3.8: Expectation Values

An important deduction can be made if we multiply the left-hand side of the Schrödinger equation by $\psi^*(x)$, integrate over all values of x, and examine the potential energy term that arises. We can deduce that the potential energy integral provides the average value for the potential energy. Likewise we can deduce that the kinetic energy integral provides the average value for the kinetic energy. This is shown in Equation 3.8.1. If we generalize this conclusion, such integrals give the average value for any physical quantity by using the operator corresponding to that physical observable in the integral. In the equation below, the symbol $\langle H \rangle$ is used to denote the average value for the total energy.

$$\langle H \rangle = \int_{-\infty}^{\infty} \psi^*(x) \hat{H} \psi(x) dx = \int_{-\infty}^{\infty} \psi^*(x) \left(\frac{-\hbar^2}{2m} \right) \frac{\partial^2}{\partial x^2} \psi(x) dx + \int_{-\infty}^{\infty} \psi^*(x) V(x) \psi(x) dx \tag{3.8.1}$$

kinetic energy term — Potential energy term

Example 3.8.1

Evaluate the two integrals in Equation 3.8.1 for the wavefunction $\psi(x) = \sin(kx)$ and the potential function $V(x) = x$.

The Hamiltonian operator consists of a kinetic energy term and a potential energy term. The kinetic energy operator involves differentiation of the wavefunction to the right of it. This step must be completed before multiplying by the complex conjugate of the wavefunction. The potential energy, however, usually depends only on position and not momentum. The potential energy operator therefore only involves the coordinates of a particle and does not involve differentiation. For this reason we do not need to use a caret over V in Equation 3.8.1. For example, the harmonic potential in one dimension is $½kx^2$. (Note: here k is the force constant and not the wave vector. Unfortunately just like words, a symbol can have more than one meaning, and the meaning must be gotten from the context.) The potential energy integral then involves only products of functions, and the order of multiplication does not affect the result, e.g. 6×4 = 4×6 = 24. This property is called the commutative property. The potential energy integral therefore can be written as

$$\langle V \rangle = \int_{-\infty}^{\infty} V(x) \psi^*(x) \psi(x) dx \tag{3.8.2}$$

This integral is telling us to take the probability that the particle is in the interval dx at x, which is $\psi^*(x)\psi(x)dx$, multiply this probability by the potential energy at x, and sum (i.e. integrate) over all possible values of x. This procedure is just the way to calculate the average potential energy $\langle V \rangle$ of the particle. This integral therefore is called the average-value integral or the expectation-value integral because it gives the average result of a large number of measurements of the particle's potential energy.

When an operator involves differentiation, it does not commute with the wavefunctions, e.g.

$$\psi^*(x) \frac{\partial^2}{\partial x^2} \psi(x) \neq \psi^*(x) \psi(x) \frac{\partial^2}{\partial x^2} \neq \frac{\partial^2}{\partial x^2} (\psi^*(x) \psi(x)) \tag{3.8.3}$$

but the interpretation of the kinetic energy integral in Equation 3.8.1 is the same as for the potential energy. This integral gives the average kinetic energy of the particle.

These expectation value integrals are very important in Quantum Mechanics. They provide us with the average values of physical properties (e.g. like energy, momentum, or position) because in many cases precise values cannot, even in principle, be determined. If we know the average of some quantity, it also is important to know whether the distribution is narrow, i.e. all values are close to the average, or broad, i.e. many values differ considerably from the average. The width of a distribution is characterized by its variance.