator p generates translations in space, the invariance of H under translations by a n

$$\exp(ia\boldsymbol{n}\cdot\boldsymbol{p})\,H\exp(-ia\boldsymbol{n}\cdot\boldsymbol{p}) = H \tag{2.152}$$

implies that $e^{ian \cdot p}$ and H are compatible normal operators $[e^{ian \cdot p}, H] = 0$. As explained in section 1.31, it follows that we may choose the eigenstates of H also to be eigenstates of $e^{ian \cdot p}$

$$e^{ia\boldsymbol{p}\cdot\boldsymbol{n}/\hbar}|\psi\rangle = e^{ia\boldsymbol{k}\cdot\boldsymbol{n}}|\psi\rangle \tag{2.153}$$

which implies that

$$\psi(\boldsymbol{x} + a\boldsymbol{n}) = \langle \boldsymbol{x} + a\boldsymbol{n} | \psi \rangle = \langle \boldsymbol{x} | e^{ia\boldsymbol{p} \cdot \boldsymbol{n}/\hbar} | \psi \rangle = \langle \boldsymbol{x} | e^{ia\boldsymbol{k} \cdot \boldsymbol{n}/\hbar} | \psi \rangle = e^{ia\boldsymbol{k} \cdot \boldsymbol{n}} \psi(\boldsymbol{x}).$$
(2.154)

Setting

$$\psi(\boldsymbol{x}) = e^{i\boldsymbol{k}\cdot\boldsymbol{x}} u(\boldsymbol{x}) \tag{2.155}$$

we see that condition (2.154) implies that u(x) is periodic

$$u(\boldsymbol{x} + a\boldsymbol{n}) = u(\boldsymbol{x}). \tag{2.156}$$

For a general Bravais lattice, this **Born–von Karman** periodic boundary condition is

$$u\left(\boldsymbol{x} + \sum_{i=1}^{3} n_i \boldsymbol{a}_i, t\right) = u(\boldsymbol{x}, t).$$
(2.157)

Equations (2.154) and (2.156) are known as **Bloch's theorem**.

Exercises

- 2.1 Show that $\sin \omega_1 x + \sin \omega_2 x$ is the same as (2.9).
- 2.2 Find the Fourier series for the function $\exp(ax)$ on the interval $-\pi < x \le \pi$.
- 2.3 Find the Fourier series for the function $(x^2 \pi^2)^2$ on the same interval $(-\pi, \pi]$.
- 2.4 Find the Fourier series for the function $(1 + \cos x) \sin ax$ on the interval $(-\pi, \pi]$.
- 2.5 Show that the Fourier series for the function $x \cos x$ on the interval $[-\pi, \pi]$ is

$$x\cos x = -\frac{1}{2}\sin x + 2\sum_{n=2}^{\infty} \frac{(-1)^n n}{n^2 - 1}\sin nx.$$
 (2.158)

2.6 (a) Show that the Fourier series for the function |x| on the interval $[-\pi,\pi]$ is

$$|x| = \frac{\pi}{2} - \frac{4}{\pi} \sum_{n=0}^{\infty} \frac{\cos(2n+1)x}{(2n+1)^2}.$$
 (2.159)

(b) Use this result to find a neat formula for $\pi^2/8$. Hint: set x = 0.

2.7 Show that the Fourier series for the function $|\sin x|$ on the interval $[-\pi, \pi]$ is

$$|\sin x| = \frac{2}{\pi} - \frac{4}{\pi} \sum_{n=1}^{\infty} \frac{\cos 2nx}{4n^2 - 1}.$$
 (2.160)

- 2.8 Show that the Fourier coefficients of the C^0 function (2.58) on the interval $[-\pi, \pi]$ are given by (2.59).
- 2.9 Find by inspection the Fourier series for the function $\exp[\exp(-ix)]$.
- 2.10 Fill in the steps in the computation (2.27) of the Fourier series for x^2 .
- 2.11 Do the first integral in equation (2.64). Hint: differentiate $\ln\left(\frac{\sin \pi x}{\pi x}\right)$.
- 2.12 Use the infinite-product formula (2.65) for the sine and the relation $\cos \pi x = \sin 2\pi x/(2\sin \pi x)$ to derive the infinite-product formula (2.66) for the cosine. Hint:

$$\prod_{n=1}^{\infty} \left[1 - \frac{x^2}{\frac{1}{4}n^2} \right] = \prod_{n=1}^{\infty} \left[1 - \frac{x^2}{\frac{1}{4}(2n-1)^2} \right] \left[1 - \frac{x^2}{\frac{1}{4}(2n)^2} \right].$$
 (2.161)

2.13 What's the general solution to the equation $x^3 f(x) = a$?

Exercises

2.14 Suppose we wish to approximate the real square-integrable function f(x) by the Fourier series with N terms

$$f_N(x) = \frac{a_0}{2} + \sum_{n=1}^N \left(a_n \cos nx + b_n \sin nx \right).$$
 (2.162)

Then the error

$$E_N = \int_0^{2\pi} \left[f(x) - f_N(x) \right]^2 dx \qquad (2.163)$$

will depend upon the 2N+1 coefficients a_n and b_n . The best coefficients minimize this error and satisfy the conditions

$$\frac{\partial E_N}{\partial a_n} = \frac{\partial E_N}{\partial b_n} = 0. \tag{2.164}$$

By using these conditions, find them.

2.15 Find the Fourier series for the function

$$f(x) = \theta(a^2 - x^2)$$
(2.165)

on the interval $[-\pi,\pi]$ for the case $a^2 < \pi^2$. The **Heaviside step** function $\theta(x)$ is zero for x < 0, one-half for x = 0, and unity for x > 0 (Oliver Heaviside, 1850–1925). The value assigned to $\theta(0)$ seldom matters, and you need not worry about it in this problem.

- 2.16 Derive or infer the formula (2.116) for the stretched Dirac comb.
- 2.17 Use the commutation relation $[q, p] = i\hbar$ to show that the annihilation and creation operators (2.123) satisfy the commutation relation $[a, a^{\dagger}] = 1$.
- 2.18 Show that the state $|n\rangle = (a^{\dagger})^n |0\rangle / \sqrt{n!}$ is an eigenstate of the hamiltonian (2.124) with energy $\hbar \omega (n + 1/2)$.
- 2.19 Show that the coherent state $|\alpha\rangle$ (2.137) is an eigenstate of the annihilation operator *a* with eigenvalue α .
- 2.20 Derive equations (2.144 & 2.145) from the expansion (2.143) and the integral formula (2.142).
- 2.21 Consider a string like the one described in section 2.12, which satisfies the boundary conditions (2.139) and the wave equation (2.140). The string is at rest at time t = 0

$$y(x,0) = 0 \tag{2.166}$$

and is struck precisely at t = 0 and x = a so that

$$\left. \frac{\partial y(x,t)}{\partial t} \right|_{t=0} = L v_0 \delta(x-a).$$
(2.167)

Find y(x,t) and $\dot{y}(x,t)$, where the dot means time derivative. 2.22 Same as exercise (2.21), but now the initial conditions are

$$u(x,0) = f(x)$$
 and $\dot{u}(x,0) = g(x)$ (2.168)

in which f(0) = f(L) = 0 and g(0) = g(L) = 0. Find the motion of the amplitude u(x,t) of the string.

2.23 (a) Find the Fourier series for the function $f(x) = x^2$ on the interval $[-\pi, \pi]$. (b) Use your result at $x = \pi$ to show that

$$\sum_{n=1}^{\infty} \frac{1}{n^2} = \frac{\pi^2}{6} \tag{2.169}$$

which is the value of Riemann's zeta function (4.99) $\zeta(x)$ at x = 2.