APPENDIX A

The Dirac delta function

A.1 Definition and basic properties

The Dirac delta function $\delta(x)$ is a function defined to have the following properties:

$$\begin{aligned} \delta(x) &= 0 \qquad x \neq 0, \\ \delta(x) &= \infty \qquad x = 0, \\ \int_{-\infty}^{\infty} \delta(x)\,\mathrm{d}x &= 1. \end{aligned} \tag{A.1}$$

$\delta(x)$ is not a proper mathematical function but is nevertheless a very useful tool in mathematical physics. Note that the function gives a meaningful result only after the integration process.

From the definition we have

$$\int_{-\infty}^{\infty} f(x)\delta(a-x)\,\mathrm{d}x = f(a), \tag{A.2}$$

$$\delta(cx) = \frac{1}{c}\,\delta(x), \tag{A.3}$$

where c is a positive constant,

$$\delta(x) = \delta(-x). \tag{A.4}$$

A.2 Representation in terms of an infinite integral

There are several ways of representing the delta function as the limit of a proper mathematical function. The most useful one for our purposes is in terms of an infinite integral. Consider the function

$$\begin{aligned} f(x) = \int_{-k_0}^{k_0} \exp(\mathrm{i}kx)\,\mathrm{d}k &= \frac{1}{\mathrm{i}x}\{\exp(\mathrm{i}k_0x) - \exp(-\mathrm{i}k_0x)\} \\ &= \frac{2}{x}\sin k_0x. \end{aligned} \tag{A.5}$$

$f(x)$ is shown for a particular value of k_0 in Fig. A.1. The total area under the curve is

$$2\int_{-\infty}^{\infty} \frac{1}{x}\sin k_0x\,\mathrm{d}x = 2\int_{-\infty}^{\infty} \frac{\sin y}{y}\,\mathrm{d}y = 2\pi. \tag{A.6}$$

Now consider the function $f(x)$ as k_0 increases. The height of the peak at $x = 0$ increases, and the first zero occurs at smaller and smaller values of x. But the value of $\int_{-\infty}^{\infty} f(x)\,\mathrm{d}x$ remains constant. So, as $k_0 \to \infty$ the function $f(x)/2\pi$ becomes more and more like a δ function, i.e.

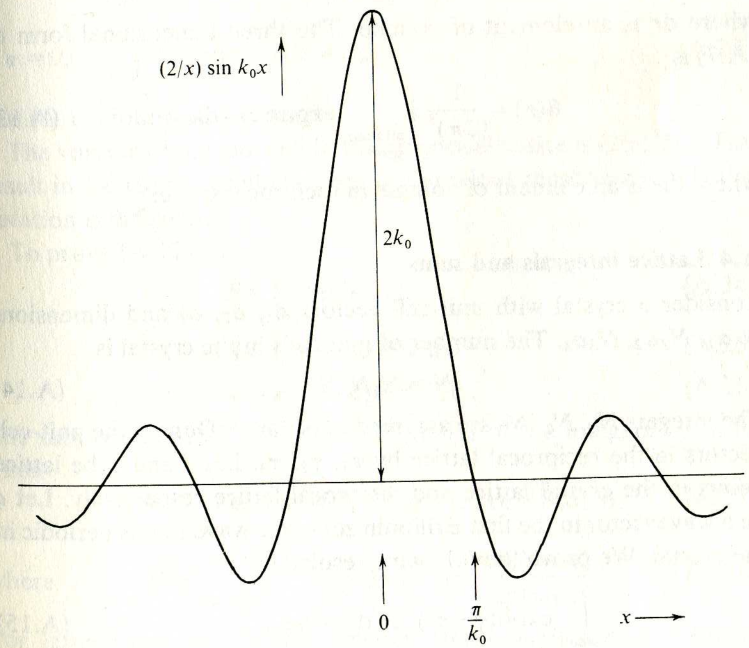
$$\delta(x) = \frac{1}{2\pi}\int_{-\infty}^{\infty} \exp(\mathrm{i}kx)\,\mathrm{d}k. \tag{A.7}$$

Similarly

$$\delta(k) = \frac{1}{2\pi}\int_{-\infty}^{\infty} \exp(\mathrm{i}kx)\,\mathrm{d}x, \tag{A.8}$$

$$\delta(\hbar\omega) = \frac{1}{\hbar}\delta(\omega) = \frac{1}{2\pi\hbar}\int_{-\infty}^{\infty} \exp(\mathrm{i}\omega t)\,\mathrm{d}t, \tag{A.9}$$

Fig. A.1 Plot of the function $(2/x)\sin k_0x$.



and

$$\delta(E_\lambda - E_{\lambda'} + \hbar\omega) = \frac{1}{2\pi\hbar}\int_{-\infty}^{\infty} \exp\{i(E_{\lambda'} - E_\lambda)t/\hbar\}\exp(-i\omega t)\,dt, \tag{A.10}$$

where E_λ and $E_{\lambda'}$ are constants.

A.3 Three-dimensional delta function

If $\boldsymbol{r}$ is a vector with components x, y, z, we define the three-dimensional δ-function by

$$\delta(\boldsymbol{r}) = \delta(x)\delta(y)\delta(z). \tag{A.11}$$

$\delta(\boldsymbol{r})$ has the following properties:

$$\begin{aligned} &\delta(\boldsymbol{r}) = 0 \qquad \boldsymbol{r} \neq 0,\\ &\delta(\boldsymbol{r}) = \infty \qquad \boldsymbol{r} = 0,\\ &\int_{\substack{\text{all}\\ \text{space}}} \delta(\boldsymbol{r})\,d\boldsymbol{r} = 1,\\ &\int_{\substack{\text{all}\\ \text{space}}} f(\boldsymbol{r})\delta(\boldsymbol{r}-\boldsymbol{r}_0)\,d\boldsymbol{r} = f(\boldsymbol{r}_0), \end{aligned} \tag{A.12}$$

where $d\boldsymbol{r}$ is an element of volume. The three-dimensional form of (A.7) is

$$\delta(\boldsymbol{r}) = \frac{1}{(2\pi)^3}\int_{\substack{\text{all recip}\\ \text{space}}} \exp(i\boldsymbol{\kappa}\,.\,\boldsymbol{r})\,d\boldsymbol{\kappa}, \tag{A.13}$$

where $d\boldsymbol{\kappa}$ is an element of volume in reciprocal space.

A.4 Lattice integrals and sums

Consider a crystal with unit-cell vectors $\boldsymbol{a}_1$, $\boldsymbol{a}_2$, $\boldsymbol{a}_3$ and dimensions N_1a_1, N_2a_2, N_3a_3. The number of unit cells in the crystal is

$$N = N_1N_2N_3. \tag{A.14}$$

The integers N_1, N_2, N_3 are assumed to be large. Denote the unit-cell vectors in the reciprocal lattice by $\boldsymbol{\tau}_1$, $\boldsymbol{\tau}_2$, $\boldsymbol{\tau}_3$. Let $\boldsymbol{l}$ and $\boldsymbol{\tau}$ be lattice points in the crystal lattice and reciprocal lattice respectively. Let $\boldsymbol{q}$ be a wavevector in the first Brillouin zone of a wave that is periodic in the crystal. We prove the following results:

$$\int_{\text{cell}} \exp\{i(\boldsymbol{\tau}-\boldsymbol{\tau}')\,.\,\boldsymbol{r}\}\,d\boldsymbol{r} = v_0\delta_{\boldsymbol{\tau}\boldsymbol{\tau}'}, \tag{A.15}$$

$$\int_{\text{cell}} \exp\{i\boldsymbol{\kappa}\,.\,(\boldsymbol{l}-\boldsymbol{l}')\}\,d\boldsymbol{\kappa} = \frac{(2\pi)^3}{v_0}\delta_{\boldsymbol{l}\boldsymbol{l}'}, \tag{A.16}$$

$$\sum_{\boldsymbol{l}} \exp(i\boldsymbol{\kappa}\,.\,\boldsymbol{l}) = \frac{(2\pi)^3}{v_0}\sum_{\boldsymbol{\tau}}\delta(\boldsymbol{\kappa}-\boldsymbol{\tau}), \tag{A.17}$$

$$\sum_{\boldsymbol{l}} \exp\{i(\boldsymbol{q}-\boldsymbol{q}')\,.\,\boldsymbol{l}\} = N\delta_{\boldsymbol{q}\boldsymbol{q}'}. \tag{A.18}$$

v_0 is the volume of the unit cell in the crystal lattice, and $\int_{\text{cell}}$ means integrate over the unit cell of the crystal or reciprocal lattice.

To prove (A.15) put $\boldsymbol{\tau}' = 0$ and let

$$\boldsymbol{\tau} = t_1\boldsymbol{\tau}_1 + t_2\boldsymbol{\tau}_2 + t_3\boldsymbol{\tau}_3, \tag{A.19}$$

$$\boldsymbol{r} = r_1\boldsymbol{a}_1 + r_2\boldsymbol{a}_2 + r_3\boldsymbol{a}_3, \tag{A.20}$$

where t_1, t_2, t_3 are integers. Then

$$\int_{\text{cell}} \exp(i\boldsymbol{\tau}\,.\,\boldsymbol{r})\,d\boldsymbol{r} = 0, \tag{A.21}$$

unless $\boldsymbol{\tau} = 0$. This is readily seen by considering a one-dimensional component of the integral along one side of the unit cell. If t_i ($i = 1, 2, 3$) is an integer other than zero,

$$\int_0^1 \exp(2\pi i t_i r_i)\,dr_i = \frac{1}{2\pi i t_i}\{\exp(2\pi i t_i) - 1\} = 0. \tag{A.22}$$

If $\boldsymbol{\tau} = 0$,

$$\int_{\text{cell}} \exp(i\boldsymbol{\tau}\,.\,\boldsymbol{r})\,d\boldsymbol{r} = v_0, \tag{A.23}$$

and (A.15) follows immediately.

The volume of the unit cell in the reciprocal lattice is $(2\pi)^3/v_0$. The result in (A.16) then follows from the previous reasoning – only the notation is different.

To prove (A.17) put

$$S = \sum_{\boldsymbol{l}} \exp(i\boldsymbol{\kappa}\,.\,\boldsymbol{l}), \tag{A.24}$$

$$\boldsymbol{l} = l_1\boldsymbol{a}_1 + l_2\boldsymbol{a}_2 + l_3\boldsymbol{a}_3, \tag{A.25}$$

$$\boldsymbol{\kappa} = \kappa_1\boldsymbol{\tau}_1 + \kappa_2\boldsymbol{\tau}_2 + \kappa_3\boldsymbol{\tau}_3. \tag{A.26}$$

The sum over $\boldsymbol{l}$ in (A.24) is over all values of the integers l_1, l_2, l_3. Then

$$S = \sum_{l_1l_2l_3} \exp\{2\pi i(\kappa_1l_1 + \kappa_2l_2 + \kappa_3l_3)\} = S_1S_2S_3, \tag{A.27}$$

where

$$S_i = \sum_{l_i=-(N_i-1)/2}^{(N_i-1)/2} \exp(2\pi i\kappa_il_i) = \frac{\sin(N_i\pi\kappa_i)}{\sin(\pi\kappa_i)}. \tag{A.28}$$

For large values of N_i the function $\sin(N_i\pi\kappa_i)/\sin(\pi\kappa_i)$ is highly peaked as κ_i varies, and is effectively zero unless

$$\kappa_i = n_i, \tag{A.29}$$

where n_i is an integer. Thus S is effectively zero unless κ_1, κ_2, κ_3 are simultaneously integers, i.e. unless $\boldsymbol{\kappa}$ is a vector in the reciprocal lattice. Thus

$$S = \sum_{l} \exp(\mathrm{i}\boldsymbol{\kappa} \,.\, \boldsymbol{l}) = c \sum_{\boldsymbol{\tau}} \delta(\boldsymbol{\kappa} - \boldsymbol{\tau}). \tag{A.30}$$

To determine the constant c we integrate both sides of (A.30) over a unit cell in the reciprocal lattice. The integral on the right-hand side is equal to c. From (A.16) the integral on the left-hand side is equal to $(2\pi)^3/v_0$, which gives the required result.

Similar reasoning gives (A.18). Since $\boldsymbol{q}$ represents a wave periodic in the crystal,

$$\boldsymbol{q} = q_1\boldsymbol{\tau}_1 + q_2\boldsymbol{\tau}_2 + q_3\boldsymbol{\tau}_3, \tag{A.31}$$

where
$$q_i = \frac{n_i}{N}, \tag{A.32}$$

with n_i an integer ($|n_i| < N_i/2$). Put

$$S = \sum_{l} \exp(\mathrm{i}\boldsymbol{q} \,.\, \boldsymbol{l}) = S_1 S_2 S_3, \tag{A.33}$$

where
$$S_i = \sum_{l_i = -(N_i-1)/2}^{(N_i-1)/2} \exp(2\pi \mathrm{i} q_i l_i) = \frac{\sin(n_i\pi)}{\sin(n_i\pi/N_i)}. \tag{A.34}$$

Thus
$$\begin{aligned} S_i &= 0 \qquad \text{for } n_i \neq 0, \\ &= N_i \qquad \text{for } n_i = 0, \end{aligned} \tag{A.35}$$

and
$$\begin{aligned} \sum_{l} \exp(\mathrm{i}\boldsymbol{q} \,.\, \boldsymbol{l}) &= 0 \qquad \text{for } \boldsymbol{q} \neq 0, \\ &= N \qquad \text{for } \boldsymbol{q} = 0, \end{aligned} \tag{A.36}$$

which is equivalent to (A.18).