3.1: Introduction to the Schrödinger Equation

A scientific postulate is a generally accepted statement, which is accepted because it is consistent with experimental observation and serves to predict or explain a variety of observations. These postulates also are known as physical laws. Postulates cannot be derived by any other fundamental considerations. Newton's second law, $f = ma$, is an example of a postulate that is accepted and used because it explains the motion of objects like baseballs, bicycles, rockets, and cars. One goal of science is to find the smallest and most general set of postulates that can explain all observations. A whole new set of postulates was added with the invention of Quantum Mechanics. The Schrödinger equation is the fundamental postulate of Quantum Mechanics. In the previous chapter we saw that many individual quantum postulates were introduced to explain otherwise inexplicable phenomena. We will see that quantization and the relations $E = h\nu$ and $p = \frac{h}{\lambda}$, discussed in the last chapter, are consequences of the Schrödinger equation. In other words the Schrödinger equation is a more general and fundamental postulate.

A differential equation is a mathematical equation involving one or more derivatives. The analytical solution to a differential equation is the expression or function for the dependent variable that gives an identity when substituted into the differential equation. A mathematical function is a rule that assigns a value to one quantity using the values of other quantities. Any mathematical function can be expressed not only by a mathematical formula, but also in words, as a table of data, or by a graph. Numerical solutions to differential equations also can be obtained. In numerical solutions, the behavior of the dependent variable is expressed as a table of data or by a graph; no explicit function is provided.

Example 3.1.1

The differential equation $\frac{dy(x)}{dx} = 2$ has the solution $y(x) = 2x + b$, where b is a constant. This function $y(x)$ defines the family of straight lines on a graph with a slope of 2. Show that this function is a solution to the differential equation by substituting for $y(x)$ in the differential equation. How many solutions are there to this differential equation? For one of these solutions, construct a table of data showing pairs of x and y values, and use the data to sketch a graph of the function. Describe this function in words.

Some differential equations have the property that the derivative of the function gives the function back multiplied by a constant. The differential equation for a first-order chemical reaction is one example. This differential equation and the solution for the concentration of the reactant are given below.

$$\frac{dC(t)}{dt} = -kC(t) \tag{3.1.1}$$

$$C(t) = C_0 e^{-kt} \tag{3.1.2}$$

Example 3.1.2

Show that C(t) is a solution to the differential equation.

Another kind of differential equation has the property that the second derivative of the function yields the function multiplied by a constant. Both of these types of differential equations are found in Quantum Mechanics.

$$\frac{d^2\psi(x)}{dx^2} = k\psi(x) \tag{3.1.3}$$

Example 3.3

What is the value of the constant in the above differential equation when $\psi(x) = \cos(3x)$?

Example 3.1.4

What other functions, in addition to the cosine, have the property that the second derivative of the function yields the function multiplied by a constant?

Since some mathematical functions, such as the sine and cosine, go through repeating periodic maxima and minima, they produce graphs that look like waves. Such functions can themselves be thought of as waves and can be called wavefunctions. We now make a mathematically intuitive leap. If electrons, atoms, and molecules have wave-like properties, then there must be a mathematical function that is the solution to a differential equation that describes electrons, atoms, and molecules. This differential equation is called the wave equation, and the solution is called the wavefunction. Such thoughts may have motivated Erwin Schrödinger to argue that the wave equation is a key component of Quantum Mechanics.
