Quantum Mechanics 2

Robert C. Roleda
Physics Department

Three Dimensions

De La Salle University

Schrodinger Equation

To move from one-dimension to three-dimensions, the Schrodinger Equation

$$-\frac{\hbar^2}{2m}\frac{\partial^2 u(x)}{\partial x^2} + V(x)u(x) = Eu(x)$$

is generalized to

$$-\frac{\hbar^2}{2m}\nabla^2 u(x,y,z) \ + V(x,y,z)u(x,y,z) = Eu(x,y,z)$$

where the Laplacian in Cartesian coordinates is

$$\nabla^2 u = \frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} + \frac{\partial^2 u}{\partial z^2}$$

Separable Potentials

If the potential can be decomposed as

$$V(x,y,z) = V_1(x) + V_2(y) + V_3(z)$$

variables of the differential equation can be separated. If we let

$$u(x,y,z) = u_1(x)u_2(y)u_3(z)$$

then

$$-\frac{\hbar^2}{2m}\left[u_2(y)u_3(z)\frac{d^2u_1(x)}{dx^2} + u_1(x)u_3(z)\frac{d^2u_2(y)}{dy^2} + u_1(x)u_2(y)\frac{d^2u_3(z)}{dz^2}\right]$$
$$+ [V_1(x) + V_2(y) + V_3(z)\ ]u_1(x)u_2(y)u_3(z) = Eu_1(x)u_2(y)u_3(z)$$

Dividing by $u_1(x)u_2(y)u_3(z)$, we get

$$-\frac{\hbar^2}{2m}\left[\frac{1}{u_1(x)}\frac{d^2u_1(x)}{dx^2} + \frac{1}{u_2(y)}\frac{d^2u_2(y)}{dy^2} + \frac{1}{u_3(z)}\frac{d^2u_3(z)}{dz^2}\right]$$
$$+ [V_1(x) + V_2(y) + V_3(z)\ ] = E$$

Separation of Variables

Each term now contains only one variable, and would remain unchanged when other variables change. We may thus write

$$-\frac{\hbar^2}{2m}\frac{1}{u_1(x)}\frac{d^2u_1(x)}{dx^2}+V_1(x)=\epsilon_1$$

$$-\frac{\hbar^2}{2m}\frac{1}{u_2(y)}\frac{d^2u_2(y)}{dy^2}+V_2(y)=\epsilon_2$$

$$-\frac{\hbar^2}{2m}\frac{1}{u_3(z)}\frac{d^2u_3(z)}{dz^2}+V_3(z)=\epsilon_3$$

such that

$$\epsilon_1+\epsilon_2+\epsilon_3=E$$

3 copies of one-dimensional equation

Rearranging, we get three copies of the one-dimensional Schrodinger Equation

$$-\frac{\hbar^2}{2m}\frac{d^2u_1(x)}{dx^2}+V_1(x)u_1(x)=\epsilon_1 u_1(x)$$
$$-\frac{\hbar^2}{2m}\frac{d^2u_2(y)}{dy^2}+V_2(y)u_2(y)=\epsilon_2 u_2(y)$$
$$-\frac{\hbar^2}{2m}\frac{d^2u_3(z)}{dz^2}+V_3(z)u_3(z)=\epsilon_3 u_3(z)$$

which can be solved separately, and then put together to give the energy eigenfunctions

$$u(x,y,z)=u_1(x)u_2(y)u_3(z)$$

and the eigenenergies

$$E=\epsilon_1+\epsilon_2+\epsilon_3$$

Example

De La Salle University

Oscillators

For example, take the three-dimensional oscillator with potential

$$V(x, y, z) = \frac{1}{2}m\omega_1^2x^2 + \frac{1}{2}m\omega_2^2y^2 + \frac{1}{2}m\omega_3^2z^2$$

The solutions to the one-dimensional oscillator problem are

$$u_n(x) = (2^n n!)^{-1/2}\left(\frac{m\omega}{\pi\hbar}\right)^{1/4}\exp\left(-\frac{m\omega}{2\hbar}x^2\right)H_n\left(\sqrt{\frac{m\omega}{\hbar}}x\right)$$

$$E = (n + 1/2)\hbar\omega$$

Oscillators

The eigenfunctions of the three-dimensional oscillator problem are therefore

$$u_{n_1 n_2 n_3}(x,y,z) = (2^{n_1} n_1!)^{-1/2} \left(\frac{m\omega_1}{\pi\hbar}\right)^{1/4} \exp\left(-\frac{m\omega_1}{2\hbar}x^2\right) H_{n_1}\left(\sqrt{\frac{m\omega_1}{\hbar}}x\right)$$
$$(2^{n_2} n_2!)^{-1/2} \left(\frac{m\omega_2}{\pi\hbar}\right)^{1/4} \exp\left(-\frac{m\omega_2}{2\hbar}y^2\right) H_{n_2}\left(\sqrt{\frac{m\omega_2}{\hbar}}y\right)$$
$$(2^{n_3} n_3!)^{-1/2} \left(\frac{m\omega_3}{\pi\hbar}\right)^{1/4} \exp\left(-\frac{m\omega_3}{2\hbar}z^2\right) H_{n_3}\left(\sqrt{\frac{m\omega_3}{\hbar}}z\right)$$

and the eigenenergies are

$$E = (n_1 + 1/2)\hbar\omega_1 + (n_2 + 1/2)\hbar\omega_2 + (n_3 + 1/2)\hbar\omega_3$$

Special Case: Isotropic Oscillators

For isotropic oscillators, $\omega_1 = \omega_2 = \omega_3 = \omega$, the energy eigenfunctions are

$$u_{n_1 n_2 n_3}(x, y, z)$$
$$= \left[2^{(n_1+n_2+n_3)} n_1!\, n_2!\, n_3!\right]^{-1/2} \left(\frac{m\omega}{\pi\hbar}\right)^{3/4} \exp\left[-\frac{m\omega}{2\hbar}(x^2 + y^2 + z^2)\right]$$
$$H_{n_1}\left(\sqrt{\frac{m\omega}{\hbar}}x\right) H_{n_2}\left(\sqrt{\frac{m\omega}{\hbar}}y\right) H_{n_3}\left(\sqrt{\frac{m\omega}{\hbar}}z\right)$$

and the eigenenergies are

$$E = (n_1 + n_2 + n_3 + 3/2)\hbar\omega$$

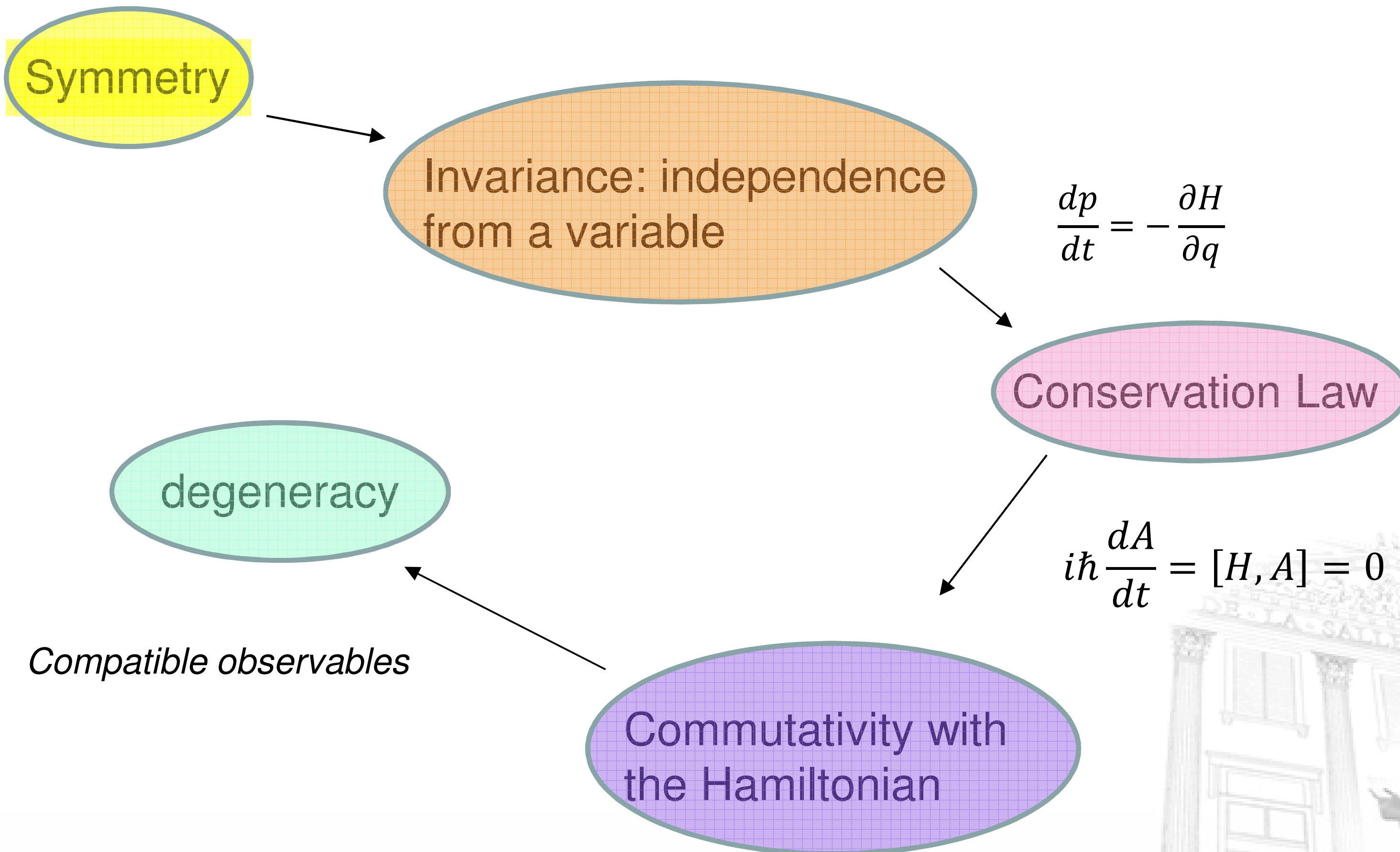
Note that different combinations of n_1, n_2, n_3 can give a specific value of $n = n_1 + n_2 + n_3$. Thus, it is possible for many states to have the same energy. This is called **degeneracy**.

Degeneracies

Let's take for example the four lowest energy levels of the 3-D oscillators

Energy	n_1	n_2	n_3	degeneracy
$3\hbar\omega/2$	0	0	0	1
$5\hbar\omega/2$	0	0	1	3
	0	1	0	
	1	0	0	
$7\hbar\omega/2$	0	1	1	6
	1	0	1	
	1	1	0	
	0	0	2	
	0	2	0	
	2	0	0	
$9\hbar\omega/2$	1	1	1	10
	0	1	2	
	0	2	1	
	1	0	2	
	2	0	1	
	1	2	0	
	2	1	0	
	0	0	3	
	0	3	0	
	3	0	0	

Noether's Theorem



$$\frac{dp}{dt} = -\frac{\partial H}{\partial q}$$

$$i\hbar \frac{dA}{dt} = [H, A] = 0$$

Isotropy: invariance under rotation

Another Example

Particle in a Box

The solutions to the particle in a one-dimensional box with size L problem are

$$u_n(x) = \sqrt{\frac{2}{L}} \sin \frac{n\pi x}{L}; \qquad E = \frac{n^2 \pi^2 \hbar^2}{2mL^2}$$

For a three-dimensional box with lengths a, b, c on each side, the eigenfunctions are

$$u_{n_1 n_2 n_3}(x, y, z) = \sqrt{\frac{8}{abc}} \sin \frac{n_1 \pi x}{a} \sin \frac{n_2 \pi y}{b} \sin \frac{n_3 \pi z}{c}$$

and the eigenenergies are

$$E_{n_1 n_2 n_3} = \frac{\pi^2 \hbar^2}{2m} \left(\frac{n_1^2}{a^2} + \frac{n_2^2}{b^2} + \frac{n_3^2}{c^2} \right)$$