Lecture $\boxed{42}$, Dec. 11 (Fri.)

$\boxed{\text{Outline}}$ for $\boxed{\text{today}}$ & last lecture on Mon.

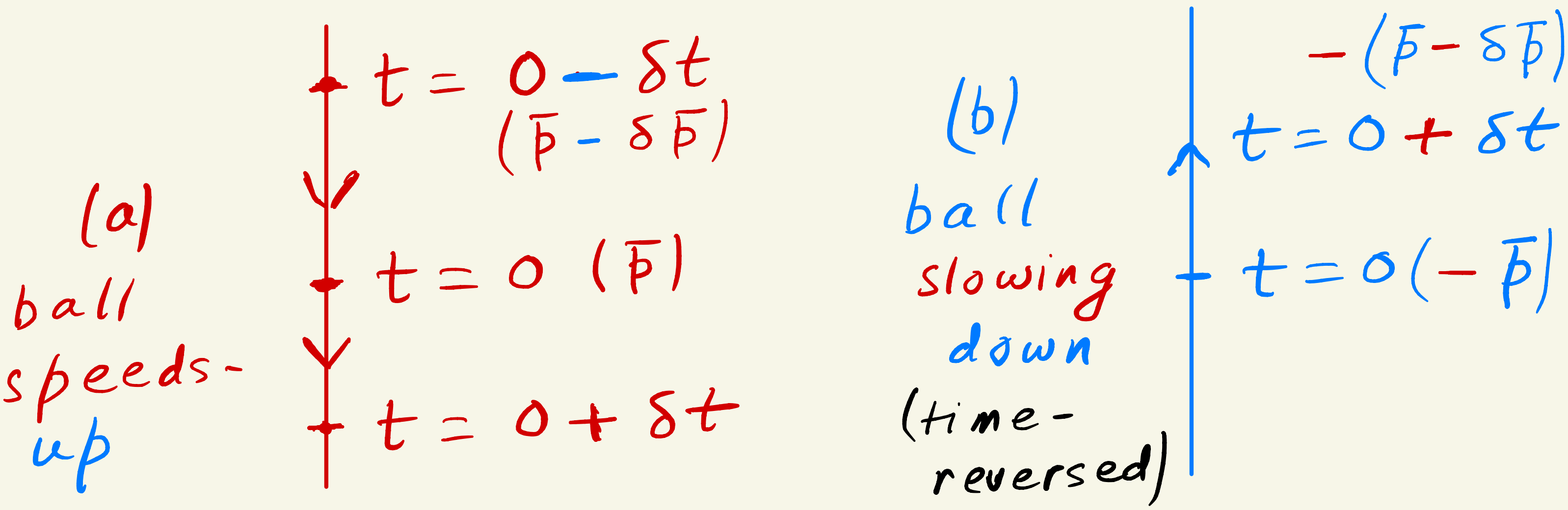
(After getting warmed-up to anti-unitary operator)

- Back to time-reversal: must be anti-unitary (based on how Hamiltonian transforms for time-reversal symmetry)
- how other operators $(\hat{x}, \hat{p})$, expectation values, wavefunctions transform (matching intuition / educated guess of before)
- H is time-reversal invariant $\Rightarrow$ wavefunction is "real" (up to phase independent of x')
- Time-reversal for spin-1/2 system

Time-reversal operation is anti-unitary (denoted by Θ)

— start with fixed time: time-reversed state is really "motion-reversed", e.g.,

$|\vec{p}\,'\rangle \longrightarrow |-\vec{p}\,'\rangle$ (in general, $|\alpha\rangle \to \Theta|\alpha\rangle$)



— Consider (infinitesimal) time-evolution:

— original ket: $|\alpha, t_0 = 0; t = \delta t\rangle$

$$= \left(1 - iH\,\delta t/\hbar\right) \underbrace{|\alpha\rangle}_{\text{at } t_0 = 0} \qquad \text{(usual)} \qquad \ldots(1)$$

... $\boxed{\text{similarly}}$, for time-reversed state

$$(\Theta|\alpha\rangle) \xrightarrow{\text{after } \delta t} \left(1 - \frac{iH\,\delta t}{\hbar}\right)(\Theta|\alpha\rangle)$$

- $\boxed{\text{Next}}$, assume time-reversal symmetry, as for ball falling under gravity (neglecting air resistance!) [but not for ball rolling on ground with friction]: time-reversed state at later time $(+\delta t)$

= start with original state at earlier time $(-\delta t)$; then reverse its momentum $\Rightarrow$

$$\underbrace{\left(1 - \frac{iH}{\hbar}\delta t\right)\left(\Theta|\alpha\rangle\right)}_{\text{(later) time-evolved version of time-reversed state}} = \underbrace{\Theta\left(|\alpha, t_0 = 0; t = -\delta t\rangle\right)}_{\text{time-reversed version of original state in past}} \quad \ldots (2)$$

Combining (1) & (2) gives (for any $|\alpha\rangle$):

$$\left(1 - \frac{iH}{\hbar}\delta t\right)\Theta|\alpha\rangle = \Theta\left[1 - \frac{iH}{\hbar}(-\delta t)\right]|\alpha\rangle$$

$\Rightarrow \boxed{(-i)\, H\Theta = \Theta\,(i) H}$ $\boxed{\text{Suppose}}$ Θ was unitary

$\Rightarrow i\,\Theta = \Theta\, i \Rightarrow H\Theta = -\Theta H$: "strange" for H being time-reversal invariant [cf. $\pi H = +H\pi$ for parity-invariant]

... so what?! Apply to energy eigenket:

$H\left(\Theta|n\rangle\right) = -\Theta H|n\rangle = -E_n\left(\Theta|n\rangle\right) \Rightarrow$

energy eigenvalue < 0 (starting with positive): does not make sense for free particle

[later: $\bar{p}$ is odd under time-reversal: $\Theta^{-1}\bar{p}\,\Theta = -\bar{p} \Rightarrow |\bar{p}|^2/(2m) = H_{free}$ is even:

$\Theta^{-1} H_{free}\,\Theta = H_{free} \Rightarrow H_{free}\,\Theta = \Theta H_{free}$]

So, assumption of Θ is unitary invalid: Θ must be anti-unitary so that

$(-i) H\,\Theta = \Theta\, i\, H$ (of before)

$= -i\,\Theta H$ (Θ anti-unitary)

$\Rightarrow \boxed{H\,\Theta = \Theta H}$ $(\Theta^{-1} H \Theta = H)$: again, that's H having time-reversal symmetry, like with H being parity invariant: $[H, \pi] = 0$ / $(H\pi = \pi H)$

[do not get negative energy eigenvalue, cf. if Θ were unitary]

[Having concluded time-reversal is anti-unitary based on H being invariant, this property valid in general, i.e., even if H is not time-reversal invariant ...]

$\boxed{\text{How do other operators } (\bar{x}, \bar{p}, \bar{J} \ldots), \text{ their expectation values transform under time-reversal?}}$

- Recall Θ taken to act on kets from left: no need to define (directly) Θ acting on bras from right

$\Rightarrow \langle\beta|\Theta|\alpha\rangle$ "interpreted" as $(\langle\beta|) \cdot (\Theta|\alpha\rangle)$, not as $(\langle\beta|\Theta) \cdot (|\alpha\rangle)$

- Useful result for transition amplitude / expectation value, related to transformation of operator under Θ

$$\langle\beta|X|\alpha\rangle = \langle\tilde{\alpha}|\Theta X^{\dagger}\Theta^{-1}|\tilde{\beta}\rangle \quad (X \text{ is linear})$$

(Note $\tilde{\alpha}$, $\tilde{\beta}$ order "switched")

Proof : $|\gamma\rangle \equiv X^{\dagger}|\beta\rangle \leftrightarrow \langle\beta|X = \langle\gamma|$

so that $\langle\beta|X|\alpha\rangle = \langle\gamma|\alpha\rangle = \langle\alpha|\gamma\rangle^{*} = \langle\tilde{\alpha}|\tilde{\gamma}\rangle$

$= \langle\tilde{\alpha}|\Theta|\gamma\rangle = \langle\tilde{\alpha}|\Theta X^{\dagger}|\beta\rangle = \langle\tilde{\alpha}|\Theta X^{\dagger}\Theta^{-1}\underbrace{\Theta|\beta\rangle}_{|\tilde{\beta}\rangle}$

- Special case : Hermitian operator/observable

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

- Operators/observables even/odd under time-reversal : $\boxed{\Theta A \Theta^{-1} = \pm A}$ ...(b)

- Combining (a) & (b) : $\langle\beta|A|\alpha\rangle = \pm\langle\tilde{\alpha}|A|\tilde{\beta}\rangle$

$= \pm\langle\tilde{\beta}|A|\tilde{\alpha}\rangle^{*}$ ("think "A is Hermitian matrix : interchange row & column)

- More specifically, $|\beta\rangle = |\alpha\rangle$ (expectation values) : $\langle\alpha|A|\alpha\rangle = \pm\langle\tilde{\alpha}|A|\tilde{\alpha}\rangle^{*}$ diagonal element of A

(expectation values are even/odd with A...) $= \pm\langle\tilde{\alpha}|A|\underbrace{\tilde{\alpha}\rangle}_{\text{time-reversed state}}$ Hermitian matrix

$\boxed{\text{Example}}$ $A = \boxed{\vec{p}}$: classically, time-reversed particle has opposite $\vec{p}$ (really "motion"-reversed)

$\Rightarrow$ (Ehrenfest theorem) "impose" $\langle\vec{p}\rangle$ flips :

$\langle\alpha|\vec{p}|\alpha\rangle = -\langle\tilde{\alpha}|\vec{p}|\tilde{\alpha}\rangle \Rightarrow \vec{p}$ is odd :

$\boxed{\Theta \bar{p} \Theta^{-1} = -\bar{p}}$ Sanity check: expect $(\Theta|\bar{p}'\rangle)$

to have eigenvalue $-\bar{p}'$: $\bar{p}$

$$\bar{p}(\Theta|\bar{p}'\rangle) = \overbrace{-(\Theta \bar{p} \Theta^{-1})}^{\bar{p}}(\Theta|\bar{p}'\rangle) = -\Theta \underbrace{\bar{p}'}_{\text{real}}|\bar{p}'\rangle$$

$$= -\bar{p}'(\Theta|\bar{p}'\rangle)$$

$\Rightarrow$ (upto phase) $\Theta|\bar{p}'\rangle = |-p'\rangle$

[In general, eigenvalue "flips" for odd operator]

- Whereas, impose $\langle\alpha|\bar{x}|\alpha\rangle = +\langle\tilde{\alpha}|\bar{x}|\tilde{\alpha}\rangle$

(position not reversed) $\Rightarrow$ $\bar{x}$ is even

$\Theta|x'\rangle = |x'\rangle$ upto phase

... cf. both $\bar{x}, \bar{p}$ are odd under parity $\Rightarrow$

$\boxed{\text{fundamental commutation relation}}$ easily

preserved under parity ...

... also under time-reversal due to $\overbrace{\ }^{\text{arbitrary}}$

anti-unitary : $[x_i, p_j]|\alpha\rangle = i\hbar\delta_{ij}\underbrace{|\alpha\rangle}_{}$ $\Rightarrow$

$$\underbrace{\Theta[x_i,p_j]\Theta^{-1}}\Theta|\alpha\rangle = \Theta i\hbar\delta_{ij}|\alpha\rangle = -i\Theta\delta_{ij}\hbar|\alpha\rangle$$

$$\underbrace{\Theta x_i \Theta^{-1}}_{x_i}\underbrace{\Theta p_j \Theta^{-1}}_{-p_j} - \dots \Rightarrow (-x_i p_j + p_j x_i)\Theta|\alpha\rangle = -i\hbar\delta_{ij}\Theta|\alpha\rangle$$

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

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

if $\bar{J}$ is odd : $\boxed{\Theta J \Theta^{-1} = -J}$

... reasonable, since $\bar{L}$ (= one realization of $\bar{J}$) $= (\bar{x} \times \bar{p})$ is odd

$\bar{x}$ → even, $\bar{p}$ → odd

How do wavefunctions transform under time-reversal?

Educated guess (earlier): complex conjugate

Check formally now: $\psi_\alpha(x') = \langle x'|\alpha\rangle$

(no spin: see later) (expansion coefficient with $|x'\rangle$ basis)

[now, know how $|x'\rangle, |\alpha\rangle$ change]

$$\underbrace{\Theta|\alpha\rangle}_{\text{time-reversed}} = \Theta \int d^3x' \langle x'|\alpha\rangle |x'\rangle$$

$$= \int d^3x' \langle x'|\alpha\rangle^* \underbrace{\Theta|x'\rangle}_{|x'\rangle}$$

$$= \int d^3x' |x'\rangle \langle x'|\alpha\rangle^* \Rightarrow \psi_{\tilde{\alpha}}(x') = \psi_\alpha(x')^*$$

Recall: general anti-unitary $= U K$

U = unitary, K = c.c.

So, based on $\underbrace{\Theta|\alpha\rangle}_{\int d^3x' |x'\rangle\langle x'|\alpha\rangle} = \int d^3x' \langle x'|\alpha\rangle^* |x'\rangle$ (again, $\Theta|x'\rangle = |x'\rangle$)

it seems $U = \mathbb{1}$: $\Theta = $ (only) K ... but if base kets $|x'\rangle$ ... but basis-dependence : not quite valid for base kets $|p'\rangle$ instead, since $\Theta |\bar{p}'\rangle = |-\bar{p}'\rangle$ (cf. $\Theta |\bar{x}'\rangle = |\bar{x}'\rangle$) :

$$\underbrace{\phi_{\tilde{\alpha}}}_{}(\bar{p}') = \phi_{\alpha}^{*}(-\bar{p}') \leftarrow \text{... of original state}$$

momentum-space wavefunction of time-reversed state

(c.c. and "flip" $\bar{p}'$)

$$\Big[\ \Theta\,|\alpha\rangle = \Theta \int d^3p'\, |\bar{p}'\rangle\langle\bar{p}'|\alpha\rangle$$
$$= \int d^3p'\, \langle\bar{p}'|\alpha\rangle^{*}\, \Theta\,|\bar{p}'\rangle$$
$$= \int d^3p'\, \langle\bar{p}'|\alpha\rangle^{*}\, |-\bar{p}'\rangle \underset{p' \to -p'}{=} \int d^3p' \langle -\bar{p}'|\alpha\rangle^{*} \times |\bar{p}'\rangle\ \Big]$$

– $\boxed{\text{Angular}}$ part of $\psi_\alpha(\bar{x}') = \underbrace{R(r)}_{\text{real}}\, Y_\ell^m(\theta,\phi)$

$$Y_\ell^m(\theta,\phi)\,(m>0) = \left[e^{im\phi}\right](-1)^m P_\ell^m(\cos\theta)\sqrt{\frac{(2\ell+1)(\ell-m)!}{4\pi\,(\ell+m)!}}$$

time-reversal $\longrightarrow$ $Y_\ell^{m\,*}(\theta,\phi) = \boxed{(-1)^m\ Y_\ell^{(-m)}(\theta,\phi)}$ (Note: changes in "2 places")

since (convention) $Y_\ell^{-m}(\theta,\phi)\,(m>0) = (-1)^m\left[Y_\ell^m(\theta,\phi)\right]^{*}$

- $Y_\ell^m(\theta, \phi)$ is wavefunction of $|\ell, m\rangle$

$\Rightarrow$ $\boxed{\Theta\, |\ell, m\rangle = (-1)^m\, |\ell, -m\rangle}$ (again, 2 changes)

- Sanity check: probability current density $\propto \mathrm{Im}\left(\psi^* \bar{\nabla} \psi\right)$: for $\psi(x') \sim R(r)\, Y_\ell^m$, current counter-clockwise for $m > 0$, vs. clockwise expected for time-reversed: agrees with flip of sign of m

Consequence (for wavefunction) of H being time-reversal invariant

(so far, H having time-reversal symmetry only "used" to deduce Θ is anti-unitary)

Claim: (spin-less particle: include it later) wavefunction of energy eigenstate is **real**, up to $\bar{x}$-independent phase for $\Theta H \Theta^{-1} = H$ and no degeneracy

Intuition: "eigenket" of Θ also $\Rightarrow$ "Θ" on $\psi_n \propto \psi_n$,

but $\psi_n \to \psi_n^*$ also, so $\psi_n = \psi_n^*$
(in general)

$\boxed{\text{Proof}}$: $H\,\theta\,\underbrace{|n\rangle}_{\text{energy eigenket}} = \theta H\,|n\rangle = E_n\,\theta|n\rangle$

$\Rightarrow$ $\theta|n\rangle$ has same energy as $|n\rangle$, but

no degeneracy $\Rightarrow$

$\theta|n\rangle = |n\rangle$, upto $\underbrace{\boxed{\text{constant}}\text{ phase}}_{\text{neglect it}}$

$\Rightarrow$ wavefunctions of $|n\rangle$ & $\underbrace{\theta|n\rangle}$ $\boxed{\text{same}}$:

(in general) $\boxed{\text{c.c.}}$ of $|n\rangle$'s wavefunction

$\Rightarrow$ wavefunction real

$H = |\bar{p}|^2/(2m)$ invariant

e.g. (1): free particle wavefunction

$\sim \exp\left(i\,\bar{p}'\cdot\bar{x}'/\hbar\right)$ (position-dependent phase?!)

... but degenerate with $\exp\left(-i\,\bar{p}'\cdot\bar{x}'/\hbar\right)$

e.g. (2): One-electron atom: for $m \neq 0$,
(H is invariant)

wavefunction $\propto \exp(i m \phi)$ (not constant phase?!)
(of $|n, \ell, m\rangle$)
... but degenerate with $|n, \ell, -m\rangle$
(actually, for spherically symmetric potential, $m = -\ell, -\ell+1 \ldots \ell-1, \ell$ all degenerate)

Time-reversal for spin-½ system

- Earlier twist for spin-½ state: 2π rotation ("full circle") flips sign
- Another (related) one with time-reversal: for orbital angular momentum (only),

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

$$\Theta^2\,|\ell, m\rangle = (-1)^m\left[(-1)^m\,|\ell, -(-m)\rangle\right] = +|\ell, +m\rangle$$

$\Theta^2 = \mathbb{1}$ for orbital angular momentum,
but $\boxed{\Theta^2 = -\mathbb{1} \text{ for spin-}1/2}$

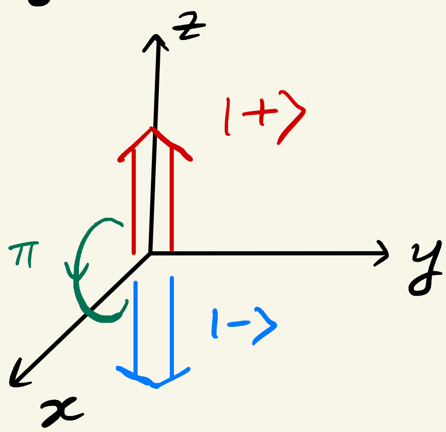
Proof: Use $\vec{J}$ is odd under time-reversal
$\Rightarrow$ eigenvalue "flips" (like for $\vec{p}$) ... $\boxed{(\mathrm{I})}$

$$S_z\,(\Theta\,|+\rangle) = -\Theta S_z\,|+\rangle \quad \left(\Theta^{-1} S_z \Theta = S_z \Rightarrow S_z\Theta = -\Theta S_z\right)$$

$= -\theta\, \hbar/2\, |+\rangle = -\hbar/2\, (\theta|+\rangle)$

$\Rightarrow \theta|+\rangle = \eta\,(\text{phase})\,|-\rangle \quad \cdots (1)$

- Now, $|-\rangle$, upto phase, obtained by "rotating" $|+\rangle$ about y-axis by π $\boxed{(II)}$



$$|-\rangle\, \tilde{\eta} = \exp(-i\pi S_y/\hbar)\,|+\rangle \quad \cdots (2)$$

θ "on" Eq. (2) gives

$$\theta|-\rangle = \theta\, \frac{1}{\tilde{\eta}} \exp\left(-\frac{i\pi S_y}{\hbar}\right)|+\rangle$$

$$= \frac{1}{\tilde{\eta}^*}\, \theta \exp\left(-\frac{i\pi S_y}{\hbar}\right)|+\rangle \quad \cdots (3)$$

- Need $[\theta, iS_y]$ to move θ to right past $\exp(-i\pi S_y/\hbar)$ (power series in iS_y):

$$\theta(iS_y) - (iS_y)\theta = -i\theta S_y - iS_y\theta$$

$$= -i(\theta S_y + S_y\theta) = 0, \text{ since } S_i\theta = -\theta S_i$$

$$\Rightarrow \theta(\exp -i\pi S_y/\hbar) = \exp(-i\pi S_y/\hbar)\,\theta$$

$\Rightarrow$ Eq. (3) gives

$$\theta|-\rangle = \frac{1}{\tilde{\eta}^*} \exp\left(-\frac{i\pi S_y}{\hbar}\right) \underbrace{\theta|+\rangle}_{\text{use (1)}}$$

$$= \frac{1}{\tilde{\eta}^*} \exp\left(-\frac{i\pi S_y}{\hbar}\right) \eta \underbrace{|-\rangle}_{\text{use (2)}}$$

$$= \frac{1}{\tilde{\eta}^*} \eta \exp\left(-\frac{i\pi S_y}{\hbar}\right) \frac{1}{\tilde{\eta}} \exp\left(-\frac{i\pi S_y}{\hbar}\right)|+\rangle$$

$$= \eta \underbrace{\exp\left(-\frac{i\,2\pi S_y}{\hbar}\right)|+\rangle}_{-|+\rangle \ (\boxed{\text{III}}.\ 2\pi \text{ rotation flips sign})} = -\eta|+\rangle \quad \ldots (4)$$

$$\boxed{\tilde{\eta}^*\tilde{\eta} = 1}$$

So, $\theta \underbrace{(c_+|+\rangle + c_-|-\rangle)}_{\text{arbitrary ket}} = c_+^* \theta|+\rangle + c_-^* \theta|-\rangle$

$$= c_+^* \eta|-\rangle - c_-^* \eta|+\rangle \quad [\text{use (1), (4)}]$$

$$\theta^2 \boxed{(c_+|+\rangle + c_-|-\rangle)} = \theta\, c_+^* \eta|-\rangle - \theta\, c_-^* \eta|+\rangle$$

general ket

$$= c_+ \eta^* \underbrace{\theta|-\rangle}_{-\eta|+\rangle\ (4)} - c_- \eta^* \underbrace{\theta|+\rangle}_{+\eta|-\rangle\ (1)}$$

$$= -\underbrace{|\eta|^2}_{1}(c_+|+\rangle + c_-|-\rangle) = (-)\boxed{(c_+|+\rangle + c_-|-\rangle)}$$

Generalize above results for spin-$\frac{1}{2}$ & orbital angular momentum (l = integer) to arbitrary angular momentum:

$$\Theta^2 |j \text{ half-integer}\rangle = -|j \text{ half-integer}\rangle$$

(like for spin-$\frac{1}{2}$)

$$\Theta^2 |j \text{ integer}\rangle = +|j \text{ integer}\rangle$$

(like for orbital angular momentum)

(see Sakurai for proof)

Note: j integer above can be (purely) orbital or made up of even number of spin-$\frac{1}{2}$ (e.g., two electron total spin can be 0, 1)...

Similarly, j half-integer can be odd number of spin-$\frac{1}{2}$ or orbital angular momentum, plus one spin-$\frac{1}{2}$ ...

- Actually, any state of even number of spin-$\frac{1}{2}$ is even under Θ^2, no matter their spin or spatial orientations (latter determining orbital angular momentum), even if not $|\vec{J}|^2$ eigenstate: such combination "decomposes" into components with $|\vec{J}|^2$ eigenvalues integer, since orbital angular momentum always integer (total $L = L_1 + L_2 + \cdots$), while even number of spin-$\frac{1}{2}$ gives integer total spin ($= S_1 + S_2 + \cdots$)

- Similarly, any state with odd number of spin-$\frac{1}{2}$ is odd under Θ^2...

- $\boxed{\text{generalize}}$ $\Theta^{1}|\ell, m\rangle = (-1)^m |\ell, -m\rangle$ for orbital angular momentum to

$$\boxed{\Theta^{1}|j, m\rangle = (-1)^m |j, -m\rangle \quad (j \text{ integer})}$$

orbital or even number of spin-$\frac{1}{2}$ ...

further to $\boxed{\Theta^{1}|j, m\rangle = (i)^{2m} |j, -m\rangle}$

(Sakurai problem 4.10 for proof)

for any j (integer or half-integer)

consistent with $\eta = +i$ for spin-$\frac{1}{2}$ and $|j, m\rangle$ made up of $2j$ spin-$\frac{1}{2}$'s

(Schwinger's oscillator model)