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) : $\mathcal{L}$.

$\mathcal{L}^{+}\mathcal{L} = I$ ← unitary.

G is constant of motion.

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

Heinsenberg

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

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

G → generator of symmetry.

G → Hermitian, $G^{+} = G$

~ ← approximate

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

Schrodinger:

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

↳ eigenket of G.

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

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

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

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

$G(t) = UGU^\dagger = G$

$UG = GU.$

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

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

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

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

$$H\mathcal{L}|n\rangle \overset{!}{=} E_n\underbrace{\mathcal{L}|n\rangle}$$

is also an eigenket of H.

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

↑ allow phase difference.

Ex: $\left[\underset{\sim}{\mathcal{D}}(R), H\right] = 0$ 2

↳ $[\vec{J}, H] = 0$
G

↳ $[J^2, H] = 0$

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.

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

↑ $2j+1$ degenerate.

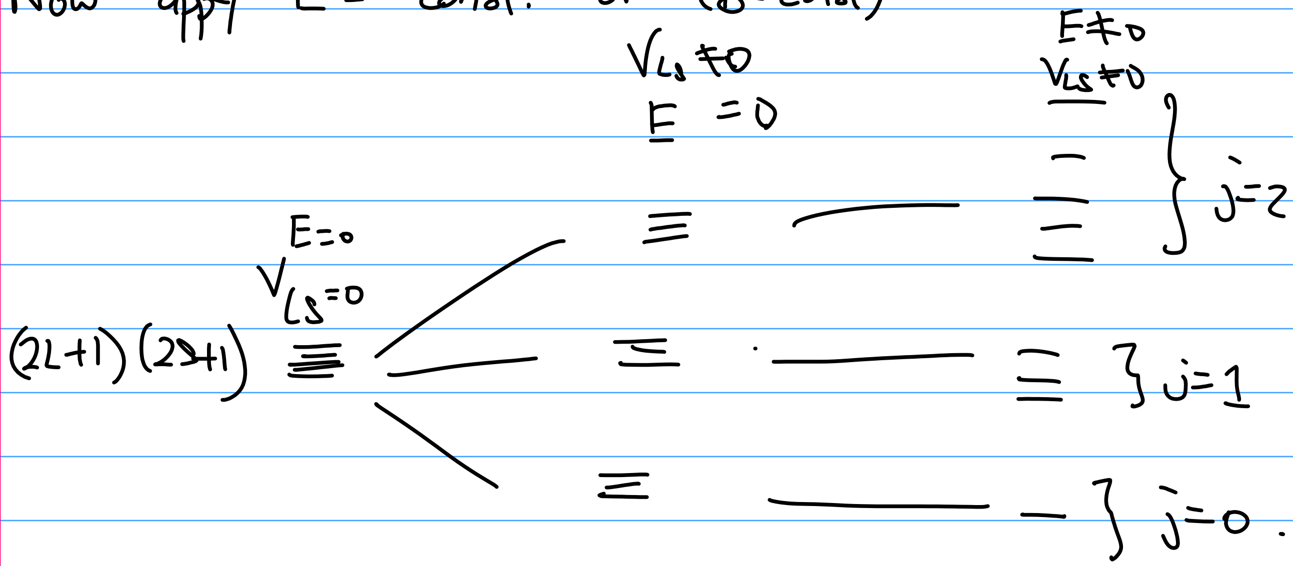
Application : $V = \underset{\substack{\uparrow \\ \text{central} \\ \text{potential}}}{V(r)} + \underbrace{V_{LS}\, \vec{L} \cdot \vec{S}}_{\text{spin-orbit interaction.}}$

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

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

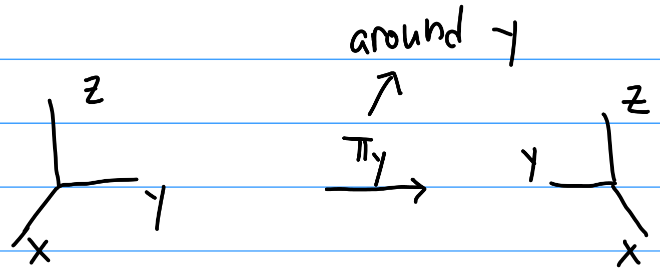
then $(2j+1)$ degenerate.

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

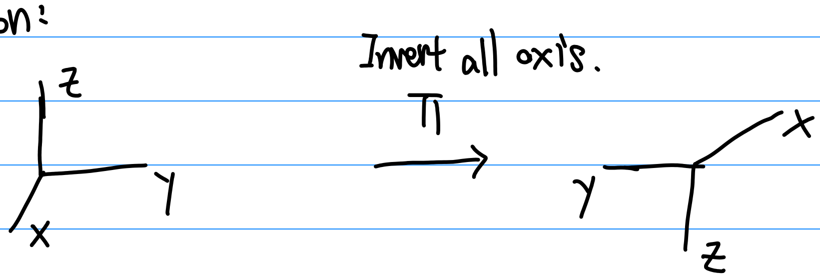


Discrete Symmetries:

→ Parity :



→ Space Inversion:



→ Corresponding transformation of ket state:

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

parity operator (unitary)

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

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

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

odd operator.

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

$|x'\rangle$: 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.

$\hookrightarrow$ $\Pi \, \mathcal{D}(R) = \mathcal{D}(R) \, \Pi$ $\leftarrow$ postulate the same for operator.

$$\mathcal{D}(R) = 1 - \frac{i}{\hbar} \varepsilon \hat{n} \cdot \vec{J}$$

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

$\uparrow$ 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:

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

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

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

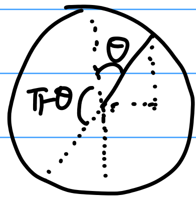
Eigenstate of parity: $\boxed{\pi | \alpha \rangle = \pm | \alpha \rangle}$

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

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

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

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

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

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

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

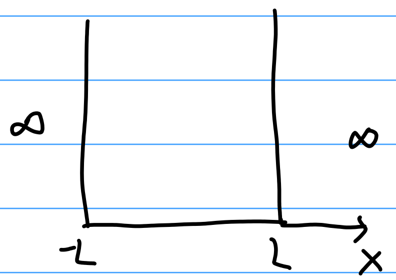
$\hookrightarrow \Pi|n_\pm\rangle = \pm\left(\frac{1\pm\Pi}{2}\right)|n\rangle = \pm|n_\pm\rangle$

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

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

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

Ex: free particle in 3d

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

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

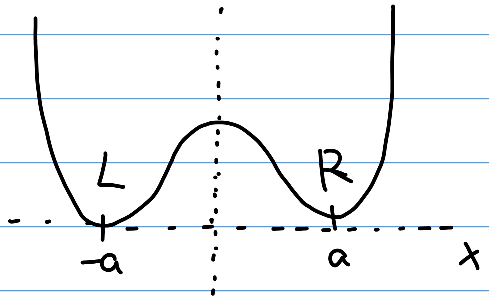
Also $E_p = \frac{p^2}{2m} = E_{-p}$, so it is degenerate.

So theorem doesn't apply.

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

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

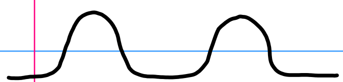
Ex: Symmetrical double-well potential:

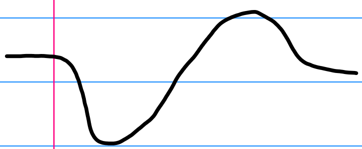


Since $U(x) = U(-x)$

$[\Pi, H] = 0$

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

Not eigenstate of H
so its not stationary

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

overall phase.

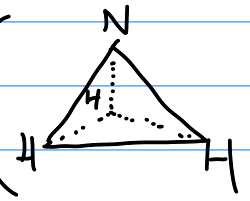
$$|R\rangle = \frac{1}{\sqrt{2}}\left(e^{-\frac{i}{\hbar}E_S t}|S\rangle + e^{-\frac{i}{\hbar}E_A t}|A\rangle\right)$$ ← has extra interference so state changes.

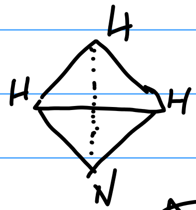
$$= \frac{1}{\sqrt{2}} e^{-\frac{i}{\hbar}E_S t}\left(|S\rangle + e^{-\frac{i}{\hbar}\Delta t}|A\rangle\right)$$

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

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

Ex: Ammonic Molecule: NH_3:

$\frac{1}{\sqrt{2}}\Big($ 

$\pm$ 

$\Big)$

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

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.

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

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

→ 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 $\varepsilon_\alpha \varepsilon_\beta = -1$.

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

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

Rotational selection rule:

$\hookrightarrow \quad l = \begin{cases} l'-1 \\ l' \\ l+1 \end{cases} \xrightarrow[\text{selection}]{\text{with parity}} \boxed{l = l' \pm 1}$

Other discrete symetry:

- 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:
$$m\ddot{\vec{x}} = e(\vec{E} + \tfrac{1}{c}\vec{v}\times\vec{B})$$
$$\vec{\nabla}\cdot\vec{E} = 4\pi\rho$$
$$\vec{\nabla}\times\vec{B} - \tfrac{1}{c}\partial_t\vec{E} = \tfrac{4\pi}{c}\vec{j}$$
$$\vec{\nabla}\times\vec{E} = -\tfrac{1}{c}\partial_t B$$
$$\vec{\nabla}\cdot\vec{B} = 0$$

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 $\to \psi^* = \langle x|\alpha\rangle^*$

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

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

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

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

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 $\theta(c_1|\alpha\rangle + c_2|\beta\rangle) = c_1^*\theta|\alpha\rangle + c_2^*\theta|\beta\rangle$

complex conjugate.

Write $\theta = UK$

unitary complex conjugate.

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

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.

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

$$\Theta^{-1}\frac{p^2}{2m}\Theta = -\frac{p^2}{2m}$$ ← can't be, so Θ is not unitary.

If Θ is anti-unitary:

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

complex conjugate since anti-unitary.

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

↳ $\boxed{[H, \Theta] = 0}$ 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.

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

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

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

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

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

$$\stackrel{!}{=} \langle\tilde{\alpha}|\theta A^\dagger|\beta\rangle$$

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

$$\langle\beta|A|\alpha\rangle \stackrel{!}{=} \langle\tilde{\alpha}|\theta A\theta^{-1}|\tilde{\beta}\rangle \quad \text{if } A = A^\dagger$$

If $\boxed{\tilde{A} = \theta A \theta^{-1} = \pm A}$ then A is even (+) or odd (−) under time reversal.

then $\theta A = \pm A\theta$

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Wavefunction:

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

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

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

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

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

$$\theta^2|l,m\rangle = \theta(-1)^m|l,-m\rangle \overset{!}{=} (-1)^m \theta|l,-m\rangle \overset{!}{=} (-1)^m(-1)^m|l,m\rangle$$

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

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

Theorem: if $[H,\Theta]=0$, 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 $\Theta|n\rangle = |n\rangle$

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

Form of Θ depends on representation:

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

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

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

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

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

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

$$\text{Spin-}\tfrac{1}{2}: \qquad \text{note } \Theta|\hat{n},+\rangle = \overset{\swarrow \text{phase.}}{\eta}\,|\hat{n},-\rangle$$

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

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

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

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

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

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

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 $\boxed{\Theta = \eta\,\sigma^2 K}$

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

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

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

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

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

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

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

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

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

$\stackrel{!}{=} e^{-\frac{i}{\hbar}2\pi m}$ $\qquad J_y = (-j, -j+1 \cdots, j)\hbar$

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

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

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

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

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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 $\Theta^2|n\rangle = |n\rangle$

↳ $(-1)^{2j}|n\rangle = |n\rangle$ ← 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.

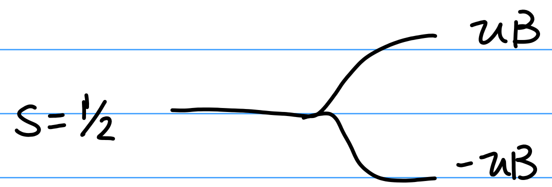
Magnetic field: $\vec{V}_1 = \vec{S} \cdot \vec{B}$ ← $\vec{B}$ is real ← zeeman-coupling.

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

← $\vec{A}$ 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 $S = 1\frac{7}{2}$

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

$$[n_i, n_j] = i\left(\frac{\hbar}{S}\right)\varepsilon^{ijk} n_k$$ ← if $S \to \infty$, RHS is 0 so basically classical.