Schrödinger equation

In the last article, we have seen that a particle is a wave with wavelength given by h/p. Since it is a wave, it has a displacement. From now on, we will call this displacement "wave function." But, what is a wave? Recall that in our earlier article "Travelling wave," we learned that wave can be expressed in terms of sine and cosine functions. Also, remember that sine and cosine functions can be expressed in terms of exponential function using Euler's theorem. These considerations yield following for the wave function $\psi(x)$:

$$\psi(x,t) = e^{i(\frac{2\pi}{\lambda}x - \frac{2\pi}{T}t)} \tag{1}$$

where λ is the wavelength, and T is period. Certainly, this is a wave moving in positive x-direction. Now, using de Broglie's formula and Planck's formula, the above equation can be re-expressed as follows:

$$\psi(x,t) = e^{i(\frac{p}{h/(2\pi)}x - \frac{E}{h/(2\pi)}t)} \tag{2}$$

If we define $\hbar = h/(2\pi)$, the above equation can be re-expressed as:

$$\psi(x,t) = e^{i(\frac{p}{\hbar}x - \frac{E}{\hbar}t)} \tag{3}$$

Now, notice following:

$$\begin{aligned} \frac{\partial^2\psi}{\partial x^2} &= -\frac{p^2}{\hbar^2}\psi \\ -\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2}\psi &= \frac{p^2}{2m}\psi \qquad (4) \end{aligned}$$

The above equation is derived when p is constant. For example, if there is a potential energy that depends on the position x, p would not be a constant, but depends on the position x. However, we will assume that the above equation is valid generally. (After all, the derivation of Schrödinger equation in this article is heuristic, rather than rigorous. If you want to know a rigorous derivation, please read my "short introduction to quantum mechanics" series. However, you would need to know linear algebra.)

Now, let's use the following fact:

$$E = \frac{p^2}{2m} + V(x) \tag{5}$$

where E is the total energy and $V(x)$ is potential energy. Then, we have:

$$\frac{p^2}{2m}\psi(x) + V(x)\psi(x) = E\psi(x)$$
$$-\frac{\hbar^2}{2m}\frac{\partial^2\psi(x)}{\partial x^2} + V(x)\psi(x) = E\psi(x) \tag{6}$$

where in the last step we used (4). This equation is called "time-independent Schrödinger equation" in 1-dimension. In 3 dimensions, it is given as follows:

$$-\frac{\hbar^2}{2m}(\frac{\partial^2\psi}{\partial x^2} + \frac{\partial^2\psi}{\partial y^2} + \frac{\partial^2\psi}{\partial z^2})\psi(x,y,z,t) + V(x,y,z)\psi(x,y,z,t) = E\psi(x,y,z,t) \tag{7}$$

Here, the double partial derivatives with respect to y and z come from the momentum squared components of y and z. In other words,

$$-\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial y^2}\psi = \frac{p_y^2}{2m}\psi, \qquad -\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial z^2}\psi = \frac{p_z^2}{2m}\psi \tag{8}$$

Using these relations, it is easy to check () can be obtained from following 3-dimensional formula:

$$\frac{p_x^2}{2m} + \frac{p_y^2}{2m} + \frac{p_z^2}{2m} + V = E \tag{9}$$

Now, notice also that (3) implies:

$$i\hbar\frac{\partial\psi}{\partial t} = E\psi \tag{10}$$

Plugging this into (), we get:

$$-\frac{\hbar^2}{2m}(\frac{\partial^2\psi}{\partial x^2} + \frac{\partial^2\psi}{\partial y^2} + \frac{\partial^2\psi}{\partial z^2})\psi(x,y,z,t) + V(x,y,z)\psi(x,y,z,t) = i\hbar\frac{\partial\psi(x,y,z,t)}{\partial t} \tag{11}$$

This is called "time-dependent Schrödinger equation."

You might wonder what the interpretation of ψ is. As advertised in our earlier article "Probability density function," the answer is that its absolute value squared is the probability density. Considering that we explained that the displacement squared is proportional to the intensity in our earlier article "Young's interference experiment, revisited," this sounds very reasonable. If you shoot electrons through double slit, it is more probable for the electrons to end up in the locations where constructive interference occurs than any other locations, since the intensity of the wave is high there. Also, the electrons will never end up in the locations where destructive interference occurs since the intensity is zero there. In other words, $|\psi|^2$ denotes the probability density function that particles will be found there. The only difference between the case in this article and the case in our articles on

Young's interference is that ψ can be a complex number, while the displacements in the earlier articles were always a real number. The square of a real number, such as the displacement in our earlier articles, is always real, while the square of a complex number such as ψ, the wave function, is not always real. As the probability density function is always real, we need $|\psi|^2$ instead of ψ^2.

The wave function that satisfies $\int dx|\psi(x)|^2 = 1$ (which implies that the total probability is 1, as explained in that article) is called a "normalized" wave function.

Problem 1. Let a wave function of a particle with a mass m given as follows by a Gaussian form:

$$\psi(x,t) = Ae^{-x^2} \tag{12}$$

By normalizing the wave function find A. Also find the potential $V(x)$.

Summary

- From
$$\frac{p_x^2}{2m} + \frac{p_y^2}{2m} + \frac{p_z^2}{2m} + V = E$$
and de Broglie's matter wave formula, one can infer the following Schrödinger equation:
$$-\frac{\hbar^2}{2m}(\frac{\partial^2\psi}{\partial x^2}+\frac{\partial^2\psi}{\partial y^2}+\frac{\partial^2\psi}{\partial z^2})\psi(x,y,z,t)+V(x,y,z)\psi(x,y,z,t) = E\psi(x,y,z,t)$$

- $|\psi|^2$ denotes the probability density function that particles will be found there.

- Normalized wave function satisfies
$$\int dx|\psi|^2 = 1$$