Appendix

A. The Dirac Delta Function and the Normalisation of the Wavefunction of a Free Particle in Unbounded Space

The English physicist *Dirac* introduced a function which is extremely useful for many purposes of theoretical physics and mathematics. Precisely speaking, it is a generalised function which is only defined under an integral. We shall first give its definition, and then discuss its uses. The delta function (δ function) is defined by the following properties (x is a real variable, $-\infty \leqq x \leqq \infty$):

$$1) \quad \delta(x) = 0 \quad \text{for} \quad x \neq 0\,, \tag{A.1}$$

$$2) \quad \int_a^b \delta(x)\,dx = 1 \quad \text{for} \quad a < 0 < b\,. \tag{A.2}$$

The δ function thus vanishes for all values of $x \neq 0$, and its integral over every interval which contains $x = 0$ has the value 1. The latter property means, speaking intuitively, that the δ function must become infinitely large at $x = 0$. The unusual properties of the δ function become more understandable when we consider it as the limiting case of functions which are more familiar. Such an example is given by the function

$$\frac{1}{\sqrt{\pi}u}\,\mathrm{e}^{-x^2/u^2}\,, \tag{A.3}$$

which is shown in Fig. A.1.

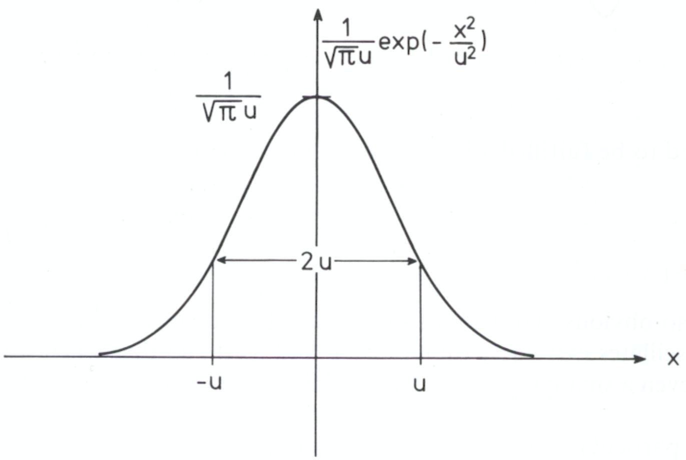

Fig. A.1. The function $(1/\sqrt{\pi}u)\exp(-x^2/u^2)$ plotted against the variable x. If we let the parameter u become smaller, the value of the function at $x = 0$ gets larger and larger and the decrease to both sides gets steeper, until the function has finally pulled itself together into a δ function

If we allow u to go to zero, the function becomes narrower and higher until it is finally just a "vertical line". We thus have

$$\text{for} \quad x \neq 0: \lim_{u \to 0} \frac{1}{\sqrt{\pi} u} e^{-x^2/u^2} = 0 . \tag{A.4}$$

On the other hand, one can find in any integral table the following fact:

$$\int_{-\infty}^{+\infty} \frac{1}{\sqrt{\pi} u} e^{-x^2/u^2} dx = 1 , \tag{A.5}$$

independently of the value of u. If the limit $u \to 0$ is calculated it becomes clear that because of (A.4), we can write the integral (A.5) with any finite limits a and b with $a < 0 < b$ without changing its value. This is just the relation (A.2).

In many practical applications in quantum mechanics, the δ function occurs as the following limit:

$$\delta(x) = \lim_{u \to \infty} \frac{1}{\pi} \frac{\sin ux}{x} . \tag{A.6}$$

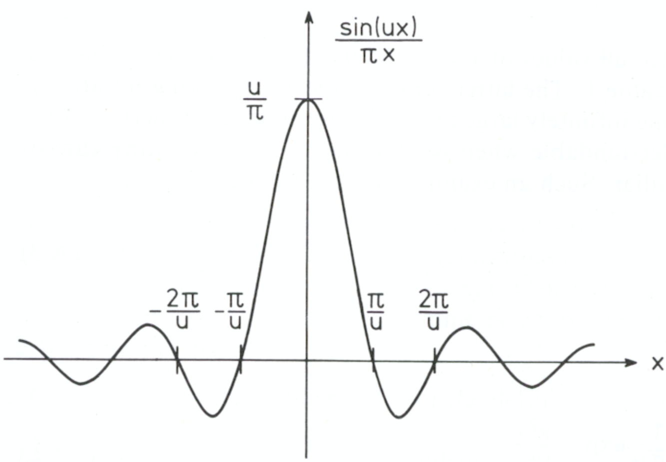

Fig. A.2. The function $\sin(ux)/\pi x$ plotted against x. If we allow u to go to the limit infinity, the value of the function at $x = 0$ becomes larger and larger. At the same time, the position of the zero-crossing moves towards $x = 0$

The property (A.2) is found to be fulfilled when we take into account that

$$\int_{-\infty}^{+\infty} \frac{1}{\pi} \frac{\sin(ux)}{x} dx = 1 . \tag{A.7}$$

The property (A.1) is not so obvious. To demonstrate it, one has to consider that for $u \to \infty$, $x \neq 0$, $\sin(ux)/x$ oscillates extremely rapidly back and forth, so that when we average the function over even a small region, the value of the function averages out to zero (Fig. A.2).

The δ function has, in particular, the following properties:

for a continuous function $f(x)$,

$$\int_a^b f(x)\,\delta(x-x_0)\,dx = f(x_0)\,, \qquad a < x_0 < b \qquad \text{is valid}\,. \tag{A.8}$$

For a function $f(x)$ which is n times continuously differentiable,

$$\int_a^b f(x)\,\delta^{(n)}(x-x_0)\,dx = (-1)^n f^{(n)}(x_0)\,, \qquad a < x_0 < b \tag{A.9}$$

holds. Here $f^{(n)}$ and $\delta^{(n)}$ mean the nth derivatives w.r.t. x. The proof of (A.8) follows immediately from (A.1, 2). The proof of (A.9) is obtained by n-fold partial integration. Furthermore,

$$\delta(cx) = \frac{1}{|c|}\,\delta(x)\,, \qquad c \text{ real} \tag{A.10}$$

is valid. The relation (A.1) is seen to be fulfilled on both sides. If we insert (A.10) in (A.2), we find

$$\int_a^b \delta(cx)\,dx\,,$$

which, after changing variables using $cx = x'$, becomes

$$\int_{a'}^{b'} \frac{1}{c}\,\delta(x')\,dx'\,, \qquad a' \lesseqgtr b' \qquad \text{for} \qquad c \gtrless 0\,,$$

which is thus, according to (A.2), equal to $1/|c|$.

We now turn to the question of the normalisation of wavefunctions in unbounded space, where we can limit ourselves to the one-dimensional case without missing any essentials. We start with wavefunctions which are normalised in the interval L,

$$\psi_k(x) = (1/\sqrt{L})\,e^{ikx}\,, \tag{A.11}$$

for which we have the normalisation integral

$$\int_{-L/2}^{L/2} |\psi(x)|^2\,dx = 1\,. \tag{A.12}$$

If we furthermore assume that $\psi(x)$ is periodic, $\psi(x+L) = \psi(x)$, the k's must have the form

$$k = \frac{2\pi n}{L}\,, \qquad n = 0, \pm 1, \pm 2, \ldots\,. \tag{A.13}$$

It is easy to convince oneself that

$$\int_{-L/2}^{L/2} \psi_k^*(x)\, \psi_{k'}(x)\, dx = \delta_{k,k'} \tag{A.14}$$

$$= \begin{cases} 1 & \text{for} \quad k = k' \\ 0 & \text{for} \quad k \neq k' . \end{cases} \tag{A.15}$$

To prove this relation, the integral must be computed, taking account of (A.13). The integral yields

$$\frac{1}{L} \int_{-L/2}^{L/2} e^{-ikx+ik'x} dx = \frac{1}{iL(k'-k)} (\exp[i(k'-k)L/2] - \exp[-i(k'-k)L/2]) . \tag{A.16}$$

If we now abbreviate $k'-k$ with ξ and $L/2$ with u, we may write (A.16) in the form

$$\sin(\xi u)/\xi u . \tag{A.17}$$

This is, however, apart from the factor $2\pi/L$, just the function which appears in (A.6) on the right under the limit, if we identify ξ with x. If we thus divide (A.16) by $2\pi/L$ and form $\lim_{L\to\infty}$, we obtain on the left side of (A.16)

$$\frac{1}{2\pi} \lim_{L\to\infty} \int_{-L/2}^{L/2} \exp(-ikx + ik'x)\, dx , \tag{A.18}$$

which we may also write somewhat differently:

$$\int_{-\infty}^{+\infty} \left[\frac{1}{\sqrt{2\pi}} e^{ikx} \right]^* \left[\frac{1}{\sqrt{2\pi}} e^{ik'x} \right] dx . \tag{A.19}$$

The right-hand side of (A.16), using (A.17) and (A.6), goes to $\delta(k'-k)$. We thus finally obtain

$$\int_{-\infty}^{+\infty} \psi_k^*(x)\, \psi_{k'}(x)\, dx = \delta(k'-k) , \tag{A.20}$$

where

$$\psi_k(x) = \frac{1}{\sqrt{2\pi}} e^{ikx} . \tag{A.21}$$

Equation (A.20) with (A.21) generalises the relation (A.14) [with (A.11)] to the case of wavefunctions without finite boundary conditions and thus to the corresponding case of continuous k values. As may be seen in all practical applications, the δ function in (A.20) always occurs under further integrals over k or k' (or both), so that we have found a self-consistent formalism.

Let the wavefunctions in (A.21) depend not upon k, but upon $p = \hbar k$; then we must observe (A.10). In order to normalise the new wavefunctions

$$\psi_p(x) = N e^{ipx/\hbar}$$

correctly, we must set N equal to $(1/\sqrt{\hbar})(1/\sqrt{2\pi}) = (1/\sqrt{h})$. The normalised wavefunction is now given by

$$\psi_p(x) = \frac{1}{\sqrt{h}} e^{ipx/\hbar} .$$

B. Some Properties of the Hamiltonian Operator, Its Eigenfunctions and Its Eigenvalues

We write the time-independent Schrödinger equation in the form

$$\mathscr{H}\psi_n = E_n \psi_n \tag{B.1}$$

with the Hamiltonian

$$\mathscr{H} = -\frac{\hbar^2}{2m_0}\nabla^2 + V(\boldsymbol{r}) , \qquad V(\boldsymbol{r}) \text{ real} .$$

The $\psi_n(\boldsymbol{r})$ are square-integrable eigenfunctions with the eigenvalues E_n. Here, $\psi_n = 0$ is excluded. The eigenvalues E_n may be discrete or they may be continuous.

In the following, we denote by ψ_μ and ψ_ν the wavefunctions on which the operator $\mathscr{H}$ can act. We can now easily read off the following properties:

a) $\mathscr{H}$ is a linear operator, i.e. the relation

$$\mathscr{H}(c_\mu \psi_\mu + c_\nu \psi_\nu) = c_\mu \mathscr{H}\psi_\mu + c_\nu \mathscr{H}\psi_\nu$$

holds, where c_μ and c_ν are some complex numbers. In particular, it follows from this that every linear combination of eigenfunctions of $\mathscr{H}$ with the same eigenvalue E is itself an eigenfunction of $\mathscr{H}$ with the eigenvalue E.

b) $\mathscr{H}$ is Hermitian, i.e. the equation

$$\int \psi_\mu^*(\boldsymbol{r})[\mathscr{H}\psi_\nu(\boldsymbol{r})]\,dV = \int [\mathscr{H}\psi_\mu(\boldsymbol{r})]^* \psi_\nu(\boldsymbol{r})\,dV \tag{B.2}$$

is valid. It follows from (B.2) that for the operator of the potential energy, $V^*(\boldsymbol{r}) = V(\boldsymbol{r})$. For the kinetic energy operator, (B.2) can be proved by double partial integration, taking into account the fact that the wavefunctions vanish at infinity.

c) The eigenvalues E_n are real. This is a consequence of (B.2), if one inserts for ψ_μ and ψ_ν the same *eigenfunction* ψ_n and utilises (B.1).

d) Eigenfunctions with different eigenvalues are orthogonal.

We take the following scalar products (different eigenvalues belong to the functions ψ_m and ψ_n):