Lecture 13

Tuesday, October 29, 2024 11:33

November 28 : puzzle challenge !

potential bonus marks !!

Chapter 6 : The Hydrogen Atom

6.1 The One-Particle Central-Force Problem

Central force : spherically symmetric

$$V = V(r)$$

$$\vec{F} = -\nabla V(x,y,z)$$

$$= -\left(\frac{\partial V}{\partial x}\right)\vec{i} - \left(\frac{\partial V}{\partial y}\right)\vec{j} - \left(\frac{\partial V}{\partial z}\right)\vec{k}$$

$$g(x,y,z) = f\left[r(x,y,z), \theta(x,y,z), \phi(x,y,z)\right]$$

$$\left(\frac{\partial g}{\partial x}\right)_{y,z} = \left(\frac{\partial f}{\partial r}\right)_{\theta,\phi}\left(\frac{\partial r}{\partial x}\right)_{y,z} + \left(\frac{\partial f}{\partial \theta}\right)_{r,\phi}\left(\frac{\partial \theta}{\partial x}\right)_{y,z} + \left(\frac{\partial f}{\partial \phi}\right)_{r,}$$

$$\left(\frac{\partial V}{\partial \theta}\right)_{r,\phi} = 0 \quad \text{and} \quad \left(\frac{\partial V}{\partial \phi}\right)_{r,\theta} = 0$$

for spherically symmetric V

$$\left(\frac{\partial V}{\partial x}\right)_{y,z} = \frac{dV}{dr}\left(\frac{\partial r}{\partial x}\right)_{y,z}$$

$$r = (x^2 + y^2 + z^2)^{\frac{1}{2}}$$

$$\left(\frac{\partial r}{\partial x}\right)_{y,z} = \frac{1}{2}(x^2 + y^2 + z^2)^{-\frac{1}{2}} \cdot 2$$

$$\left(\frac{\partial r}{\partial y}\right)_{x,z} = \frac{1}{2}(x^2 + y^2 + z^2)^{-\frac{1}{2}} \cdot 2y$$

$$\left(\frac{\partial r}{\partial z}\right)_{x,y} = \frac{1}{2}(x^2 + y^2 + z^2)^{-\frac{1}{2}} \cdot 2z$$

$$\left(\frac{\partial r}{}\right) \quad \frac{x}{} =$$

$$\left(\frac{\partial V}{\partial x}\right)_{y,z} = \frac{\cdots}{(x^2+y^2+z^2)^{\frac{1}{2}}}$$

$$\left(\frac{\partial V}{\partial x}\right)_{y,z} = \frac{x}{r}\frac{dV}{dr}, \left(\frac{\partial V}{\partial y}\right)_{x,z} = \frac{y}{r}\frac{dV}{dr}, \left(\frac{\partial V}{\partial z}\right)_{x,y} =$$

$$\vec{F} = -\frac{1}{r}\frac{dV}{dr}(x\vec{i}+y\vec{j}+z\vec{k}) = -\frac{dV(r)}{dr}\boxed{\frac{\vec{r}}{r}}$$

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Hamiltonian :

$$\hat{H} = \hat{T} + \hat{V} = -\frac{\hbar^2}{2m}\nabla^2 + V(r)$$

$$\frac{\partial}{\partial x} = \sin\theta\cos\phi\frac{\partial}{\partial r} + \frac{\cos\theta\cos\phi}{r}\frac{\partial}{\partial\theta} - \frac{\sin\phi}{r\sin\theta}\frac{\partial}{\partial\phi}$$

$$\frac{\partial}{\partial y} = \sin\theta\sin\phi\frac{\partial}{\partial r} + \frac{\cos\theta\sin\phi}{r}\frac{\partial}{\partial\theta} + \frac{\cos\phi}{r\sin\theta}\frac{\partial}{\partial\phi}$$

$$\frac{\partial}{\partial z} = \cos\theta\frac{\partial}{\partial r} - \frac{\sin\theta}{r}\frac{\partial}{\partial\theta}$$

$$\nabla^2 = \frac{\partial^2}{\partial r^2} + \frac{2}{r}\frac{\partial}{\partial r} + \frac{1}{r^2}\frac{\partial^2}{\partial\theta^2} + \frac{1}{r^2}\cot\theta\frac{\partial}{\partial\theta} + \frac{1}{r^2\sin^2\theta}\cdots$$

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

$$\hat{L}^2 = -\hbar^2\left(\frac{\partial^2}{\partial\theta^2} + \cot\theta\frac{\partial}{\partial\theta} + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2}\right)$$

$$\boxed{\nabla^2 = \frac{\partial^2}{\partial r^2} + \frac{2}{r}\frac{\partial}{\partial r} - \frac{1}{r^2\hbar^2}\hat{L}^2}$$

$$\boxed{\hat{H} = -\frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial r^2} + \frac{2}{r}\frac{\partial}{\partial r}\right) + \frac{1}{2mr^2}\hat{L}^2 + V(}$$

Does $\hat{H}$ commute with $\hat{L}^2$?

$$[\hat{H}, \hat{L}^2] = [\hat{T} + \hat{V}, \hat{L}^2]$$

$$= [\hat{T}, \hat{L}^2] + \underbrace{[\hat{V}, \hat{L}^2]}_{0}$$

$$[\hat{T}, \hat{L}^2] = -\frac{\hbar^2}{2m}\cancel{\left[\frac{\partial^2}{\partial r^2} + \frac{2}{r}\frac{\partial}{\partial r}, \hat{L}^2\right]}$$

$$+ \frac{1}{2m}\cancel{[r^2\hat{L}^2, \hat{L}^2]}$$

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

$$[\hat{H}, \hat{L}^2] = 0 \quad \text{if } V = V(r)$$

$$\hat{L}_z = -i\hbar\frac{\partial}{\partial\phi}$$

$$[\hat{H}, \hat{L}_z] = 0 \quad \text{if } V = V(r)$$

$$\hat{H}\Psi = E\Psi$$

$$\hat{L}^2\Psi = l(l+1)\hbar^2\Psi, \quad l = 0, 1, 2, \ldots$$

$$\hat{L}_z\Psi = m\hbar\Psi, \quad m = -l, -l+1, \ldots, 0, \ldots, l-1,$$

$$-\frac{\hbar^2}{2m}\left(\frac{\partial^2\psi}{\partial r^2} + \frac{2}{r}\frac{\partial\psi}{\partial r}\right) + \frac{1}{2mr^2}\hat{L}^2\psi + V(r)\psi =$$

$$-\frac{\hbar^2}{2m}\left(\frac{\partial^2\psi}{\partial r^2}+\frac{2}{r}\frac{\partial\psi}{\partial r}\right)+\frac{l(l+1)\hbar^2}{2mr^2}\psi+V(r)\psi=$$

$$\boxed{\psi=R(r)Y_l^m(\theta,\phi)}$$

$$\boxed{-\frac{\hbar^2}{2m}\left(R''+\frac{2}{r}R'\right)+\frac{l(l+1)\hbar^2}{2mr^2}R+V(r)R=}$$

6.2 Noninteracting Particles and Separa of Variables

$$E=E_x+E_y+E_z$$

three-dimensio particle-in-a-b

$$E=E_1+E_2$$

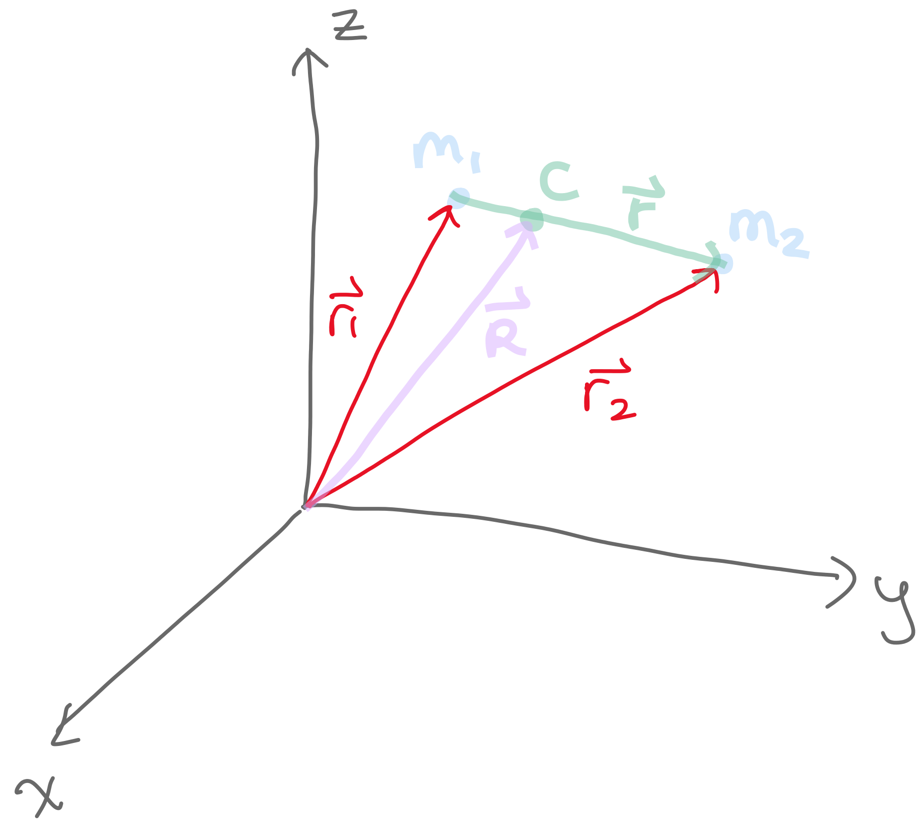
$$\hat{H}=\hat{H}_1+\hat{H}_2$$

$$\boxed{\psi(q_1,q_2,\cdots,q_n)=G_1(q_1)\,G_2(q_2)\cdots G_n(q_n)}$$

$$E = E_1 + E_2 + \cdots + E_n$$

$$\hat{H}_i G_i = E_i G_i, \quad i = 1, 2, 3, \ldots, n$$

6.3 Reduction of the Two-Particle Problem to Two One-Particle Problem



Relative coordinates: $x_2 - x_1$,

$y_2 - y_1$,

$z_2 - z_1$

$$\boxed{\vec{r} = \vec{r}_2 - \vec{r}_1} \quad , \quad \vec{R} = X\vec{i} + Y\vec{j} +$$

$$X = \frac{m_1 x_1 + m_2 x_2}{m_1 + m_2}$$

$$\boxed{\vec{R} = \frac{m_1 \vec{r}_1 + m_2 \vec{r}}{m_1 + m_2}}$$

$$Y = \frac{m_1 y_1 + m_2 y_2}{m_1 + m_2}$$

$$Z = \frac{m_1 z_1 + m_2 z_2}{m_1 + m_2}$$

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

$$\vec{R} = \frac{m_1(\vec{r}_2 - \vec{r}) + m_2 \vec{r}_2}{m_1 + m_2}$$

$$\vec{R} = \frac{m_1 \vec{r}_2 - m_1 \vec{r} + m_2 \vec{r}_2}{m_1 + m_2}$$

$$(m_1 + m_2)\vec{R} = (m_1 + m_2)\vec{r}_2 - m_1 \vec{r}$$

$$\boxed{\vec{r}_2 = \vec{R} + \frac{m_1}{m}\vec{r}}$$

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

$$= \vec{R} + \frac{m_1}{m_1+m_2}\vec{r} - \vec{r}$$

$$= \vec{R} + \frac{m_1}{m_1+m_2}\vec{r} - \frac{m_1+m_2}{m_1+m_2}\vec{r}$$

$$\boxed{\vec{r}_1 = \vec{R} - \frac{m_2}{m_1+m_2}\vec{r}}$$

transformation of coordinates from

$x_1, y_1, z_1, x_2, y_2, z_2$ to x, y, z, X, Y, Z

What happens to the Hamiltonian?

$$T = \frac{1}{2}m_1|\dot{\vec{r}}_1|^2 + \frac{1}{2}m_2|\dot{\vec{r}}_2|^2$$

$$\vec{v}_1 = \frac{d\vec{r}_1}{dt} = \dot{\vec{r}}_1 \qquad |\vec{A}|^2 = \vec{A}$$

$$T = \frac{1}{2}m_1\left(\dot{\vec{R}} - \frac{\quad}{m_1+m_2}\dot{\vec{r}}\right)\cdot\left(\dot{\vec{R}} \quad \frac{\quad}{m_1+m_2}\right)$$

$$+\frac{1}{2}m_2\left(\dot{\vec{R}} + \frac{m_1}{m_1+m_2}\dot{\vec{r}}\right)\cdot\left(\dot{\vec{R}} + \frac{m_1}{m_1+m_2}\right.$$

$$= \frac{1}{2}m_1\left(\dot{\vec{R}}\cdot\dot{\vec{R}} - \frac{2m_2}{m_1+m_2}\dot{\vec{r}}\cdot\dot{\vec{R}} + \frac{m_2{}^2}{(m_1+m_2)^2}\dot{\vec{r}}\cdot\right.$$

$$+\frac{1}{2}m_2\left(\dot{\vec{R}}\cdot\dot{\vec{R}} + \frac{2m_1}{m_1+m_2}\dot{\vec{r}}\cdot\dot{\vec{R}} + \frac{m_1{}^2}{(m_1+m_2)^2}\dot{\vec{r}}\cdot\dot{\vec{r}}\right.$$

$$= \frac{1}{2}\left(m_1\dot{\vec{R}}\cdot\dot{\vec{R}} - \cancel{\frac{2m_1m_2}{m_1+m_2}\dot{\vec{r}}\cdot\dot{\vec{R}}} + \frac{m_1m_2{}^2}{(m_1+m_2)^2}\dot{\vec{r}}\right.$$

$$m_2\dot{\vec{R}}\cdot\dot{\vec{R}} + \cancel{\frac{2m_1m_2}{m_1+m_2}\dot{\vec{r}}\cdot\dot{\vec{R}}} + \frac{m_2m_1{}^2}{(m_1+m_2)^2}\dot{\vec{r}}\cdot\dot{\vec{r}}$$

$$= \frac{1}{2}(m_1+m_2)\left|\dot{\vec{R}}\right|^2 + \frac{\cancel{(m_1+m_2)}m_1m_2}{2(m_1+m_2)^{\cancel{2}}}\left|\dot{\vec{r}}\right.$$

$$\boxed{T = \frac{1}{2}(m_1+m_2)\left|\dot{\vec{R}}\right|^2 + \frac{1}{2}\frac{m_1m_2}{m_1+m_2}\left|\dot{\vec{r}}\right.}$$

$$M \equiv m_1 + m_2$$ total mass

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

$$\boxed{T = \underbrace{\frac{1}{2} M |\dot{\vec{R}}|^2}_{} + \underbrace{\frac{1}{2} \mu |\dot{\vec{r}}|^2}_{}}$$

translational motion of the whole system

kinetic energy of the relative motion of the two particles

$$\boxed{\hat{H} = \frac{\hat{p}_M^2}{2M} + \left[\frac{\hat{p}_\mu^2}{2\mu} + V(x, y, z) \right]}$$