Chapter 7
Angular momentum and Rotation
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Section 7.2: Rotations in Quantum Mechanics

A rotation is specified by an angle of rotation (α) and by an axis of rotation (unit vector $\vec{n}(\theta,\phi)$) about which the rotation is performed. (i.e $R_{\vec{n}}(\alpha)$)

Knowing the rotation operator $\hat{R}$, we can determine how state vectors and operators transform under rotations

$$\psi' = R\psi \quad \text{and} \quad \hat{A}' = \hat{R} A R^{\dagger} \quad ; \quad R^{\dagger} = R^{-1} \text{ or } R^{\dagger}R = I$$

$\hat{R}$ is unitary as it preserveses the lengths and angles between vectors $\Rightarrow$ $RI = IR = R$; I : identity operator.

and $RR^{-1} = R^{-1}R = I$

- the product of any two rotations is just the rotation obtained by performing each rotation in a sequence for example $R_{\vec{n}}(\alpha)\, R_{\vec{n}'}(\alpha')$ corresponds to a rotation through an angle α' about the axis $\vec{n}'$, followed by a rotation through an angle α about the axis $\vec{n}$. Note that the identity rotation correspond to $\alpha = 0$.

- The inverse of $R_{\vec{n}}(\alpha)$ is the rotation $R_{\vec{n}}^{-1}(\alpha)$ which can be written as

$$R_{\vec{n}}^{-1}(\alpha) = R_{\vec{n}}(-\alpha)$$ $\Rightarrow$ rotates the system in the opposite direction about the same axis.

it is well known that in 3D, Rotations (in general) are not commute i.e it depends upon the order in which they are performed $[R_1, R_2] \neq 0 \Rightarrow R_1 R_2 \neq R_2 R_1$

the rotation group is said non commutative or (non-Abelian group). However, there are two exceptions

i) Rotations about the same fixed axis are commutative (Abelian group)

$$R_{\vec{n}}(\alpha)\, R_{\vec{n}}(\beta) = R_{\vec{n}}(\beta)\, R_{\vec{n}}(\alpha) = R_{\vec{n}}(\alpha+\beta)$$

ii) Infinitesmal rotations $R_{\vec{n}}(\delta\alpha)$ are also commutative (Abelian group)

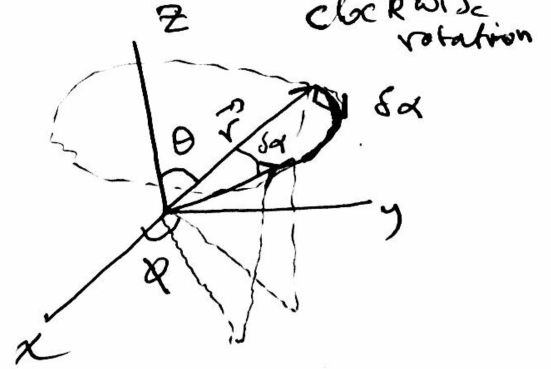
- <u>Infinitesmal Rotation:</u>

consider a rotation of the coordinates of a spinless particle over an infinitesmal angle $\delta\alpha$ about the z-axis

$$\hat{R}_z(\delta\alpha)\,\psi(r,\theta,\phi) = \psi(r,\theta,\phi-\delta\alpha)$$

notice that ϕ decreases

$$\phi \to \phi - \delta\alpha$$



Now expanding the new wavefunction in a Taylor series to first order in $\delta\alpha$, we get

$$\psi(r,\theta,\phi-\delta\alpha) \approx \psi(r,\theta,\phi) - \delta\alpha \frac{\partial \psi}{\partial \phi} = \left(1 - \delta\alpha \frac{\partial}{\partial \phi}\right)\psi(r,\theta,\phi)$$

$$\therefore \quad \hat{R}_z(\delta\alpha)\,\psi(r,\theta,\phi) = \left(1 - \delta\alpha \frac{\partial}{\partial\phi}\right)\psi(r,\theta,\phi)$$

$$\Rightarrow \quad \hat{R}_z(\delta\alpha) = 1 - \delta\alpha \frac{\partial}{\partial\phi}$$

$$\hat{R}_z(\delta\alpha) = 1 - \frac{i}{\hbar}\delta\alpha\,\hat{L}_z$$, Recall that $L_z = -i\hbar\frac{\partial}{\partial\phi}$

we may generalize this relation to a rotation of an angle $\delta\alpha$ about an arbitrary axis whose direction is given by the unit vector $\vec{n} = (\sin\theta\cos\phi, \sin\theta\sin\phi, \cos\theta)$

$$\Rightarrow \quad R_{\vec{n}}(\delta\alpha) = 1 - \frac{i}{\hbar}\delta\alpha\,\vec{n}\cdot\vec{L}$$

$\Rightarrow$ the orbital angular momentum $\vec{L}$ is thus the generator of infinitesmal spatial rotations

<u>Finite rotations</u>: The operator $\hat{R}_z(\alpha)$ corresponding to a rotation over a finite angle α about the z-axis. this can be constructed in terms of the infinitesmal rotations as follows: we divide the angle α into N infinitesmal angles $\delta\alpha$ $\Rightarrow$ $\alpha = N\delta\alpha$, so the rotation over the angle α can be seen as a series of N consecutive infinitesmal rotations about the same axis (z-axis)

$$R_z(\alpha) = \hat{R}_z(N\delta\alpha) = \left(R_z(\delta\alpha)\right)^N = \left(1 - \frac{i}{\hbar}\delta\alpha L_z\right)^N$$

since $\delta\alpha = \alpha/N$ $\Rightarrow$

$$\hat{R}_z(\alpha) = \lim_{N\to\infty} \left(1 - \frac{i}{\hbar}\frac{\alpha}{N} L_z\right)^N \quad ; \quad e^{-x} \approx 1 - x \text{ to } 1^{st} \text{ order}$$

$$= \left(e^{-\frac{i}{\hbar}\frac{\alpha}{N} L_z}\right)^N \qquad \sum_{n=0}^{\infty} \frac{x^n}{n!} = 1 - x$$

$$= e^{-\frac{i}{\hbar}\alpha L_z} \qquad \therefore \quad \hat{R}_z(\alpha) = e^{-\frac{i}{\hbar}\alpha L_z}$$

for finite rotation over a finite angle α around an axis $\vec{n}$:

$$\hat{R}_{\vec{n}}(\alpha) = e^{-\frac{i}{\hbar}\alpha \vec{n}.\vec{L}} \quad ; \quad \vec{L} = l_x\hat{i} + l_y\hat{j} + l_z\hat{k}$$

orbital angular momentum

$\Downarrow$

for spinless particle

if the spin is taken into account, we have the last eq^n modified to a more general one

$$\hat{R}_{\vec{n}}(\alpha) = e^{-\frac{i}{\hbar}\alpha \vec{n}.\vec{J}} \quad ; \text{ when } \vec{J} = \vec{L} + \vec{S}$$

L: orbital angular momentum

S spin " "

J total " " (or shortly angular momentum)

$$\hat{R}_x(\alpha) = e^{-i/\hbar\, \alpha \hat{J}_x} \quad ; \quad \hat{R}_y(\alpha) = e^{-i/\hbar\, \alpha \hat{J}_y} \quad ; \quad \hat{R}_z(\alpha) = e^{-\frac{i}{\hbar}\alpha \hat{J}_z}$$

notice that $\hat{R}_{\vec{n}}(\alpha)$ is unitary as (for finite rotation)

$$R_{\vec{n}} R_{\vec{n}}^{\dagger} = e^{-\frac{i}{\hbar}\alpha \vec{n}.\vec{J}}\, e^{+\frac{i}{\hbar}\alpha \vec{n}.\vec{J}} = 1$$

- $\hat{R}_{\vec{n}}(\delta\alpha)$ is also unitary for infinitesimal rotations as

$$R_{\vec{n}}(\delta\alpha) R_{\vec{n}}^{\dagger}(\delta\alpha) = \left(1 - \frac{i}{\hbar}\delta\alpha \vec{n}.\vec{J}\right)\left(1 + \frac{i}{\hbar}\delta\alpha \vec{n}.\vec{J}\right)$$

$$= 1 + \cancel{\frac{i}{\hbar}\delta\alpha \vec{n}.\vec{J}} - \cancel{\frac{i}{\hbar}\delta\alpha \vec{n}.\vec{J}} + \underbrace{\frac{1}{\hbar^2}(\delta\alpha)^2(\vec{n}.\vec{J})^2}_{\text{small}} \approx 1$$

we know from classical physics that when-ever a system is invariant under rotation, its angular momentum is conserved. let us demonstrate this for an infinitesmal rotation about an arbitrary axis $\vec{n}$ (for spinless particl $s=0$)

$$R_{\vec{n}}(\delta\alpha) = 1 - \frac{i}{\hbar}\delta\alpha\, \vec{n}.\vec{L}$$

under rotation H transforms to H' as

$$\hat{H}' = R_{\vec{n}}(\delta\alpha)\, H\, R^{\dagger}_{\vec{n}}(\delta\alpha) = (1-\frac{i}{\hbar}\delta\alpha\,\vec{n}.\vec{L})\,\hat{H}\,(1+\frac{i}{\hbar}\delta\alpha\,\vec{n}.\vec{L})$$

$$= (1-\frac{i}{\hbar}\delta\alpha\,\vec{n}.\vec{L})\,(\hat{H} + \frac{i}{\hbar}\delta\alpha\,\hat{H}\,\vec{n}.\vec{L})$$

$$= \hat{H} + \frac{i}{\hbar}\delta\alpha\,\hat{H}\,n.\vec{L} - \frac{i}{\hbar}\delta\alpha\,\vec{n}.\vec{L}\,\hat{H} + \underbrace{O(\delta\alpha)^2}_{\text{small}}$$

$$\hat{H}' = \hat{H} + \frac{i}{\hbar}\delta\alpha\,[\hat{H}, \vec{n}.\vec{L}]$$

This means that if H is invariant under arbitrary rotation around an axis $\vec{n}$ (i.e $\hat{H} = \hat{H}'$), then the component of the angular momentum in that direction is preserved. for example if $\vec{n} = \vec{e}_z \Rightarrow l_z$ is conserved. i.e $[\hat{H}, l_z] = 0$

This statement is true in the opposite direction. i.e if $[\hat{H}, l_z] = 0$, then H is invariant $(H' = H)$

Recall that for central potentials $H = \frac{p^2}{2m} + V(r)$, H is invariant under rotations around any axis ($[H, l_x] = [H, l_y] = [H, l_z] = 0$), meaning any component of the angular momentum is conserved i.e the total angular momentum is conserved.

∴ for a spinless particle moving in a central potential $\hat{H}_0 = \frac{\hat{P}^2}{2m} + V(r)$, the orbital angular momentum is conserved, because H_0 is invariant under rotations around an arbitrary axis. However, for an electron in the real hydrogen atom, this is half of the truth. The reason is that the electron possesses an internal degree of freedom, the spin, and therefore there have ~~ha~~ to be an additional ~~terms~~ in H operator. This term is due to the coupling between $\vec{S}$ and $\vec{L}$ of the electron.

let us call this term $H_1 \propto \vec{L}\cdot\vec{S}$

$\Rightarrow H = H_0 + H_1$ total Hamiltonian

here neither $\vec{L}$ nor $\vec{S}$ are conserved

<u>check??</u> $[H, \vec{L}] \neq 0$ $\quad [H, \vec{S}] \neq 0$

$$[\vec{L}, H] = \cancel{[L, H_0]}^{0} + [L, H_1] = [\vec{L}, \vec{L}\cdot\vec{S}] \neq 0$$

also

$$[\vec{S}, H] = \cancel{[\vec{S}, H_0]}^{0} + [\vec{S}, H_1] = [\vec{S}, \vec{L}\cdot\vec{S}] \neq 0$$

proof: $[l_z, \vec{l}\cdot\vec{s}] = [l_z, l_x S_x + l_y S_y + l_z S_z] = [l_z, l_x S_x] + [l_z, l_y S_y] + [l_z, l_z S_z]$

$$= l_x \cancel{[l_z, S_x]}^{0} + [l_z, l_x] S_x + l_y \cancel{[l_z, S_y]}^{0} + [l_z, l_y] S_y$$

$$+ l_z \cancel{[l_z, S_z]}^{0} + \cancel{[l_z, l_z]}^{0} S_z$$

$$= i\hbar l_y S_x - i\hbar l_x S_y \neq 0$$

in general $[\vec{L}, \vec{L}\cdot\vec{S}] = i\hbar\, \vec{S}\times\vec{L}$

now $[S_z, \vec{l}\cdot\vec{s}] = [S_z, l_x S_x + l_y S_y + l_z S_z] = i\hbar l_x S_y - i\hbar l_y S_x$

in general $[\vec{S}, \vec{L}\cdot\vec{S}] = i\hbar\, \vec{L}\times\vec{S}$

Now $[l_z + S_z, \vec{l}.\vec{s}] = [l_z, \vec{l}.\vec{s}] + [S_z, \vec{l}.\vec{s}]$

$= i\hbar l_y S_x - i\hbar l_x S_y + i\hbar l_x S_y - i\hbar l_y S_x$

$= 0$

so the quantity $l_z + S_z \equiv j_z$ is conserved.

$\therefore [j_z, \vec{l}.\vec{s}] = 0$, similarly $[j_x, \vec{l}.\vec{s}] = [j_y, \vec{l}.\vec{s}] = 0$

$\Rightarrow [j, \vec{l}.\vec{s}] = 0 \Rightarrow j$ is conserved.

$\therefore \vec{J} = \vec{L} + \vec{S}$ is the total angular momentum

$J_z = L_z + S_z$: the z-component of the total angular momentum.

$\therefore$ when two angular momenta ($\vec{L}$ and $\vec{S}$ for example or $\vec{J_1}$ and $\vec{J_2}$) are present and when there is an interaction between them, then each one separately will not be conserved, but their sum (the total angular momentum $\vec{J} = \vec{J_1} + \vec{J_2}$ or $\vec{J} = \vec{L} + \vec{S}$) will be conserved.

- for a particle with spin moving in a central potential $V(r)$

in the ~~presence~~ absence of spin-orbit coupling

$$H = \frac{P^2}{2m} + V(r)$$

then $[L, H] = 0$ and $[S, H] = 0$ the two angular momenta are separately constants of the motion

- in the presence of spin-orbit coupling

$$H = \frac{P^2}{2m} + V(r) + \underbrace{A}_{\text{constant}} \vec{L}.\vec{S}$$

then $[L, H] \neq 0$, $[S, H] \neq 0$ Not constants of the motion

but $[\vec{L} + \vec{S}, H] = [J, H] = 0$ J is constant of the motion

See back