Symmetry in QM:

Classical Physics: $L(q_i, \dot{q}_i)$

$$q_i \to q_i + \delta q_i \quad , \quad \frac{\partial L}{\partial q_i} = 0$$

$$\frac{d}{dt}\left(\frac{\partial L}{\partial \dot{q}_i}\right) = \frac{\partial L}{\partial q_i} = 0$$

so $p_i = \text{const.}$

In Hamilton: $$\frac{dp_i}{dt} = \{H, p_i\} = \frac{\partial H}{\partial q_i}\{q_i, p_i\} = 0$$

Symmetry: If $\{H, p_i\} = 0$, then $p_i = \text{const.}$

QM: symmetry operator (unitary) : $\mathcal{L}$.

$$\mathcal{L}^{+}\mathcal{L} = I \quad \leftarrow \text{unitary.}$$

G is constant of motion.

$$[H, \mathcal{L}] = 0 \rightleftharpoons \boxed{\mathcal{L}^{+} H \mathcal{L} = H} \quad \to \; i\hbar \frac{dG}{dt} = [G, H] = 0$$

Heinsenberg

If $\mathcal{L}$ depends on continuous parameter

$$\mathcal{L} \sim 1 - \frac{i}{\hbar}\varepsilon G$$

G → generator of symmetry.

→ Hermitian, $G^{+} = G$

$\sim$ ← approximate

$$\mathcal{L} = e^{-\frac{i}{\hbar}\varepsilon G}$$

Schrodinger:

$$G|g\rangle = g|g\rangle$$

↳ eigenket of G.

$$|g\rangle \to U(t,t_0)|g\rangle_{t_0}$$

↳ $= e^{-\frac{i}{\hbar}H(t-t_0)}$ if time independent V.

$$G|g\rangle_t = GU(t,t_0)|g\rangle_{t_0}$$

↳ $\overset{!}{=} U(t,t_0)\underbrace{G|g\rangle_{t_0}}_{g|g\rangle_{t_0}}$ ↙ $G(t) = UGU^{+} = G$

$UG = GU$.

$$G|g\rangle_t = g|g\rangle_t$$

Suppose $[H, \mathcal{L}] = 0$

$$H|n\rangle = E_n|n\rangle$$

↳ $H\mathcal{L}|n\rangle = \mathcal{L}H|n\rangle$

$$H\mathcal{L}|n\rangle \overset{!}{=} E_n\underbrace{\mathcal{L}|n\rangle}_{\text{is also an eigenket of } H.}$$

If $|n\rangle \neq \mathcal{L}|n\rangle$, then E_n is degenerate.

↑ allow phase difference.

Ex: $[\underset{\sim}{\mathcal{D}}(R), H] = 0$ $\leftarrow L$

$\hookrightarrow [\vec{J}, H] = 0$ $\leftarrow G$

$\hookrightarrow [J^2, H] = 0$

Introduce : $|n, j, m\rangle$: eigenket of H, J^2, J_z

$\mathcal{D}(R)|n, j, m\rangle$ has the same E_n for all R.

$$\hookrightarrow = \sum_{m'=-j}^{j} |n, j, m'\rangle \mathcal{D}^{(j)}_{m', m}(R)$$

$\uparrow$ $2j+1$ degenerate.

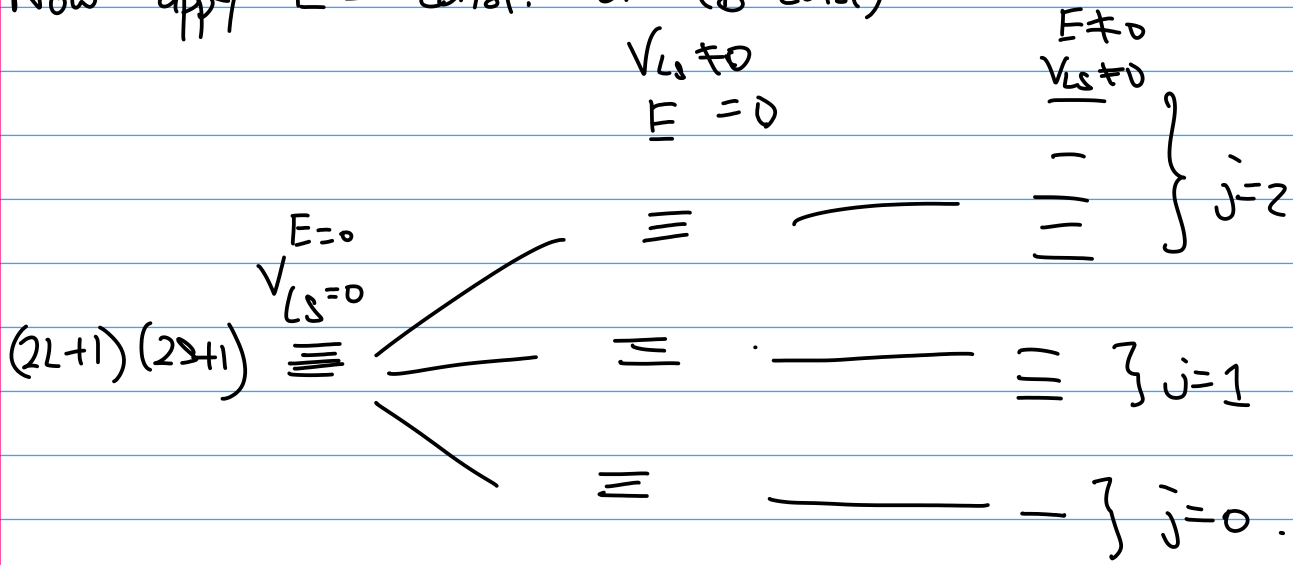
Application: $V = \underset{\substack{\uparrow \\ \text{central} \\ \text{potential}}}{V(r)} + \underbrace{V_{LS}\, \vec{L} \cdot \vec{S}}_{\text{spin-orbit interaction.}}$

If $V_{LS} = 0$ then we have $(2l+1)(2s+1)$ degenerate.

If $V_{LS} \neq 0$, $[V_{LS}(\vec{r})\, \vec{L} \cdot \vec{S}, \vec{J}] = 0$.

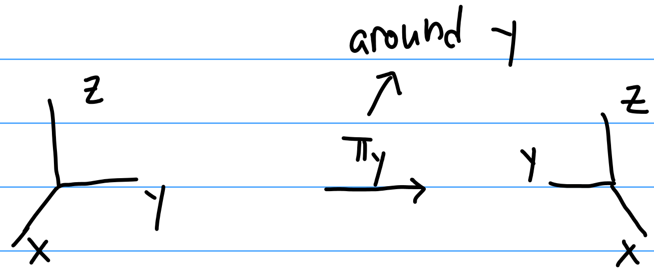
then $(2j+1)$ degenerate.

Now apply $E =$ const. or ($B =$ const)

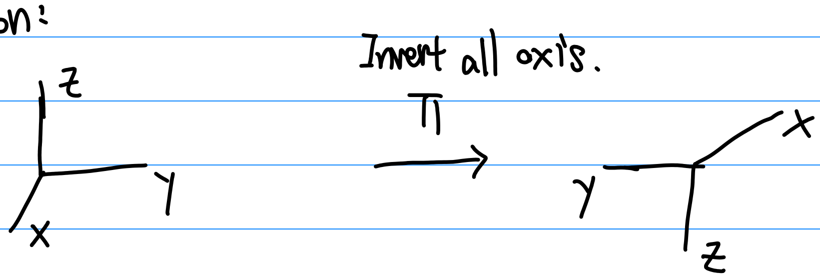


Discrete Symmetries:

→ Parity :



→ Space Inversion:



→ Corresponding transformation of ket state:

$$|\alpha\rangle \rightarrow \Pi|\alpha\rangle$$

$\uparrow$ parity operator (unitary)

$$\langle\alpha|\Pi^{\dagger}\vec{x}\,\Pi|\alpha\rangle = -\langle\alpha|\vec{x}|\alpha\rangle$$

$$\Pi^{\dagger}\vec{x}\,\Pi = -\vec{x}$$

$\hookrightarrow$ $\vec{x}\,\Pi = -\Pi\vec{x}$ $\rightarrow$ $\{\vec{x}, \vec{\Pi}\} = 0$

$\uparrow$ odd operator.

Odd operator if:	Even operator if:
$\{\Pi, \mathcal{L}\} = 0$	$[\Pi, \mathcal{L}] = 0$

$|x'\rangle$: position eigenket.

$$\vec{x}(\pi|\vec{x}'\rangle) = -\pi(\vec{x}|\vec{x}'\rangle) = -\vec{x}'\,\pi|\vec{x}'\rangle$$

$$\boxed{\pi|\vec{x}'\rangle = |-\vec{x}'\rangle}$$ ← convention, no phase $e^{i\phi}$

$$\boxed{\pi = \pi^{-1} = \pi^{\dagger}}$$ ← unitary and Hermitian.

$$\pi^2|x'\rangle = \pi|-x'\rangle = |x'\rangle$$

Eigenvalue of $\pi = \pm 1$

Translation:

$J(d\vec{x}')$: translation by $d\vec{x}'$

$$\boxed{\pi\, J(d\vec{x}') = J(-d\vec{x}')\,\pi}$$

$$\pi J(d\vec{x}')|\vec{x}'\rangle = J(-d\vec{x}')\,\pi|x'\rangle = |-x' - d\vec{x}'\rangle$$

$$\pi\left(1 - \frac{i}{\hbar}\vec{p}\cdot d\vec{x}'\right)\pi^{\dagger} = \left(1 + \frac{i}{\hbar}\vec{p}\cdot d\vec{x}'\right)$$

$$\left.\begin{aligned} \pi\vec{p}\,\pi^{\dagger} &= -p \\ \pi^{\dagger}\vec{p}\,\pi &= -\vec{p} \end{aligned}\right\}$$

$\{\pi, \vec{p}\} = 0$

So p is odd under parity

Angular Momentum:

$$[\Pi, \vec{L}] = 0 \quad , \quad \vec{L} = \vec{r} \times \vec{p}$$

$\uparrow$ $\vec{L}$ is even.

Rotation of 3d space:

$$R^{(parity)} = \begin{pmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{pmatrix} = -\hat{1}$$

$$R^{(parity)} R^{(rot)} = R^{(rot)} R^{(parity)}$$ $\leftarrow$ for matrix.

$\hookrightarrow \Pi \underbrace{\mathcal{D}(R)}_{= 1 - \frac{i}{\hbar}\epsilon \hat{n}\cdot\vec{J}} = \mathcal{D}(R) \Pi$ $\leftarrow$ postulate the same for operator.

$\hookrightarrow$ $\boxed{[\Pi, J] = 0 \quad \text{so} \quad \Pi^{\dagger}\vec{J}\Pi = \vec{J}}$

$\uparrow$ even operator.

	Rotation (J)	Parity (Π)	
$\vec{x}, \vec{p}$	vector	odd	Polar Vector
$\vec{J}, \vec{S}, \vec{L}$	vector	even	axial vector (pseudovector)
$\vec{S}\cdot\vec{x}, \vec{S}\cdot\vec{p}$	scalar	odd	pseudoscalar
$\vec{L}\cdot\vec{S}, \vec{x}\cdot\vec{p}$	scalar	even	True Scalar.

Wave function under parity:

$$\psi_\alpha(\vec{x}) = \langle \vec{x} | \alpha \rangle$$

$$\langle \vec{x} | \pi | \alpha \rangle = \langle -\vec{x} | \alpha \rangle = \psi_\alpha(-\vec{x}) = \psi_{parity}(x)$$

$$\boxed{\psi(x) \xrightarrow{\pi} \psi(-x)}$$

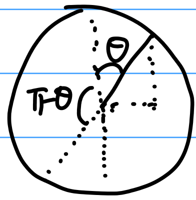
Eigenstate of parity: $\boxed{\pi | \alpha \rangle = \pm | \alpha \rangle}$

$$\langle \vec{x} | \pi | \alpha \rangle = \pm \langle \vec{x} | \alpha \rangle = \pm \psi_\alpha(x)$$

$$\langle -\vec{x} | \alpha \rangle = \boxed{\psi_\alpha(-\vec{x}) = \pm \psi_\alpha(x)} \rightarrow \begin{cases} + : \text{parity even} \\ - : \text{parity odd} \end{cases}$$

In spherical coordinate:

$r \to r$
$\theta \to \pi - \theta$
$\phi \to \pi + \phi$



$\cos\theta \to -\cos\theta$
$e^{im\phi} \to (-1)^m e^{im\phi}$

note:

$\pi|\alpha; l\, m\rangle = \delta|\alpha; l\, m\rangle$, $[\pi, L] = 0$

so Apply L_+ : $\pi|\alpha; l\; m+1\rangle = \delta|\alpha; l\; m+1\rangle$

so δ doesn't depend on m

$\langle\theta, \phi, r|\alpha; l\, m\rangle = R_{\alpha l}(r)\, Y_l^m(\theta, \phi)$

$\langle\theta, \phi|\pi|l, m\rangle = \langle\pi - \theta, \phi + \pi|l, m\rangle$

$\stackrel{!}{=} Y_l^m(\pi - \theta, \phi + \pi) = (-1)^l\, Y_l^m(\theta, \phi)$

so $\boxed{\pi|\alpha; l\, m\rangle = (-1)^l\, |\alpha; l\, m\rangle}$

Theorem: If $[H, \pi] = 0$, $H|n\rangle = E_n|n\rangle$ and $|n\rangle$ is non-degenerate.

then $|n\rangle$ is an eigenstate of π, so $|n\rangle$ must be either even or odd.

Take $|n_\pm\rangle = \frac{1\pm\Pi}{2}|n\rangle$ $\qquad \Pi\left(\frac{1\pm\Pi}{2}\right) = \frac{\Pi\pm1}{2} = \pm\left(\frac{1\pm\Pi}{2}\right)$

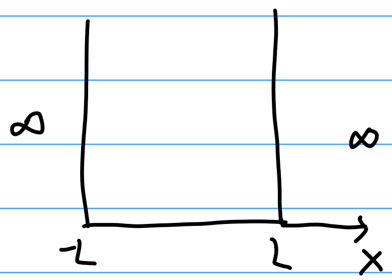
↳ $\Pi|n_\pm\rangle = \pm\left(\frac{1\pm\Pi}{2}\right)|n\rangle = \pm|n_\pm\rangle$

$H|n_\pm\rangle = E_n|n_\pm\rangle$

then $|n_+\rangle = |n_-\rangle$? $\qquad$ or $\qquad |n_+\rangle = 0$

$|n_-\rangle = 0 \qquad\qquad |n_-\rangle = |n_+\rangle$

Ex:



$\psi_n(x) = \frac{1}{\sqrt{L}}\sin\left(\frac{\pi}{2L}n(x+L)\right)$

$E_n = \frac{\hbar^2}{2m}\frac{\pi^2 n^2}{4L^2}$

When n = odd, then its even under parity
n = even, odd under parity.

odd: $\psi_{2k+1}(x) = \frac{(-1)^k}{\sqrt{L}}\cos\left(\frac{\pi}{L}(n+\frac{1}{2})x\right) \to \Pi\psi_{2k+1} \underset{\text{even}}{=} \psi_{2k+1}$

even: $\psi_{2k}(x) = \frac{(-1)^k}{\sqrt{L}}\sin\left(\frac{\pi}{L}kx\right) \to \Pi\psi_{2k} \underset{\text{odd}}{=} -\psi_{2k}$

Ex: free particle in 3d

$H = \frac{p^2}{2m}$ $\quad [H, \Pi] = 0$ $\quad$ with eigenstate $|\vec{p}\rangle$

but $\Pi|\vec{p}\rangle = |-\vec{p}\rangle$ so $|\vec{p}\rangle$ is not eigenstate of $|\pi\rangle$

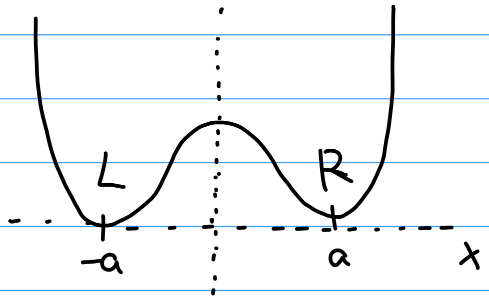
Also $E_p = \frac{p^2}{2m} = E_{-p}$, so it is degenerate.

So theorem doesn't apply.

We can use $\frac{|\vec{p}\rangle \pm |-\vec{p}\rangle}{\sqrt{2}}$ $\leftarrow$ eigenstate of Π, but not for $\vec{p}$

$|\vec{p}\rangle \leftarrow$ eigenstate of p, but not Π.

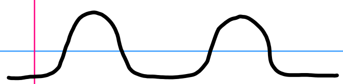
Ex: Symmetrical double-well potential:

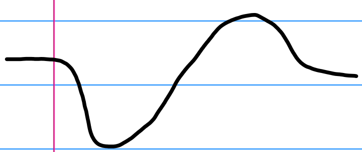


Since $U(x) = U(-x)$

$[\Pi, H] = 0$

So eigenstate have definite parity.

$\psi_0 =$  $= |S\rangle$

$\psi_1 =$  $= |A\rangle$

$$\left.\begin{aligned} \Pi|S\rangle &= |S\rangle \\ \Pi|A\rangle &= -|A\rangle \end{aligned}\right\} E_A > E_S$$

and $\Delta = E_A - E_S$ very small

then let
$$\left.\begin{aligned} |R\rangle &= \frac{1}{\sqrt{2}}(|S\rangle + |A\rangle) \\ |L\rangle &= \frac{1}{\sqrt{2}}(|S\rangle - |A\rangle) \end{aligned}\right\}$$

Not eigenstate of H

so its not stationary

overall phase.

$$|S\rangle \to e^{-\frac{i}{\hbar}E_S t}|S\rangle \quad , \quad |A\rangle \to e^{-\frac{i}{\hbar}E_A t}|A\rangle$$

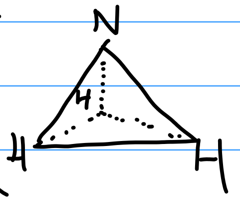
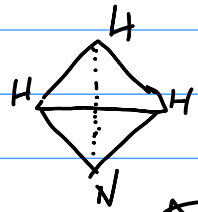
$$|R\rangle = \frac{1}{\sqrt{2}}\left(e^{-\frac{i}{\hbar}E_S t}|S\rangle + e^{-\frac{i}{\hbar}E_A t}|A\rangle\right)$$ ← has extra interference so state changes.

$$\doteq \frac{1}{\sqrt{2}} e^{-\frac{i}{\hbar}E_S t}\left(|S\rangle + e^{-\frac{i}{\hbar}\Delta t}|A\rangle\right)$$

period: $T = \frac{2\pi\hbar}{\Delta}$

After $t = T/2$ $\quad |R\rangle \xrightarrow{T/2} |L\rangle$

Ex: Ammonic Molecule: NH_3:

$\frac{1}{\sqrt{2}}\Bigg($  $\pm$  $\Bigg)$

$\sim |R\rangle$ $\sim |L\rangle$

Not eigenstate of H

since after Π it is not the same.

Parity Selection Rule:

suppose $[H, \Pi] = 0$

eigenvalues of Π, (± 1)

$\Pi |\alpha\rangle = \varepsilon_\alpha |\alpha\rangle$

$\Pi |\beta\rangle = \varepsilon_\beta |\beta\rangle$

If $\vec{x}$ is odd $\rightarrow$ $\Pi^\dagger x \Pi = -x = \Pi x \Pi^\dagger$

$$\langle\beta| x |\alpha\rangle = \langle\beta| \Pi^\dagger \Pi x \Pi^\dagger \Pi |\alpha\rangle$$

$$= \varepsilon_\alpha \varepsilon_\beta \langle\beta| \Pi x \Pi^\dagger |\alpha\rangle$$

$$\langle\beta|x|\alpha\rangle \overset{!}{=} -\varepsilon_\alpha \varepsilon_\beta \langle\beta| x |\alpha\rangle$$

$\hookrightarrow$ $\boxed{\langle\beta|x|\alpha\rangle (1 + \varepsilon_\alpha \varepsilon_\beta) = 0}$

* parity selection rule.

$$\boxed{\text{So } \langle\beta|x|\alpha\rangle = 0 \text{ unless } \varepsilon_\alpha\varepsilon_\beta = -1 \text{ or } \varepsilon_\alpha = -\varepsilon_\beta}$$

$$\langle\beta|x|\alpha\rangle = \int \psi_\alpha^* x \psi_\beta \, d^3x.$$

$\rightarrow$ Implys non-degenerate energy state cannot posess a permanent dipole moment.

$$\langle\alpha| \vec{x} \cdot \vec{r} |\alpha\rangle = 0$$

$\rightarrow \quad \langle \alpha'; l' m' | \vec{X} | \alpha; l. m \rangle = 0$ unless $\varepsilon_\alpha \varepsilon_\beta = -1.$

$\hookrightarrow \varepsilon_\alpha = (-1)^{l'} \qquad \varepsilon_\beta = (-1)^{l}$

$\hookrightarrow \quad \varepsilon_\alpha \varepsilon_\beta = (-1)^{l}(-1)^{l'} \Rightarrow \boxed{l - l' = \text{odd.}}$ ← parity selection rule.

Rotational selection rule:

$\hookrightarrow \; l = \begin{cases} l'-1 \\ l' \\ l+1 \end{cases} \xRightarrow{\text{with parity selection}} \boxed{l = l' \pm 1}$

Other discrete symettry:

- Point group
- Lattice translational.

Time Reversal Symmetry:

Newton: If $m\ddot{x} = -\vec{\nabla}V$: and $x(t)$ is a solution
then $x(-t)$ is also a solution.

Maxwell:
$$\left.\begin{aligned} m\ddot{\vec{x}} &= e\left(\vec{E} + \tfrac{1}{c}\vec{v}\times\vec{B}\right) \\ \vec{\nabla}\cdot\vec{E} &= 4\pi\rho \\ \vec{\nabla}\times\vec{B} - \tfrac{1}{c}\partial_t\vec{E} &= \tfrac{4\pi}{c}\vec{J} \\ \vec{\nabla}\times\vec{E} &= -\tfrac{1}{c}\partial_t B \\ \vec{\nabla}\cdot\vec{B} &= 0 \end{aligned}\right\}$$

if $t \to -t$, then
$\vec{E} \to \vec{E}$
$\vec{B} \to -\vec{B}$
$\rho \to \rho$
$\vec{J} \to -\vec{J}$
$\vec{v} \to -\vec{v}$

Now Schrodinger : $i\hbar\,\partial_t\psi = \left[-\frac{\hbar^2}{2m}\nabla^2 + V(\vec{x})\right]\psi$

If $\psi(x,t)$ is a solution, then
$\psi^*(x,-t)$ is a solution, notice that complex conjugate.

at $t=0$: $\psi = \langle x|\alpha\rangle$ - time reversal $\to \psi^* = \langle x|\alpha\rangle^*$

$$\langle\alpha|\pi^\dagger\pi|\beta\rangle = \langle\alpha|\beta\rangle$$

$\hookrightarrow \int \psi_\alpha^*(-x)\,\psi_\beta(-x)\,d\vec{x} = \int \psi_\alpha^*(x)\,\psi_\beta(x)\,d\vec{x}$ ← parity.

but $\int dx\, \underbrace{(\psi_\alpha^*(x))^*}_{\langle\tilde{\alpha}|}\ \underbrace{(\psi_\beta(x)^*)}_{|\tilde{\beta}\rangle} = \left(\int dx\,\psi_\alpha^*(x)\psi_\beta(x)\right)^*$ ← Time Reversal

$$\boxed{\hookrightarrow \langle\tilde{\alpha}|\tilde{\beta}\rangle = \langle\alpha|\beta\rangle^*}$$

time reversal of $|\alpha\rangle$ and $|\beta\rangle$

implies time reversal is not unitary.

Def: $|\alpha\rangle \rightarrow |\tilde{\alpha}\rangle = \Theta|\alpha\rangle$

$|\beta\rangle \rightarrow |\tilde{\beta}\rangle = \Theta|\beta\rangle$) Transformation.

anti-unitary.

$\boxed{\text{If i) } \langle\tilde{\beta}|\tilde{\alpha}\rangle = \langle\beta|\alpha\rangle^*}$

ii) antlinear $\Theta(c_1|\alpha\rangle + c_2|\beta\rangle) = \underset{\substack{\uparrow \\ \text{complex conjugate.}}}{c_1^*}\Theta|\alpha\rangle + c_2^*\Theta|\beta\rangle$

Write $\Theta = \underset{\substack{\uparrow \\ \text{unitary}}}{U}\underset{\substack{\uparrow \\ \text{complex conjugate.}}}{K}$

where $K\,c|\alpha\rangle = c^* K|\alpha\rangle$

let $|\alpha\rangle = \sum_a |a\rangle\langle a|\alpha\rangle$

$\xrightarrow{K}$ $K|\alpha\rangle = \sum_a \langle a|\alpha\rangle^* |a\rangle$

→ K: depends on basis, $K|a\rangle = |a\rangle$

Ex: check $\Theta = UK$ antiunitary holds?

$$|\alpha\rangle \xrightarrow{\Theta} |\tilde{\alpha}\rangle = \sum_a \langle a|\alpha\rangle^* \underbrace{UK}_{\Theta} |a\rangle$$

$$= \sum_a \langle a|\alpha\rangle^* U|a\rangle$$

$$|\tilde{\alpha}\rangle \overset{!}{=} \sum \langle\alpha|a\rangle U|a\rangle$$

Similarly $\langle\tilde{\beta}| = \sum_a \langle a|\beta\rangle \langle a|U^\dagger$

then $\langle\tilde{\beta}|\tilde{\alpha}\rangle = \sum_{a_1 a_2} \langle a_2|\beta\rangle \underbrace{\langle a_2|U^\dagger U|a_1\rangle}_{\substack{\langle a_2|a_1\rangle \\ a_1 = a_2}} \langle\alpha|a_1\rangle$

$$= \sum_{a_2} \langle a_2|\beta\rangle\langle\alpha|a_2\rangle$$

$$\overset{!}{=} \langle\alpha|\beta\rangle$$

$\langle\tilde{\beta}|\tilde{\alpha}\rangle \overset{!}{=} \langle\beta|\alpha\rangle^*$ ← proves anti-unitary.

but → $|\langle\tilde{\beta}|\tilde{\alpha}\rangle| = |\langle\beta|\alpha\rangle|$ absolute value don't change.

either unitary or antiunitary.

Time reversal operator:

$$|\alpha\rangle \longrightarrow \Theta|\alpha\rangle = |\tilde{\alpha}\rangle$$

expect $\Theta|\vec{p}\rangle \longrightarrow |-\vec{p}\rangle$

$$\vec{J} \xrightarrow{\Theta} -\vec{J}$$

$$|\alpha\rangle_{\delta t} = \left(1 - \frac{i}{\hbar}H\delta t\right)|\alpha\rangle$$

$$\left(1 - \frac{i}{\hbar}H\delta t\right)\Theta|\alpha\rangle = \Theta\left(1 - \frac{i}{\hbar}H(-\delta t)\right)|\alpha\rangle$$

$$-iH\Theta = \Theta iH$$

If Θ is unitary, so i doesn't get conjugated.

$$-iH\Theta = i\Theta H \quad \rightarrow \quad H\Theta = -\Theta H$$

$$\Theta^{-1}\frac{p^2}{2m}\Theta = -\frac{p^2}{2m} \quad \leftarrow \text{can't be, so}$$

Θ is not unitary.

If Θ is anti-unitary:

$$-iH\Theta = \Theta iH$$

complex conjugate since anti-unitary.

$$-iH\Theta = -i\Theta H$$

$\hookrightarrow$ $\boxed{[H,\Theta] = 0}$ Θ commutes with H.

If there is time reversal symmetry in the system (H) then Θ commutes $[H,\Theta]=0$

How does Θ act on operators:

$$\langle\beta|\Theta|\alpha\rangle = \langle\beta|\left(\Theta|\alpha\rangle\right)$$, let Θ always act to the right.

$$|\tilde{\alpha}\rangle = \Theta|\alpha\rangle$$
$$|\tilde{\beta}\rangle = \Theta|\beta\rangle$$

if A is Hermitian

$*$ $$\boxed{\text{Identity: } \langle\beta|A|\alpha\rangle = \langle\tilde{\alpha}|\Theta A^{\dagger}\Theta^{-1}|\tilde{\beta}\rangle = \langle\tilde{\alpha}|\Theta A\Theta^{-1}|\tilde{\beta}\rangle}$$

proof: $$\langle\beta|A|\alpha\rangle = \left(\langle\beta|A\right)|\alpha\rangle = \langle\gamma|\alpha\rangle$$

$$\langle\gamma|\alpha\rangle = \langle\tilde{\gamma}|\tilde{\alpha}\rangle^{*} = \langle\tilde{\alpha}|\tilde{\gamma}\rangle$$

$$\overset{!}{=} \langle\tilde{\alpha}|\Theta\,\underbrace{(A^{\dagger}|\beta\rangle)}_{|\gamma\rangle}$$

$$\overset{!}{=} \langle\tilde{\alpha}|\Theta A^{\dagger}|\beta\rangle$$

$$\overset{!}{=} \langle\tilde{\alpha}|\Theta A^{\dagger}\Theta^{-1}|\tilde{\beta}\rangle$$

$$\langle\beta|A|\alpha\rangle \overset{!}{=} \langle\tilde{\alpha}|\Theta A\Theta^{-1}|\tilde{\beta}\rangle$$ if $A = A^{\dagger}$ $\leftarrow$ always true if A is observable.

If $$\boxed{\tilde{A} = \Theta A^{\dagger}\Theta^{-1} = \Theta A\,\Theta^{-1} = \pm A}$$

then $\Theta A = \pm A\Theta$ then A is even $(+)$ or odd $(-)$ under time reversal.

$$\langle\beta|A|\alpha\rangle = \langle\tilde{\alpha}|\Theta A\Theta^{-1}|\tilde{\beta}\rangle$$

$$\stackrel{|}{=} \pm \langle\tilde{\alpha}|A|\tilde{\beta}\rangle$$

or $\langle\alpha|A|\alpha\rangle = \pm\langle\tilde{\alpha}|A|\tilde{\alpha}\rangle$ ← restriction on exp value in time reversal state.

$$\Theta\vec{p}\Theta^{-1} = -\vec{p}$$

↳ $\langle\alpha|\vec{p}|\alpha\rangle = -\langle\tilde{\alpha}|\vec{p}|\tilde{\alpha}\rangle$

$$\vec{p}\,\Theta|\vec{p}\rangle = -\Theta\vec{p}|\vec{p}'\rangle = -\Theta\vec{p}'|\vec{p}'\rangle = -p'(\Theta|\vec{p}'\rangle$$

$$\boxed{\Theta|\vec{p}'\rangle = |-\vec{p}'\rangle \quad \text{up to phase.}}$$

$\Theta\vec{x}\Theta^{-1} = \vec{x}$ → $\boxed{\Theta|\vec{x}'\rangle = |\vec{x}'\rangle}$

↳ $|\vec{x}'\rangle$ is even under time reversal.

$$[x_i, p_j] = i\hbar\delta_{ij}$$

$$\Theta[x_i, p_j]\Theta^{-1} = \Theta x_i p_j \Theta^{-1} - \Theta p_j x_i \Theta^{-1}$$

$$\stackrel{|}{=} \underbrace{\Theta x_i\Theta^{-1}}_{x_i}\underbrace{\Theta p_j\Theta^{-1}}_{-p_j} - \underbrace{\Theta p_j\Theta^{-1}}_{-p_j}\underbrace{\Theta x_i\Theta^{-1}}_{x_i} \leftarrow$$

$$\stackrel{|}{=} -i\hbar\delta_{ij}$$

B131, 5:00 PM:

$$[J_i, J_j] = i\hbar \varepsilon_{ijk} J_k$$

$$[\tilde{J}_i, \tilde{J}_j] = \Theta\, i\hbar \varepsilon_{ijk} J_k \Theta^{-1}$$

$$\stackrel{!}{=} -i\hbar \varepsilon_{ijk} \tilde{J}_k$$

$$\boxed{\tilde{J}_i = \Theta J_i \Theta^{-1} = -J_i}$$

<u>Wavefunction</u>:

$t=0$ $$|\alpha\rangle = \int d^3x' \; |x'\rangle\langle x'|\alpha\rangle$$

$$\Theta|\alpha\rangle = \int d^3x' \; \langle x'|\alpha\rangle^* \, \Theta|x'\rangle$$

so $$\Theta \psi_\alpha(x') = \psi_\alpha(x')^*$$

so $$Y_l^m(\theta,\phi) \xrightarrow{\Theta} Y_l^{m*}(\theta,\phi) = (-1)^m Y_l^{-m}(\theta,\phi)$$

$$\Theta|l,m\rangle = (-1)^m |l,-m\rangle$$

$$\Theta^2|l,m\rangle = \Theta(-1)^m|l,-m\rangle$$

$$\stackrel{!}{=} (-1)^m \Theta|l,-m\rangle$$

$$\stackrel{!}{=} (-1)^m(-1)^m|l,m\rangle$$

$$\Theta^2|l,m\rangle = |l,m\rangle$$

$$\boxed{\Theta^2 = 1 \text{ when applied to } \psi(\vec{r})}$$

$\boxed{\text{Theorem: if } [H,\Theta]=0\text{, then wavefunction of nondegenerate states are real (up to overall phase)}}$

proof: $H\,\Theta|n\rangle = \Theta H|n\rangle = \Theta E_n|n\rangle = E_n\,\Theta|n\rangle$

then $\Theta|n\rangle$ and $|n\rangle$ have the same eigenvalue E_n.

If non degenerate, then $\Theta|n\rangle = \Theta|x\rangle\langle x|n\rangle = |n\rangle$

then $\langle x|n\rangle^* = \langle x|n\rangle \rightarrow$ so $\psi_n(x)$ is real

Form of Θ depends on representation:

$$\Theta|\alpha\rangle = \sum_a \Theta|a\rangle\langle a|\alpha\rangle = \sum_a \Theta|a\rangle\langle a|\alpha\rangle^*$$

$$\overset{!}{=} \int d^3x\ \langle x|\alpha\rangle^*\ \Theta|x\rangle = \int d^3x\ \underbrace{\langle x|\alpha\rangle^*}_{\psi_\alpha(x)^*}\ |x\rangle$$

$\boxed{\psi_\alpha(x) \xrightarrow{\Theta} \psi_\alpha^*(x)}$ in position basis, we just complex conjugate under Θ.

$$\Theta|\alpha\rangle = \int d^3p\ \langle p|\alpha\rangle^*\ \Theta|p\rangle = \int d^3p\ \langle p|\alpha\rangle^*\ |-p\rangle$$

$$\overset{!}{=} \int d^3p\ \langle -p|\alpha\rangle^*\ |p\rangle$$

so $\boxed{\psi_\alpha(p) \xrightarrow{\Theta} \psi_\alpha^*(-p)}$ In momentum basis, complex conjugate and $-p$

Spin $-\frac{1}{2}$: note $\Theta|\hat{n},+\rangle = \underset{\text{phase.}}{\eta}\,|\hat{n},-\rangle$

$$(\vec{\sigma}\cdot\hat{n})\,|\hat{n},+\rangle = |\hat{n},+\rangle$$

$$(\vec{\sigma}\cdot\hat{n})\,\chi(\hat{n},+) = +\chi(\hat{n},+)$$

$$(\vec{\sigma}^*\cdot\hat{n})\,\chi^*(\hat{n},+) = \chi^*(\hat{n},+)$$

using identity: $\vec{\sigma}^* = -\sigma^2\vec{\sigma}\sigma^2$ for Pauli-Matrices.

$$\hookrightarrow -\sigma^2(\vec{\sigma}\cdot\hat{n})\sigma^2\chi^*(\hat{n},+) = \chi^*(\hat{n},+)$$

$$\hookrightarrow (\vec{\sigma}\cdot\hat{n})\underbrace{\sigma^2\chi^*(\hat{n},+)} = -\sigma^2\chi^*(\hat{n},+)$$

note: $(\vec{\sigma}\cdot\hat{n})\tilde{\chi}(\hat{n},\pm) = \pm\tilde{\chi}(\hat{n},\pm)$

then we see: $\sigma^2\chi^*(\hat{n},+) = \eta\,\chi(\hat{n},-)$

By comparing $\Theta|\hat{n},+\rangle = \eta|\hat{n},-\rangle$

then $\boxed{\Theta = \eta\sigma^2 K \quad \text{for spin } 1/2}$

then $\Theta^2 = \eta\sigma^2 K\eta\sigma^2 K$

$$\overset{!}{=} \underbrace{\eta\eta^*}_{=1}\sigma^2 K\sigma^2 K$$

$$\overset{!}{=} \sigma^2\sigma^{2*}K^2$$

$\boxed{\Theta^2 \overset{!}{=} -1}$ for spin 1/2 (actually applies for any half-integer spin)

For general j:

$|\hat{n}, m\rangle$: $\quad (\vec{J}\cdot\hat{n})|\hat{n}, m\rangle = \hbar m |\hat{n}, m\rangle$

$$J^2 |\hat{n}, m\rangle = \hbar^2 j(j+1) |\hat{n}, m\rangle$$

$$|\hat{n}, m\rangle = e^{-\frac{i}{\hbar}J_z\alpha} e^{-\frac{i}{\hbar}J_y\beta} |\hat{z}, m\rangle$$

Θ: $J_i \xrightarrow{\Theta} -J_i$, $\quad i \xrightarrow{\Theta} -i$

$$\Theta|\hat{n}, m\rangle = e^{\frac{i}{\hbar}J_z\alpha} e^{\frac{i}{\hbar}J_y\beta}\, \Theta|\hat{z}, m\rangle$$

$$\shortparallel$$

$$\eta|\hat{n}, -m\rangle = \eta e^{-\frac{i}{\hbar}J_z\alpha} e^{-\frac{i}{\hbar}J_y\beta} - |\hat{z}, m\rangle$$

$$\overset{!}{=} \eta e^{-\frac{i}{\hbar}J_z\alpha} e^{-\frac{i}{\hbar}J_y(\beta+\pi)} K|\hat{z}, m\rangle$$

then $\boxed{\Theta = \eta e^{-\frac{i}{\hbar}J_y\pi} K = UK.}$

assuming $\hat{z}$ axis is real.

For $S = 1/2$: $\quad e^{-i\frac{\pi}{2}\sigma^2} = \cos\frac{\pi}{2} - i\sigma^2 \sin\left(\frac{\pi}{2}\right) = -i\sigma^2$

then $\quad \Theta = \eta e^{-i\pi\frac{\sigma^2}{2}} K$

$$\overset{!}{=} \eta(-i\sigma^2)K \leftarrow \text{same as } s=1/2 \text{ case.}$$

Find $\theta^2 = \eta e^{-\frac{i}{\hbar}\pi J_y} K \eta e^{\frac{i}{\hbar}\pi J_y} K$

$$\stackrel{!}{=} \eta e^{\frac{-i}{\hbar}\pi J_y} \eta^* e^{\frac{-i}{\hbar}\pi J_y} K^2$$

$$\stackrel{!}{=} |\eta|^2 e^{\frac{-i}{\hbar}2\pi J_y} K^2$$

$$\stackrel{!}{=} e^{\frac{-i}{\hbar}2\pi J_y}$$

$$\stackrel{!}{=} e^{\frac{-i}{\hbar}2\pi m}$$

$J_y = (-j, -j+1 \cdots, j)\hbar$

$2m = (-2j, -2j+1 \cdots 2j)$

$$\stackrel{!}{=} (-1)^{2m} = (-1)^{2j}$$

* then $\boxed{\theta^2 = (-1)^{2j}}$ $\begin{cases} 1 & j = \text{integer} \\ -1 & j = \text{half-integer.} \end{cases}$

ex: if $j = \frac{1}{2}$, $\theta^2 = 1$ $\leftarrow$ half integer

Kramers Degeneracy.

suppose $[H, \theta] = 0$

Note that it ~~doesn't~~ does NOT form conservation laws. because θ is anti-unitary.

since $$e^{\frac{i}{\hbar}Ht}\,\theta\, e^{\frac{-i}{\hbar}Ht} = e^{\frac{2i}{\hbar}Ht}\,\theta \neq \theta$$

unlike parity $$e^{\frac{i}{\hbar}Ht}\,\pi\, e^{\frac{-i}{\hbar}Ht} = \pi.$$

If $[H, \theta] = 0$ and $|n\rangle$ is nondegenerate eigenket of H.

then $\psi_n(x)$ is Real.

→ Suppose $[\theta, H] = 0$, then $|n\rangle$ and $\theta|n\rangle$ are degenerate.

→ If $|n\rangle$ is not degenerate, then $\theta|n\rangle = e^{i\delta}|n\rangle$

then $$\theta^2|n\rangle = \theta e^{i\delta}|n\rangle = e^{-i\delta}\theta|n\rangle = e^{-i\delta}e^{i\delta}|n\rangle$$

then $$\theta^2|n\rangle = |n\rangle$$

$\hookrightarrow (-1)^{2j}|n\rangle = |n\rangle$ ← this is impossible for j = half integer.

So If j = half-integer, then $|n\rangle$ and $\theta|n\rangle$ must be different state with same eigenenergy. so they must be at least 2-fold degeneracy when $[H, \theta] = 0$.

Consider example:

E-field: $V(x) = e\,\varphi(x)$ since its real

then $[\Theta, V] = 0$

So we can conclude E-field cannot lift kramer degeneracy.

Magnetic field: $\vec{V}_1 = \vec{S} \cdot \vec{B}$ ← $\vec{B}$ is real ← zeeman-coupling.

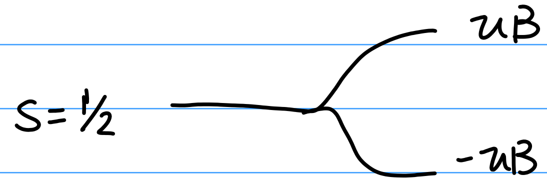
$$H \sim (\vec{p} - \vec{A})^2 = p^2 - (\vec{p} \cdot \vec{A} + \vec{A} \cdot \vec{p}) + A^2$$

$\vec{A}$ is real

$$\Theta S \Theta^{-1} = -\vec{S} \quad \rightarrow \quad [\vec{S} \cdot \vec{B}, \Theta] \neq 0$$

$$\Theta p \Theta^{-1} = -\vec{p} \quad \rightarrow \quad [(\vec{p} - \vec{A})^2, \Theta] \neq 0$$

Since Θ don't commute with H, then it lifts degeneracy.



If S is large, suppose $S = 17/2$

$$\frac{1}{S^2} [S_i, S_j] = i\hbar\, \varepsilon^{ijk} S_k \frac{1}{S^2}$$

$$[n_i, n_j] = i\left(\frac{\hbar}{S}\right) \varepsilon^{ijk} n_k$$

← if $S \to \infty$, RHS is 0
so basically classical.