with coefficients

$$f_n = \frac{2}{L} \int_0^L \sin \frac{n\pi x}{L} f(x) dx \tag{2.145}$$

and the representation

$$\sum_{m=-\infty}^{\infty} \delta(x - z - 2mL) = \frac{2}{L} \sum_{n=1}^{\infty} \sin \frac{n\pi x}{L} \sin \frac{n\pi z}{L} \tag{2.146}$$

for the Dirac comb on S_L.

2.13 Periodic Boundary Conditions

Periodic boundary conditions are often 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

$$\psi(x \pm L, t) = \psi(x, t). \tag{2.147}$$

In three dimensions, the analogous conditions are

$$\begin{aligned} \psi(x \pm L, y, z, t) &= \psi(x, y, z, t) \\ \psi(x, y \pm L, z, t) &= \psi(x, y, z, t) \\ \psi(x, y, z \pm L, t) &= \psi(x, y, z, t). \end{aligned} \tag{2.148}$$

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

$$\psi_{\boldsymbol{p}}(\boldsymbol{x}) = \langle \boldsymbol{x}|\boldsymbol{p}\rangle = e^{i\boldsymbol{x}\cdot\boldsymbol{p}/\hbar}/(2\pi\hbar)^{3/2}. \tag{2.149}$$

The periodic boundary conditions (2.148) require that each component p_i of momentum satisfy $Lp_i/\hbar = 2\pi n_i$ or

$$\boldsymbol{p} = \frac{2\pi\hbar\boldsymbol{n}}{L} = \frac{h\boldsymbol{n}}{L} \tag{2.150}$$

where $\boldsymbol{n}$ is a vector of integers, which may be positive or negative or zero.

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

$$\boldsymbol{x}_i = \boldsymbol{x}_0 + \sum_{i=1}^{3} n_i \boldsymbol{a}_i \tag{2.151}$$

in which the three vectors $\boldsymbol{a}_i$ 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

$$\sum_{i=1}^{3} n_i \boldsymbol{a}_i. \tag{2.152}$$

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

$$\exp(ia\boldsymbol{n}\cdot\boldsymbol{p})H\exp(-ia\boldsymbol{n}\cdot\boldsymbol{p}) = H \tag{2.153}$$

implies that $\exp(ia\boldsymbol{n}\cdot\boldsymbol{p})$ and H are compatible observables $[\exp(ia\boldsymbol{n}\cdot\boldsymbol{p}), H] = 0$. As explained in section 1.30, it follows that we may choose the eigenstates of H also to be eigenstates of $\boldsymbol{p}$

$$e^{ia\boldsymbol{p}\cdot\boldsymbol{n}/\hbar}|\psi\rangle = e^{ia\boldsymbol{k}\cdot\boldsymbol{n}}\,|\psi\rangle \tag{2.154}$$

which implies that

$$\psi(\boldsymbol{x}+a\boldsymbol{n},t) = e^{ia\boldsymbol{k}\cdot\boldsymbol{n}}\,\psi(\boldsymbol{x},t). \tag{2.155}$$

Setting

$$\psi(\boldsymbol{x}) = e^{i\boldsymbol{k}\cdot\boldsymbol{x}}\,u(\boldsymbol{x}) \tag{2.156}$$

we see that condition (2.155) implies that $u(\boldsymbol{x})$ is periodic

$$u(\boldsymbol{x}+a\boldsymbol{n}) = u(\boldsymbol{x}). \tag{2.157}$$

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

$$u\left(\boldsymbol{x}+\sum_{i=1}^{3} n_i\boldsymbol{a}_i, t\right) = u(\boldsymbol{x},t). \tag{2.158}$$

Equations (2.155) and (2.157) 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 $(-\pi,\pi]$.