Quantum Mechanics - 2

More on symmetry

① discrete sym on the lattice / double well / NH_3 -
② Parity
③ Time reversal
④ Some remarks on C, & CPT

$\boxed{\text{Periodic potential}}$

$$V(x) = V(x+a) \Rightarrow H(x) = H(x+a)$$

$$T\psi(x) = \psi(x+a)$$

$$\& \quad H\psi(x) = E\psi(x)$$

$$[T, H] = 0 \quad \text{because}$$

$$HT\psi(x) = H\psi(x+a) = H(x+a)\psi(x+a) = E\psi(x+a)$$

$\Rightarrow T\psi(x)$ is also an eigenstate, (T: unitary)

λ: eigenvalue of T such that $T\psi(x) = \lambda\psi(x)$

define $\lambda = \exp(ika) \Rightarrow k$: real

$$u_k(x) = \exp(-ikx)\psi(x)$$

$$\begin{aligned} \Rightarrow u_k(x+a) &= e^{-ikx} e^{-ika} \psi(x+a) \\ &= e^{-ikx} e^{-ika} T\psi(x) \\ &= e^{-ikx}\psi(x) = u_k(x) \end{aligned}$$

$$\Rightarrow \boxed{u_k(x) = u_k(x+a)}$$

$u_k(x)$ is periodic and $\psi(x)$ can always be expressed in the "Block wave" form

$\psi(x) = e^{ikx} u_k(x)$, also $-\frac{\pi}{a} < k < \frac{\pi}{a}$ is a sufficient range for k

A simple example is the Kronig-Penney model

$$V(x) = \sum_{n=-\infty}^{\infty} V_0 \, \delta(x-na), \quad V_0 : \text{positive const.}$$

We seek a solution to this $V(x)$ with energy E

In the region $0 < x < a$, $V(x) = 0$

$$\Rightarrow \quad \psi = A e^{i g x} + B e^{-i g x}, \quad E = \frac{\hbar^2 g^2}{2m}$$

Thus $u = A e^{i(g-k)x} + B e^{-i(g+k)x}$

The boundary conditions determine A, B and g

$$\int_{a-\epsilon}^{a+\epsilon} dx \left[\frac{-\hbar^2}{2m} \frac{d^2}{dx^2} \psi + V(x) \psi \right] = E \int_{a-\epsilon}^{a+\epsilon} dx \, \psi$$

ϵ: arbitrary infinitesimal parameter for the integral to cover the delta-function potential at $x = a$

$$\Rightarrow \quad -\frac{\hbar^2}{2m} \psi' \Big|_{a-\epsilon}^{a+\epsilon} + V_0 \psi(a) \simeq 2\epsilon E \psi(a)$$

or $\quad \psi'(a+\epsilon) \simeq \psi'(a-\epsilon) + \frac{2m V_0}{\hbar^2} \psi(a)$

at $x = a$, we require the ψ to satisfy the following B.C.

$$\left\{ \begin{array}{l} \psi(a-\epsilon) = \psi(a+\epsilon) \\ \psi'(a+\epsilon) = \psi'(a-\epsilon) + \frac{2m V_0}{\hbar^2} V(a) \end{array} \right.$$

$\psi(a-\epsilon) = (A e^{igx} + B e^{-igx}) \Big|_{x=a-\epsilon}$

$\psi(a+\epsilon) = e^{ika} \psi(\epsilon)$

$$\Rightarrow \quad \cos ka = \cos ga + \frac{m a V_0}{\hbar^2} \frac{\sin ga}{ga}$$

$|LHS| < 1$

Solution for ga if $|RHS| < 1$

$$\Rightarrow \boxed{\text{Energy band, Energy gap}}$$

✱ Parity

$\boxed{\text{spatial inversion in 3D physical space}}$

$$\vec{r} = \begin{pmatrix} x \\ y \\ z \end{pmatrix} \longrightarrow -\vec{r} = -\begin{pmatrix} x \\ y \\ z \end{pmatrix} = \begin{pmatrix} -1 & & \\ & -1 & \\ & & -1 \end{pmatrix}\begin{pmatrix} x \\ y \\ z \end{pmatrix} = P\begin{pmatrix} x \\ y \\ z \end{pmatrix}$$

$$P = \begin{pmatrix} -1 & & \\ & -1 & \\ & & -1 \end{pmatrix} = -\mathbb{1}_{3\times 3}.$$

$P^2 = 1$ and $PRP^{-1} = R$ for all proper rotation $R \in SO(3)$

$(\because P \propto \mathbb{1}_{3\times3})$

P : improper rotation, $\in O(3)$, $(\det(P) \neq +1)$

$$\left(\begin{array}{l} O(3) : \quad O O^T = O^T O = \mathbb{1}, \quad (O : \text{any } 3\times3 \text{ real matrix.}) \\ \Rightarrow \det \mathbb{1} = (\det O)^2 \Rightarrow \det O = \begin{cases} +1 & \text{proper} \\ -1 & \text{improper} \end{cases} \end{array} \right)$$

Every (proper rotation)$\cdot P$ $\rightarrow$ improper rotation

$\boxed{\text{Parity in QM}}$

What is the corresponding operator π in QM ?

recall that $\quad R \longmapsto U(R)$

3D rotation $\longmapsto$ operator in the Hilbert space
unitary representation of the classical rotation group $SO(3)$

Same spirit for finding π, we require that π statisfies the following postulates:

$$\begin{cases} \pi^\dagger \pi = 1 & (\text{unitary}) \\ \pi^2 = 1 \end{cases} \quad \text{and} \quad \pi U(R) \pi^\dagger = U(R) \quad \text{for all } R \in SO(3)$$

$\hookrightarrow \pi = \pi^\dagger = \pi^{-1}$

π is both unitary & Hermitian

$\Rightarrow [\pi, J] = 0$

$\because$ angular momentum is the generator of the rotation operators $U(R)$.

for $R \in SO(3)$

$U(R)$ and $\Pi U(R)$ form a unitary representation of the full rotation group $O(3)$.

We can say $\Pi = U(P)$

$\boxed{\text{Parity for a spinless particle in 3D}}$

The basis states can be taken to be the position eigenstates $|\vec{r}\rangle$ and the Hilbert space is isomorphic to the space of configuration space wave functions $\psi(\vec{r}) = \langle \vec{r}|\psi\rangle$

$$U(R)\,|\vec{r}\rangle = |R\vec{r}\rangle$$

so we guess

$$\Pi\,|\vec{r}\rangle = |P\vec{r}\rangle = |-\vec{r}\rangle$$

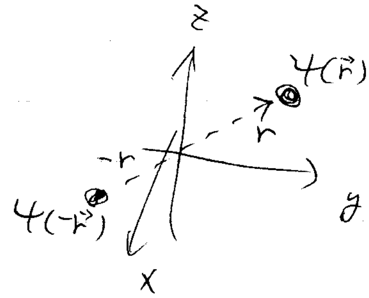
Therefore,

$$\psi(\vec{r}) \xrightarrow{\Pi} (\Pi\psi)(\vec{r}) = \langle \vec{r}|\,\Pi\psi\rangle = \langle \vec{r}|\Pi|\psi\rangle$$
$$= \langle -\vec{r}|\psi\rangle = \psi(-\vec{r})$$

$$\boxed{\psi(\vec{r}) \xrightarrow{\Pi} \psi(-\vec{r})}$$

check:

① $\Pi^2|\vec{r}\rangle = |\vec{r}\rangle$



② $\int d\vec{r}^{\,3}\,|\psi(\vec{r})|^2 = \int d\vec{r}^{\,3}\,|\psi(-\vec{r})|^2$

for all wave functions $\Rightarrow$ Π is unitary

it preserves the normalization of states.

③ $\Pi U(R)|\vec{r}\rangle = \Pi|R\vec{r}\rangle = |-R\vec{r}\rangle = U(R)|-\vec{r}\rangle$
$= U(R)\Pi|\vec{r}\rangle$

$$\Rightarrow \quad \Pi U(R) \Pi^{+} = U(R)$$

Therefore, we can take $\Pi|\vec{r}\rangle = |-\vec{r}\rangle$ as the definition of parity operator for a spinless particle in 3D.

* For a spinless particle, $\vec{J} = \vec{L} = \vec{r} \times \vec{p}$

$$\Rightarrow \quad \pi L \pi^{+} = L \quad \text{and} \quad [\pi, J] = 0$$

* $\pi \hat{r} \pi^{+} |\vec{r}\rangle = \pi \hat{r} |-\vec{r}\rangle = \underbrace{-\vec{r}}_{\text{c-\#}} \pi |-\vec{r}\rangle = -\vec{r} |\vec{r}\rangle$

$$\Rightarrow \quad \boxed{\pi \hat{r} \pi^{+} = -\hat{r}}$$

Similarly we have

$$\boxed{\pi \hat{p} \pi^{+} = -\hat{p}}$$

Parity for spin systems

First ignore the spatial D.O.F for the moment.
The Hilbert space is

$$\mathcal{E}_{spin} = \text{span}\{ |s, m\rangle, \ m = -s \cdots +s \}$$

What's the reasonable definition of π here?

$\vec{J} = \vec{S}$ in this case.

$$\Rightarrow \quad [\pi, \vec{S}] = 0, \quad [\pi, \hat{S}_z] = 0$$

$$\hat{S}_z (\pi |s\, m\rangle) = \pi \hat{S}_z |s\, m\rangle = m\hbar (\pi |s\, m\rangle)$$

But in $\mathcal{E}_{spin}$, the eigenstates of $\hat{S}_z$ are nondegenerate.

$$\Rightarrow \quad \pi |s\, m\rangle = \underbrace{\eta_m}_{\text{some factor depending on } m} |s\, m\rangle$$

$$S_{\pm} (\pi |s\, m\rangle) = \pi S_{\pm} |s\, m\rangle = \hbar \sqrt{s(s+1) - m(m\pm 1)} \ |s, m\pm 1\rangle$$

$$= \eta_m \hbar \sqrt{s(s+1) - m(m\pm 1)} \ |s, m\pm 1\rangle$$

$$\Rightarrow \quad \boxed{\pi |s, m\pm 1\rangle = \eta_m |s, m\pm 1\rangle} \quad \Rightarrow \eta_m = \eta_{m\pm 1} = \eta_{m\pm 2} = \cdots$$

$\Rightarrow$ η is independent of m for all $2s+1$ values.

$\Rightarrow \boxed{\Pi|s\,m\rangle = \eta|s\,m\rangle}$ all kets in $\mathcal{E}_{spin}$ are eigenstates of Π with eigenvalue η.

Since $\Pi^2 = 1 \Rightarrow \eta^2 = 1$, or $\eta = \pm 1$

We have $\boxed{\Pi|s, m\rangle = \pm|s\,m\rangle}$

☆ In non relativistic QM, there is no way to determine the sign by either theory or experiments. The sign is totally unphysical. We can simply assume

$$\boxed{\Pi|s\,m\rangle = |s\,m\rangle}$$

☆ However, in relativistic QM, particles can be created or annihilated $\Rightarrow$ intrinsic parity is fixed by requiring initial state parity = final state parity in the parity conserving processes (QED, QCD)

total parity $= P_1 \times P_2 \cdots P_n \times P_{spatial}$

$\Rightarrow$ photon has negative intrinsic parity $\Rightarrow$ Laporte's rule

☆ Returning to NR QM, if we include the spatial D.O.F. the Hilbert space is spanned by the basis kets

$$|\vec{r}\rangle \otimes |s\,m\rangle \equiv |\vec{r}, s\,m\rangle$$

$$\Pi|\vec{r}, s\,m\rangle = |-\vec{r}, s\,m\rangle$$

It is equivalent to the action on the W.F.:

$$\psi_m(\vec{r}) \xrightarrow{\Pi} \psi_m(-\vec{r})$$

$\vec{r}, \vec{p}$ change sign when conjugated by parity

$\vec{L}, \vec{S}$ do not

All are transformed in the same way under conjugated by proper rotations, but are diffent under improper rotations.

$\hat{V}$: vector operator $\quad \pi \hat{V} \pi^{\dagger} = \begin{cases} -\hat{V} : & \text{vector} \\ +\hat{V} : & \text{pseudo-vector} \\ & \text{axial-vector} \end{cases}$

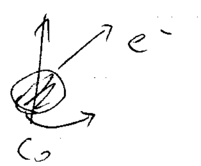
Other examples $\quad \vec{E}$: vector $\quad \sim \vec{\nabla}\phi$

$\vec{B}$: pseudo vector $\quad \sim \nabla \times \vec{A}$

Similarly, if O_s a scalar operator

$$\pi O_s \pi^{\dagger} = \begin{cases} +O_s & : \text{scalar} \\ -O_s & : \text{pseudo-scalar} \end{cases} \qquad \begin{matrix} \text{example} \\ \vec{r}\cdot\vec{p} \\ \vec{p}\cdot\vec{s} \end{matrix}$$

~~Before~~ Unitl 1956, Lee & Yang, C. S. Wu
parity nonconservation in weak interaction
(maximally)



$$\vec{p}_e \cdot \vec{S}_{Co} \xrightarrow{\pi} -\vec{p}_e \cdot \vec{S}_{Co}$$

However, the effect is very small at low energy.

$H = \frac{p^2}{2m} + V(r)$, $\quad [H, \pi] = 0$, $\quad \vec{p}^2 \to (-\vec{p})^2$, $\quad |\vec{r}| \to |-\vec{r}| = |\vec{r}|$

$\Rightarrow$ parity is a good quantum number for a wide variety of approximate Hamiltonians for atoms, molecules, and other system.