Lecture $\boxed{39}$, Dec. 4 (Fri.)

Outline for $\boxed{\text{remaining}}$ lectures:

— symmetries (and their consequences: constants of motion & degeneracies) in QM (ch. 4 of Sakurai)

— continuous (e.g., rotations): sec. 4.1

vs. — discrete (e.g. parity/space inversion: sec. 4.2 & time-reversal: sec. 4.4)

$\boxed{\text{Outline / motivation}}$ for continuous symmetry

— In study of rotations, angular momentum (ch. 3), central potential was a focus: $H = \frac{|\bar{p}|^2}{2m} + V(r(=|\bar{x}|))$:

$\boxed{\text{rotationally}}$ invariant: symmetry $SO(3)$

$[H, \bar{L}] = 0 = [H, |\bar{L}|^2]$

Consequences:

(i). constant of motion / conservation law for expectation value of $\vec{L}$: in H-picture,

$$\frac{d}{dt}\underbrace{\langle\alpha|}_{\text{arbitrary}}\ \overset{\text{only}}{L}\ |\alpha\rangle = \langle\alpha|\frac{dL}{dt}|\alpha\rangle$$

$$= \langle\alpha|\frac{1}{i\hbar}[L, H]|\alpha\rangle = 0$$

(ii) energy eigenkets are also eigenkets of angular momentum: $|\underset{\text{radial}}{\alpha}, \underbrace{l\ m}_{\text{angular}}\rangle$

Energy eigenvalues (E) from radial equation:

$$\left[-\frac{\hbar^2}{2mr^2}\frac{d}{dr}\left(r^2\frac{d}{dr}\right) + \frac{l(l+1)\hbar^2}{2mr^2} + U(r)\right]R_{El}(r)$$
$$= E\,R_{El}(r)$$

$\Rightarrow$ E depends on l: no degeneracy (in general, e.g., ∞ spherical well)

... but not on $\boxed{m}$: $m = -l \ldots$ to $+l$ (for given l) degenerate: $\boxed{(2l+1)\text{-fold}}$

... $\boxed{\text{generalize}}$: symmetry

$\Rightarrow$ constant of motion & degeneracy

— Back to Coulomb potential $\left(\frac{1}{r}\right)$:

more than $(2l+1)$-fold degeneracy

E depends only on n : for fixed n, $l = 0, \ldots n-1$

(n^2 - fold degeneracy), larger than expected from $SO(3)$ [rotational invariance]

... can't be accident : must be due to larger symmetry: indeed $SO(4$

$\boxed{\text{Continuous}}$ symmetry :

- classically (Hamiltonian formulation) : if $H(q_i, p_i)$ does not explicitly depend on q_i [x "generalized"] (H has symmetry under transformation $q_i \to q_i + \delta q_i$), then

$$\underbrace{d p_i / dt = \partial H / \partial q_i}_{\text{Hamilton's}} = 0$$

(constant of motion)

Onto $\boxed{\text{QM}}$: transformations (e.g., translations, rotations) correspond to unitary operator $\mathcal{S}$ ($\mathcal{S}^{+} = \mathcal{S}^{-1}$)

$\boxed{\mathcal{S}^{-1} H \mathcal{S}}$ is transformed H, e.g.

$$\mathcal{D}^{+}(R) \underbrace{T_q^{(K)}}_{\text{tensor}} \underbrace{\mathcal{D}(R)}_{\text{rotation operator}}$$

- $\boxed{\text{Continuous}}$ transformation has infinitesimal version : $\mathcal{S} = \left(\mathbb{1} - i \frac{\varepsilon}{\hbar} G\right)$,

where G (generator) is Hermitian

- $\mathcal{S}$ is $\boxed{\text{symmetry}}$ if H is invariant:

$$\mathcal{S}^{-1} H \mathcal{S} = H = \overbrace{\left(1 + i\frac{\varepsilon}{\hbar} G\right)}^{\mathcal{S}^{-1}} H \overbrace{\left(1 - i\frac{\varepsilon}{\hbar} G\right)}^{\mathcal{S}}$$

$$\Rightarrow [H, G] = 0 \qquad \Rightarrow \frac{dG}{dt} = \frac{1}{i\hbar} \underbrace{[H, G]}_{=0}$$

(Heisenberg picture)

only

$$\Rightarrow \frac{d}{dt} \langle \alpha | G | \alpha \rangle = \langle \alpha | \tfrac{d}{dt} G | \alpha \rangle$$

expectation value of G is $\boxed{\text{constant of motion}}$

(Ehrenfest theorem) [consequence (i)]

e.g. invariance under translation/rotation $\Rightarrow$ constant expectation value of linear/angular momentum

- Relatedly, if system is in eigenket of G at t_0 (given by $|g'\rangle$), then it evolves at time t into $\mathcal{U}(t, t_0)|g'\rangle$ which is also (like $|g'\rangle$) eigenket of G with same eigenvalue (g') ("constant of motion"): $[G, \mathcal{U}(t, t_0)] = 0$

$\mathcal{U}(t,t_0) = \exp[iH(t-t_0)/\hbar]$

$$\Rightarrow G \underbrace{\mathcal{U}(t, t_0)|g'\rangle}_{\text{time-evolved } |g'\rangle} = \mathcal{U}(t, t_0) G |g'\rangle = \mathcal{U} g' |g'\rangle = g' (\mathcal{U} |g'\rangle)$$

[Equivalently, $|g'\rangle$ is also eigenket of H
$\Rightarrow$ $|g'\rangle$ is energy eigenket $\Rightarrow$ phase only upon time-evolution]

Consequence (ii): $\boxed{\text{degeneracies}}$

If $[H, G] = 0$, then $H \underbrace{|n\rangle}_{\text{energy eigenket}} = E_n |n\rangle \Rightarrow H(G|n\rangle)$

$$= G\, H|n\rangle$$
$$= E_n\, (G|n\rangle)$$

$G|n\rangle$ is also energy eigenket with same energy as $|n\rangle$

If $G|n\rangle \neq |n\rangle$, then degeneracy

e.g., $\mathcal{G}$ is rotation operator $\mathcal{D}(R)$, with H being rotationally invariant:

$\mathcal{D}^{-1}(R)\, H\, \mathcal{D}(R) = H$ (e.g., spherically symmetric potential; no spin)

$\Rightarrow [\vec{J}, H] = 0 = [|\vec{J}|^2, H] \Rightarrow$ eigenkets simultaneously of $H, |\vec{J}|^2, J_z$

generator (G) [of rotations here]

Degeneracy in m follows from $\in G$

$[H, J_\pm] = 0$, with $J_\pm$ raising/lowering m (but same j) $\Rightarrow (2l+1)$-fold degeneracy [for only angular momentum being orbital]

(saw it earlier using radial equation, but here follows from general principles)

– include spin-orbit interaction:

$$V(r) + V_{LS}(r) \underbrace{\bar{L}\cdot\bar{S}}_{\text{(also) rotationally-invariant}}$$

$\Rightarrow (2j+1)$-fold degeneracy

e.g., based on $\bar{L}\cdot\bar{S}$ eigenvalues in Eq. 3.8.66 (Sakurai)

$(\bar{L}+\bar{S}=)\ \bar{J}$ eigenvalue

(degeneracy in l by itself broken)

Onto $\boxed{\text{Coulomb}}$ potential (special case of spherically symmetric potential)

Why are different ℓ's for given n degenerate? Additional symmetry of $1/r$ potential (not for 3D isotropic SHO) $\Rightarrow$ another constant of motion

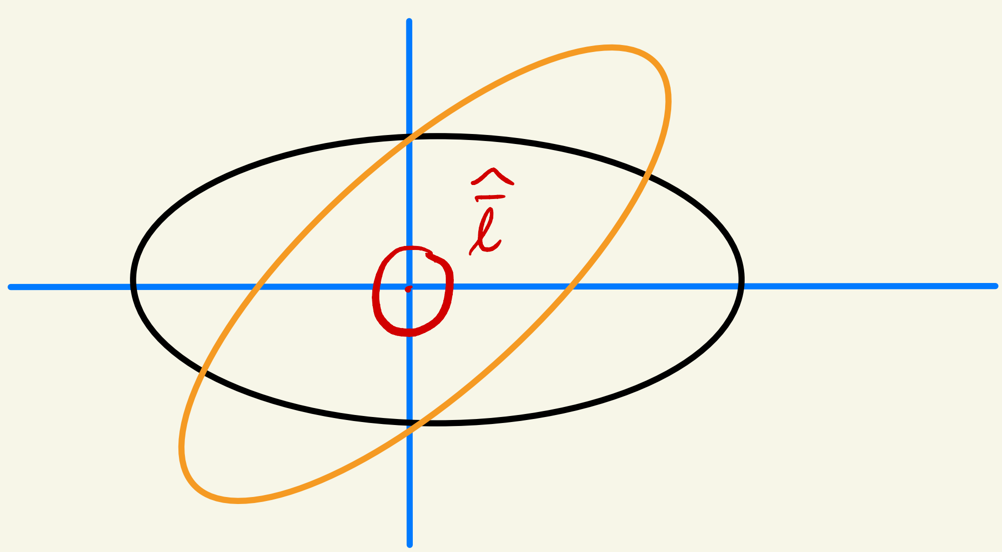
... even classically: $\boxed{\text{Kepler problem}}$

"obvious" constants of motion:

$\hat{\ell}$ (unit vector): fixes plane of orbit ($\perp \hat{\ell}$)

$|\vec{\ell}|$, E: fix size, shape of orbit

... what else? orientation of ellipse in plane



or direction of major axis of ellipse, given by Laplace-Runge-Lenz vector:

$$\boxed{\bar{M} = \frac{\bar{p} \times \bar{l}}{m} - Ze^2\bar{r}/r}$$ (Goldstein sec. 3.9)

(another/new constant of motion)

Onto QM: define Hermitian operator corresponding to $\bar{M}$: $\boxed{[\bar{M}, H] = 0}$

Summary (details in Sakurai):

(a). obtain algebra (commutators) of M & L

(b). above algebra similar to that of rotations in 4d [SO(4)], i.e., symmetry enhanced from SO(3)

(c). relate SO(4) to larger degeneracy

Onto parity / space inversion as example of discrete symmetry (not continuously connected to $\mathbb{1}$: no infinitesimal version

Preview in SHO and linear potential:

energy eigenstates wavefunctions classified as even/odd under $x' \to -x'$): not accident, due to H invariant under $x \to -x$

[parity transformation, $\boxed{\Pi}$ (operator)]:

parity is symmetry of H

$\boxed{\text{Outline}}$ for parity discussion

- properties of Π: $\{\Pi, x\} = 0$ ...

anti-commutator

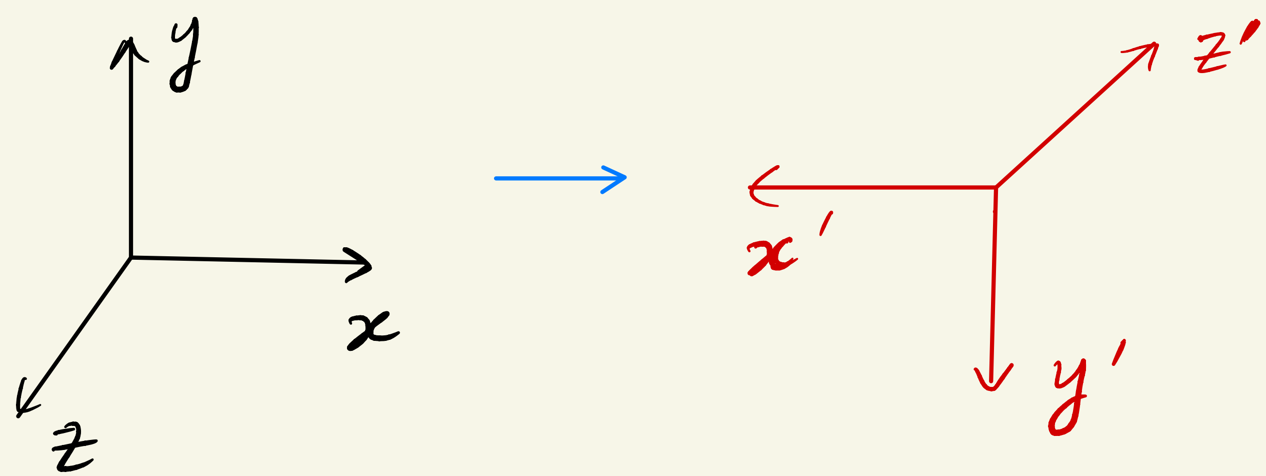
- behavior of $\boxed{\psi(x'), Y_\ell^m(\theta, \phi)}$ under Π

$\Rightarrow$ e.g. of selection rule combining parity transformation (even if not symmetry) and angular momentum conservation (rotational symmetry)

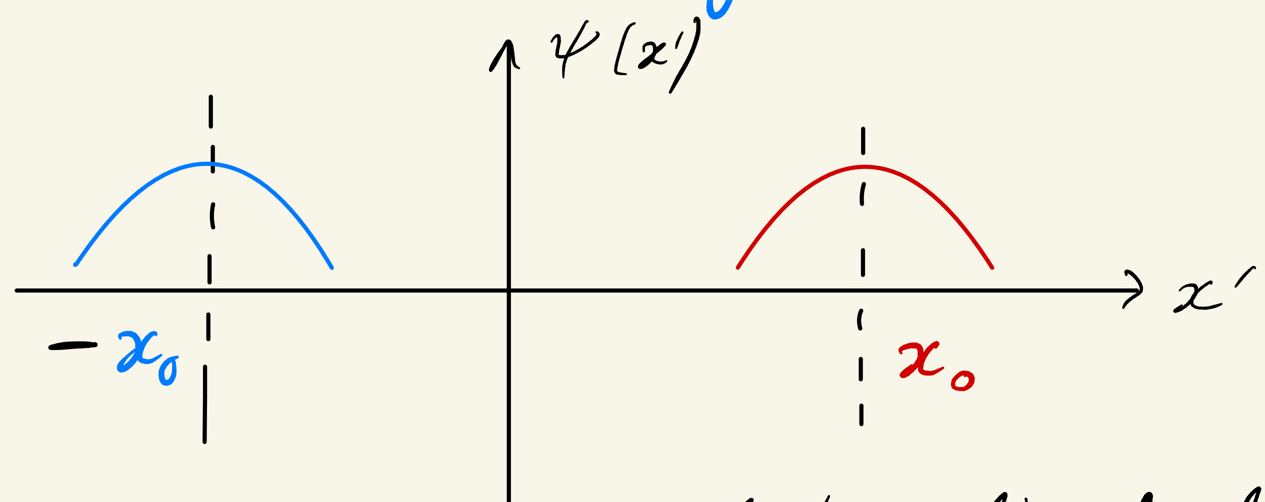
– Consequences of parity symmetry: $[\Pi, H] = 0$

Getting to know Π

– often, parity/space inversion as passive operation: RH $\longrightarrow$ LH coordinate system (state unchanged)



... vs. $\boxed{\text{active}}$ here: transform state kets, with coordinate system fixed



Π transforms wavepacket localized at

x_0 to $(-x_0)$

$$\underset{\text{(old)}}{|\alpha\rangle} \longrightarrow \underbrace{\pi}_{\text{unitary}} |\alpha\rangle$$ (new, parity-transformed/space inverted state)

– classically, $\bar{x}$ (coordinates) $\rightarrow -\bar{x}$ $\Rightarrow$ in QM, require expectation value of $\bar{x}$ (Ehrenfest theorem), e.g., above wavepacket

$$\underbrace{\underbrace{\langle \pi\alpha |}_{\text{new bra}} x | \pi\alpha\rangle}_{\text{new expectation value}} = - \underbrace{\langle \alpha | x | \alpha \rangle}_{\text{old} \ldots}$$

$= \langle \alpha | \pi^{\dagger} x \, \pi | \alpha \rangle$ ... for all $|\alpha\rangle \Rightarrow$

(as expected) $\boxed{\pi^{\dagger} x \, \pi = -x}$ $\Rightarrow x\pi = -\pi x$ $\boxed{\{x, \pi\} = 0}$

– transformation of position eigenket:

expect $\pi |x'\rangle = e^{i\delta} |-x'\rangle$:

$$x \left(\pi |x'\rangle\right) = -\pi x |x'\rangle = -x' \left(\pi |x'\rangle\right)$$

$\Rightarrow$ $\pi|x'\rangle$ has eigenvalue $-x'$: must be $|-x'\rangle$ (upto phase)

$\boxed{\text{choose}}$ $e^{i\delta} = 1 \Rightarrow \pi|x'\rangle = +|-x'\rangle$

$$\Rightarrow \pi^2 \underbrace{|x'\rangle}_{\text{base kets}} = \pi|-x'\rangle = +|x'\rangle \Rightarrow \boxed{\pi^2 = \mathbb{1}}$$

$\Rightarrow \pi$ eigenvalues $= \pm 1$

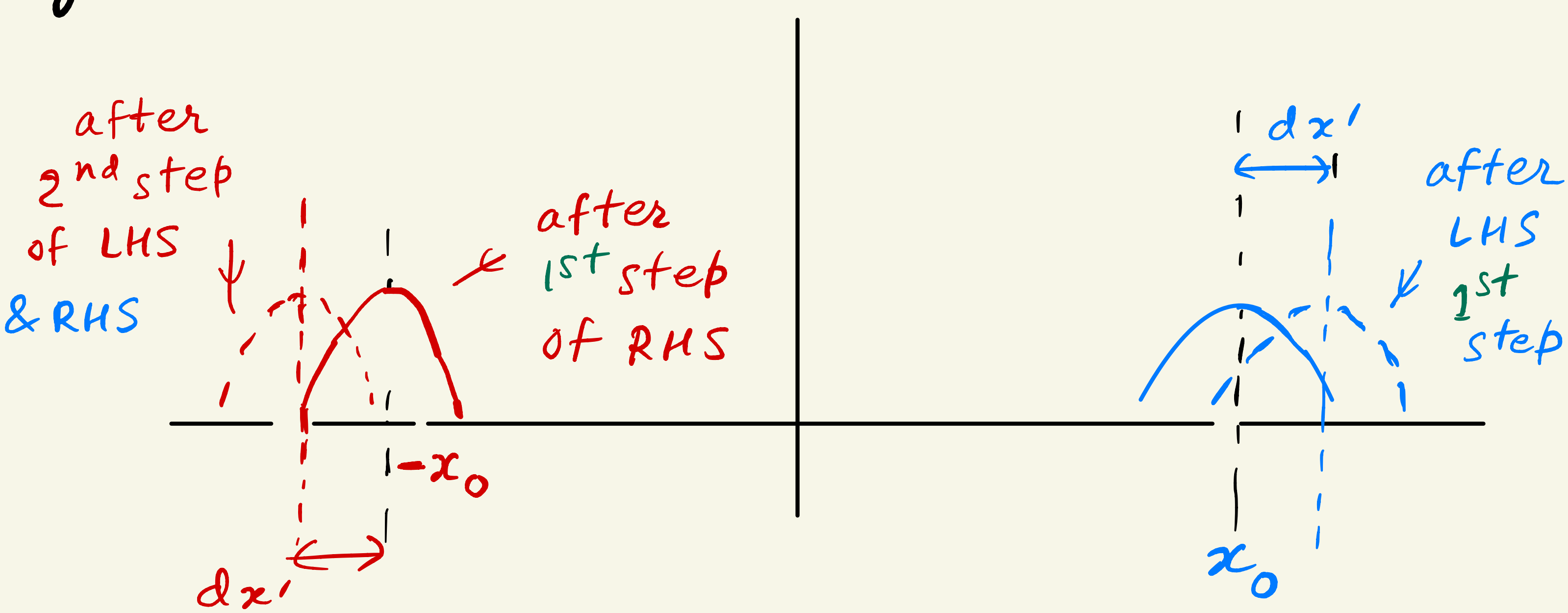
but π unitary : $\pi^{+}\pi = \mathbb{1}$ (on general grounds:

$\langle \pi\alpha | \pi\alpha\rangle = \langle\alpha|\alpha\rangle$) ... & $\pi^2 = \mathbb{1}$ $(= \pi^{+}\pi)$

$\Rightarrow \pi$ also Hermitian $\Rightarrow$ eigenvalues real

How does $\bar{p}$ transform under π ?

$\bar{p}$ "like" $m\dfrac{d\bar{x}}{dt}$, so expect odd under parity, but check using $\bar{p}$ is generator of (infinitesimal) translation:



2 paths should give same result:

$$\underbrace{\pi}_{\text{then parity}} \quad \underbrace{T(dx')}_{\text{translate } 1^{st}} = \underbrace{T(-dx')}_{\substack{\text{followed by translation} \\ \text{in opposite direction}}} \quad \underbrace{\pi}_{\text{parity } 1^{st}}$$

$$\Rightarrow \pi \left(\mathbb{1} - \frac{i\,dx'}{\hbar} p \right) \pi^{+} = \left(\mathbb{1} + \frac{i\,dx'}{\hbar} p \right) \underbrace{\pi \pi^{+}}_{\mathbb{1}}$$

$$\Rightarrow \pi^{+} p\, \pi = -p \quad \text{or} \quad \{\pi, p\} = 0 \quad \left(p \text{ is ``parity odd''} \right)$$

– What else? Transformation under parity of $\bar{J}$: e.g. $\bar{L} = \bar{x} \times \bar{p}$, with $\bar{x}, \bar{p}$ being odd under parity, so L is even $\Rightarrow [\pi, \bar{L}] = 0$

$$\left[\begin{aligned} \pi^{+} L_i \pi &= \pi^{+} \varepsilon_{ijk} x_j p_k \pi = \varepsilon_{ijk} (\pi^{+} x_j \pi)(\pi^{+} p_k \pi) \\ &= \varepsilon_{ijk} (-x_j)(-p_k) = +\varepsilon_{ijk} x_j p_k = L_i \end{aligned} \right]$$

... but spin ($\bar{S}$) not expressed in terms of $\bar{x}, \bar{p}$?! Think of $\bar{J}$ as generator of rotation (not just as $\bar{L} = \bar{x} \times \bar{p}$)

– start with rotation, parity transformation of classical vector: both parametrized by 3×3 orthogonal matrix

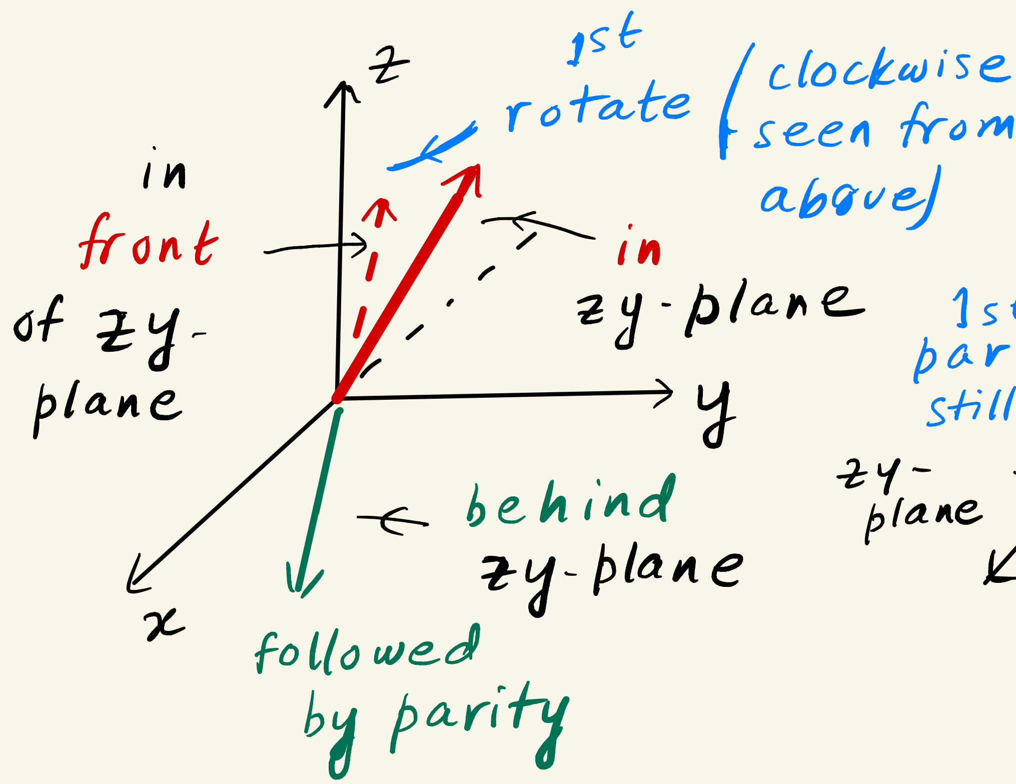
$$R^{\text{parity}} = \begin{pmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{pmatrix} \qquad \det R^{\text{parity}} = -1$$

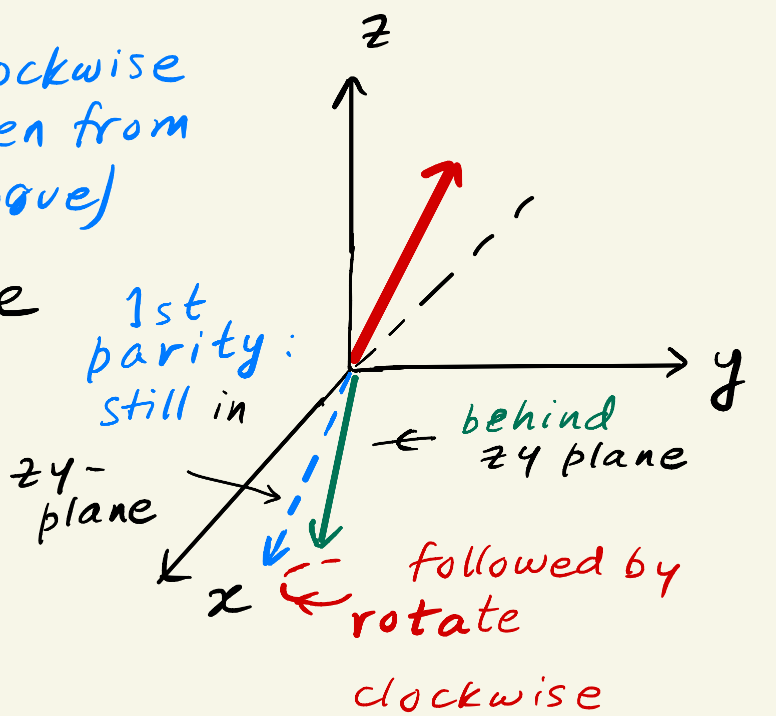
$\Rightarrow O(3)$, not $SO(3)$

Clearly, parity commutes with rotation:

$$R^{\text{parity}} R^{\text{rotation}} = R^{\text{rotation}} R^{\text{parity}}$$

Picture it:





So, in QM, same for correspoinding rotation operators $\mathcal{D}(R)$: like $R_1 R_2 = R_3 \Rightarrow \mathcal{D}(R_1)\mathcal{D}(R_2) = \mathcal{D}(R_3)$

$$\mathcal{D}(R)\,\pi = \pi\,\mathcal{D}(R), \text{ with } \mathcal{D}_R = 1 - i\frac{\varepsilon}{\hbar}\bar{J}\cdot\bar{\Phi}$$

$\Rightarrow [\pi, \bar{J}] = 0$, but $\bar{J} = \bar{L} + \bar{S}$

and $[\pi, \bar{L}] = 0 \quad \Rightarrow \quad [\pi, \bar{S}] = 0$

- Under rotations $[SO(3)]$, $\bar{x}, \bar{p}, \bar{J}$ are vectors (spherical tensor rank 1), but $\bar{x}, \bar{p}$ odd under parity (pseudo-vectors) vs. $\bar{J}$ (even parity: vector)

- Scalars under rotations : $\bar{S}\cdot\bar{x}$ or $\bar{S}\cdot\bar{p}$

... but under parity, $\pi^{-1}(\bar{S}\cdot\bar{x})\pi = \pi^{-1} S_i x_i \pi$ odd

$= \pi^{-1} S_i \pi \pi^{-1} x_i \pi = + S_i(-x_i) = -\bar{S}\cdot\bar{x}$ (similarly, $\bar{S}\cdot\bar{p}$)

(called pseudo-scalar) vs. $\pi^{-1}(\bar{L}\cdot\bar{S})\pi = \bar{L}\cdot\bar{S}$

or $\pi^{-1}(\bar{x}\cdot\bar{p})\pi = \bar{x}\cdot\bar{p}$ are even (called scalars)

Wavefunctions under parity : if

$\underbrace{\psi_\alpha(x')}_{\text{wavefunction of } |\alpha\rangle} = \langle x'|\alpha\rangle$, then wavefunction of space-inverted ket is

$$\langle x' | \underbrace{\pi | \alpha\rangle}_{\text{parity-transformed}} = \langle -x' | \alpha \rangle = \psi_\alpha(-x')$$

e.g. wavepacket localized at $x_0 \longrightarrow$ ... at $-x_0$

Eigenket of parity operator:

$$\underbrace{\pi\,|\pm\rangle}_{\text{not spin-up/down!}} = \underbrace{\pm 1}_{\text{only allowed eigenvalues}}|\pm\rangle$$

$$\Rightarrow \quad \underbrace{\langle x'|\pi|\pm\rangle}_{\text{in general, } \langle -x'|\pm\rangle = \psi_\pm(-x')} = \pm\langle x'|\pm\rangle = \boxed{\pm}\,\psi_\pm(x')$$

$\Rightarrow$ state $\boxed{\text{ket}}$ even/odd under parity operator if its expansion in $|x'\rangle$ basis, $\psi(x')$, is even/odd in x'

[earlier, e.g., SHO, linear potential, discussed $\psi_\alpha(x')$ being odd/even ... vs. here ket under parity operator]

— $\boxed{\text{Not}}$ all wavefunctions are odd/even, e.g., wavepacket localized at $x_0\ (\neq 0)$

or $|p'\rangle \propto e^{-\frac{ip'x'}{\hbar}}$: expected since

$[\bar{p}, \pi] \neq 0$ (given $\{\pi, p\} = 0$), so

no simultaneous eigenkets

... better luck with $Y_\ell^m(\theta,\phi)$, since $[\pi, \bar{L}] = 0$

and eigenkets of $\bar{L}$ are $\langle x' | \alpha, \ell, m\rangle = R(r) Y_\ell^m$,

so must be parity odd/even (simultaneous eigenkets)

– Under parity,

$r \rightarrow r \Rightarrow R(r)$ invariant, so $Y_\ell^m(\theta,\phi)$

even/odd

$\theta \rightarrow (\pi - \theta)$ since $z \rightarrow -z$ ($z = r\cos\theta$)
[and want to keep $0 \leq \theta(\text{new}) \leq \pi$]

$\phi \rightarrow \phi + \pi$ since $x = r\sin\theta\cos\phi \rightarrow -x$
($\sin\theta$ unchanged, both $\sin\phi$, $\cos\phi$ flip) $\longrightarrow$ $y = r\sin\theta\sin\phi \rightarrow -y$

– Determine parity of $Y_\ell^m(\theta,\phi)$:

start with $m = \boxed{0}$: $Y_\ell^0(\theta,\phi) \propto P_\ell(\cos\theta)$,

which are even/odd in $\cos\theta$ for even/odd

ℓ, so is $Y_\ell^0(\theta,\phi)$ then even/odd with

ℓ), thus $|\ell, 0\rangle$ ...

And $Y_\ell^m(\theta,\phi)$ $(m>0) \sim (L_+)^m$ "on" Y_ℓ^0

... but $[\pi, (L_+)^m] = 0 \Rightarrow$

$$\pi (L_+)^m |\ell, 0\rangle = (L_+)^m \underbrace{\pi |\ell, 0\rangle}_{(-1)^\ell |\ell, 0\rangle}$$

$$\Rightarrow \pi \underbrace{\left((L_+)^m |\ell, 0\rangle\right)}_{|\ell, m\rangle \text{: also eigenket}} = (-1)^\ell \left((L_+)^m |\ell, 0\rangle\right)$$

$|\ell, m\rangle$: also eigenket of π with $(-1)^\ell$

$\Rightarrow$ $\boxed{\underbrace{Y_\ell^m(\theta,\phi)}_{\text{wavefunction of } |\ell, m\rangle} \text{ even/odd with } \ell}$

wavefunction of $|\ell, m\rangle$

(again, independent of m)