Lecture $\boxed{40}$, Dec. 7 (Mon.)

(continued from lecture 39 notes)

Outline

- consequeaces of H being parity-invariant
- parity selection rule
- onto time-reversal symmetry
  - classically: is "reversed" particle trajectory also valid?
  - implication for wavefunction in QM

—— x ——

Consequenses of H being parity-invariant: simultaneous eignekets of energy & parity

- Claim: if $[H, \pi] = 0$ and $H|n\rangle = E_n|n\rangle$ (non-degenerate), then $|n\rangle$ is also parity eigenket

Proof : follows from general theorem 1.2 (page 29) of Sakurai : if $[A, B]=0$, then simultaneous eigenkets of A & B (assuming non-degenerate A eigenvalues)

Anyway, from scratch : $\frac{1}{2}(1 \pm \pi)\underbrace{|\alpha\rangle}_{\text{general ket}}$ is parity eigenket (whether $|\alpha\rangle$ is or not) :

$$\pi\left(\frac{1}{2}(1 \pm \pi)|\alpha\rangle\right) = \frac{1}{2}(\pi \pm \pi^2)|\alpha\rangle$$

$$= \frac{1}{2}(\pi \pm 1)|\alpha\rangle = \pm 1\left[\left(\frac{1}{2} \pm \pi\right)|\alpha\rangle\right]$$

(eigenvalues : as expected)

Suppose $|\alpha\rangle$ is also energy eigenket, $|n\rangle$ with eigenvalue E_n :

$$H\left[\frac{1}{2}(1 \pm \pi)|n\rangle\right] = \left(\frac{H}{2} \pm \pi H\right)|n\rangle$$

use $[\pi, H] = 0$

$= \frac{1}{2}(1 \pm \pi) E_n |n\rangle$ (use $H|n\rangle = E_n|n\rangle$)

$$= E_n \left[\frac{1}{2}(1 \pm \pi)|n\rangle\right]$$

$\to$ also eigenket of H with E_n

Non-degeneracy

$$\Rightarrow \frac{1}{2}(1 \pm \pi)|n\rangle \propto |n\rangle \Rightarrow$$

$\pi|n\rangle \propto |n\rangle$, i.e., $|n\rangle$ is parity eigenket

e.g (1), SHO ($V = \frac{1}{2} m\omega x^2$) and linear potential ($V = k|x|$) H's are parity-invariant : earlier, $\psi_n(x')$ even/odd under $x' \to -x'$ for n = even/odd

$\Rightarrow |n\rangle$ is even/odd under parity

[e.g., $|1\rangle = a^{+}|0\rangle \sim (\underbrace{x}_{\text{odd}}$ "+" $\underbrace{p}_{\text{odd}})\underbrace{|0\rangle}_{\text{even}}$ is odd under parity]

e.g. (2) : One-electron atom: H is parity-invariant (since $1/r$ is), but energy depends on n only $\Rightarrow$
$2s\ (\ell=0)$ (parity even)
& $2p\ (\ell=1)$ (odd)
are degenerate

$\Rightarrow$ linear combination : $c_p|2p\rangle + c_s|2s\rangle$ is not eigenket of parity, but is energy eigenket

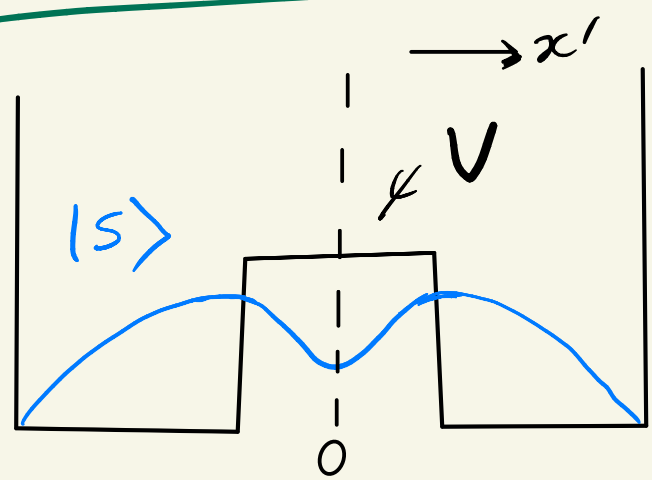
e.g. (3) : $[H_{\text{free}}, \pi] = 0$, since $[\pi, p^2] = 0$ (p is parity-odd $\Rightarrow p^2$ is even)

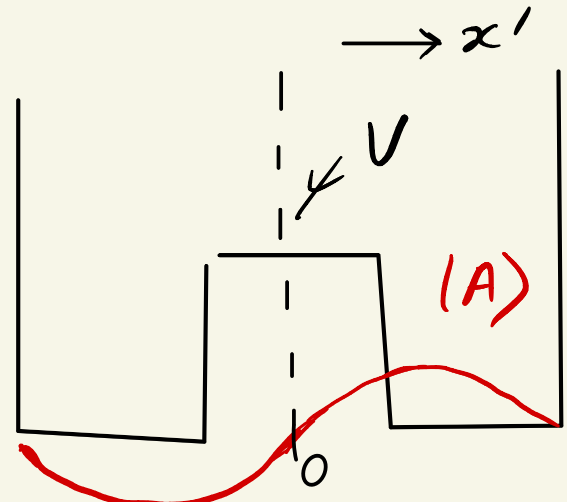
plane wave (momentum & energy eigenket) $\propto \boxed{e^{ip'\cdot x'/\hbar}}$ is not parity eigenket (expected, since

$[\pi, p] \neq 0$) ... theorem OK, since $\exp\left(-\frac{ip'\cdot x'}{\hbar}\right)$ $\boxed{\text{degenerate}}$ with it

[combinations : $\exp\left(-\frac{ip'\cdot x'}{\hbar}\right) \pm \exp\left(+\frac{ip'\cdot x'}{\hbar}\right)$ are cos or sin $\left(\frac{p'x'}{\hbar}\right)$: even/odd parity] & energy eigenkets

e.g. (4) (also illustrates broken symmetry & degeneracy) Symmetrical double-well potential





- V, thus H is parity-invariant
- ground $|S\rangle$ (symmetric : parity-even) & 1st excited $|A\rangle$ (asymmetric : parity odd)

[obtained using cos/sin in allowed region/bottom of wells, vs. cosh/sinh in forbidden ; match at boundaries]

(no node for ground state)

- Both are de-localized : build

$|R \text{ or } L\rangle = \frac{1}{\sqrt{2}}\left(|S\rangle \pm |A\rangle\right)$ localized

in RHS/LHS "wells" : not parity eigenkets:

$\pi|R\rangle = |L\rangle$ since $\pi|S \text{ or } A\rangle = \pm |S \text{ or } A\rangle$;

no energy eigenkets :

$H\left(|S\rangle \pm |A\rangle\right) = E_S|S\rangle \pm E_A|A\rangle$, with $E_S < E_A$

$\Rightarrow |R \text{ or } L\rangle$ not stationary : start

in $|R\rangle$ at $t=0$ $\longrightarrow$ at time t :

$$\frac{1}{\sqrt{2}}\left[\exp\left(-i\frac{E_S t}{\hbar}\right)|S\rangle + \exp\left(-i\frac{E_A t}{\hbar}\right)|A\rangle\right]$$

$$= \frac{1}{\sqrt{2}}\exp\left(-iE_S t/\hbar\right)\left(|S\rangle + \exp\left(-i\frac{(E_A - E_S)t}{\hbar}\right) \times |A\rangle\right)$$

$\Rightarrow$ at $t = T/2 = 2\pi\hbar/\left[2(E_A - E_S)\right]$, system in $|L\rangle$; back to $|R\rangle$ at $t=T$

[oscillates between $|R\rangle, |L\rangle$ with frequency, $\omega = (E_A - E_S)/\hbar$: from "tunneling" : start on RHS, go thru' barrier to LHS ...]

→ what happens as $\boxed{\text{barrier height}}$ → $\boxed{\infty}$? $|S\rangle, |A\rangle$ are degenerate ⇒

$|R\rangle, |L\rangle$ are energy eigenkets

(system beginning in $|R\rangle$ will not tunnel thru' ∞ barrier),

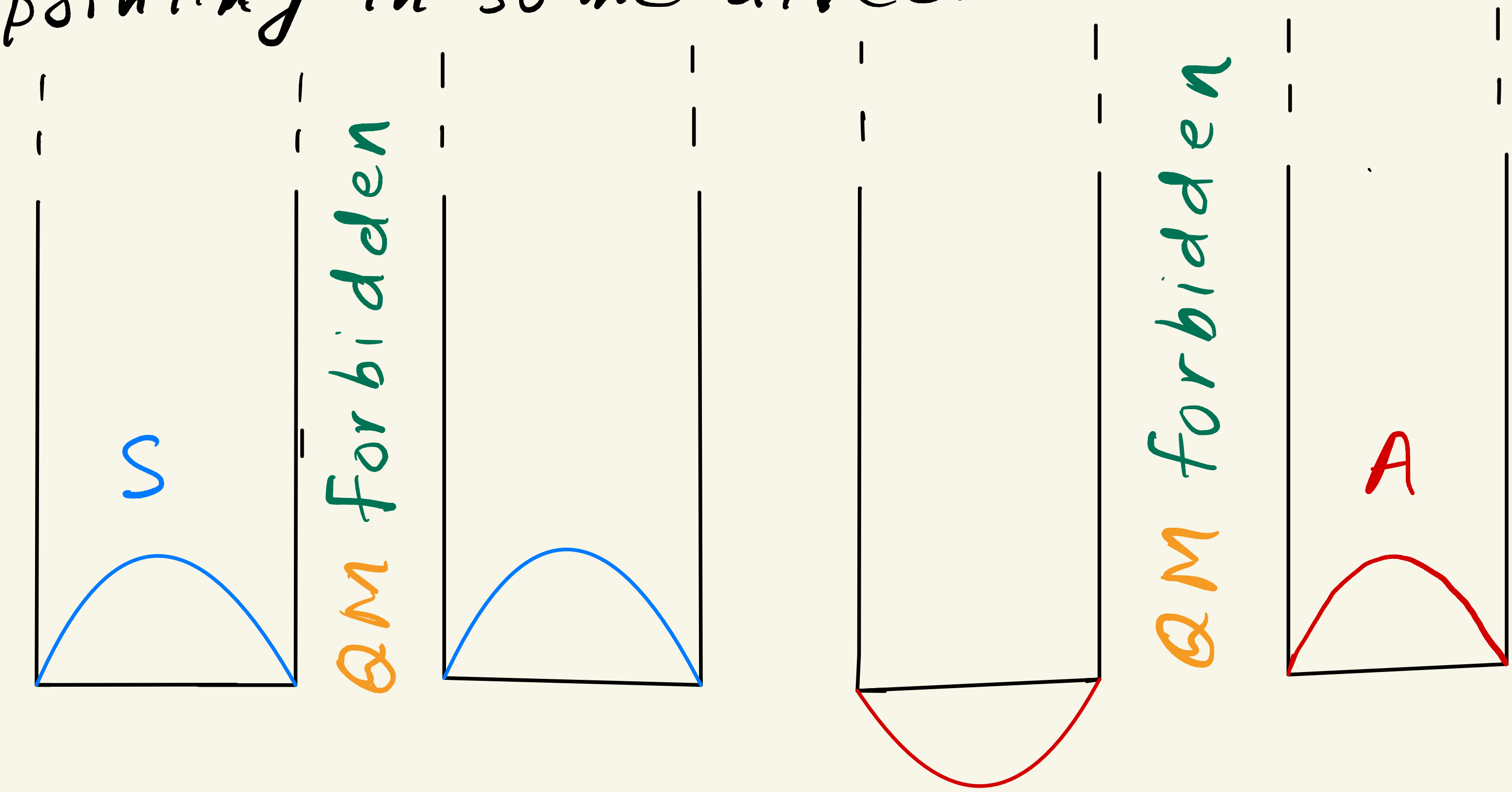
but still not parity eigenkets

("ok" due to degeneracy)

– Also, ground state does not "respect" parity, e.g. $|R\rangle$ or $|L\rangle$,

even though H is parity invariant:
e.g. of symmetry being "broken"
(degeneracy needed)

another e.g.: ferromagnet; H is rotationally invariant, but ground state has spins pointing in some direction



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Parity selection rule for process.

$|\alpha\rangle, |\beta\rangle$ parity eigenstates:

$\pi|\alpha \text{ or } \beta\rangle = (\varepsilon_{\alpha \text{ or } \beta})\,|\alpha \text{ or } \beta\rangle$, with $\varepsilon_{\alpha \text{ or } \beta} = \pm 1$

$\Rightarrow$ Claim: $\langle \alpha | A_{odd} | \beta \rangle = 0$, unless $\varepsilon_\alpha \varepsilon_\beta = -1$

(odd parity operators only connects states of opposite parity : even ... same ...)

Proof : $\langle\alpha|A_{odd}|\beta\rangle = \langle\alpha|\underbrace{\pi\pi^{-1}}_{\mathbb{1}}A_{odd}\underbrace{\pi\pi^{-1}}_{\mathbb{1}}|\beta\rangle$ (ε_α, ε_β)

$$= \varepsilon_\alpha \varepsilon_\beta (-1) \langle\alpha|A_{odd}|\beta\rangle$$

[using $\pi^{-1}A_{odd}\pi = -A_{odd}$]

$\Rightarrow (1+\varepsilon_\alpha\varepsilon_\beta)\langle\alpha|A_{odd}|\beta\rangle = 0 \Rightarrow$

$\langle\alpha|A_{odd}|\beta\rangle \neq 0$ only if $\varepsilon_\alpha\varepsilon_\beta = -1$

(above is whether or not H is parity-invariant)

— Suppose H is parity-invariant and $|n\rangle$ is non-degenerate energy eigenket $\Rightarrow$ $|n\rangle$ is parity eigenket

$$\Rightarrow \langle n|\bar{x}|n\rangle = 0$$

$\hookrightarrow$ parity odd

Now, $\boxed{\text{electric dipole moment}}$ (classically)

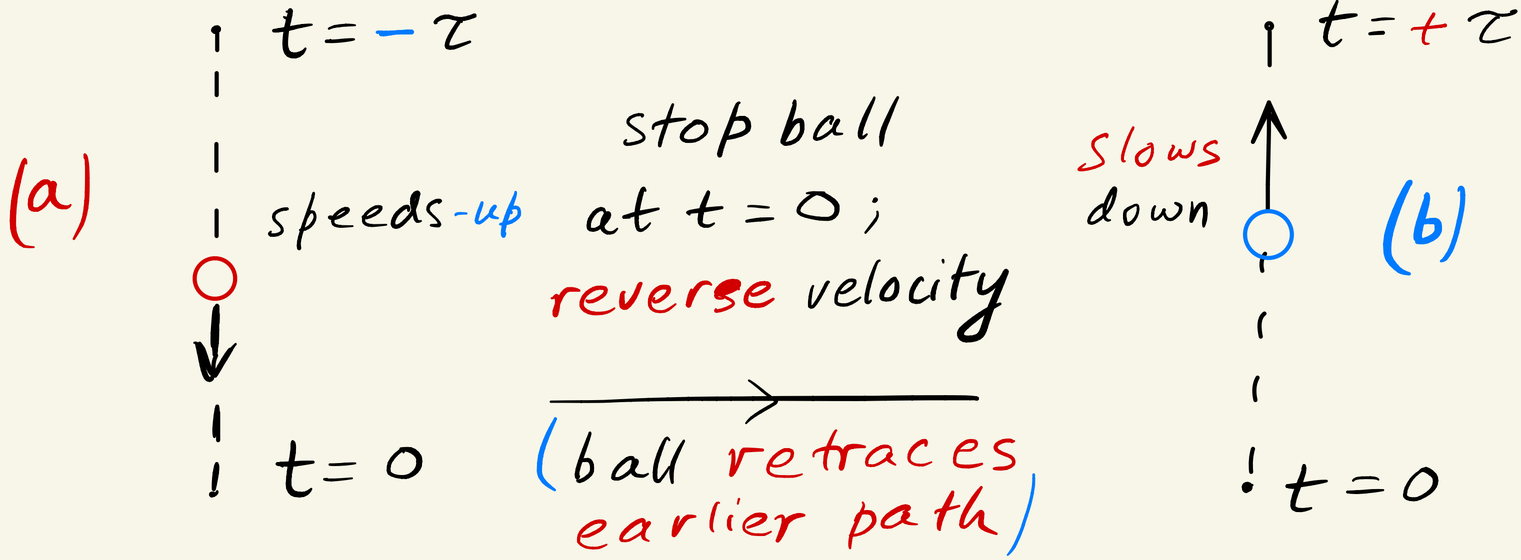
= charge × distance between (opposite) charges

$\longrightarrow \bar{x}$ operator in QM

$\Rightarrow$ vanishing electric dipole moment

Time-reversal symmetry (sec. 4.4)

classical intuition/motivation: ball falling under gravity



$$\Rightarrow \quad x_b\left[t\,(>0)\right] = x_a(-t)$$

"shoot movie" of (a); run it in reverse to get (b)

— $\boxed{\text{crucial}}$ point: (a) & (b) both valid trajectories (solve equation of motion): cannot tell which was original/"foward" in real time (no "arrow" of time) (e.g., just put hard wall at bottom) cf. release gas thru' hole in container: molecules spread:

run movie in reverse, but gas molecules "collecting" "never" happens

(entropy always increases: "arrow" of time)