A short introduction to quantum mechanics XI: Schrödinger equation in 3-dimensional space

So far we have considered a 1-dimensional problem. But in reality, a particle can move in three dimensions, on which we will now focus. In this case, we have the position operators X, Y, Z, which act by multiplying x, y, z respectively. Also, we now have three momentum operators: the x,y,z-components of momentum, which we denote by P_x,P_y,P_z. Naturally, they act by $-i\hbar\frac{\partial}{\partial x}$,$-i\hbar\frac{\partial}{\partial y}$,$-i\hbar\frac{\partial}{\partial z}$. With this information, it is easy to check the following:

$$[X, P_x] = [Y, P_y] = [Z, P_z] = i\hbar \tag{1}$$

$$[X, Y] = [Y, Z] = [Z, X] = 0 \tag{2}$$

$$[P_x, P_y] = [P_y, P_z] = [P_z, P_x] = 0 \tag{3}$$

The last one can be shown from the fact that partial derivatives commute.

Problem 1. Check $[Y, P_x] = 0$ using Leibniz rule and the property of partial derivatives. (Hint[1]) Thus, we have

$$[Y, P_x] = [Z, P_x] = [X, P_y] = [Z, P_y] = [X, P_z] = [Y, P_z] = 0 \tag{4}$$

In 3d, the energy of a particle is given by

$$E = \frac{p_x^2 + p_y^2 + p_z^2}{2m} + V(x, y, z) \tag{5}$$

which implies

$$-\frac{\hbar^2}{2m}\left(\frac{\partial^2\psi(x,y,z)}{\partial x^2} + \frac{\partial^2\psi(x,y,z)}{\partial y^2} + \frac{\partial^2\psi(x,y,z)}{\partial z^2}\right) + V(x,y,z)\psi(x,y,z) = E\psi(x,y,z) \tag{6}$$

This is the Schrödinger equation for 3-dimensional case.

If the potential can be written in the following form

$$V(x, y, z) = V(x) + V(y) + V(z), \tag{7}$$

solving 3d Schrödinger equation can be reduced to solving three 1d Schrödinger equations. For simplicity, I will show this in case of 2d Schrödinger equation instead of the 3d case. The 3d case is similar. Let

$$V(x, y) = V(x) + V(y), \qquad \psi(x, y) = \psi_x(x)\psi_y(y) \tag{8}$$

[1] Show $[Y, P_x]\psi = 0$

Then, the Schrödinger equation is given by

$$-\frac{\hbar^2}{2m}\left(\frac{\partial^2\psi(x,y)}{\partial x^2}+\frac{\partial^2\psi(x,y)}{\partial y^2}\right)+V(x,y)\psi(x,y)=E\psi(x,y). \tag{9}$$

If we divide both hand sides by $\psi(x,y)$, we get

$$\frac{1}{\psi_x(x)}\left(-\frac{\hbar^2}{2m}\frac{\partial^2\psi_x(x)}{\partial x^2}+V(x)\psi_x(x)\right)+\frac{1}{\psi_y(y)}\left(-\frac{\hbar^2}{2m}\frac{\partial^2\psi_y(y)}{\partial x^2}+V(x)\psi_y(y)\right)=E \tag{10}$$

Thus, the first part on the left-hand side is a function of x only and the second part on the right-hand side is a function of y only. As their sum is E, a number that depends neither on x nor on y, each part on the left-hand side must be a number. If we call these numbers E_x and E_y, we have

$$-\frac{\hbar^2}{2m}\psi_x(x)+V(x)\psi_x(x)=E_x\psi_x(x) \tag{11}$$

$$-\frac{\hbar^2}{2m}\psi_y(y)+V(y)\psi_y(y)=E_y\psi_y(y) \tag{12}$$

where $E_x+E_y=E$. Therefore, we divided one 2d Schrödinger equation to two 1d Schrödinger equations.

Now, let's see an example. Consider the following Hamiltonian of 2d harmonic oscillator:

$$H=\frac{p_x^2+p_y^2}{2m}+\frac{1}{2}mw(x^2+y^2) \tag{13}$$

What are the allowed energies?

We have $E=E_x+E_y$, where

$$E_x=\hbar\omega(n_x+\frac{1}{2}), \qquad E_y=\hbar\omega(n_y+\frac{1}{2}), \qquad n_x,n_y=0,1,2,3\cdots \tag{14}$$

The ground state (i.e., the lowest energy state) is given by $n_x=n_y=0$. Therefore, the ground state energy is $E=\hbar\omega$. The first excited state (i.e., the second lowest energy state) is given by $n_x=1,n_y=0$ and $n_x=0,n_y=1$. Its energy is $E=2\hbar\omega$. Notice that there are two such states. We say that the first excited state has degeneracy 2. Any linear combination of these two states is the first excited state. In other words, if $\psi_n(x)$ is a solution to the Schrödinger equation of 1d harmonic oscillator with the eigenvalue of $(n+\frac{1}{2})\hbar\omega$, the following state is the first excited state:

$$\psi(x,y)=c_1\psi_1(x)\psi_0(y)+c_2\psi_0(x)\psi_1(y) \tag{15}$$

Note that we need $|c_1|^2+|c_2|^2=1$, if $\psi(x,y)$ is normalized.

The second excited state (i.e., the third lowest energy state) is given by $n_x=2,n_y=0$ and $n_x=1,n_y=1$ and $n_x=0,n_y=2$ and its degeneracy is 3.

Problem 1. Consider the following Hamiltonian of 3d harmonic oscillator:

$$H=\frac{p_x^2+p_y^2+p_z^2}{2m}+\frac{1}{2}mw(x^2+y^2+z^2) \tag{16}$$

What is the degeneracy of the first excited state?

Summary

- The 3d Schrödinger equation is given by

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

- If $V(x,y,z) = V(x) + V(y) + V(z)$, the solution to the 3d Schrödinger equation is given by

$$\psi(x,y,z) = \psi_x(x)\psi_y(y)\psi_z(z)$$

  where $\psi_x(x)$ is the solution to the 1d Schrödinger equation with the potential $V(x)$, and similarly for $\psi_y(y)$ and $\psi_z(z)$. The energy is given by

$$E = E_x + E_y + E_z$$

  where E_x, E_y, E_z are the energy eigenvalues of each 1d Schrödinger equation.

- The ground state is the lowest energy state. The first excited state is the second lowest energy state and the second excited state is the third lowest energy state and so on.

- If n linearly independent states have the same energy, we say the state with that energy has degeneracy n.