Phys 570A Lecture 26

Rotations

$$[L_i, r_j] = i\hbar\, \varepsilon_{ijk} r_k$$

$$[\hat{n}\cdot\vec{L}, \vec{r}] = i\hbar(\vec{r}\times\hat{n})$$

consider an infinitessimal rotation

$$\vec{r}\,' = \vec{r} + d\vec{\alpha}\times\vec{r},$$

where $d\vec{\alpha}$ is an infinitessimal vector.

We can write

$$\vec{r}\,' = \vec{r} + \frac{i}{\hbar}[d\vec{\alpha}\cdot\vec{L}, \vec{r}]$$

$$\vec{r}\,' = \left(1+\frac{i}{\hbar}d\vec{\alpha}\cdot\vec{L}\right)\vec{r}\left(1-\frac{i}{\hbar}d\vec{\alpha}\cdot\vec{L}\right)$$

to first order in $d\vec{\alpha}$. This is the leading order result for a unitary transformation

$$\vec{r}\,' = e^{\frac{i}{\hbar}d\vec{\alpha}\cdot\vec{L}}\,\vec{r}\,e^{-\frac{i}{\hbar}d\vec{\alpha}\cdot\vec{L}}$$

In fact, this expression even works for finite rotations:

$$\vec{r}\,' = e^{\frac{i}{\hbar}\vec{\alpha}\cdot\vec{L}}\ \vec{r}\ e^{-\frac{i}{\hbar}\vec{\alpha}\cdot\vec{L}}.$$

To see that this is true, notice that

$$\vec{r}\,'(|\alpha| + d|\alpha|) = \vec{r}\,'(|\alpha|) + d|\alpha|\,\hat{\alpha}\times\vec{r}\,'(|\alpha|)$$

$$\frac{d\vec{r}\,'}{d\alpha} = \hat{\alpha}\times\vec{r}\,'(\alpha) \quad \text{with b.c. } \vec{r}\,'(0) = \vec{r}.$$

Differentiating the above expression for $\vec{r}\,'$ gives:

$$\frac{d\vec{r}\,'}{d\alpha} = e^{\frac{i}{\hbar}\vec{\alpha}\cdot\vec{L}}\left(\frac{i}{\hbar}\hat{\alpha}\cdot\vec{L}\,\vec{r} - \vec{r}\,\frac{i}{\hbar}\hat{\alpha}\cdot\vec{L}\right)e^{-\frac{i}{\hbar}\vec{\alpha}\cdot\vec{L}}$$

$$= e^{\frac{i}{\hbar}\vec{\alpha}\cdot\vec{L}}(\hat{\alpha}\times\vec{r})e^{-\frac{i}{\hbar}\vec{\alpha}\cdot\vec{L}} = \hat{\alpha}\times\vec{r}\,' \checkmark$$

What effect does the unitary operator $e^{\frac{i}{\hbar}\vec{\alpha}\cdot\vec{L}}$ have on the states?

$$\langle \vec{r}_0 | e^{\frac{i}{\hbar}\vec{\alpha}\cdot\vec{L}} \, \vec{r} \, e^{-\frac{i}{\hbar}\vec{\alpha}\cdot\vec{L}} = \langle \vec{r}_0 | \, \vec{r}\,'$$

$$= \langle \vec{r}_0 | \, \vec{r}_0\,' ,$$

where $\vec{r}_0\,'$ is the vector $\vec{r}_0$ rotated about the axis $\hat{\alpha}$ by $|\alpha|$.

Multiplying on the right by $e^{\frac{i}{\hbar}\vec{\alpha}\cdot\vec{L}}$,

$$\langle \vec{r}_0 | e^{\frac{i}{\hbar}\vec{\alpha}\cdot\vec{L}} \, \vec{r} = \vec{r}_0\,' \langle \vec{r}_0 | e^{\frac{i}{\hbar}\vec{\alpha}\cdot\vec{L}} .$$

Thus $\langle \vec{r}_0 | e^{\frac{i}{\hbar}\vec{\alpha}\cdot\vec{L}}$ is an eigenstate of $\vec{r}$ with eigenvalue $\vec{r}_0\,'$.

$$\langle \vec{r}_0 | e^{\frac{i}{\hbar}\vec{\alpha}\cdot\vec{L}} = \langle \vec{r}_0\,' | .$$

In particular, for an infinitessimal rotation

$$\langle \vec{r}_0 | \left(\mathbb{1} + \frac{i}{\hbar} \delta\vec{\alpha}\cdot\vec{L} \right) = \langle \vec{r}_0 + \delta\vec{\alpha} \times \vec{r}_0 |$$

For this reason, the operator $\vec{L}$ is referred to as the generator of rotations.

Let $|\psi'\rangle = e^{\frac{i\vec{\alpha}\cdot\vec{L}}{\hbar}} |\psi\rangle$

$$\psi'(\vec{r}_0) = \langle \vec{r}_0 | \psi' \rangle = \langle \vec{r}_0 | e^{\frac{i\vec{\alpha}\cdot\vec{L}}{\hbar}} |\psi\rangle$$

$$= \langle \vec{r}_0{}' | \psi \rangle = \psi(\vec{r}_0{}'),$$

which is the wavefunction at the rotated position.

Compare the role of angular momentum in generating rotations with the role of linear momentum in generating translations:

$$e^{\frac{i\vec{p}\cdot\vec{\lambda}}{\hbar}} \, \vec{r} \, e^{\frac{-i\vec{p}\cdot\vec{\lambda}}{\hbar}} = \vec{r} + \vec{\lambda}.$$

$$\langle \vec{r} | e^{\frac{i\vec{p}\cdot\vec{\lambda}}{\hbar}} = \langle \vec{r} + \vec{\lambda} |$$

Differential operator representation

We can use the relation

$$\langle \vec{r}_0 | \left(1 + \frac{i}{\hbar} \delta\vec{\alpha} \cdot \vec{L}\right) = \langle \vec{r}_0 + \delta\vec{\alpha} \times \vec{r}_0 |$$

to construct explicit differential operator representations of $\vec{L}$, analogous to the representation $\vec{p} = \frac{\hbar}{i} \nabla$. In spherical polar coordinates r, θ, φ, where

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

we can denote $\langle \vec{r} | = \langle r, \theta, \varphi |$. Under a rotation, r is unchanged. For a rotation about the z-axis

$$\theta \to \theta \quad , \quad \varphi \to \varphi + \delta\alpha.$$

$$\langle r,\theta,\varphi|\left(1+\frac{i}{\hbar}\delta\alpha L_z\right)=\langle r,\theta,\varphi+\delta\alpha|$$

$$=\langle r,\theta,\varphi|+\delta\alpha\frac{\partial}{\partial\varphi}\langle r,\theta,\varphi|$$

Thus

$$\boxed{\langle r,\theta,\varphi|L_z=\frac{\hbar}{i}\frac{\partial}{\partial\varphi}\langle r,\theta,\varphi|}$$

Now, for an infinitessimal rotation about the x-axis,

$$x\to x,\quad y\to y-\delta\alpha z,\quad z\to z+\delta\alpha y$$

$$\delta z=\delta\alpha y=\delta\alpha r\sin\theta\sin\varphi=r\,\delta\cos\theta$$
$$=-r\sin\theta\,\delta\theta$$

Thus, under this infinitessimal rotation,

$$\theta\to\theta+\delta\theta=\theta-\delta\alpha\sin\varphi$$

x is unchanged, so $\delta(\sin\theta\cos\varphi)=0$.

$$\cos\theta\cos\varphi\,\delta\theta-\sin\theta\sin\varphi\,\delta\varphi=0$$

$$\delta\varphi=\cot\theta\cot\varphi\,\delta\theta=-\cot\theta\cos\varphi\,\delta\alpha$$

$$\langle r,\theta,\varphi|\left(1+i\,\frac{\delta\alpha\, L_x}{\hbar}\right) = \langle r,\theta-\delta\alpha\sin\varphi,\ \varphi-\delta\alpha\cot\theta\cos\varphi|$$

$$\boxed{\langle r,\theta,\varphi|\,L_x = \frac{\hbar}{i}\left(-\sin\varphi\,\frac{\partial}{\partial\theta}-\cot\theta\cos\varphi\,\frac{\partial}{\partial\varphi}\right)\langle r,\theta,\varphi|}$$

Under an infinitessimal rotation about the y-axis, one has

$$\langle r,\theta,\varphi| \rightarrow \langle r,\ \theta+\delta\alpha\cos\varphi,\ \varphi-\delta\alpha\cot\theta\sin\varphi|.$$

Therefore

$$\boxed{\langle r,\theta,\varphi|\,L_y = \frac{\hbar}{i}\left(\cos\varphi\,\frac{\partial}{\partial\theta}-\cot\theta\sin\varphi\,\frac{\partial}{\partial\varphi}\right).}$$

The operators $L_\pm = L_x \pm i L_y$ have the representation

$$\boxed{\langle r,\theta,\varphi|\,L_\pm = \frac{\hbar}{i}\,e^{\pm i\varphi}\left[\pm i\frac{\partial}{\partial\theta}-\cot\theta\frac{\partial}{\partial\varphi}\right]\langle r,\theta,\varphi|}$$

Furthermore, $\vec{L}^2 = L_x^2+L_y^2+L_z^2$ has the rep.

$$\boxed{\langle r,\theta,\varphi|\,\vec{L}^2 = -\hbar^2\left[\frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\varphi^2}+\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right)\right]\langle r,\theta,\varphi|}$$

The Laplacian takes the simple form

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

Eigenfunctions

$$\langle \theta, \varphi | l m \rangle \equiv Y_{lm}(\theta, \varphi)$$

$$L_z | l m \rangle = m \hbar \, | l m \rangle$$

$$\langle \theta, \varphi | L_z | l m \rangle = \frac{\hbar}{i} \frac{\partial}{\partial \varphi} Y_{lm}(\theta, \varphi) = m \hbar \, Y_{lm}$$

$$\boxed{Y_{lm}(\theta, \varphi) = e^{i m \varphi} \, Y_{lm}(\theta, 0)}$$

Y_{lm} must be single-valued under $\varphi \to \varphi + 2\pi$ for the wave function to be continuous.

$$e^{im2\pi} = \mathbb{1} \Rightarrow m \in \mathbb{Z}.$$

This implies, in particular, that $l \equiv m_{max}$ must be an integer. <u>Orbital angular momentum is described by integer quantum numbers only.</u>

<u>Rotations in spin space ($s = 1/2$)</u>

By analogy with rotations discussed above, consider the operator

$$\boxed{\vec{S}' = e^{\frac{i}{\hbar}\vec{\alpha}\cdot\vec{S}}\, \vec{S}\, e^{-\frac{i}{\hbar}\vec{\alpha}\cdot\vec{S}}}$$

$$\frac{d\vec{S}'}{d\alpha} = e^{\frac{i}{\hbar}\vec{\alpha}\cdot\vec{S}}\left(\frac{i}{\hbar}(\hat{\alpha}\cdot\vec{S})\vec{S} - \vec{S}\frac{i}{\hbar}\hat{\alpha}\cdot\vec{S}\right)e^{-\frac{i}{\hbar}\vec{\alpha}\cdot\vec{S}}$$

$$= e^{\frac{i}{\hbar}\vec{\alpha}\cdot\vec{S}}(\hat{\alpha}\times\vec{S})e^{-\frac{i}{\hbar}\vec{\alpha}\cdot\vec{S}} = \hat{\alpha}\times\vec{S}'$$

Thus the operator

$e^{\frac{i}{\hbar}\vec{\alpha}\cdot\vec{S}}$ plays the same role in spin-space as $e^{\frac{i}{\hbar}\vec{\alpha}\cdot\vec{L}}$ does in 3-space. For $s = 1/2$,

$$e^{\frac{i}{\hbar}\vec{\alpha}\cdot\vec{S}} = e^{i\frac{\vec{\alpha}\cdot\vec{\sigma}}{2}}.$$

What is the effect on the states?

Consider a rotation about the z-axis,

$$e^{-\frac{i S_z \phi}{\hbar}}|\chi\rangle = e^{-i\frac{\sigma_z\phi}{2}}\left(|\uparrow\rangle\langle\uparrow|\chi\rangle + |\downarrow\rangle\langle\downarrow|\chi\rangle\right)$$

$$= e^{-i\frac{\phi}{2}}|\uparrow\rangle\langle\uparrow|\chi\rangle + e^{i\frac{\phi}{2}}|\downarrow\rangle\langle\downarrow|\chi\rangle$$

What about a 2π rotation?

$$\phi \rightarrow \phi + 2\pi$$

$$e^{-i\sigma_z\pi}|\chi\rangle = e^{-i\pi}|\uparrow\rangle\langle\uparrow|\chi\rangle + e^{i\pi}|\downarrow\rangle\langle\downarrow|\chi\rangle$$

$$= -|\chi\rangle$$

Thus, the spin state changes sign under a 2π rotation! This does not violate the postulates of QM because there is no requirement that $|\chi\rangle$ be "continuous." It is simply a 2-component object representing an internal, purely quantum degree of freedom. The sign change can be observed using interferometry, and this strange prediction of QM has been confirmed!

$$e^{-i\frac{\vec{\sigma}\cdot\hat{\alpha}\,\alpha}{2}} = \mathbb{1}\cos\frac{\alpha}{2} - i\,\vec{\sigma}\cdot\hat{\alpha}\sin\frac{\alpha}{2}$$

$$= \begin{pmatrix} \cos\frac{\alpha}{2} - i\hat{\alpha}_z\sin\frac{\alpha}{2} & (-i\hat{\alpha}_x - \hat{\alpha}_y)\sin\frac{\alpha}{2} \\ (-i\hat{\alpha}_x + \hat{\alpha}_y)\sin\frac{\alpha}{2} & \cos\frac{\alpha}{2} + i\hat{\alpha}_z\sin\frac{\alpha}{2} \end{pmatrix}$$

(using $(\vec{\sigma}\cdot\hat{\alpha})^n = \begin{cases} 1, & n \text{ even} \\ \vec{\sigma}\cdot\hat{\alpha}, & n \text{ odd} \end{cases}$)

Group properties of rotations: SO(3), SU(2)

The usual way to represent rotations is with orthogonal matrices:

$$\vec{r}\,' = R\vec{r} \quad , \quad R^T R = R R^T = \mathbb{1}.$$

A rotation can be specified by the 3-Cartesian components of the $\vec{\alpha}$; $\hat{\alpha}$ = axis of rotation, $|\alpha|$ = angle of rotation about the axis

$$3 \text{ real parameters} = \underbrace{3\times 3}_{\text{elements}} - \underbrace{6}_{\text{constraints}}$$

The set of all rotation matrices forms a group known as SO(3).

They satisfy the 4 group axioms:

1. $R_1 R_2 = R_3 \in G$

$$(R_1 R_2)(R_1 R_2)^T = R_1 R_2 R_2^T R_1^T = \mathbb{1}$$

2. $R_1 (R_2 R_3) = (R_1 R_2) R_3$

3. $\mathbb{1} \in G \qquad \mathbb{1}^T = \mathbb{1}$

4. $R^{-1} = R^T \in G$

The group G is denoted $SO(3)$, special orthogonal group, because it omits some orthogonal transformations (like the parity operation $\vec{r} \to -\vec{r}$ that are not reachable through rotations alone). $\Pi = \begin{pmatrix} -1 & & \\ & -1 & \\ & & -1 \end{pmatrix} = -\mathbb{1}$.

In QM, we have seen that rotations can also be represented by unitary matrices:

$$D(\vec{\alpha}) = e^{-i\frac{\vec{\alpha}\cdot\vec{J}}{\hbar}},$$

where $\vec{J}$ can represent orbital, spin or a combination.

For $s = 1/2$, we saw

$$D(\vec{\alpha}) = e^{\frac{i\vec{\alpha}\cdot\vec{\sigma}}{2}} = 2\times2 \text{ unitary matrix}$$

which is also unimodular (determinant $= 1$). These matrices also form a group obeying the 4 group axioms.

This group is known as $SU(2)$, a subgroup of $U(2)$, the group of all unitary 2×2 matrices (not necesarilly unimodular).

Since rotations can be represented by both the groups $SO(3)$ and $SU(2)$, one might assume that $SO(3)$ and $SU(2)$ are isomorphic, but this is not the case, due to the fact that for half-odd integer representations of $SU(2)$, 2π rotations give $-\mathbb{1}$.