PHYS 621 Lecture Notes 19

16.3 Rotations and Wave Functions

$$\hat{L}_i = \epsilon_{ijk} \hat{X}_j \hat{P}_k$$

Einstein-summation convention: Repeated indices are summed, e.g.

$$\epsilon_{ijk} \hat{X}_j \hat{P}_k \equiv \sum_{j=1}^{3} \sum_{k=1}^{3} \epsilon_{ijk} \hat{X}_j \hat{P}_k .$$

$$\langle \vec{x} | \hat{L}_i | \vec{x}' \rangle = \epsilon_{ijk} \langle \vec{x} | \hat{X}_j \hat{P}_k | \vec{x}' \rangle$$

$$= \epsilon_{ijk} x_j \langle \vec{x} | \hat{P}_k | \vec{x}' \rangle$$

$$= -i\hbar \epsilon_{ijk} x_j \delta(\vec{x} - \vec{x}') \frac{\partial}{\partial x_k'}$$

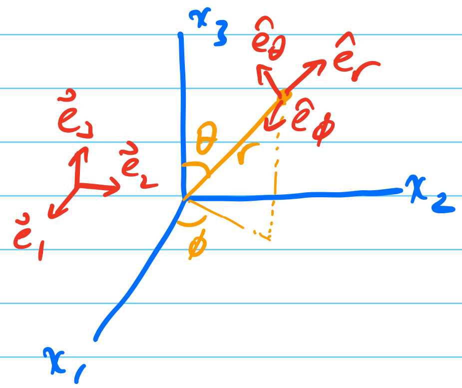
Then,

$$\langle \vec{x} | \hat{L}_i | \psi \rangle = \int d^3x' \langle \vec{x} | \hat{L}_i | \vec{x}' \rangle \langle \vec{x}' | \psi \rangle$$

$$= -i\hbar \epsilon_{ijk} x_j \frac{\partial}{\partial x_k} \psi(\vec{x})$$

$$= -i\hbar (\vec{r} \times \nabla \psi)_i$$

Spherical Coordinates:



$$x_1 = r \sin\theta \cos\phi$$
$$x_2 = r \sin\theta \sin\phi$$
$$x_3 = r \cos\theta$$

Unit basis vectors: $\vec{e}_r, \vec{e}_\theta, \vec{e}_\phi$

$$\vec{e}_r = \vec{e}_\theta \times \vec{e}_\phi, \quad \vec{e}_\theta = \vec{e}_\phi \times \vec{e}_r,$$

$$\vec{e}_\phi = \vec{e}_r \times \vec{e}_\theta$$

$$\vec{\nabla} = \vec{e}_r \frac{\partial}{\partial r} + \vec{e}_\theta \frac{1}{r}\frac{\partial}{\partial \theta} + \vec{e}_\phi \frac{1}{r\sin\theta}\frac{\partial}{\partial \phi}$$

$$\vec{L} = -i\hbar \vec{r} \times \nabla = -i\hbar r \vec{e}_r \times \nabla$$

$$= -i\hbar \left[\vec{e}_\phi \frac{\partial}{\partial \theta} - \vec{e}_\theta \frac{1}{\sin\theta} \frac{\partial}{\partial \phi} \right]$$

In terms of $\vec{e}_1, \vec{e}_2, \vec{e}_3$:

$$\vec{e}_r = \sin\theta\cos\phi\, \vec{e}_1 + \sin\theta\sin\phi\, \vec{e}_2 + \cos\theta\, \vec{e}_3$$

$$\vec{e}_\theta = \cos\theta\cos\phi\, \vec{e}_1 + \cos\theta\sin\phi\, \vec{e}_2 - \sin\theta\, \vec{e}_3$$

$$\vec{e}_\phi = -\sin\phi\, \vec{e}_1 + \cos\phi\, \vec{e}_2$$

$\rightarrow$

$$\boxed{\begin{aligned} L_1 &= -i\hbar\left(-\sin\phi \frac{\partial}{\partial\theta} - \cos\phi\cot\theta\frac{\partial}{\partial\phi}\right) \\ L_2 &= -i\hbar\left(\cos\phi\frac{\partial}{\partial\theta} - \sin\phi\cot\theta\frac{\partial}{\partial\phi}\right) \\ L_3 &= -i\hbar\frac{\partial}{\partial\phi} \end{aligned}}$$

Angular-momentum raising and lowering operators:

$$\boxed{\begin{aligned} L_+ &= L_1 + iL_2 = \hbar e^{i\phi}\left[\frac{\partial}{\partial\theta} + i\cot\theta\frac{\partial}{\partial\phi}\right] \\ L_- &= L_1 - iL_2 = \hbar e^{-i\phi}\left[-\frac{\partial}{\partial\theta} + i\cot\theta\frac{\partial}{\partial\phi}\right] \end{aligned}}$$

Write coordinate basis states in spherical coordinates:

$|\vec{x}\rangle \equiv |r, \vec{n}\rangle$, where $\vec{n}(\theta,\phi)$ is a unit vector in the direction of $\vec{r}$.

Some states have factorized wavefunctions:

$$\langle r, \vec{n}|\psi\rangle = \psi_r(r)\, \psi(\theta,\phi)$$

For eigenstates of angular momentum, we can suppress the dependence on r, and consider basis states $|\vec{n}(\theta,\phi)\rangle$

$$\langle \vec{n}(\theta,\phi)|\psi\rangle \equiv \psi(\theta,\phi)$$

For eigenstates of $\hat{L}^2$ and $\hat{L}_z$, write:

$$\boxed{\begin{aligned} Y_{\ell m}(\theta,\phi) &\equiv \langle \vec{n}(\theta,\phi)|\ell m\rangle \\ L^2 Y_{\ell m}(\theta,\phi) &= \hbar^2 \ell(\ell+1)\, Y_{\ell m}(\theta,\phi) \\ L_z Y_{\ell m}(\theta,\phi) &= m\hbar\, Y_{\ell m}(\theta,\phi) \end{aligned}}$$

Since $L_z = -i\hbar \frac{\partial}{\partial\phi}$,

$$-i\hbar\frac{\partial}{\partial\phi} Y_{\ell m}(\theta,\phi) = m\hbar\, Y_{\ell m}(\theta,\phi)$$

solution: $\boxed{Y_{\ell m}(\theta,\phi) = e^{im\phi}\, y_{\ell m}(\theta)}$

for some function $y_{\ell m}(\theta)$.

Rotation of States

Under a rotation described by rotation matrix R, the vector $\vec{n}$ transforms (actively) into $\vec{n}' = R\vec{n}$.

We would like to know how the state $|\vec{n}\rangle$ transforms under the same rotation.

matrix that acts on vectors in 3D

Write $|\vec{n}'\rangle = \underbrace{D(R)}_{\text{Operator that acts on states in Hilbert space.}} |\vec{n}\rangle$

$$\langle \vec{n}' | lm\rangle = \langle \vec{n} | D(R)^\dagger | lm\rangle$$

$$Y_{lm}(\vec{n}') \equiv \langle \vec{n}' | lm\rangle = \langle \vec{n} | D(R)^\dagger | lm\rangle$$

$$\equiv D^{(l)*}_{mm'}(R) \langle \vec{n} | lm'\rangle$$

(summed over m')

Note: Rotation affects L_z, but not $\hat{L}^2$.

$\Rightarrow$ Label transformation matrix $D^{(l)}_{mm'}$ by $\hat{L}^2$ quantum number l.

Under a rotation, $|\psi\rangle \to D(R)|\psi\rangle$, we must have

$$\underbrace{\langle \psi | \hat{x}_i | \psi\rangle}_{\text{Components of a spatial vector}} \to \langle \psi | D(R)^\dagger \hat{x}_i D(R) | \psi\rangle$$

$$= R_{ik} \langle \psi | \hat{x}_k | \psi\rangle$$

For states with definite l, $D^{(l)}(R(\vec{e}_R, \varphi)) = e^{-\frac{i}{\hbar}\vec{e}_R\cdot\hat{\vec{L}}\varphi}$

rotation axis

rotation angle

Angular momentum generates rotations in the same way momentum generates translations

Example:

$$\langle lm| D^{(l)}(R(\vec{e}_z, \varphi))|lm'\rangle = \langle m| e^{-\frac{i}{\hbar}\hat{L}_z \varphi}|m'\rangle$$

rotation about z-axis

$$= e^{-im\varphi}\,\delta_{mm'}$$

$$\langle \vec{n}'|lm\rangle = Y_{lm}[\underbrace{R(\vec{e}_z,\varphi)\vec{n}}_{\vec{n}'}] = e^{im\varphi}\,Y_{lm}[\vec{n}(\theta,\phi)]$$

$$= e^{im(\varphi+\phi)}\,y_{lm}(\theta)$$

Note:

Since $Y_{lm}(\theta,\phi) \propto e^{im\phi}$, for periodicity in $\phi \to \phi + 2\pi$ we must have $m \in \mathbb{Z}$ (integer)

so $l \in \mathbb{N}$ (natural number 0, 1, 2, ...)

Integer m → wavefunctions are periodic:

$$Y_{lm}(\theta,\phi) \xrightarrow{\phi\to\phi+2\pi} Y_{lm}(\theta,\phi)$$

because $e^{2m\pi i} = 1$

Half-odd-integer m, e.g. $m = 1/2$:

$$Y_{lm}(\theta,\phi) \xrightarrow{\phi\to\phi+2\pi} -Y_{lm}(\theta,\phi)$$

because $e^{(2m+1)\pi i} = -1$

Experiment → orbital angular momentum always has $l \in \mathbb{N}$, no half-odd-integral orbital ∡ mom.

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Free particle in Spherical Coordinates

$\hat{H} = \frac{\hat{\vec{P}}^2}{2m}$, eigenstates $|\vec{p}\rangle = |p_x\, p_y\, p_z\rangle$.

$$\text{eigenvalues } E = \frac{\vec{p}^2}{2m}$$

$$\hat{P}_i |\vec{p}\rangle = p_i |\vec{p}\rangle.$$

Since $[\hat{H}, \hat{L}_z] = [\hat{H}, \hat{\vec{L}}^2] = 0$, we can find simultaneous eigenstates of $\hat{H}, \hat{L}_z, \hat{\vec{L}}^2$.

Use the identity $\sum_i \epsilon_{ijk}\epsilon_{ilm} = \delta_{jl}\delta_{km} - \delta_{jm}\delta_{kl}$

to show $\hat{L}_i \hat{L}_i = (\hat{x}_j \hat{x}_j)(\hat{P}_k \hat{P}_k) - (\hat{x}_j \hat{P}_j)^2 - i\hbar \hat{x}_j \hat{P}_j$

$$= \hat{r}^2 \hat{\vec{P}}^2 - \hat{r}\hat{P}_r \hat{r}\hat{P}_r - i\hbar \hat{r}\hat{P}_r$$

$$= \hat{r}^2 \hat{\vec{P}}^2 - \hat{r}^2 \hat{P}_r^2 - \hat{r}\underbrace{[\hat{P}_r, \hat{r}]}_{-i\hbar}\hat{P}_r \quad - i\hbar \hat{r}\hat{P}_r$$

$$\hat{\vec{L}}^2 = \hat{r}^2(\hat{\vec{P}}^2 - \hat{P}_r^2)$$

$$\boxed{\hat{\vec{P}}^2 = \hat{P}_r^2 + \frac{1}{r^2}\hat{\vec{L}}^2} \quad \text{(in coordinate basis)}$$

$$\hat{P}_r = \vec{e}_r \cdot (-i\hbar \nabla)$$

$$= -i\hbar \frac{1}{r}\frac{\partial}{\partial r} r$$

$\Rightarrow$ Schrödinger Eq: $\frac{\vec{P}^2}{2m}\psi(r,\theta,\phi) = \frac{1}{2m}\left(P_r^2 + \frac{\vec{L}^2}{r^2}\right)\psi(r,\theta,\phi)$

$$= E\,\psi(r,\theta,\phi)$$

Separation of variables: write

$$\psi_{\ell m}(r,\theta,\phi) = f_\ell(r)\, Y_{\ell m}(\theta,\phi)$$

The Schrödinger Eq. becomes:

$$\left[\frac{\hat{P}_r^{\,2}}{2m} + \frac{\hbar^2 \ell(\ell+1)}{2mr^2}\right] f_\ell(r) = E f_\ell(r)$$

$$\boxed{\frac{\hbar^2}{2m}\left[-\left(\frac{1}{r}\frac{\partial}{\partial r} r\right)^2 + \frac{\ell(\ell+1)}{r^2} - \frac{2mE}{\hbar^2}\right] f_\ell(r) = 0}$$

Define $k^2 \equiv \dfrac{2mE}{\hbar^2}$, $\rho \equiv kr$

The Schrödinger Eq. is now

$$\boxed{\left[\frac{\partial^2}{\partial \rho^2} + \frac{2}{\rho}\frac{\partial}{\partial \rho} + \left(1 - \frac{\ell(\ell+1)}{\rho^2}\right)\right] f_\ell(\rho) = 0}$$

– Spherical Bessel Eq.

– Solutions are spherical Bessel functions $j_\ell(\rho)$

Regular at $\rho =$

So, $\langle r,\theta,\phi | E,\ell,m\rangle = Y_{\ell m}(\theta,\phi)\, j_\ell(kr)$

$k = \dfrac{2mE}{\hbar^2}$

Change of basis: $\langle \vec{x} | \vec{k} \rangle = e^{i\vec{k}\cdot\vec{r}}$

$$= \sum_{\ell=0}^{\infty} \sum_{m=-\ell}^{\ell} a_{\ell m}(\vec{k}) Y_{\ell m}(\theta,\phi)\, j_\ell(kr)$$

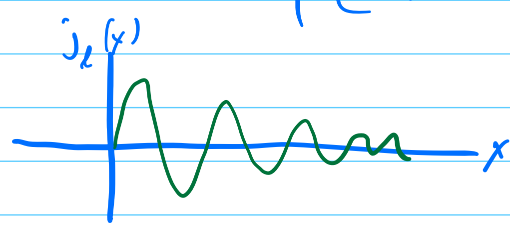
Results: $e^{ikr\cos\theta} = \sum_{\ell=0}^{\infty} (2\ell+1)\, i^\ell j_\ell(kr) P_\ell(\cos\theta)$

$$= 4\pi \sum_{\ell=0}^{\infty} \sum_{m=-\ell}^{\ell} (2\ell+1)\, i^\ell j_\ell(kr)\, Y^*_{\ell m}(\vec{n}_1)\, Y_{\ell m}(\vec{n}_2)$$

$\vec{n}_1, \vec{n}_2$ have angle θ between them.

Asymptotic behavior:

$$j_\ell(x) \xrightarrow[x\to\infty]{} \begin{cases} (-1)^{\ell/2} \dfrac{\sin x}{x}, & \ell \text{ even} \\ (-1)^{(\ell-1)/2} \dfrac{\cos x}{x}, & \ell \text{ odd} \end{cases}$$



Independent solution:

$$n_\ell(x) \xrightarrow[x\to\infty]{} \begin{cases} -(-1)^{\ell/2} \dfrac{\cos x}{x} & \ell \text{ even} \\ -(-1)^{(\ell-1)/2} \dfrac{\sin x}{x} & \ell \text{ odd} \end{cases}$$