Schrodinger eqn with central potential

We considered 2D or 3D square well
What did we learn?

1. The components of the wave function corresponding to independent degrees of freedom are reflected in the factorization of the wave function

   3D square well → x, y, z are independent

   $$\psi(x,y,z) = X(x)\, Y(y)\, Z(z)$$

2. Bound states in 2D or 3D potential require 2 or 3 indices to characterize them

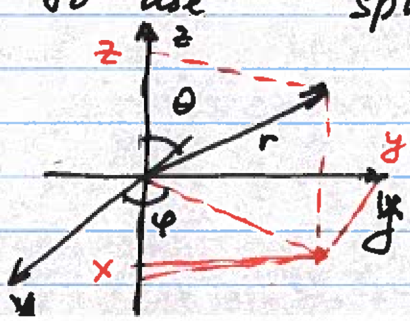
   $$\psi_{nsj} = \left(\frac{2}{L}\right)^{3/2} \sin\frac{\pi n x}{L_x} \sin\frac{\pi s y}{L_y} \sin\frac{\pi j z}{L_z}$$

   $$E_{nsj} = \frac{\pi^2 \hbar^2}{2m}\left[\frac{n^2}{L_x^2} + \frac{s^2}{L_y^2} + \frac{j^2}{L_z^2}\right]$$

3. Energy states can be degenerate, i.e. same energy corresponds to two or more physically distinguishable states

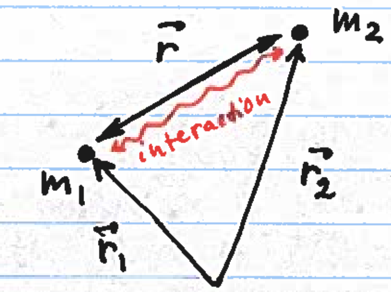
4. Geometry and symmetry of the boundary conditions reflects in the preferred coordinate systems

For many systems it is convenient to use spherical coordinates



$$x = r\cos\theta\cos\varphi$$
$$y = r\cos\theta\sin\varphi$$
$$z = r\sin\theta$$

Why it is convenient? It is applicable for most two-particle interactions!



$$\hat{H} = \hat{K}_1 + \hat{K}_2 + U(\hat{\vec{r}}_1, \hat{\vec{r}}_2) =$$

$$= \frac{\hat{p}_1^2}{2m_1} + \frac{\hat{p}_2^2}{2m_2} + \underbrace{U(|\hat{\vec{r}}_1 - \hat{\vec{r}}_2|)}_{\text{for vast majority of systems}}$$

$\vec{r} = \vec{r}_1 - \vec{r}_2$

Motion of two interacting particles:

center of mass motion + rotation around CM

$$\vec{R}_{CM} = \frac{m_1\vec{r}_1 + m_2\vec{r}_2}{m_1+m_2} \qquad \vec{r} = \vec{r}_1 - \vec{r}_2 \quad \text{(relative position)}$$

$$\underbrace{\vec{P}_{CM} = \vec{p}_1 + \vec{p}_2}_{\text{"external"}} \qquad \underbrace{\vec{p} = \frac{m_2\vec{p}_1 - m_1\vec{p}_2}{m_1+m_2}}_{\text{"internal"}}$$

Two independent motions

We can present the wavefunction as a product of two terms: one describing CM motion $\psi_{ex}(\vec{R}_{cm})$ and one of internal motion $\psi_{int}(\vec{r})$

Total kinetic energy $\hat{K}_1 + \hat{K}_2 = \frac{\hat{p}_1^2}{2m_1} + \frac{\hat{p}_2^2}{2m} = \frac{\hat{P}_{cm}^2}{2(m_1+m_2)} + \frac{\hat{\vec{p}}}{2\mu}$

$\mu = \frac{m_1 m_2}{m_1+m_2}$ reduced mass

$$\hat{H} = \hat{H}_{ext} + \hat{H}_{int} = \underbrace{\frac{\hat{P}_{cm}^2}{2(m_1+m_2)}}_{\text{freely moving compound object}} + \underbrace{\frac{\hat{\vec{p}}^2}{2\mu} + U(\hat{r})}_{\text{"single" particle in a spherically symmetric potential}}$$

$$\hat{H} = \frac{\hat{p}^2}{2m} + U(r)$$

no angular dependence in $U(r) \longrightarrow$ spherically symmetrical potential

This symmetry is reflected in wave function
will use spherical coordinates!

1D: $\hat{p}_x = -i\hbar \frac{\partial}{\partial x}$

3D: $\vec{p} = (\hat{p}_x, \hat{p}_y, \hat{p}_z) = \left(-i\hbar \frac{\partial}{\partial x}, -i\hbar \frac{\partial}{\partial y}, -i\hbar \frac{\partial}{\partial z}\right)$

$= -i\hbar \nabla$ vector operator

$\nabla \psi = \vec{i} \frac{\partial \psi}{\partial x} + \vec{j} \frac{\partial \psi}{\partial y} + \vec{k} \frac{\partial \psi}{\partial z}$ (grad)

$\hat{\vec{p}}^2 \psi = -\hbar^2 \nabla^2 \psi = -\hbar^2 \left[\frac{\partial^2 \psi}{\partial x^2} + \frac{\partial^2 \psi}{\partial y^2} + \frac{\partial^2 \psi}{\partial z^2} \right]$

scalar operator

In spherical coordinates

$$\frac{1}{2m} \hat{p}^2 \psi(r,\theta,\varphi) = \frac{\hat{L}^2}{2mr^2} \psi - \frac{\hbar^2}{2m} \left[\frac{\partial^2 \psi}{\partial r^2} + \frac{2}{r} \frac{\partial \psi}{\partial r} \right]$$

$\hat{L}^2$ – angular momentum^2 operator

$\hat{\vec{L}} = \hat{\vec{r}} \times \hat{\vec{p}}$ – vector operator

$\hat{L}_x = \hat{y}\hat{p}_z - \hat{z}\hat{p}_y$, $\hat{L}_y = \hat{z}\hat{p}_x - \hat{x}\hat{p}_z$, $\hat{L}_z = \hat{x}\hat{p}_y - \hat{y}\hat{p}_x$

Three components, that do not commute with each other

$[\hat{L}_x, \hat{L}_y] = i\hbar \hat{L}_z$, $[\hat{L}_y, \hat{L}_z] = i\hbar \hat{L}_x$, $[\hat{L}_z, \hat{L}_x] = i\hbar \hat{L}_y$

$\hat{L}^2 = \hat{L}_x^2 + \hat{L}_y^2 + \hat{L}_z^2$

Close relative of $\hat{\vec{S}}$ and $\hat{\vec{J}}$ operators
orbital vs spin vs total angular momentum

As before, we can find the common eigenstates of $\hat{L}^2$ and $\hat{L}_z$ $|\ell, m\rangle$

$$\hat{L}^2 |\ell, m\rangle = \hbar^2 \ell(\ell+1) |\ell, m\rangle$$
$$\hat{L}_z |\ell, m\rangle = \hbar m \; |\ell, m\rangle$$

$|\ell, m\rangle$ – spherical functions, in x-representation $Y_{\ell,m}(\theta, \varphi)$

In a centrally symmetric potential

$$\hat{H}\psi(\vec{r}) = \frac{\hat{p}^2}{2m}\psi + U(r)\psi = -\frac{\hbar^2}{2m}\left[\frac{\partial^2\psi}{\partial r^2} + \frac{2}{r}\frac{\partial\psi}{\partial r}\right] + \frac{\hat{L}^2}{2mr^2}\psi + U(r)\psi$$

$$[\hat{H}, \hat{L}^2] = [\hat{H}, \hat{L}_z] = 0$$

It is possible to find a common basis for $\hat{H}$, $\hat{L}^2$ and $\hat{L}_z$ $|n, \ell, m\rangle$

$$\hat{H}|n, \ell, m\rangle = E_{n\ell m}|n, \ell, m\rangle$$

n – principle quantum #

$$\langle \vec{r} | n, \ell, m\rangle = \psi_{n\ell m}(r, \theta, \varphi) \qquad \hat{L}^2 \psi_{n\ell m} = \hbar^2 \ell(\ell+1)\psi$$

$$\hat{H}\psi_{n\ell m}(r, \theta, \varphi) = -\frac{\hbar^2}{2m}\left[\frac{\partial^2\psi}{\partial r^2} + \frac{2}{r}\frac{\partial\psi}{\partial r}\right] + \frac{\hbar^2 \ell(\ell+1)}{2mr}\psi_{n\ell m} + U(r)\psi_{n\ell m}$$
$$= E_{n\ell m}\psi_{n\ell m}$$

Stationary Schrodinger equation

Assuming $\psi_{n\ell m}(r, \theta, \varphi) = R(r)\, Y_{\ell m}(\theta, \varphi)$

$$-\frac{\hbar^2}{2m}\left[\frac{d^2R}{dr^2} + \frac{2}{r}\frac{dR}{dr}\right] + \frac{\hbar^2\ell(\ell+1)}{2mr}R + U(r)R = E_{n\ell m} R$$

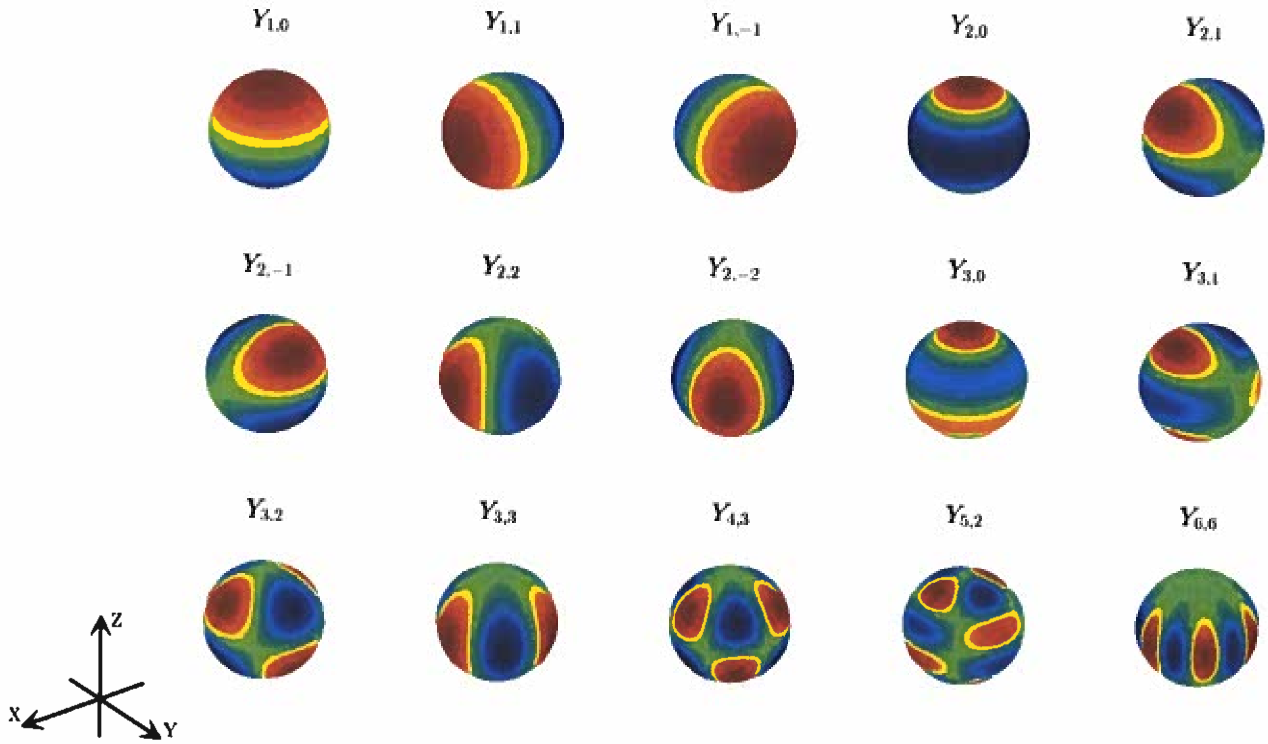
$$R = \frac{u(r)}{r} \qquad \frac{dR}{dr} = \frac{u'}{r} - \frac{u}{r^2} \qquad \frac{d^2R}{dr^2} = \frac{u''}{r^2} - \frac{2u'}{r^2} - \frac{2u}{r^3}$$

$$-\frac{\hbar^2}{2m}\frac{d^2u}{dr^2} + \left[\frac{\hbar^2 \ell(\ell+1)}{2mr^2} + U(r)\right]u = E_{n\ell m} \cdot u(r)$$

Quazi - one dimentional ~~potential~~ motion in an effective one-D potential

$$U_{eff}(r) = \frac{\hbar^2 \ell(\ell+1)}{2mr^2} + U(r)$$

Full wavefunction $\psi_{n\ell}(r,\theta,\varphi) = \frac{u_{n\ell}(r)}{r} Y_{\ell m}(\theta,\varphi)$



Spherical functions

$$Y_l^m(\theta, \phi) \equiv \sqrt{\frac{2l+1}{4\pi} \frac{(l-m)!}{(l+m)!}} \, P_l^m(\cos\theta) \, e^{im\phi},$$

Associate Legandre polynomials

$$P_n^m(x) = \frac{(1-x^2)^{\frac{m}{2}}}{2^n n!} \frac{d^{n+m}}{dx^{n+m}} (x^2-1)^n .$$

$$Y_0^0(\theta,\phi)=\frac{1}{2}\frac{1}{\sqrt{\pi}}$$

$$Y_1^{-1}(\theta,\phi)=\frac{1}{2}\sqrt{\frac{3}{2\pi}}\sin\theta\, e^{-i\phi}$$

$$Y_1^0(\theta,\phi)=\frac{1}{2}\sqrt{\frac{3}{\pi}}\cos\theta$$

$$Y_1^1(\theta,\phi)=-\frac{1}{2}\sqrt{\frac{3}{2\pi}}\sin\theta\, e^{i\phi}$$

$$Y_2^{-2}(\theta,\phi)=\frac{1}{4}\sqrt{\frac{15}{2\pi}}\sin^2\theta\, e^{-2i\phi}$$

$$Y_2^{-1}(\theta,\phi)=\frac{1}{2}\sqrt{\frac{15}{2\pi}}\sin\theta\cos\theta\, e^{-i\phi}$$

$$Y_2^0(\theta,\phi)=\frac{1}{4}\sqrt{\frac{5}{\pi}}\left(3\cos^2\theta-1\right)$$

$$Y_2^1(\theta,\phi)=-\frac{1}{2}\sqrt{\frac{15}{2\pi}}\sin\theta\cos\theta\, e^{i\phi}$$

$$Y_2^2(\theta,\phi)=\frac{1}{4}\sqrt{\frac{15}{2\pi}}\sin^2\theta\, e^{2i\phi}$$

$$Y_3^{-3}(\theta,\phi)=\frac{1}{8}\sqrt{\frac{35}{\pi}}\sin^3\theta\, e^{-3i\phi}$$

$$Y_3^{-2}(\theta,\phi)=\frac{1}{4}\sqrt{\frac{105}{2\pi}}\sin^2\theta\cos\theta\, e^{-2i\phi}$$

$$Y_3^{-1}(\theta,\phi)=\frac{1}{8}\sqrt{\frac{21}{\pi}}\sin\theta\left(5\cos^2\theta-1\right)e^{-i\phi}$$

$$Y_3^0(\theta,\phi)=\frac{1}{4}\sqrt{\frac{7}{\pi}}\left(5\cos^3\theta-3\cos\theta\right)$$

$$Y_3^1(\theta,\phi)=-\frac{1}{8}\sqrt{\frac{21}{\pi}}\sin\theta\left(5\cos^2\theta-1\right)e^{i\phi}$$

$$Y_3^2(\theta,\phi)=\frac{1}{4}\sqrt{\frac{105}{2\pi}}\sin^2\theta\cos\theta\, e^{2i\phi}$$

$$Y_3^3(\theta,\phi)=-\frac{1}{8}\sqrt{\frac{35}{\pi}}\sin^3\theta\, e^{3i\phi}.$$