Symmetries IV : Discrete Symmetries in Q.M.

To complete the 'symmetries' topic in this course, we will discuss 2 important discrete symmetries in Q.M: parity and time reversal symmetries.

In contrast to the continuous Lie Groups we have been studying in past few weeks, parity and time reversal are both discrete groups - similar to those we discussed at the start of the course when we first introduced concept of a group.

You have studied Parity symmetry in QMB - and have seen it's importance in solving the Schroedinger Equation for systems where the potential is parity invariant.

Here we will focus on formal properties of this symmetry in relation to the Dirac formalism.

Parity:

Classically, parity is just space inversion

i.e. $\vec{x} \to -\vec{x}$.

In Q.M. let's represent parity operator by $\hat{\pi}$

(following notation of Sakurai)

Now the observable related to the classical position $\vec{x}$ is the expectation value $\langle\alpha|\hat{\vec{x}}|\alpha\rangle$

where $\hat{\vec{x}}$ is the position operator and $|\alpha\rangle$ some state in our Hilbert space.

The parity transformed state $|\alpha\rangle' \equiv \hat{\pi}|\alpha\rangle$

By comparison with how $\vec{x}$ transforms it's natural to require:-

$$'\langle\alpha|\hat{\vec{x}}|\alpha'\rangle = \langle\alpha|\hat{\pi}^{+}\hat{\vec{x}}\hat{\pi}|\alpha\rangle$$

$$= -\langle\alpha|\hat{\vec{x}}|\alpha\rangle.$$

$\forall\ |\alpha\rangle \in \mathcal{H}$

$$\Rightarrow \quad \hat{\pi}^{+}\hat{\vec{x}}\hat{\pi} = -\hat{\vec{x}}$$

Clearly $\hat{\pi}^{+} = \hat{\pi}^{-1}$ if we require $\langle\alpha'|\alpha'\rangle = \langle\alpha|\alpha\rangle$

and so $\hat{\pi}^{-1}\,\hat{\vec{x}}\,\hat{\pi} = -\hat{\vec{x}}$

$$\Rightarrow \{\hat{\vec{x}}, \hat{\pi}\} = 0$$

so $\hat{\pi}$ anti-commutes with $\hat{\vec{x}}$.

How does $\hat{\pi}$ act on momentum $\hat{\vec{p}}$?

Recall that $\hat{\vec{p}}$ is the generator of space translations:

$$\hat{T}(\vec{a}) \equiv e^{-i(\vec{a}\cdot\hat{\vec{P}}/\hbar)}$$ generates translation group.

is the group transformation that shifts $\vec{x} \to \vec{x}+\vec{a}$

Proof: $\hat{T}(\vec{a})\,|\vec{x}\rangle$

$$\hat{\vec{x}}\;\hat{T}(\vec{a})|\vec{x}\rangle = \hat{T}(\vec{a})\;\hat{\vec{x}}\,|\vec{x}\rangle + [\hat{\vec{x}}, \hat{T}(\hat{a})]\,|\vec{x}\rangle$$

$$= \vec{x}\;\hat{T}(\vec{a})|\vec{x}\rangle + \hat{a}\;\hat{T}(\vec{a})\,|\vec{x}\rangle$$

(since $[\hat{\vec{x}}, \hat{T}(\vec{a})] = \vec{a}\;\hat{T}(\vec{a})$)

$$\Rightarrow \quad \hat{\vec{x}}\left(\hat{T}(\vec{a})|\vec{x}\rangle\right) = (\vec{x}+\vec{a})\left(\hat{T}(\hat{a})|\vec{x}\rangle\right)$$

Hence up to an overall phase (which we choose $=1$)

$$e^{-i\vec{a}\cdot\vec{\hat{P}}/\hbar}\,|\vec{x}\rangle = |\vec{x}+\vec{a}\rangle.$$

Thus confirming that $\vec{\hat{P}}$ is the generator of space translations. Indeed from what we have learned about Lie Groups and Lie Algebra's we recognize that expanding $\hat{T}(\vec{a})$ for small $\hat{a}$:-

$$\hat{T}(\hat{a}) \simeq 1 - i\vec{a}\cdot\vec{\hat{P}}/\hbar + O(\hat{a}^2)$$

$\Rightarrow$ $\left(\vec{\hat{P}}/\hbar\right)$ generates the Lie Algebra :-

$$[\hat{P}_i, \hat{P}_j] = 0.$$

\- Abelian algebra. The corresponding Lie Group is also abelian. It has dimension 3 and it's easy to check that $\{\hat{T}(\vec{a})\}$ satisfies axioms required for a group.

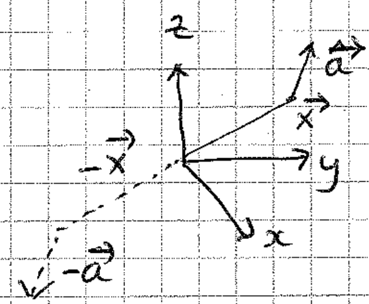
The group is isomorphic to $\mathbb{R}^3$ since the parameters $\vec{a} = (a_x, a_y, a_z)$ can have any real value $a_i \in (-\infty, \infty)$ $i = 1, 2, 3$.

This is an example of a <u>non-compact group</u>

By comparison group like $SO(3)$, $SU(2)$ or $U(1)$ are <u>compact</u> in that the group parameters are angles so that e.g. $g(\theta) \equiv e^{-i\theta}$ is an element of the group $U(1)$ ("1×1" unitary matrices).

$$g^{\dagger} = g^{*} = e^{i\theta} = g^{-1}. \qquad \underbrace{0 \leq \theta \leq 2\pi}$$

Consider the two operations of Parity transformation and shift in co-ordinate $\vec{x} \to \vec{x} + \vec{a}$



$$\Rightarrow \begin{pmatrix}\text{Parity}\\ \text{transformation}\end{pmatrix}\begin{pmatrix}\text{translation}\\ \text{by } \vec{a}\end{pmatrix} = \begin{pmatrix}\text{translation}\\ \text{by}\\ -\vec{a}\end{pmatrix}\begin{pmatrix}\text{Parity}\\ \text{transformation}\end{pmatrix}$$

$$\Rightarrow \hat{\Pi}\,\hat{T}(\hat{a}) = \hat{T}(-\vec{a})\,\hat{\Pi}$$

If we take $\vec{a}$ to be infinitesimal, then

$$\Rightarrow \hat{\vec{P}}\,\hat{\Pi} = -\hat{\Pi}\,\hat{\vec{P}}$$

$$\text{or} \quad \{\hat{\Pi}, \hat{\vec{P}}\} = 0$$

This is what we might expect – i.e. action of parity on $\vec{\hat{p}}$ is similar to it's action on $\vec{\hat{x}}$.

From this it follows that for orbital angular momentum $\vec{\hat{L}} = \vec{\hat{x}} \times \vec{\hat{p}}$; $\boxed{\hat{\Pi}^{-1} \vec{\hat{L}} \hat{\Pi} = \vec{\hat{L}}}$

we might guess the same would hold for spin angular momentum $\vec{\hat{S}}$: $\hat{\Pi}^{-1} \vec{\hat{S}} \hat{\Pi} = \vec{\hat{S}}$

so that $\hat{J} \equiv \hat{L} + \hat{S}$ transforms : $\boxed{\hat{\Pi}^{-1} \vec{\hat{J}} \hat{\Pi} = \vec{\hat{J}}.}$

Infact if we think about rotation group in 3d

$R_i(\theta_i)$ defined rotations by angle θ_i about i^{th} axis.

and were explicitly given as a 3×3 matrices (see previous lecture)

$$\vec{x} \xrightarrow{R} \vec{x}' = R\vec{x}$$

The parity transformation is just $R_\pi = \begin{pmatrix} -1 & & 0 \\ & -1 & \\ 0 & & -1 \end{pmatrix}$

and it's clear that $\underline{[R_\pi, R_i(\theta_i)] = 0}$

Infact $R_\pi, R_i(\theta_i)$ form $SO(3) \times Z_2$ group.

It follows from this that

in Q.M, - as we have seen, group SO(3)

generated by $R_i(\theta_i)$ is represented by $\mathcal{D}(\hat{R}_i(\theta_i))$

where $\hat{R}_i(\theta_i) = e^{-i\hat{J}_i\theta_i/\hbar}$. The representation of

R_π is $\hat{\Pi}$ in our notation.

$\therefore$ it is necessary that $[\hat{\Pi}, \mathcal{D}(\hat{R}_i(\theta_i))] = 0$

$\Rightarrow$ (taking θ_i small) $\boxed{[\hat{\Pi}, \hat{J}_i] = 0}$

which is confirmation of what we guessed before

- but now we have proven this.

Parity Eigenstates.

$\hat{\Pi}|\alpha\rangle = \lambda_\alpha|\alpha\rangle$; Clearly since $\hat{\Pi}^2 = \hat{I}$

(identity operator) $\lambda_\alpha^2 = 1$. $\Rightarrow$ $\lambda_\alpha = \pm 1$.

'even' parity ('+'); 'odd' parity ('−').

We can derive certain selection rules for the matrix elements of an operator $\hat{O}$ between parity eigenstates.

Let $|\alpha\rangle$, $|\beta\rangle$ be parity eigenstates : $\hat{\Pi}|\alpha\rangle = \lambda_\alpha |\alpha\rangle$

$\hat{\Pi}|\beta\rangle = \lambda_\beta |\beta\rangle$

$(\lambda_\alpha^2 = \lambda_\beta^2 = 1)$. Consider the case when $\hat{O}$ transforms with well defined parity :-

$$\hat{\Pi}^{-1}\hat{O}\hat{\Pi} = \lambda_0 \hat{O} \qquad (\lambda_0^2 = 1).$$

Then $$\langle\beta|\hat{O}|\alpha\rangle = \langle\beta|\hat{\Pi}^{+}(\hat{\Pi}^{+})^{-1}\hat{O}\hat{\Pi}^{-1}\hat{\Pi}|\alpha\rangle$$
$$= \lambda_\beta\lambda_\alpha \langle\beta|(\hat{\Pi}^{+})^{-1}\hat{O}\hat{\Pi}^{-1}|\alpha\rangle.$$

but $\hat{\Pi}^{+} = \hat{\Pi}^{-1}$ ($\hat{\Pi}$ is unitary)

and $\hat{\Pi}\hat{O}\hat{\Pi}^{-1} = \lambda_0 \hat{O}$

$$\therefore \langle\beta|\hat{O}|\alpha\rangle = (\lambda_\alpha\lambda_\beta\lambda_0)\langle\beta|\hat{O}|\alpha\rangle$$

$\Rightarrow \boxed{\lambda_\alpha\lambda_\beta\lambda_0 = 1} \longrightarrow$ Selection rule.

otherwise $\langle\beta|\hat{O}|\alpha\rangle = 0$.

e.g. consider matrix element

$\langle\alpha|\,\hat{\vec{x}}\,|\beta\rangle$. Then $\hat{O} = \hat{\vec{x}}$ with $\lambda_0 = -1$.

so $\langle\alpha|\,\hat{\vec{x}}\,|\beta\rangle \neq 0$ iff $\boxed{\lambda_\alpha \lambda_\beta = -1}$

This implies states $|\alpha\rangle$, $|\beta\rangle$ must have opposite parity assignments.

Infact matrix elements like this are related to process of photon emission by atoms, where $\langle\alpha|\,\hat{\vec{x}}\,|\beta\rangle$ is related to amplitude of a process where an atom in state $|\alpha\rangle$ emits a photon and in doing so ends up in the new state $|\beta\rangle$. The above selection rule tells us that such a photon emission necessarily requires atom to change its parity state odd $\to$ even or vise-versa.

Time-reversal invariance

So far, we have considered symmetries in Q.M. that are realized via <u>unitary</u> transformation on ket vectors:-

$$|\alpha\rangle \longrightarrow \hat{S}|\alpha\rangle.$$

$$|\beta\rangle \longrightarrow \hat{S}|\beta\rangle \quad \text{such that}$$

amplitude $\langle\beta|\alpha\rangle \rightarrow \langle\beta|\hat{S}^{\dagger}\hat{S}|\alpha\rangle$

$$= \langle\beta|\alpha\rangle \quad \text{remains unchanged}$$

since $\boxed{\hat{S}^{\dagger}\hat{S} = \hat{I}}$

We can always write $\hat{S} = e^{i\hat{G}}$

where $\hat{G}$ is some <u>Hermitian operator</u> $\left(\Rightarrow \hat{S}^{\dagger} = \hat{S}^{-1}\right)$

The fact that $\hat{S}$ is a symmetry of the theory implies that $\langle\beta|\hat{G}|\alpha\rangle$ remains unchanged in time, that is under time evolution:

$$\langle\beta|\hat{G}|\alpha\rangle \xrightarrow[\text{evolution}]{\text{time}} \langle\beta|e^{+it\hat{H}/\hbar}\hat{G}\,e^{-it\hat{H}/\hbar}|\alpha\rangle$$

$$= \langle\beta|\hat{G}|\alpha\rangle.$$

It follows that

$$e^{it\hat{H}/\hbar}\,\hat{G}\,e^{-it\hat{H}/\hbar} = \hat{G}$$

i.e. $[\hat{H}, \hat{G}] = 0$.

for any symmetry of the theory.

We then recognize a "conservation law"

(from Hamilton's Equations of motion)

that $\frac{d}{dt}\langle\beta|\hat{G}|\alpha\rangle = 0$.

Here $\hat{G}$ could represent angular momentum,

Parity*, or e.g. $\vec{\hat{p}}$ in the case

where our system is <u>translationally</u> <u>invariant</u>.

* [In the case of parity we could write
$\hat{\Pi} = e^{i\pi\hat{n}}$ where $\hat{n}|\alpha\rangle = n|\alpha\rangle$ with n an <u>even</u> integer

for parity even states and n = odd integer for

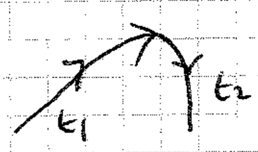
odd parity states]

As we shall see in the case of <u>time-reversal symmetry</u>, this requirement of the symmetry being 'realized' via unitary transformations, can be relaxed slightly....

First consider classically what we would understand by time reversal invariance:

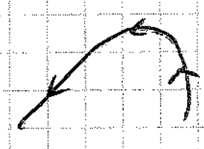
time reversal simply means operation $t \to -t$.

Assuming a non-dissipative system (so mechanical energy is conserved) then if $\vec{x}(t)$ is a solution to the equations of motion e.g. of a point particle in some potential $V(\vec{x})$; then $\vec{x}(-t)$ is <u>also</u> a solution.



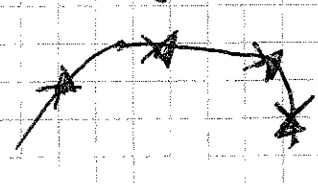
$t_1 < t_2$

$\vec{x}(t)$



time reversed solution $\vec{x}(-t)$

In fact if one imagined a situation where at some time t^*, the particles velocity was reversed – then it would follow precisely time reversed solution for $t > t_*$



What about Q.M.?

Well the Schroedinger equation plays the role of classical equations of motion.

However we have already seen that at a deeper level, the evolution operator $\hat{U}(t,t_0) = e^{-i(t-t_0)\hat{H}/\hbar}$ defines time-evolution in Q.M. Thus we need to focus on this operator to learn about time-reversal in Q.M.

Let $|\alpha\rangle$ be an state in our Hilbert space at $t=t_0$.

Then define $\hat{\Theta}|\alpha\rangle$ to be the time reversed state at $t=t_0$. For simplicity set $t_0=0$.

Now consider evolving the state $\Theta|\alpha\rangle$ in time by an amount $t=\delta t$:- $(\delta t \ll 1)$

The evolved state is $\left(1 - \frac{i\hat{H}}{\hbar}\delta t\right)\hat{\Theta}|\alpha\rangle$

This new state can equally be thought of as being obtained by first taking $|\alpha\rangle$ at $t=0$, evolving it by $t=-\delta t$ and then performing time reversal:-

$$\hat{\Theta}\left(1+i\frac{\hat{H}}{\hbar}\delta t\right)|\alpha\rangle.$$

e.g. Consider $|\alpha\rangle = |\vec{p}\rangle$ - a state in the momentum basis. $\Theta|\vec{p}\rangle = |-\vec{p}\rangle$ since $\hat{\vec{P}} \to -\hat{\vec{P}}$ under t-reversal. Then $\left(1-i\frac{\hat{H}}{\hbar}\delta t\right)|-\vec{p}\rangle$

$$= |-\vec{p}, t=\delta t\rangle$$

whereas $\hat{\Theta}\left(1+i\frac{H\delta t}{\hbar}\right)|\vec{p}\rangle = \Theta|\vec{p}, t=-\delta t\rangle$

$$= |-\vec{p}, t=+\delta t\rangle$$

Thus, quite generally, we have:-

$$\left(1-i\frac{\hat{H}}{\hbar}\delta t\right)\hat{\Theta} = \hat{\Theta}\left(1+i\frac{\hat{H}}{\hbar}\delta t\right).$$

$$\Rightarrow \quad -i\hat{H}\hat{\Theta} = \hat{\Theta}(i\hat{H})$$

cf. similar eq^n we had for $\hat{\Pi}$ and $\hat{\vec{P}}$

Now a subtlety!

If $\hat{\Theta}$ is a unitary operator then

$$\hat{\Theta}(i\hat{H}) = i\,\hat{\Theta}\hat{H}$$

and we can cancel the i factors so that

$$-\hat{H}\hat{\Theta} = \hat{\Theta}\hat{H} \qquad \text{i.e. } \{\hat{H}, \hat{\Theta}\} = 0 .$$

But this is physically unacceptable!
It implies that if e.g. $|\psi\rangle$ is an energy eigenstate with eigenvalue $E \geq 0$:-

$\hat{H}|\psi\rangle = E|\psi\rangle$, the time-reversed state $\hat{\Theta}|\psi\rangle$ has -ve energy!

$$\hat{H}(\hat{\Theta}|\psi\rangle) = -\hat{\Theta}(\hat{H}|\psi\rangle) = -\hat{\Theta}(E|\psi\rangle)$$
$$= -E(\hat{\Theta}|\psi\rangle).$$

The only consistent choice is to make $\hat{\Theta}$ anti-unitary

Anti-Unitary Operators

Definition: $\hat{\Theta}$ is an anti-unitary operator if $\forall\, |\alpha\rangle, |\beta\rangle$ and for $|\alpha'\rangle = \hat{\Theta}|\alpha\rangle$; $|\beta'\rangle = \hat{\Theta}|\beta\rangle$

(1) $\langle \beta' | \alpha' \rangle = \overline{\langle \beta | \alpha \rangle}$

(2) $\hat{\Theta}(a \cdot |\alpha\rangle + b|\beta\rangle) = \bar{a}\,\hat{\Theta}|\alpha\rangle + \bar{b}\,\hat{\Theta}|\beta\rangle \quad , \forall\, a,b \in \mathbb{C}$

notice $a, b \to \bar{a}, \bar{b}$. This also means $\hat{\Theta}$ is anti-linear

(1) + (2) $\Rightarrow$ decompose $\hat{\Theta} = \hat{O}\hat{K}$

where $\hat{K}$ is the 'complex conjugate' operator

$\hat{K}(a|\alpha\rangle) \equiv \bar{a}\,\overline{|\alpha\rangle}$ and $\hat{O}$ is any unitary operator.

Now, under the assumption that $\hat{\Theta}$ is anti-unitary

then $\hat{\Theta}(i\hat{H}) = -i\,\hat{\Theta}\hat{H}$.

$\therefore$ we learn $\hat{H}\hat{\Theta} = \hat{\Theta}\hat{H} \Rightarrow [\hat{H}, \hat{\Theta}] = 0$.

This makes more physical sense in that it shows $\hat{\Theta}$ is a symmetry in the usual sense

Acting on the state $|\psi, t=0\rangle$ we see that $\hat{\Theta}$ basically replaces $|\psi\rangle \to |\bar{\psi}\rangle$. $(\hat{O} = \hat{I})$

(for particles with spin this $\hat{\Theta}|\psi\rangle \to \hat{O}\,|\bar{\psi}\rangle$ where $\hat{O}$ is a particular unitary matrix - see later)

time-reversed wave functions

Recall configuration space wave function

$\Psi(\vec{x},t)$ is identified in Dirac formalism as:-

$$\Psi(\vec{x},t) = \langle \vec{x} \,|\, \Psi, t \rangle$$

where $|\Psi,t\rangle \equiv \hat{U}(t)\,|\Psi, t_0{=}0\rangle$ (have chosen $t_0 = 0$ for convenience)

$$\Rightarrow \quad \hat{\Theta}\,|\Psi,t\rangle = \hat{\Theta}\,\hat{U}\,\hat{\Theta}^{-1}\left(\hat{\Theta}\,|\Psi,t{=}0\rangle\right)$$

But $\hat{\Theta}\,\hat{U}(t)\,\hat{\Theta}^{-1} = \hat{U}(-t)$. (recall $\hat{\Theta}(i\hat{H}t) = -i\hat{H}t\hat{\Theta}$)

$$\Rightarrow \quad \hat{\Theta}\,|\Psi,t\rangle = \hat{U}(-t)\,\hat{\Theta}\,|\Psi,t{=}0\rangle$$

$$\langle \vec{x}\,|\,\hat{\Theta}\,|\Psi,t\rangle = \langle \vec{x}\,|\,\hat{U}(-t)\,\hat{\Theta}\,|\Psi,t{=}0\rangle$$

$$= \langle \vec{x}\,|\,\hat{U}(-t)\,|\overline{\Psi,t{=}0}\rangle$$

$$= \overline{\Psi}(\vec{x},-t)$$

So the wave function of the time-reversed state is $\overline{\Psi}(\vec{x},-t)$. This makes sense because recall the Schroedinger Eq^{n}:

$$i\hbar\frac{\partial\Psi}{\partial t}(x,t) = \hat{H}\,\Psi(\vec{x},t)$$

Given the solution $\Psi(\vec{x},t)$,

it automatically follows (by taking complex conjugate of the Equation) that $\Psi^{*}(\vec{x},-t)$ is also a solution. This represents the <u>time reversed solution</u>.

<u>Time-reversal of Operators</u>

Any observable $\hat{A}$ is even/odd under t-reversal if

$$\hat{\Theta}\,\vec{\hat{A}}\,\hat{\Theta}^{-1} = \pm\,\vec{\hat{A}}.$$

which implies that $\langle\alpha'|\,\vec{\hat{A}}\,|\alpha'\rangle = \pm\,\langle\alpha|\,\vec{\hat{A}}\,|\alpha\rangle$

where $|\alpha'\rangle = \Theta|\alpha\rangle$ is the time reversed state.

e.g. take $\vec{\hat{A}} = \vec{\hat{x}}$: the effect of $t\to -t$ should leave $\vec{\hat{x}}$ unchanged $\therefore$ $\Theta\,\vec{\hat{x}}\,\hat{\Theta}^{-1} = \vec{\hat{x}}$ – even under $t\to -t$.

$\hat{A} = \vec{\hat{p}}$ then $\hat{\Theta}\,\vec{\hat{p}}\,\hat{\Theta}^{-1} = -\vec{\hat{p}}$ $\quad$ $\vec{\hat{p}}$ – odd under $t\to -t$.

Similarly for orbital angular momentum

$$\hat{\Theta} \vec{\hat{L}} \hat{\Theta}^{-1} = \hat{\Theta} (\vec{\hat{x}} \times \vec{\hat{P}}) \hat{\Theta}^{-1}$$

$$= (\hat{\Theta} \vec{\hat{x}} \hat{\Theta}^{-1}) \times (\hat{\Theta} \vec{\hat{p}} \hat{\Theta}^{-1})$$

$$= -\vec{\hat{x}} \times \vec{\hat{P}} = -\vec{\hat{L}} .$$

Notice this odd assignment to $\vec{\hat{L}}$ is crucial

to maintain the commutation relations, because

if we start with:

$$[\hat{L}_x , \hat{L}_y] = i\hbar \hat{L}_z$$

Now act on both sides with $\hat{\Theta}$ to left and $\hat{\Theta}^{-1}$ to right

$$\hat{\Theta} [\hat{L}_x , \hat{L}_y] \hat{\Theta}^{-1} = \hat{\Theta} (i\hbar \hat{L}_z) \hat{\Theta}^{-1}$$

$$= [\hat{\Theta} \hat{L}_x \hat{\Theta}^{-1} , \hat{\Theta} \hat{L}_y \hat{\Theta}^{-1}] = -i\hbar \, \hat{\Theta} \hat{L}_z \hat{\Theta}^{-1}$$

!!

now use $\hat{\Theta} \hat{L}_i \hat{\Theta}^{-1} = -\hat{L}_i$

$$[-\hat{L}_x , -\hat{L}_y] = -i\hbar (-\hat{L}_z)$$

$\Rightarrow$ usual relations !!

If we had chosen $\hat{\Theta} \hat{L}_i \hat{\Theta}^{-1} = +\hat{L}_i$

this will violate the commutation relations!

A similar argument can be applied to spin angular momentum generators $\hat{S}_i$, namely we must demand $\hat{\Theta} \hat{S}_i \hat{\Theta}^{-1} = - \hat{S}_i$

$\Rightarrow$ $\hat{J}_i = \hat{L}_i + \hat{S}_i$ and the time-reversed

$\hat{\Theta} \hat{J}_i \hat{\Theta}^{-1} = - \hat{J}_i$ also satisfy the commutation relations.

Time-reversal of States with Angular Momentum

Since t-reversal for spinless particles $\Psi(\vec{x},t) \rightarrow \Psi^*(x,t)$

if we consider that part of the wave function describing orbital degrees of freedom naturally we think of spherical harmonics $Y_{\ell,m}(\theta,\varphi)$

Under complex conjugation $Y^*_{\ell,m_\ell}(\theta,\varphi) = Y_{\ell,-m_\ell}(\theta,\varphi)(-1)^{m_\ell}$

Hence, for kets $|\ell,m_\ell\rangle$, $\hat{\Theta}|\ell,m\rangle = (-1)^{m_\ell}|\ell,-m_\ell\rangle$

$$\hat{\Theta}^2 |\ell,m_\ell\rangle = (-1)^{2m_\ell}|\ell,m_\ell\rangle = |\ell,m_\ell\rangle$$

since $(-1)^{2m_\ell} = 1$. because m takes on integer values

$\therefore$ $\hat{\Theta}^2 = \hat{I}$ 'as one might expect'.

But what about states carrying spin angular momentum? Here we find something very surprising happens!

Consider spin $\frac{1}{2}$, and the two eigenstates of $\hat{S}_z$

namely $|j=\frac{1}{2}, m_j=+\frac{1}{2}\rangle \equiv |+\rangle$; $|j=+\frac{1}{2}, m_j=-\frac{1}{2}\rangle \equiv |-\rangle$

$\hat{S}_z |+\rangle = +\frac{\hbar}{2} |+\rangle$; $\hat{S}_z |-\rangle = -\frac{\hbar}{2} |-\rangle$.

Now consider time reversed states:-

$\hat{\Theta} |+\rangle$, $\hat{\Theta} |-\rangle$.

$$\hat{S}_z\left(\hat{\Theta}|+\rangle\right) = -\hat{\Theta}\hat{S}_z|+\rangle = -\frac{\hbar}{2}\left(\hat{\Theta}|+\rangle\right)$$ (remember $\{\hat{\Theta}, \hat{S}_i\} = 0$!)

$$\Rightarrow \quad \hat{\Theta}|+\rangle \sim |-\rangle$$
$$= e^{i\delta_+}|-\rangle$$ where δ_+ is some unknown phase.

Similarly $$\hat{S}_z\left(\hat{\Theta}|-\rangle\right) = -\hat{\Theta}\hat{S}_z|-\rangle$$
$$= +\hbar/2\left(\hat{\Theta}|-\rangle\right)$$

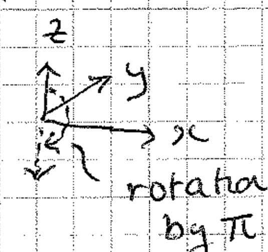
and so we can write $\hat{\Theta}|-\rangle = e^{i\delta_-}|+\rangle$

where δ_- is a second unknown phase.

Now we can learn something relating δ_+ and δ_-

The down state $|-\rangle = e^{-i\pi\hat{S}_y}|+\rangle$

where $e^{-i\pi\hat{S}_y}$ generates a rotation by π about y axis



$$\Rightarrow \hat{\Theta}|-\rangle = \hat{\Theta}\, e^{-i\pi\hat{S}_y}|+\rangle$$

$$= e^{-i\pi\hat{S}_y}\,\hat{\Theta}|+\rangle \qquad \text{(recall } \hat{\Theta} \text{ is } \underline{\text{anti}}\text{-unitary}$$

$$\text{so } \hat{\Theta}(i) = -i\,\hat{\Theta}\ !\ )$$

$$= e^{i\delta_+}\, e^{-i\pi\hat{S}_y}|-\rangle$$

but $|-\rangle = e^{-i\pi\hat{S}_y}|+\rangle$

$$\Rightarrow \quad \hat{\Theta}|-\rangle = e^{i\delta_+}\, e^{-2\pi i\hat{S}_y}|+\rangle$$

$$= e^{i\delta_-}|+\rangle$$

$e^{-2\pi i\hat{S}_y}$ represents a complete rotation (i.e. 2π) about y-axis

But in previous lectures we observed that under such a rotation, the spin states pick up a $-$ sign!

Using $\hat{S}_y = \frac{1}{2}\begin{pmatrix} 0 & i \\ -i & 0 \end{pmatrix}$, one can

check that under rotation by angle α,

$$e^{-i\alpha \hat{S}_y} |+\rangle = \cos(\alpha/2) |+\rangle - \sin(\alpha/2) |-\rangle$$

$\Rightarrow \alpha = 2\pi$, $e^{-2\pi i S_y} |+\rangle = -|+\rangle$!

$$\therefore \quad e^{i\delta_-} |+\rangle = e^{i\delta_+} (-1) |+\rangle$$

so $\boxed{\delta_+ = \delta_- + \pi}$

If we chose for simplicity $\delta_+ = 0$ so $\hat{\Theta} |+\rangle = |-\rangle$

we <u>must</u> have $\delta_- = -\pi \Rightarrow$ $\hat{\Theta} |-\rangle = - |+\rangle$

Now consider action of $\hat{\Theta}^2$:-

$$\hat{\Theta}^2 |+\rangle = \hat{\Theta}\,\hat{\Theta} |+\rangle = \hat{\Theta} |-\rangle = -|+\rangle$$

and $\hat{\Theta} |-\rangle = \hat{\Theta}\left(-|+\rangle\right) = -|-\rangle$

So for spin $\frac{1}{2}$ states, $\hat{\Theta}^2 = -\hat{I}$!!

In general, one finds that $\hat{\Theta}^2 |j, m_j\rangle = (-1)^{2j} |j, m_j\rangle$