PHY140Y

21 Enter Schrödinger and his Equation

21.1 Overview

- Fundamental Principles of Quantum Mechanics
- Schrödinger's Equation
- Probability Densities

21.2 Fundamental Principles

With the discovery of photons and particles having both wave and particle properties, the hunt was on in the late 1910's and early 1920's for a theory that could give a unified description of both matter and light. Any such theory had to find some means by which the quantization of energy could be explained or accommodated.

Underlying this search were two principles that most physicists felt had to be at the basis of this new theory:

1. The "Principle of Complementarity" postulated that the wave-particle duality associated with photons and matter particles had to be different "faces" of the same reality, *i.e.*, that any theory had to explain both sets of phenomena in a unified way.
2. The "Correspondence Principle" stated that the predictions of any new theory had to be congruent with what was already known from classical mechanics. Even though the description at the atomic level might be inconsistent with our everyday experience, the predictions of macroscopic classical phenomena had to correspond with what had already been established many centuries earlier.

These two principles helped shape the debate and the development surrounding the "new physics" that many felt had to be at play at the atomic level of matter.

21.3 Schrödinger's Equation

It was in this context that Erwin Schrödinger in 1925 postulated a new theory based on the existence of "wave functions" that described the behaviour of matter. He suggested that the behaviour of a particle with mass m influenced by a potential energy function $U(x)$ would be dictated by a wave function $\psi(x)$ that satisfied the differential equation

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + U(x)\psi(x) \quad = \quad E\psi(x), \tag{1}$$

where E is the total energy of the particle. This differential equation is the **time-independent Schrödinger's Equation**, and it forms the basis of any introduction to what we now call Quantum Mechanics.

What is this wave function $\psi(x)$? It is not an observable quantity, although it is a function of space. In principle, it is also a function of time, but we will avoid that complication here. In fact, there is still much debate about how to interpret it, but the traditional interpretation we will assume here is that we consider $\psi(x)$ to be a means of computing the probability density for the particle,

$$P(x) \quad = \quad |\psi(x)|^2. \tag{2}$$

To understand what this means, let's digress to define properly what a probability density is.

21.4 Probability Densities

Let us consider a concrete example of a single particle trapped in a one-dimensional box. For now, let's suppose we know nothing about the particle except its mass m and the fact that it must be in a 1-D box. Let L be the width of the box, so that we can define x to be the position of the particle in the box relative to one edge (thus $x \in (0, L)$).

Let us periodically take a look into the box and note where we find the particle. Let these observations form a set of N measurements of x, $(a_1, a_2, a_3, \ldots, a_N)$. Let's define a specific interval inside the box, $x \in (x_0, x_0 + \Delta x)$. Then the fraction of time we will find the particle inside this interval will be given by the ratio

$$\frac{N(a_i \in (x_0, x_0 + \Delta x))}{N}, \tag{3}$$

where the numerator is simply the number of times we have seen the particle inside this interval. If we now let N get very large, then this fraction will approach a specific number. If at the same time, we let Δx become small compared to the length L, so that we can write $\Delta x \rightarrow dx$, then we define the limit of this ratio as the probability that we will find the particle inside the given interval. Mathematically, we would write this as

$$\text{Probability} \equiv P(x)\, dx \quad = \quad \lim_{N \to \infty} \left(\frac{N(a_i \in (x_0, x_0 + \delta x))}{N} \right), \tag{4}$$

where now we have introduced the **probability density** $P(x)$.

Note that the probability density is not a probability per se, as it has units of 1/length in this case. We have to multiply it by a length to obtain a probability (which by definition is a dimensionless quantity). If for example, the particle in the box had equal probability of being anywhere in the box, we would then expect to find that the probability density for the particle in the box is constant.

One feature of any probability is that when we sum up the probabilities of anything occuring, it must equal to unity. This is clearly satisfied by our definition above. This gives us a convenient means of **normalizing** the probability density, for in this simple case of a 1-D box of length L, we would be able to write

$$1 = \sum P(x)dx \quad \rightarrow \quad \int_0^L P(x)dx. \tag{5}$$

In the case of a particle with equal probabilities of being found anywhere in the box, this relationship would give us

$$\begin{aligned} 1 &= \int_0^L P(x)dx && (6) \\ &= PL && (7) \\ \Rightarrow P &= 1/L, && (8) \end{aligned}$$

where we have now explicitly assumed that the probability density is now a constant and independent of x.

As a concrete example, suppose that $L = 1 \times 10^{-6}$ m. This means that

$$P \;=\; 1/L = 1 \times 10^{6}\ \mathrm{m}^{-1}. \tag{9}$$

The fundamental postulate of Quantum Mechanics is that $|\psi(x)|^2$ is the probability density for a particle. We'll see how this can be used to predict the quantum mechanical behaviour of a particle.