9. Central Potentials

9.1 The Orbital angular momentum in spherical coordinates

$\underline{\hat{L}} = \underline{\hat{R}} \times \underline{\hat{P}}$

where $\underline{\hat{R}} = \left(\hat{X}, \hat{Y}, \hat{Z}\right)$ and $\underline{\hat{P}} = \left(\hat{P}_x, \hat{P}_y, \hat{P}_z\right)$.

For $\Psi(x, y, z)$:

$$\hat{X}\psi(x,y,z) = X\psi(x,y,z)$$

$$\hat{Y}\psi(x,y,z) = Y\psi(x,y,z)$$

$$\hat{Z}\psi(x,y,z) = Z\psi(x,y,z)$$

$$\hat{P}_x\psi = -i\hbar\frac{\partial\psi}{\partial z}$$

$$\hat{P}_y\psi = -i\hbar\frac{\partial\psi}{\partial y}$$

$$\hat{P}_z\psi = -i\hbar\frac{\partial\psi}{\partial z}$$

$$\hat{L}_x = -i\hbar\left(Y\frac{\partial}{\partial z} - Z\frac{\partial}{\partial y}\right)$$

$$\hat{L}_y = -i\hbar\left(Z\frac{\partial}{\partial x} - X\frac{\partial}{\partial z}\right)$$

$$\hat{L}_z = -i\hbar\left(X\frac{\partial}{\partial y} - Y\frac{\partial}{\partial x}\right)$$

Cartesian / spherical geometry:

$$x = r\sin\theta\cos\phi$$

$$y = r\sin\theta\sin\phi$$

$$z = r\cos\theta$$

$$r \geq 0$$

$$0 \leq \theta \leq \pi$$

$$0 \leq \phi \leq 2\pi$$

Taking into account of spherical geometry,

$$\hat{L}_x = i\hbar\left(\sin\phi\frac{\partial}{\partial\theta} + \frac{\cos\phi}{\tan\theta}\frac{\partial}{\partial\phi}\right)$$

$$\hat{L}_y = i\hbar\left(-\cos\frac{\partial}{\partial\theta} + \frac{\sin\phi}{\tan\theta}\frac{\partial}{\partial\phi}\right)$$

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

So, the total orbital momentum,

$$\hat{L}^2 = -\hbar\left(\frac{\partial^2}{\partial\theta^2} + \frac{1}{\tan\theta}\frac{\partial}{\partial\theta} + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2}\right) \quad (9\text{-}1)$$

The eigenfunctions of $\hat{L}^2$ and $\hat{L}_z$, $\left|\ell, m_\ell\right\rangle$ in spherical coordinates are called spherical harmonics $Y_{\ell,m_\ell}(\theta,\phi)$.

$\hat{L}^2 Y_{\ell,m_\ell}(\theta,\phi) = -\hbar^2 \ell(\ell+1) Y_{\ell,m_\ell}(\theta,\phi)$ (9-2)

$\hat{L}_z Y_{\ell,m_\ell}(\theta,\phi) = \hbar m_\ell Y_{\ell,m_\ell}(\theta,\phi)$ (9-3)

To solve (9-2) and (9-3), we propose a solution using separation of variables.

i.e. $Y_{\ell,m_\ell}(\theta,\phi) = \Theta_{\ell,m_\ell}(\theta)\Phi_{\ell,m_l}(\phi)$

Replacing (9-3):

$$\cancel{\Theta(\theta)}(-i\cancel{\hbar})\frac{\partial}{\partial\phi}\Phi(\phi) = \cancel{\hbar} m_\ell \cancel{\Theta(\theta)}\Phi(\phi)$$

Leaves with $\Phi(\phi) = Ae^{im_l\phi}$

But we want $\Phi(\phi)$ to be continuous.

Then $\Phi(0) = \Phi(2\pi)$ → $1 = e^{im_\ell 2\pi}$

Which automatically implies that m_ℓ must be an integer.

ℓ runs between $m_\ell = -\ell, -\ell+1, ..., \ell$. Therefore ℓ must be an integer. (orbital angular momentum cannot be $\frac{1}{2}$ integer)

Not much can be said about the Θ part, apart from $\Theta(\theta) =$ lagrange polynomials.

9.2 Solutions of the time-independent Schrödinger equation for Central Potentials

For a particle of mass M moving in a central potential $V(r)$ and $r = |\underline{r}|$:

$$\left[-\frac{\hbar^2}{2m}\nabla^2 + V(r)\right]\psi(r,\theta,\phi) = E\phi(r,\theta,\phi)$$

Using (9-1):

$$\left[-\frac{\hbar^2}{2M}\left(\frac{\partial^2}{\partial r^2} + \frac{2}{r}\frac{\partial}{\partial r}\right) + \frac{\hat{L}^2}{2Mr} + V(r)\right]\psi(r) = E\psi(r) \quad (9\text{-}4)$$

where the part in square brackets $= \hat{H}_c$, the Hamiltonian operator of a central potential.

i.e. $\hat{H}_c\psi = E\psi$.

→ $\{\hat{H}_c, \hat{L}^2, \hat{L}_z\}$ are compatible observables, where the common eigenfunctions are $\phi_{k,\ell,m_\ell}(\underline{r})$.

$\hat{H}_c\phi_{k,\ell,m_\ell} = E_{k,\ell,m_\ell}\phi_{k,\ell,m_\ell}$

$\hat{L}^2\phi_{k,\ell,m_\ell} = \hbar^2\ell(\ell+1)\phi_{k,\ell,m_\ell}$

$\hat{L}_z\phi_{k,\ell,m_\ell} = \hbar m_\ell\phi_{k,\ell,m_\ell}$

The extra index k is to label different eigenfunctions of $\hat{H}_c$ with the same values of ℓ and m_ℓ.

We propose a solution

$\phi_{k,\ell,m_\ell}(r,\theta,\phi) = R_{k,\ell,m_\ell}(r)Y_{\ell,m}(\theta,\phi)$

Replacing (9-4);

$$\left[-\frac{\hbar^2}{2M}\left[\frac{\partial^2}{\partial r^2} + \frac{2}{r}\frac{\partial}{\partial r}\right] + \frac{\ell(\ell+1)\hbar^2}{2Mr^2} + V(r)\right]R_{k,\ell,m_\ell} = E_{k,\ell,m_\ell}R_{k,\ell,m_\ell}(r)$$

NB: now no longer depending on m_ℓ.

The bracket does not depend on m_ℓ, then we can rewrite $R_{k,\ell,m_\ell} \rightarrow R_{k,\ell}$ and $E_{k,\ell,m_\ell} \rightarrow E_{k,\ell}$.

→ $\phi_{k,\ell,m_\ell}(r,\theta,\phi) = R_{k,\ell}(r) Y_{\ell,m_\ell}(\theta,\phi)$.

$\left\{ \hat{H}_C, \hat{L}^2, \hat{L}_z, \hat{S}^2, \hat{S}_z \right\}$ are compatible observables.

$\underline{J} = \underline{L} + \underline{S}$

$\left\{ \hat{H}_c, \hat{J}^2, \hat{J}_z, \hat{L}^2, \hat{S}^2 \right\}$ are compatible observables.