7. Symmetry in QM

7.1 Symmetry groups in QM

G is a group under the operation $a \circ b$ if

- $a \circ b \in G \quad \forall a, b \in G$
- $(a \circ b) \circ c = a \circ (b \circ c) \quad \forall a, b, c$
- $\exists 1 : \; 1 \circ a = a \circ 1 = a \quad \forall a$
- $\forall a \; \exists a^{-1} : \quad a \circ a^{-1} = a^{-1} \circ a = 1$

G can be discrete (isolated points) or continuous (locally like a manifold)

Continuous groups have an associated Lie algebra

$$g = 1 + ih + \mathcal{O}(h^2) \quad \text{for } g \sim 1$$

Lie algebra $\mathfrak{g} = \{h\}$ (tangent space to G), $\quad [h_i, h_j] = i \hbar f_{ijk} h_k$ structure

$$= \lim_{\varepsilon \to 0} \frac{-1}{\varepsilon^2} \left[e^{i\varepsilon h_i} e^{i\varepsilon h_j} e^{-i\varepsilon h_i} e^{-i\varepsilon h_j} - 1 \right]$$

Ex's of groups

discrete

$\mathbb{Z}_2 : \; \{1, a\} \quad a^2 = 1$

	1	a
1	1	a
a	a	1

$\mathbb{Z} : \; \{n\} \quad n \circ m = n + m$

continuous

$U(1) : \; \{e^{i\theta}, \; \theta \in [0, 2\pi]\} \quad e^{i\theta} \circ e^{i\phi} = e^{i(\phi + \theta)}$

Lie algebra: $\mathbb{R} : [h, h] = 0$

$SU(2)$
$SO(3)$ $\Big\}$ Lie algebra: $\mathbb{R}^3 : [h_i, h_j] = i \varepsilon_{ijk} h_k$

Representations of a group G:

$$\mathcal{D}(g) : \mathcal{H} \to \mathcal{H} \quad \text{linear} \quad \forall g \in G$$
$$\mathcal{D}(g)\mathcal{D}(h) = \mathcal{D}(gh)$$
$$\mathcal{D}^{-1}(g) = \mathcal{D}(g^{-1}) \qquad (\mathcal{D}^{-1} = \mathcal{D}^{\dagger} \text{ if unitary rep.})$$
$$\mathcal{D}(\mathrm{id}) = \mathbb{1}$$

If $\mathcal{D}^{-1}(g) H \mathcal{D}(g) = H \quad \forall g \in G$,
then G is a symmetry of physical system.

Representation reducible if can put $\mathcal{D}(g) = \begin{pmatrix} \mathcal{D}^{(1)} & 0 \\ 0 & \mathcal{D}^{(2)} \end{pmatrix}$ in block-diagonal form $\forall g$, irreducible if not.

Conserved quantities

Classically, given a continuous symmetry,

$$\alpha^i \partial \mathcal{L} / \partial q^i = 0$$

$$\Rightarrow \alpha^i \frac{d}{dt} \left(\partial \mathcal{L} / \partial \dot{q}^i \right) = 0 \quad \Rightarrow \alpha^i p_i \text{ is conserved}$$

QM, $\quad \mathcal{D}(g) H \mathcal{D}(g^{-1}) = H, \qquad g = 1 + ih + \mathcal{O}(\mathcal{J}^2)$

$$\Rightarrow [h, H] = 0 \quad \Rightarrow \langle h \rangle \text{ conserved.}$$

For example, if H invariant under $SU(2)$ rotations, $\vec{J}$ is conserved.

Degeneracy:

If $H|\psi\rangle = E|\psi\rangle, \qquad \mathcal{D}^{-1}(g) H \mathcal{D}(g) = H$,

$$H \mathcal{D}(g) |\psi\rangle = \mathcal{D}(g) H |\psi\rangle = \mathcal{D}(g) E |\psi\rangle$$

so $\mathcal{D}(g)|\psi\rangle$ has same energy as $|\psi\rangle$.

G irreps give multiplets w/ fixed energy

Ex: $2p$ states in hydrogen – all 3 have degenerate energy in absence of field breaking $SU(2)$ invariance.

7.2 Parity (spatial inversion)

maps $\vec{x} \to -\vec{x}$

Discrete symmetry, group is $G = \mathbb{Z}_2$, $\{1, a\}$ $a^2 = 1$

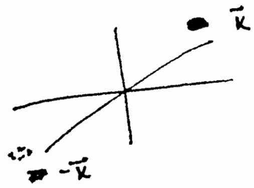
Reps of $\mathbb{Z}_2$: $\mathcal{D}(a)^2 = \mathbb{1}$, so irreps are $\mathcal{D}(a) = \pm 1$ in one-dimensional $\mathcal{H}$.

General representation: $\mathcal{D}(a) = \begin{pmatrix} \overbrace{1 \; 1 \; \ddots}^{n} & \\ & \underbrace{-1 \; -1 \; \ddots}_{m} \end{pmatrix}$

Denote $\Pi = \mathcal{D}(a)$ for parity xform.

Define $\Pi|\vec{x}\rangle = |-\vec{x}\rangle$ (phase is convention)

reflects point on all axes



Properties of Π:

$$\Pi^{+} = \Pi , \qquad \Pi^{2} = \mathbb{1}$$

($\hat{}$ = operator)

$$(\Pi \hat{\vec{x}} \Pi)\int f(\vec{x})\,|\vec{x}\rangle = \Pi \hat{\vec{x}} \int f(\vec{x})\,|-\vec{x}\rangle$$

$$= \Pi \int f(\vec{x})\,(-\vec{x})\,|-\vec{x}\rangle$$

$$= \int f(\vec{x})\,(-\vec{x})\,|\vec{x}\rangle$$

$$= -\hat{\vec{x}} \int f(\vec{x})\,|\vec{x}\rangle$$

so $\Pi^{+}\vec{X}\Pi = -\vec{X} = \Pi\vec{X}\Pi$

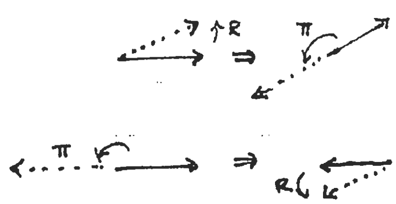
similarly, $\Pi\vec{p}\,\Pi = \Pi(-i\vec{\partial})\Pi = -\vec{p}$

so $\{\Pi, \vec{x}\} = \{\Pi, \vec{p}\} = 0.$

$L = \vec{x}\times\vec{p} \;\Rightarrow\; \Pi\vec{L} = \vec{L}\Pi, \quad [\Pi, \vec{L}] = 0.$

In general, for rotations

$$\Pi R(\hat{n},\theta) = R(\hat{n},\theta)\Pi$$



$\Rightarrow [\Pi, \vec{J}] = 0$ in general.

Thus, expect $[\Pi, \vec{S}] = 0$

so Π reverses coordinates, momentum, but not angular momentum.

Notation:

Polar vector: transforms as vector under rotation, odd parity $[\vec{x}, \vec{p}]$

Axial vector: " " vector " " even parity $[\vec{L}]$

Scalar: " " scalar " " even parity $[x^2, \vec{x}\cdot\vec{p}, \vec{L}\cdot\vec{S}]$

Pseudoscalar: " " scalar " " odd parity $[\vec{S}\cdot\vec{x}, \vec{L}\cdot\vec{p}]$

Wavefunctions under parity

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

under parity xform, $\psi(\vec{x}) \to \tilde{\psi}(\vec{x})$

$$\tilde{\psi}(\vec{x}) = \langle \vec{x} | \Pi | \psi \rangle = \langle -\vec{x} | \psi \rangle = \psi(-\vec{x})$$

If $\Pi |\psi\rangle = \pm |\psi\rangle$,

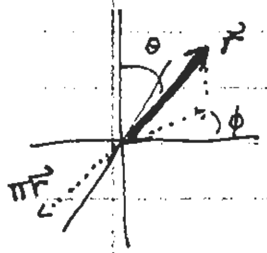
$$\psi(x) = \pm \psi(-x), \quad \psi \ \begin{matrix}\text{even}\\ \text{odd}\end{matrix} \ \text{under parity}$$

Momentum & Angular momentum eigenstates

$$\Pi |\vec{p}\rangle = |-\vec{p}\rangle \neq \pm |\vec{p}\rangle$$

since $[\vec{p}, \Pi] \neq 0$.

But since $[\vec{L}, \pi] = 0$,
 can simultaneously diagonalize $\vec{L}, \pi$.



$$\pi\,|\theta, \phi\rangle = |\pi - \theta, \phi + \pi\rangle$$

$$Y_{\ell m} = \langle \theta, \phi | \ell, m\rangle$$

Y_{00} = const : has even parity

$Y_{1m} = \sin\theta\, e^{\pm i\phi}$, $\cos\theta$ have odd parity

$\Rightarrow$ $Y_{\ell m}$ has parity $(-1)^\ell$
since $Y_{\ell m}$ is $(Y_{1m})^\ell$ by angular momentum add. using Clebsch-Gordan coefficients
(also from explicit formulae – see book)

<u>Energy eigenstates</u>

Suppose $[H, \pi] = 0$

If $H = \frac{p^2}{2m} + V(x)$

$$\pi H \pi = \frac{p^2}{2m} + V(-x)$$

so $V(x) = V(-x)$ even under parity.

If $H|\psi\rangle = E|\psi\rangle$, the same is true of $\pi|\psi\rangle$.

Thus, either a) nondegenerate
$\pi|\psi\rangle = \xi|\psi\rangle \quad \xi^2 = 1 \Rightarrow \xi = \pm 1$

or b) degenerate ...

$\pi|\psi\rangle$ may be linearly independent of $|\psi\rangle$.

If so, $|\phi\pm\rangle = |\psi\rangle \pm \pi|\psi\rangle$

$$\pi|\phi\pm\rangle = \pm|\psi\rangle + \pi|\psi\rangle = \pm|\phi\pm\rangle$$

$\rightarrow$ can simultaneously diagonalize H, π, so all ϵ eigenstates can be chosen to be π eigenstates.

Ex. free particle

$$H|\vec{p}\rangle = \frac{p^2}{2m}|\vec{p}\rangle$$

$$\pi|\vec{p}\rangle = |-\vec{p}\rangle$$

$|\phi\pm\rangle = \frac{1}{\sqrt{2}}(|\vec{p}\rangle \pm |-\vec{p}\rangle)$ are simultaneous eigenstate of H, π.

Selection rules

Consider
$$\left.\begin{aligned} \pi\Theta\pi &= \lambda\Theta \\ \pi|\psi\rangle &= \xi|\psi\rangle \\ \pi|\psi'\rangle &= \xi'|\psi'\rangle \end{aligned}\right\} \quad \lambda, \xi, \xi' \in \{-1, 1\}$$

$$\langle\psi|\Theta|\psi'\rangle = \langle\psi|\pi\pi\,\Theta\,\pi\pi|\psi'\rangle$$
$$= \lambda\xi\xi'\langle\psi|\Theta|\psi'\rangle$$

so $= 0$ unless $\lambda\xi\xi' = 1$.

Θ ~~is~~ even $\Rightarrow$ $|\psi\rangle, |\psi'\rangle$ same parity
Θ ~~is~~ odd $\Rightarrow$ $|\psi\rangle, |\psi'\rangle$ opp. parity.

Ex. E1 transitions

$\langle \psi' | \vec{x} | \psi \rangle$

only nonzero when $|\psi\rangle, |\psi'\rangle$ have opposite parity.

M1 transitions

$\langle \psi' | \vec{L} + g\vec{S} | \psi \rangle$

nonzero when $|\psi\rangle, |\psi'\rangle$ have same parity.

7.3 Time reversal

Consider classical Eom $m\ddot{x} = -\nabla V(x)$

$x(t)$ solution $\Rightarrow$ $x(-t)$ solution.

All microscopic classical systems are invariant under time reversal

$\rightarrow$ $q^i(t) \rightarrow q^i(-t)$ invariance

Quantum:

$$i\hbar \frac{\partial \psi}{\partial t} = \left(-\frac{\hbar^2}{2m}\nabla^2 + V(x)\right)\psi(x,t)$$

not satisfied by $\psi(x,-t)$

but <u>is</u> satisfied by $\psi^*(x,-t)$

$$\psi(x,t) = \sum c_n(0)\, e^{-\frac{i}{\hbar}E_n t}$$

$$\psi^*(x,-t) = \sum c_n^*(0)\, e^{-(-\frac{i}{\hbar})E_n(-t)}$$

$$= \sum c_n^*(0)\, e^{-\frac{i}{\hbar}E_n t} \quad \text{OK.}$$

Implies time reversal involves cpx conjugation.

Antiunitary transformations

Recall: Unitary xforms have $U^{+} = U^{-1}$;
preserve inner product

$$|\tilde{\alpha}\rangle = U|\alpha\rangle \;, \quad |\tilde{\beta}\rangle = U|\beta\rangle$$
$$\Rightarrow \quad \langle\tilde{\beta}|\tilde{\alpha}\rangle = \langle\beta|U^{+}U|\alpha\rangle = \langle\beta|\alpha\rangle.$$

For physical results to be invariant under a transform.,
only need $|\langle\tilde{\beta}|\tilde{\alpha}\rangle| = |\langle\beta|\alpha\rangle|$.

A transformation Θ: $|\alpha\rangle \to |\tilde{\alpha}\rangle = \Theta|\alpha\rangle$
$|\beta\rangle \to |\tilde{\beta}\rangle = \Theta|\beta\rangle$

is <u>antilinear</u> if
$$\Theta\left(c_1|\alpha\rangle + c_2|\beta\rangle\right) = c_1^{*}\,\Theta|\alpha\rangle + c_2^{*}\,\Theta|\beta\rangle.$$

<u>antiunitary</u> if antilinear &
$$\langle\tilde{\beta}|\tilde{\alpha}\rangle = \langle\beta|\alpha\rangle^{*}$$

Given a basis $|\alpha_i\rangle$ for $\mathcal{H}$, can define

<u>Complex conjugation</u> K:
$$K\left(\sum c_i|\alpha_i\rangle\right) = \sum c_i^{*}|\alpha_i\rangle$$

Note: K depends on choice of basis.

Theorem

Any antiunitary operator Θ can be written $\Theta = UK$, where U unitary.

[For different choices of basis, work of U, K reapportioned]

Pf. Choose basis $|a\rangle$,
[corresponding K: $K(\sum c_a |a\rangle) = \sum c_a^* |a\rangle$]

ΘK takes

$$|\alpha\rangle \to |\tilde{\alpha}\rangle = \Theta K |\alpha\rangle$$

$$= \sum_a \Theta K |a\rangle\langle a|\alpha\rangle$$

$$= \sum_a \langle a|\alpha\rangle \; \Theta|a\rangle$$

$$|\beta\rangle \to |\tilde{\beta}\rangle = \sum_b \langle b|\beta\rangle \; \Theta|b\rangle$$

$$\Rightarrow \quad \langle \tilde{\beta}|\tilde{\alpha}\rangle = \sum_{a,b} \langle \tilde{b}|\tilde{a}\rangle \langle \beta|b\rangle\langle a|\alpha\rangle$$

$$= \sum_{a,b} \langle \beta|b\rangle \; \delta_{ba} \; \langle a|\alpha\rangle = \langle \beta|\alpha\rangle$$

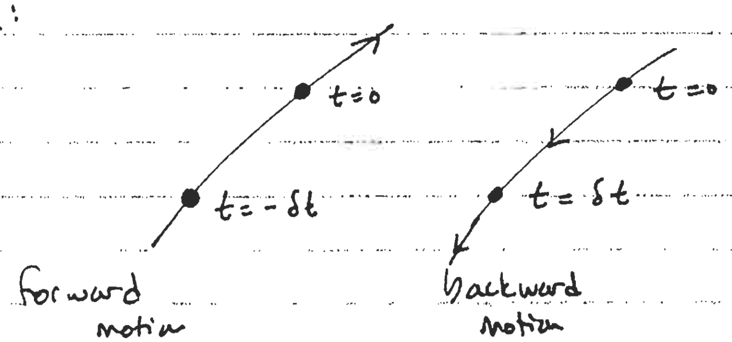
$\Rightarrow$ ΘK unitary.

Same argument $\Longrightarrow$ any UK is antiunitary, for U unitary
(see book)

Time-reversal operator Θ

Expect Θ involves K.

Check:



$$\text{want} \quad |\psi(-\delta t)\rangle_f = \Theta|\psi(\delta t)\rangle_r$$

$$|\psi(0)\rangle_f = \Theta|\psi(0)\rangle_r$$

$$|\psi(-\delta t)\rangle_f = \left(1 + \frac{iH}{\hbar}\delta t\right)|\psi(0)\rangle_f$$

$$= \left(1 + \frac{iH}{\hbar}\delta t\right)\Theta|\psi(0)\rangle_r$$

$$= \Theta|\psi(\delta t)\rangle_r$$

$$= \Theta\left(1 - \frac{iH}{\hbar}\delta t\right)|\psi(0)\rangle_r$$

$$\Rightarrow \quad iH\Theta = -\Theta iH.$$

If Θ unitary, $H\Theta = -\Theta H$

e.g. $H\Theta|\vec{p}\rangle = -\Theta H|\vec{p}\rangle = -\frac{p^2}{2m}\Theta|\vec{p}\rangle, \; E<0$

BAD.

Instead, take Θ antiunitary

$$\Rightarrow [H, \Theta] = 0.$$

<u>Behavior of operators under Θ</u>

For Θ antiunitary, A Hermitian

$$\begin{aligned}\langle\beta|A|\alpha\rangle &= \langle\alpha|A|\beta\rangle^* \\ &= \langle\tilde{\alpha}|\Theta A|\beta\rangle \\ &= \langle\tilde{\alpha}|\Theta A \Theta^{-1}|\tilde{\beta}\rangle\end{aligned}$$

An operator is even/odd under time reversal if

$$\Theta A \Theta^{-1} = \pm A.$$

$$\begin{aligned}\langle\beta|A|\alpha\rangle &= \pm\langle\tilde{\alpha}|A|\tilde{\beta}\rangle \\ &= \pm\langle\tilde{\beta}|A|\tilde{\alpha}\rangle^*.\end{aligned}$$

If $|\alpha\rangle = |\beta\rangle$,

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

Time reversal should leave $\vec{x}$ unchanged.

Choose

$$\Theta |\vec{x}\rangle = |\vec{x}\rangle \qquad \text{(phase by convention)}$$

$$\Rightarrow \quad \Theta \vec{X} \Theta^{-1} = \vec{X}.$$

For a general wavefunction $|\psi\rangle = \int \psi(x) |\vec{x}\rangle$

$$\Theta |\psi\rangle = \int \psi^*(x) |x\rangle$$

$$\text{so} \quad \psi(x) \longrightarrow \psi^*(x)$$

In particular

$$\Theta |\vec{p}\rangle = \Theta \int \frac{1}{\sqrt{2\pi\hbar}} e^{i\vec{p}\cdot\vec{x}/\hbar} |\vec{x}\rangle$$

$$= \int \frac{1}{\sqrt{2\pi\hbar}} e^{-i\vec{p}\cdot\vec{x}/\hbar} |\vec{x}\rangle = |-\vec{p}\rangle$$

Follows that

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

$$\Rightarrow \quad \Theta (\vec{X} \times \vec{P}) \Theta^{-1} = -\vec{X} \times \vec{P}.$$

More generally,

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

– consistent with spinless case, natural to extend to spins $\Rightarrow$ needed to preserve $[J_i, J_j] = i\hbar \epsilon_{ijk} J_k$.

For angular momentum eigenstates:

(Recall $Y_{\ell m}$ has $e^{im\phi}$ phase)

$$\Theta |\ell, m\rangle = (-1)^m |\ell, -m\rangle$$ ($\ell \in \mathbb{Z}$; generalize to $\ell \in \mathbb{Z}+\frac{1}{2}$ in HW)

Time-reversal & spin

Consider spin-1/2 particle

$$J_z \Theta |+\rangle = -\Theta J_z |+\rangle = -\frac{\hbar}{2}\Theta|+\rangle$$

so $\Theta|+\rangle = \eta|-\rangle$, η a phase

but $|-\rangle = e^{-i\pi S_y/\hbar}|+\rangle$

so $\Theta|-\rangle = \eta e^{-i\pi S_y/\hbar}|-\rangle = -\eta|+\rangle$

so $\Theta = \eta e^{-i\pi S_y/\hbar} K$ for spin-1/2 system.

Standard convention: $\eta = i$

so $\Theta = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} K = \sigma_y K$

Note: $\Theta^2 = \sigma_y K \sigma_y K = -\sigma_y^2 K^2 = -\sigma_y^2 = -1$.

Result independent of phase choices

$\Theta^2 = -1$ for any system w/ odd # of fermions (all fermions have 1/2-integral spin)

[Think of spin j as $2j$ spin-1/2 particles]

Consequences of time-reversal invariance

We have focused on behaviour of operators under Θ

$$\Theta A \Theta^{-1} = \pm A$$

Behaviour on states less significant, depends on phase choices.

Even if $[H, \Theta] = 0$, does not make sense to think of Θ as an observable being associated with an ~~conserved~~ quantity (unlike parity)

– no conservation law/selection rule

Ex. consider state $H|\psi\rangle = E|\psi\rangle$, $\Theta|\psi\rangle = |\psi\rangle$, $[H,\Theta]=0$ (e.g. real wavefunction for spinless state)

$$|\psi, t\rangle = e^{-\frac{i}{\hbar}Et}|\psi\rangle.$$

$$\Theta|\psi, t\rangle = e^{\frac{i}{\hbar}Et}|\psi\rangle \neq |\psi, t\rangle.$$

Time-reversal does have other consequences, though...

Assume $[H, \Theta] = 0$, $H|n\rangle = E_n|n\rangle$

$$H\Theta|n\rangle = \Theta E_n|n\rangle = E_n(\Theta|n\rangle).$$

So $|n\rangle$, $\Theta|n\rangle$ have degenerate energy.

Same state? if so, $\Theta|n\rangle = e^{i\delta}|n\rangle$.

$$\Theta^2|n\rangle = \Theta e^{i\delta}|n\rangle = e^{-i\delta}\Theta|n\rangle = |n\rangle.$$

Thus, for ½-integral spin states, must be that

$|n\rangle$, $\Theta|n\rangle$ are linearly independent.

Kramer's degeneracy:

Any system containing an odd number of fermions which is time-reversal invariant has at least 2-fold degeneracy.

What about external B field?

$\uparrow B_z$ $\quad H = \vec{S}\cdot\vec{B}$ no degeneracy

Treating $\vec{B}$ as external field, $\Theta\vec{S} = -\vec{S}\Theta$
so $[H, \Theta] \neq 0$.

If we include sources, $\vec{B}$ also reverses.

Ex. proton + electron

$H \sim \vec{I}\cdot\vec{S}$ $\quad \vec{F} = \vec{I} + \vec{S}$
$[H, \Theta] = 0$.

3 states with $F = 1$
1 state with $F = 0$ } hyperfine splitting.

But $\Theta^2 = 1$ for all states, so ok.

If $I = 1$, $S = ½$, $F = 3/2$ (4 states) $F = ½$ (2 states)
exhibit Kramer's degeneracy.