3.1: The State of a Quantum System

Let us first look at how we specify the state for a classical system. Once again, we use the ubiquitous billiard ball. As any player knows, there are three important aspects to its motion:

1. position,
2. velocity and
3. spin (angular momentum around its center).

Knowing these quantities we can in principle (no friction) predict its motion for all times. We have argued before that quantum mechanics involves an element of uncertainty. We cannot predict a state as in classical mechanics, we need to predict a probability. We want to be able to predict the outcome of a measurement of, say, position. Since position is a continuous variable, we cannot just deal with a discrete probability, we need a probability density, To understand this fact look at the probability that we measure x to be between X and $X + \Delta X$. If ΔX is small enough, this probability is directly proportional to the length of the interval

$$P(X < x < X + \Delta X) = P(X)\Delta X \tag{3.1.1}$$

Here $P(X)$ is called the *probability density*. The standard statement that the total probability is one translates to an integral statement,

$$\int_{-\infty}^{\infty} dx\, P(x) = 1 \tag{3.1.2}$$

(Here I am lazy and use the lower case x where I have used X before; this a standard practice in QM.) Since probabilities are always positive, we require $P(x) \geq 0$.

Now let us try to look at some aspects of classical waves, and see whether they can help us to guess how to derive a probability density from a wave equation. The standard example of a classical wave is the motion of a string. Typically a string can move up and down, and the standard solution to the wave equation

$$\frac{\partial^2}{\partial x^2} A(x,t) = \frac{1}{c^2}\frac{\partial^2}{\partial x^2} A(x,t) \tag{3.1.3}$$

can be positive as well as negative. Actually the square of the wave function is a possible choice for the probability (this is proportional to the intensity for radiation). Now let us try to argue what wave equation describes the quantum analog of classical mechanics, i.e., quantum mechanics.

The starting point is a propagating wave. In standard wave problems this is given by a plane wave, i.e.,

$$\psi = A \Re \exp(i(kx - \omega t + \phi)). \tag{3.1.4}$$

This describes a wave propagating in the x direction with wavelength $\lambda = 2\pi/k$, and frequency $\nu = \omega/(2\pi)$. We interpret this plane wave as a propagating beam of particles. If we define the probability as the square of the wave function, it is not very sensible to take the real part of the exponential: the probability would be an oscillating function of x for given t. If we take the complex function $A\exp(i(kx - \omega t + \phi))$, however, the probability, defined as the absolute value squared, is a constant ($|A|^2$) independent of x and t, which is very sensible for a beam of particles. Thus we conclude that the wavefunction $\psi(x,t)$ is complex, and the probability density is $|\psi(x,t)|^2$.

Using de Broglie's relation

$$p = \hbar/\lambda, \tag{3.1.5}$$

we find

$$p = \hbar k. \tag{3.1.6}$$

The other of de Broglie's relations can be used to give

$$E = h\nu = \hbar\omega. \tag{3.1.7}$$

One of the important goals of quantum mechanics is to generalize classical mechanics. We shall attempt to generalize the relation between momenta and energy,

$$E = 12mv^2 = \frac{p^2}{2m} \tag{3.1.8}$$

to the quantum realm. Notice that

$$p\psi(x,t) = \hbar k\psi(x,t) = \frac{\hbar}{i}\frac{\partial}{\partial x}\psi(x,t) \tag{3.1.9}$$

$$E\psi(x,t) = \hbar\omega\psi(x,t) = \frac{\hbar i\partial}{\partial t}\psi(x,t) \tag{3.1.10}$$

Using this we can guess a wave equation of the form

$$\frac{1}{2m}\left(\frac{\hbar}{i}\frac{\partial}{\partial x^2}\right)\psi(x,t) = \frac{\hbar i\partial}{\partial t}\psi(x,t). \tag{3.1.11}$$

Actually using the definition of energy when the problem includes a potential,

$$E = \frac{1}{2}mv^2 + V(x) = \frac{p^2}{2m} + V(x) \tag{3.1.12}$$

(when expressed in momenta, this quantity is usually called a "Hamiltonian") we find the time-dependent Schrödinger equation

$$-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\psi(x,t) + V(x)\psi(x,t) = \frac{\hbar i\partial}{\partial t}\psi(x,t). \tag{3.1.13}$$

We shall only spend limited time on this equation. Initially we are interested in the time-independent Schrödinger equation, where the probability $|\psi(x,t)|^2$ is independent of time. In order to reach this simplification, we find that $\psi(x,t)$ must have the form

$$\psi(x,t) = \phi(x)e^{-iEt/\hbar}. \tag{3.1.14}$$

If we substitute this in the time-dependent equation, we get (using the product rule for differentiation)

$$-e^{-iEt/\hbar}\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\phi(x) + e^{-iEt/\hbar}V(x)\phi(x) = Ee^{-iEt/\hbar}\phi(x). \tag{3.1.15}$$

Taking away the common factor $e^{-iEt/\hbar}$ we have an equation for ϕ that no longer contains time, the time-independent Schrödinger equation

$$\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\phi(x) + V(x)\phi(x) = E\phi(x). \tag{3.1.16}$$

The corresponding solution to the time-dependent equation is the standing wave (Equation 3.1.14).