1 Wave Functions and Expectation Values

In this section we consider how to extract quantitative information from wave functions. This information is obtained in the form of so-called *expectation values* of variables. We first explore expectation values related to the position of a particle. We then investigate how to obtain information about particle momentum from the wave function.

1.1 Expected Position

The wave function as predicted by the Schrödinger equation yields probabilistic information about the position of a particle, in that the absolute square of the wave function, $|\psi^2(x)|$, is the relative probability of finding the particle at location x. The *expectation value* of the particle position is the probability-weighted average of all the possible particle positions, x_i:

$$< x >\equiv \sum_i x_i|\psi(x_i)|^2 \bigg/ \sum_i |\psi(x_i)|^2 \ . \tag{1}$$

Since the possible particle positions are continuously distributed in x, we may wish to replace sums by integrals:

$$< x >= \int x|\psi(x)|^2 dx \bigg/ \int |\psi(x)|^2 dx \ . \tag{2}$$

For normalized wave functions the denominators in the above two equations are unity. Furthermore, since $|\psi|^2 = \psi^*\psi$, we can write

$$< x >= \sum_i \psi_i^* x_i \psi_i \tag{3}$$

or

$$< x >= \int \psi^* x \psi dx. \tag{4}$$

Sometimes the expectation value of x is insufficient information. An estimate of the size of a wave packet can be obtained by finding the expectation value

$$\sigma^2 =< (x- < x >)^2 >=< x^2 > -2 < x < x >> + < x >^2 \ . \tag{5}$$

Since $< x < x >>=< x >< x >=< x >^2$, we find that

$$\sigma = (< x^2 > - < x >^2)^{1/2}. \tag{6}$$

The variable σ is a measure of the half-width of the wave packet. In order to obtain σ, the only new thing that needs to be calculated is

$$< x^2 >= \sum_i \psi_i^* x_i^2 \psi_i. \tag{7}$$

It is clear how the expectation value of any function of x, $f(x)$, is calculated:

$$< f(x) >= \sum_i \psi_i^* f(x_i) \psi_i. \tag{8}$$

1.2 Momentum Representation

We know from the work of de Broglie that a particle has a definite momentum if the associated wave is a plane wave. Thus, for a wave function of the form

$$\psi = \exp(ikx), \tag{9}$$

the momentum is $p = \hbar k$. In this case there is no question that the expectation value of the momentum is just p.

For a wave function of the form

$$\psi = \phi_1 \exp(ik_1 x) + \phi_2 \exp(ik_2 x) \tag{10}$$

with $|\phi_1|^2 + |\phi_2|^2 = 1$, the probability of the wavenumber being k_1 is $|\phi_1|^2$, while the probability of it being k_2 is $|\phi_2|^2$. The expectation value of the wavenumber is therefore $< k >= k_1|\phi_1|^2 + k_2|\phi_2|^2$. Generalizing from this, the expectation value of the wavenumber from the superposition of an arbitrary number of plane waves with different wavenumbers,

$$\psi = \sum_i \phi_i \exp(ik_i x), \qquad \sum_i |\phi_i|^2 = 1, \tag{11}$$

is

$$< k >= \sum_i k_i |\phi_i|^2 = \sum_i \phi_i^* k_i \phi_i. \tag{12}$$

The expectation value for wavenumber written in terms of the ϕ_i is thus in the same form as the expectation value for position written in terms of the ψ_i.