7. Symmetry in QM

7.1 Symmetry groups in QM

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

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

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

Continuous groups have an associated Lie algebra

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

Lie algebra $\mathfrak{g} = \{h\}$, (tangent space to G) $\quad [h_i, h_j] = ih f_{ijk} h_k$ 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: $\mathbb{R}^3 : [h_i, h_j] = i\varepsilon_{ijk} h_k$

<u>Representations of a group G:</u>

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

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

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

<u>Consered quantities:</u>

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

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

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

<u>Degeneracy</u>:

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 $G = \mathbb{Z}_2$, $\{1, a\}$ $a^2 = 1$

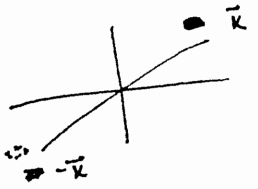
Reps of $\mathbb{Z}_2$: $\mathcal{D}(a)^2 = \mathbb{1}$, so irreps are $\mathcal{D}(a) = \pm 1$ in one-dimensional $\mathcal{H}$.

General representation: $\mathcal{D}(a) = \begin{pmatrix} \left.\begin{matrix} 1 & & \\ & 1 & \\ & & 1 \end{matrix}\right\} n & \\ & \left.\begin{matrix} -1 & & \\ & -1 & \\ & & \ddots -1 \end{matrix}\right\} m \end{pmatrix}$ $\Big\downarrow$

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:

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

(^ = operator)

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

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

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

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

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

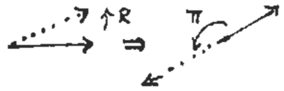
$$\text{similarly,} \quad \Pi \vec{p} \Pi = \Pi (-i \vec{\partial}) \Pi = -\vec{p}$$

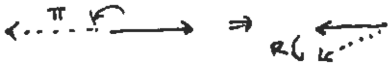
$$\text{so} \quad \{ \Pi , \vec{x} \} = \{ \Pi , \vec{p} \} = 0 .$$

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

In general, for rotations

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





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

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

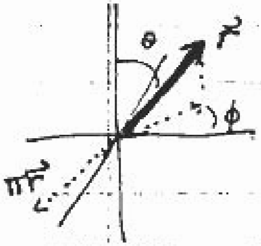
$\psi(x) = \pm \psi(-x)$, ψ $\begin{matrix}\text{even}\\ \text{odd}\end{matrix}$ under parity

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)

Energy eigenstates

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
$\pi|\psi\rangle = \xi|\psi\rangle$ $\xi^2 = 1 \Rightarrow \xi = \pm 1$
or b) degenerate ...

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

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

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

→ can simultaneously diagonalize H, π, so all ϵ eigenstates can be chosen to be π eigenstates.

Ex. free particle

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

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

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

Selection rules

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

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

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

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

Θ even $\Rightarrow$ $|\psi\rangle, |\psi'\rangle$ same parity

Θ 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 $\Longrightarrow$ $x(-t)$ solution.

All microscopic classical systems are invariant under time reversal

$\rightarrow$ $q^i(t) \to q^i(-t)$ 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 is 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

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

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

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

is antilinear if
$$\Theta(c_1|\alpha\rangle + c_2|\beta\rangle) = c_1^{*}\,\Theta|\alpha\rangle + c_2^{*}\,\Theta|\beta\rangle.$$

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

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

Complex conjugation 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

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

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

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

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

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

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

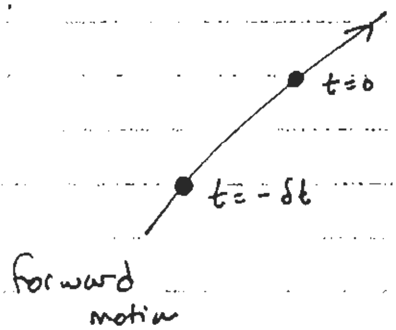
$\Rightarrow$ ΘK unitary.

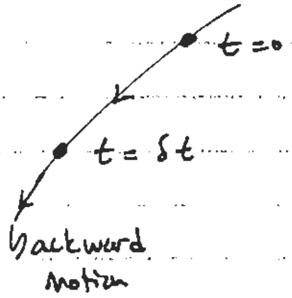
Same argument $\Longrightarrow$ any UK is antiunitary, if U unitary
(see book)

Time-reversal operator Θ

Expect Θ involves K.

Check:





want $$|\psi(-\delta t)\rangle_f = \Theta|\psi(\delta t)\rangle_r$$

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

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

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

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

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

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

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

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

Behaviour of operators under Θ

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 $\overset{\text{even}}{\text{odd}}$ 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 ⇒ 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: $\Theta^2 = \sigma_y K \sigma_y K = -\sigma_y^2 K^2 = -\sigma_y^2 = -\mathbb{1}$.

Result independent of phase choices

$\Theta^2 = -1$ for any system w/ odd # of femions (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 <u>operators</u> under Θ

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

Behaviour on states less significant, depends on phase choices.

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

- <u>no conservation law/selection rule</u>

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?

$\uparrow B_z$ $\quad H = \vec{S}\cdot\vec{B}$ $\quad$ 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

$H \sim \vec{I}\cdot\vec{S}$ $\qquad \vec{F} = \vec{I} + \vec{S}$

$[H, \Theta] = 0$.

$$\left.\begin{array}{l} 3 \text{ states with } F = 1 \\ 1 \text{ state with } F = 0 \end{array}\right\} \text{hyperfine splitting.}$$

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

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

7.4 Lattice translation as a discrete symmetry

Consider a periodic potential $V(x+a) = V(x)$

Ex: motion of an electron in a regular solid.

Want to understand spectrum, symmetry.

Review: translation operators

Define $\tau(\ell)$ through

$$\tau(\ell)\,|x\rangle = |x+\ell\rangle$$

$$\tau(\ell)^\dagger = \tau(\ell)^{-1}$$

$$\tau(\ell)^\dagger \, \overset{\nearrow}{\hat{x}} \, \tau(\ell)\,|x\rangle = \tau(\ell)^\dagger \, \hat{x} \, |x+\ell\rangle$$

distinguishes operator

$$= \tau(\ell)^\dagger \, (x+\ell)\, |x+\ell\rangle$$

$$= (x+\ell)\,|x\rangle$$

$$\Rightarrow \quad \tau(\ell)^\dagger \, \hat{x} \, \tau(\ell) = \hat{x} + \ell$$

$$\tau(\ell)\,|p\rangle = \tau(\ell) \int \frac{dx}{\sqrt{2\pi\hbar}} \, e^{ipx/\hbar} \, |x\rangle$$

$$= \int \frac{dx}{\sqrt{2\pi\hbar}} \, e^{ipx/\hbar} \, |x+\ell\rangle$$

$$= e^{-ip\ell/\hbar} \, |p\rangle$$

so $\tau(\ell) = e^{-i\hat{p}\ell/\hbar} = e^{-\ell \frac{\partial}{\partial x}}$

$$\tau^{+}(\ell)\,\hat{p}\,\tau(\ell) = \hat{p}$$

For general wavefunctn

$$\tau(\ell)\,|\psi\rangle = \tau(\ell)\int dx\ \psi(x)\,|x\rangle$$

$$= \int dx\ \psi(x)\,|x+\ell\rangle$$

$$= \int dy\ \psi(y-\ell)\,|y\rangle$$

$\Rightarrow$ when $|\psi'\rangle = \tau(\ell)\,|\psi\rangle$

$$\psi'(x) = \psi(x-\ell) = e^{-\ell\frac{\partial}{\partial x}}\,\psi(x).$$

For a particle in a periodic Hamiltonian $V(x+a) = V(x)$,

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

$$\tau^{+}(a)\,H\,\tau(a) = \tau^{+}(a)\,V(x+a)\,\tau(a) + \frac{p^2}{2m} = H.$$

so $[H, \tau(a)] = 0.$

Group theory:

Discrete translation group $\mathbb{Z}$ is generated by α,

Group elements : $\ldots, \alpha^{-1}\circ\alpha^{-1}, \alpha^{-1}, 1, \alpha, \alpha\circ\alpha, \alpha\circ\alpha\circ\alpha$

$\ldots\ \alpha^{-2}\ \ \alpha^{-1}\ \ \alpha^{0}\ \ \alpha^{1}\ \ \alpha^{2}\ \ldots$

$\{\alpha^n\}_{n\in\mathbb{Z}}$: $\alpha^n \circ \alpha^m = \alpha^{n+m}$

Group is free group on one element (no relations)

To find representations: diagonalize $\mathcal{D}(\alpha)$
irreps are 1-dimensional, $\mathcal{D}(\alpha) = e^{-i\theta}$ phase.

Since $[H, \tau(a)] = 0$, $\tau(a) = \mathcal{D}(\alpha)$,
can simultaneously diagonalize H, $\tau(a)$. Write $\theta = ka$.

States $|\psi_k\rangle$ satisfy

$$\tau(a)|\psi_k\rangle = e^{-ika}|\psi_k\rangle$$

$$\psi(x-a) = e^{-ika}\psi(x)$$

or $$\psi(x+a) = e^{ika}\psi(x).$$

write $\boxed{\psi(x) = e^{ikx}\tilde{\psi}(x),}$

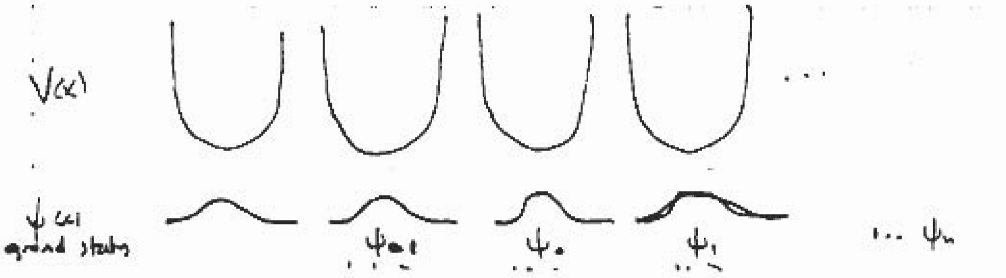
$$e^{ik(x+a)}\tilde{\psi}(x+a) = e^{ik(x+a)}\tilde{\psi}(x)$$

$$\boxed{\tilde{\psi}(x+a) = \tilde{\psi}(x)}$$

So solutions are "quasiperiodic" in $x \to x+a$

[Bloch's theorem]

Example: ∞ potential between sites



∞ potential localizes states in 1 region.

$$H|n_k\rangle = E_k|n_k\rangle$$ n = lattice site #
k = enegy level

$$\tau(a)|n_k\rangle = |(n+1)_k\rangle$$

Denote
$$|\theta_k\rangle = \frac{1}{\sqrt{2\pi}}\sum_{n=-\infty}^{\infty} e^{in\theta}|n_k\rangle$$

$$H|\theta_k\rangle = E_k|\theta_k\rangle$$

$$\tau(a)|\theta_k\rangle = \frac{1}{\sqrt{2\pi}}\sum e^{in\theta}|(n+1)_k\rangle$$
$$= e^{-i\theta}|\theta_k\rangle$$

Normalization: if $\langle n_k|m_\ell\rangle = \delta_{nm}\delta_{k\ell}$

$$\langle\theta_k|\theta'_\ell\rangle = \delta_{k\ell}\,\delta(\theta-\theta')$$

In this example, all <u>levels</u> degenerate (infinitely)

Example: free particle $(V=0)$.

Consider eigenstates $|p\rangle$. $H|p\rangle = \frac{p^2}{2m}|p\rangle$.

$$\tau(a)|p\rangle = e^{-ipa/\hbar}|p\rangle.$$

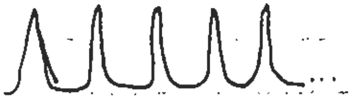
E spectrum continuous, doubly degenerate

<u>General case</u>: part way between free & localized examples.

Tight - binding approximation

A simple model:

- assume potential high, but not ∞, between lattice sites.



- associate state $|n\rangle$ with ground state of each region.

Gives lattice model

$$\langle n | n' \rangle = \delta_{nn'}$$
$$\tau |n\rangle = |n+1\rangle$$

Assume tight - binding approximation

$$\langle n' | H | n \rangle = 0 \quad \text{unless } n' \in \{n-1, n, n+1\}$$

Define $\langle n^{\pm} | H | n \rangle = -\Delta$ (assume $[\tau, H] = 0$)

so
$$H = \begin{pmatrix} \ddots & & & & \\ & E_0 & -\Delta & & 0 \\ & -\Delta & E_0 & -\Delta & \\ & & -\Delta & E_0 & -\Delta \\ & 0 & & -\Delta & E_0 & \ddots \end{pmatrix}$$

[note: many details removed in this simple model]

Define $|\theta\rangle = \sum e^{in\theta} |n\rangle$

$$\tau |\theta\rangle = e^{-i\theta} |\theta\rangle$$

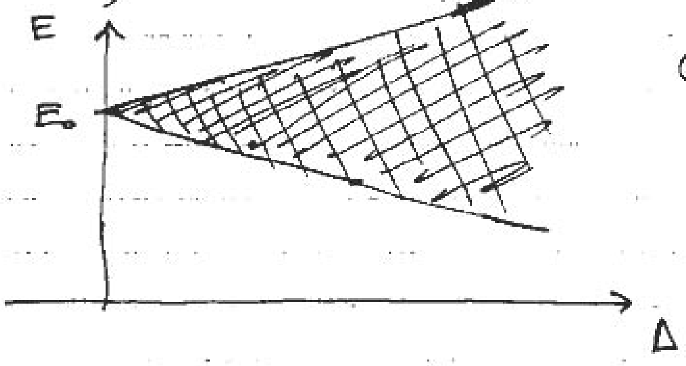
$$H |n\rangle = E_0 |n\rangle - \Delta |n-1\rangle - \Delta |n+1\rangle$$

$$H|\theta\rangle = E_0|\theta\rangle - \Delta \sum e^{in\theta}\left(|n+1\rangle + |n-1\rangle\right)$$

$$= \left[E_0 - \Delta\left(e^{i\theta} + e^{-i\theta}\right)\right]|\theta\rangle$$

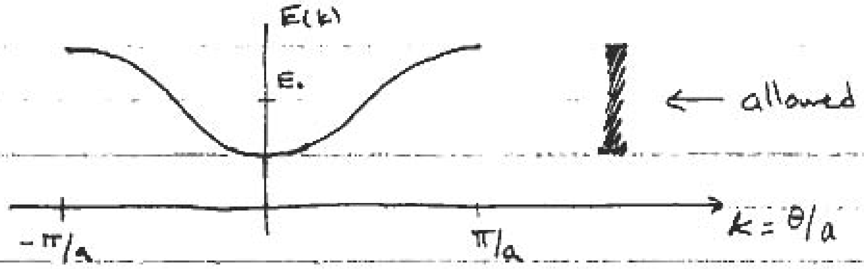
$$= \left(E_0 - 2\Delta\cos\theta\right)|\theta\rangle$$

so degeneracy is lifted by Δ



Get continuous band of E in Brillouin zone

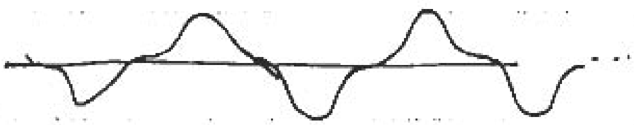
$E_0 - 2\Delta \le E \le E_0 + 2\Delta.$



Lowest E state: $|\theta = 0\rangle$

highest E state: $|\theta = \pm\pi\rangle$

$O = \sum(-1)^n|n\rangle$



Energy spectrum in general case

Want to solve $H|\psi\rangle = E\,|\psi\rangle$

$$-\frac{\hbar^2}{2m}\psi''(x) + V(x)\,\psi(x) = E\,\psi(x),$$

$$V(x+a) = U(x).$$

2nd order eq: has 2 linearly independent solutions $\psi_1(x), \psi_2(x)$ for any E.

Periodicity $\Rightarrow$ $\psi_1(x+a)$, $\psi_2(x+a)$ also solutions.

$$\Rightarrow \begin{pmatrix} \psi_1(x+a) \\ \psi_2(x+a) \end{pmatrix} = \begin{pmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{pmatrix} \begin{pmatrix} \psi_1(x) \\ \psi_2(x) \end{pmatrix}$$

$$A = \begin{pmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{pmatrix} :$$ <u>transfer matrix</u>

ψ_1, ψ_2 real @ ϕ $\Rightarrow$ A real.

Diagonalize A:

$$\phi_1(x+a) = \lambda_1\,\phi_1(x)$$
$$\phi_2(x+a) = \lambda_2\,\phi_2(x).$$

λ_1, λ_2 eigenvalues of A.

Eq. for λ: $\det(A - \lambda\mathbb{1}) = 0$

$$(A_{11} - \lambda)(A_{22} - \lambda) - A_{12}A_{21} = 0$$

$$\lambda^2 - (A_{11} + A_{22})\lambda + (A_{11}A_{22} - A_{12}A_{21}) = 0$$

$$\lambda^2 - (\mathrm{Tr}\, A)\,\lambda + \det A = 0$$

$$\Rightarrow \quad \lambda = \left[\mathrm{Tr}\, A \pm \sqrt{(\mathrm{Tr}\, A)^2 - 4 \det A}\,\right] / 2.$$

So either $\boxed{\begin{array}{ll} a) & \lambda_1, \lambda_2 \text{ both real} \\ b) & \lambda_1 = \lambda_2^*. \end{array}}$

Now: $\frac{d}{dx}(\phi_1 \phi_2' - \phi_2 \phi_1') = \phi_1 \phi_2'' - \phi_1'' \phi_2 = 0$

$$\text{so} \quad (\phi_1 \phi_2' - \phi_2 \phi_1')_{x+a} = (\phi_1 \phi_2' - \phi_2 \phi_1')_x$$

$$= \lambda_1 \lambda_2 (\phi_1 \phi_2' - \phi_2 \phi_1')_x$$

$$\text{so} \quad \boxed{\lambda_1 \lambda_2 = 1.}$$

If λ_1, λ_2 both real, $\lambda_1 = \frac{1}{\lambda_2}$.

Unless (a) and (b), then both ϕ_1, ϕ_2 grow exponentially — unphysical nonnormalizable solutions.

If $\lambda_1 = \lambda_2^*$, then ϕ_1, ϕ_2 are quasiperiodic. — physical solutions, normalization like $|p\rangle$ states.

λ's are a function of E, determined through A.

When a), $\lambda + \frac{1}{\lambda} = \mathrm{Tr}\, A \geq 2$

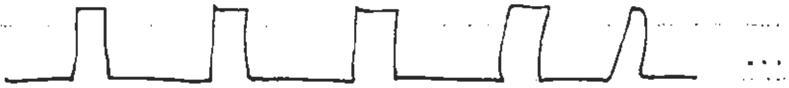
When b), $\lambda_1 + \lambda_2 = \mathrm{Tr} A = e^{i\alpha} + e^{-i\alpha} = 2\cos\alpha \leq 2.$

Thus, allowed energy bands are in regions where

$$\boxed{\mathrm{Tr}\, A \leq 2} \quad \text{(allowed bands)}$$

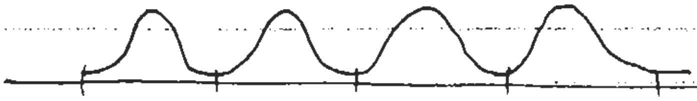
Crossover points: $A = \pm \mathbb{1}$, $\phi_i(x+a) = \pm \phi_i(x)$,
exactly periodic or antiperiodic sol'ns

Qualitative description of square well potential

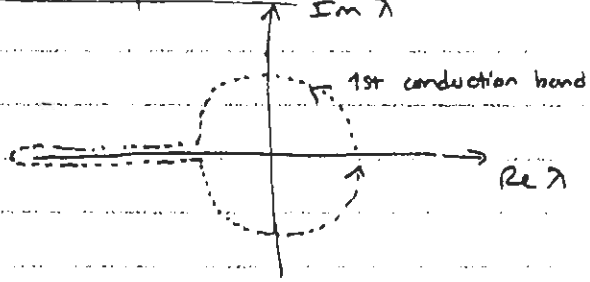


First band:

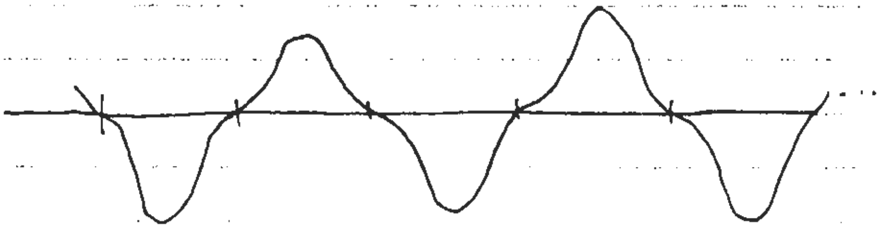
lowest state: $\lambda = 1$ periodic



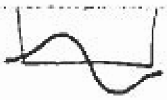
Follow λ in $\mathbb{C}$



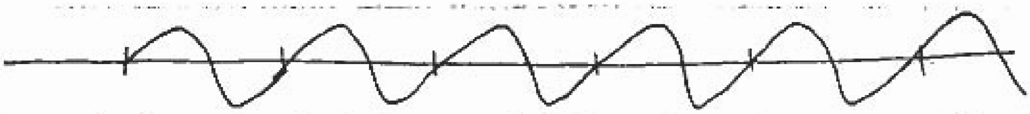
highest state $\lambda = -1$
– flips sign of ground state



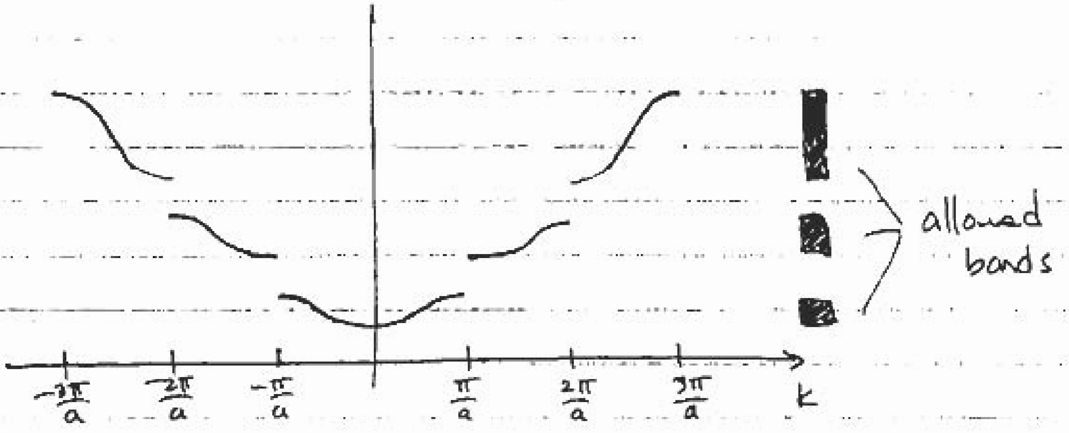
Second band:

lowest state: $\lambda = -1$, connects  in each well.

highest state: $\lambda = +1$



Spectrum



As height → 0, approaches free spectrum

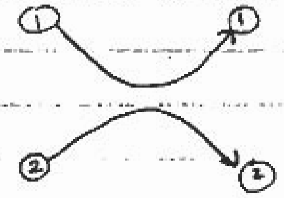
This is general form of result for any periodic potential! [HW: Kronig - Penney potential]

So far: considered 1 electron. Want to generalize → many electrons.

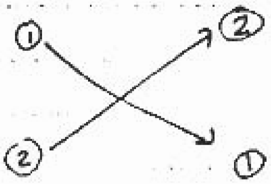
Allowed band full: insulator: allowed band partly full: conductor

7.5 Identical particles (2 particles)

Classically, electrons can be distinguished ("labelled")



is distinguishable from



Not so in Q.M. – both processes contribute.

2-particle Hilbert space

$$\mathcal{H}_{12} = \mathcal{H}_1 \otimes \mathcal{H}_2 = \mathcal{H} \otimes \mathcal{H} \quad \text{for identical particles.}$$

1-particle basis $\{|n\rangle\}$

2-particle basis $\{|n,m\rangle = |n\rangle \otimes |m\rangle\}$ (sometimes $|n\rangle|m\rangle$)

Cannot experimentally distinguish $|n,m\rangle$ from $|m,n\rangle$ for identical particles. (<u>exchange degeneracy</u>)

Recall quantization of EM field:

2-photon states

$$a^{+}_{k,\alpha}\, a^{+}_{k',\alpha'} |0\rangle = a^{+}_{k',\alpha'}\, a^{+}_{k,\alpha} |0\rangle$$

same state in multi-particle Fock space.

[degeneracy is artifact of 1st-quantized formalism]

Permutation operator

$$P_{12}\,|n,m\rangle = |m,n\rangle$$

exchanges particles.

$$P_{12} = P_{21}\,, \qquad P_{12}^{\,2} = \mathbb{1}$$

P_{12} generates a $\mathbb{Z}_2$ symmetry group, $P_{12} = \mathcal{D}(a)$, $a^2 = 1$.

Irreps of $\mathbb{Z}_2$: $P_{12} = \pm 1$, on 1D eigenspaces.

eigenstates : $|n,m\rangle_{\substack{S\\A}} = \frac{1}{\sqrt{2}}\left(|n,m\rangle \pm |m,n\rangle\right)$, $n \neq m$

for $n = m$, $P_{12}\,|n,n\rangle = +\,|n,n\rangle$, so no A state.

For identical particles, H symmetric under $1 \longleftrightarrow 2$

e.g. $$H = \frac{p_1^{\,2}}{2m} + \frac{p_2^{\,2}}{2m} + V_{ext}(x_1) + V_{ext}(x_2) + V(|x_1 - x_2|)$$

$$\underline{P_{12}\,H\,P_{12} = H}$$

Two kinds of particles appear in nature :

Bosons : $P_{12} = +1$ (Bose-Einstein statistics)

ex. photons.

Fermions : $P_{12} = -1$ (Fermi statistics)

ex. electrons, quarks
(leptons)

[note: in 2nd quant formalism, $a^{\dagger}$'s anticommute]

Spin-statistics theorem

(provable in relativistic QFT) assuming axioms of locality, etc.

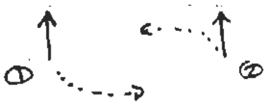
- Integer spin particles are bosons
- 1/2-integer spin particles are fermions.

[presumably can choose any statistics for e in NRQM (?)]

Theorem holds for elementary particles & composites.

→ e^- fermion
→ H atom boson.

Ex. consider 2 electrons in state $S=1$, $m=1$

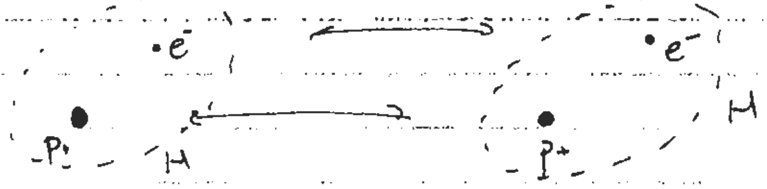


composite state rotates by 180° as $e^{im\pi} = -1$.

Rotation exchanges e^-'s, gives -1 by Fermi statistics.

Assuming thm. for elementary particles ⇒ result for composites

e.g.



$$P_{12}^{(H)} = P_{12}^{(e)} P_{12}^{(p)} = (-1)(-1) = +1$$

(−1 for each 1/2-spin particle)

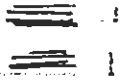
Pauli exclusion principle

2 fermions cannot be in the same state

since $P_{12} |n,n\rangle = + |n,n\rangle$

But bosons can — leads to dramatically different physics.

fermions in solids — electronics



bands, etc.

Bose - einstein condensate $|0,0,0,0,\dots\rangle$

Astrophysics — Fermi gases, etc. (neutron stars...)

Many particles

Generalize to N identical particles.

Statistics fixes one of N! states — antisymm. or symmetric

e.g. for 3 bosons / fermions

$$|n,m,p\rangle_{\substack{S\\A}} = \frac{1}{\sqrt{6}}\Big[|n,m,p\rangle \pm |n,p,m\rangle + |m,p,n\rangle \pm |m,n,p\rangle + |p,n,m\rangle \pm |p,m,n\rangle \Big]$$

has eigenvalue ±1 for P_{12}, P_{23}, P_{13}.

More on $N > 2$ later.

2 - electron systems

$\mathcal{H} = (\mathcal{H}_1 \otimes \mathcal{H}_2)_A$ restricts to -1 eigenspace of P_{12}

Can write states as

$$\psi = \sum \phi_{m,m'}(x,x') \; |m, m'\rangle \qquad m,m' \in \{-1/2, +1/2\}$$

$$\mathcal{H}_1 \otimes \mathcal{H}_2 = \mathcal{H}_1^{(x)} \otimes \mathcal{H}_2^{(x)} \otimes \mathcal{H}_1^{(s)} \otimes \mathcal{H}_2^{(s)}$$

Basis for $\mathcal{H}_1^{(s)} \otimes \mathcal{H}_2^{(s)}$ $\qquad (S = S_1 + S_2)$

$$\left.\begin{aligned} \chi_{11} &= |++\rangle \\ \chi_{10} &= \tfrac{1}{\sqrt{2}}(|+-\rangle + |-+\rangle) \\ \chi_{1-1} &= |--\rangle \end{aligned}\right\} P_{12}^{(s)} = +1 \qquad S^2 = 1$$

triplet (symmetric)

$$\chi_{00} = \tfrac{1}{\sqrt{2}}(|+-\rangle - |-+\rangle) \Big\} P_{12}^{(s)} = -1 \qquad S^2 = 0$$

singlet (antisymmetric)

For 2 particles, can choose basis for $\mathcal{H}$

$$\psi_A^{(x)} \psi_S^{(spin)} , \qquad \psi_S^{(x)} \psi_A^{(spin)}$$

- not possible for $N > 2$ particles; more complicated.

For triplet states

$$\psi = \sum_{m=\pm 1, 0} \phi_m(x,x') \; \chi_{1m}$$

$$\phi_m(x,x') = -\phi_m(x',x)$$

For singlets

$$\psi = \phi(x,x') \; \chi_{00}$$

$$\phi(x,x') = +\phi(x',x)$$

Triplets: spin symmetric, pos. antisymmetric
— particles avoid each other

Singlets: spin antisymm., pos. symmetric.
— particles can have same position.

If no interaction,

$$\phi = \frac{1}{\sqrt{2}}\left(\omega_A(x_1)\,\omega_B(x_2) \pm \omega_A(x_2)\,\omega_B(x_1) \right) \quad \begin{matrix}\text{sing.}\\ \text{trip.}\end{matrix}$$

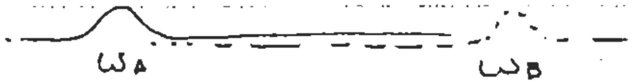
$$|\phi|^2 = \frac{1}{2}\Big[|\omega_A(x_1)|^2 |\omega_B(x_2)|^2 + |\omega_A(x_2)|^2 |\omega_B(x_1)|^2$$

$$\pm 2\,\mathrm{Re}\left(\omega_A(x_1)\,\omega_B(x_2)\,\omega_A^*(x_2)\,\omega_B^*(x_1) \right) \Big]$$

exchange density

When $x_1 = x_2$, $|\phi|^2 \to 0$ for triplets.
→ doubles for singlets
(enhances prob. @ same position)

Note that for widely separated particles



exchange density → 0,
Fermi statistics are irrelevant

2-electron atoms H^-, He, Li^+, ...

$$H = \underbrace{\frac{p_1^2}{2m} + \frac{p_2^2}{2m} - \frac{Ze^2}{r_1} - \frac{Ze^2}{r_2}}_{H_0} + \underbrace{\frac{e^2}{r_{12}}}_{V}$$

In absence of interaction, have states

$$2E_0^{(0)}\left\{\ |1s,\ 1s\rangle_s = |(100)\,(100)\rangle_s \ \chi_{00}\right.$$

$$E_0^{(0)}+E_1^{(0)}\left\{\begin{array}{lll}|1s,\ 2s\rangle_s = & |(1{,}00)\,(200)\rangle_s & \chi_{00}\\ |1s,\ 2s;\ m\rangle_A = & |(100)\,(200)\rangle_A & \chi_{1m}\\ |1s,\ 2p;\ \mu\rangle_s = & |(100)(21\mu)\rangle_s & \chi_{00}\\ |1s,\ 2p;\ \mu,m\rangle_A = & |(100)(21\mu)\rangle_A & \chi_{1m}\end{array}\right.$$

more coulomb repulsion

Spatially symmetric states (singlet) have more energy from Coulomb repulsion, since electrons tend to come together.

Can use pert. theory to estimate energies.

Helium

Ground state w/o interaction:

$$E_0 = 2\left(-\frac{Z^2e^2}{2a_0}\right) \sim -109\,\text{eV} \quad (8\cdot(-13.6\,\text{eV}))$$

adding $\left\langle \frac{e^2}{r_{12}} \right\rangle_{|1s,1s\rangle} \Rightarrow -74.8\ \text{eV} \quad \left[\left(-Z^2+\frac{5}{8}Z\right)\left(\frac{e^2}{a_0}\right)\right]$

Experimental value: -78.8 eV.

Using variational method can get to 10^{-6} accuracy, given enough params.
[~~[illegible]~~ see book] [HW: do pert, var. cal for 1D analog]
for example

Excited states of helium

$$\phi_{\substack{S\\A}}(x_1, x_2) = \frac{1}{\sqrt{2}}\Big(\psi_1(x_1)\,\psi_2(x_2) \pm \psi_1(x_2)\,\psi_2(x_1)\Big)$$

$$\left\langle \frac{e^2}{r} \right\rangle_{\substack{S\\A}} = e^2 \int d^3x_1\, d^3x_2 \Big[\psi_1(x_1)\,\psi_2(x_2)\,\frac{1}{r_{12}}\,\psi_1^*(x_1)\,\psi_2^*(x_2) \pm \psi_1(x_1)\,\psi_2(x_2)\,\frac{1}{r_{12}}\,\psi_2^*(x_1)\,\psi_1^*(x_2)\Big]$$

$$= \underset{\text{(direct)}}{V_D} \pm \underset{\text{(exchange)}}{V_E}$$

Note that:

a) $V_D \geq 0$ clearly

b) $$\int \frac{|\psi_1(x_1)\,\psi_2(x_2) \pm \psi_1(x_2)\,\psi_2(x_1)|^2}{r_{12}} = 2V_D \pm 2V_E > 0$$

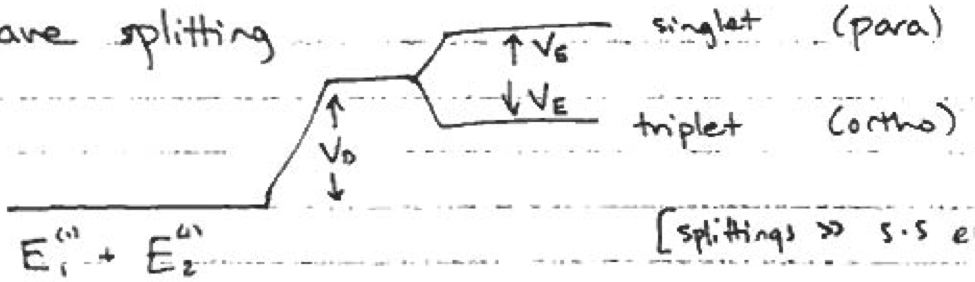
$$\Rightarrow V_D > |V_E|$$

c) Fourier xform: $$\frac{1}{r_{12}} = \int d^3k\, \frac{e^{i\vec{k}\cdot(\vec{x}_1 - \vec{x}_2)}}{k^2}$$

$$V_E = \int \frac{d^3k}{k^2} \Big(\int d^3x_1\, e^{i\vec{k}\cdot\vec{x}_1}\,\psi_1(x_1)\,\psi_2^*(x_1)\Big)^{\swarrow f(k)} \Big(\int d^3x_2\, e^{-i\vec{k}\cdot\vec{x}_2}\,\psi_2(x_2)\,\psi_1^*(x_2)\Big)^{\swarrow f^*(k)}$$

$$\geq 0$$

so have splitting



[splittings >> s.s effects]

Although Hamiltonian is spin-independent, can describe as spin-dependent interaction

$$\langle V \rangle_{\substack{S\\A}} = V_D - \tfrac{1}{2}\left(1 + \vec{\sigma}_1 \cdot \vec{\sigma}_2\right) V_E$$

$$\left[\vec{\sigma}_1 \cdot \vec{\sigma}_2 = 2(S^2 - S_1^2 - S_2^2) = 2S^2 - 3\right.$$

	S^2	$-\frac{1}{2}(1+\vec{\sigma}_1\cdot\vec{\sigma}_1)$	
triplet :	2	-1	✓]
singlet :	0	+1	

spin singlets : parahelium
spin triplets : orthohelium

Can analyze other 2-electron atoms

e.g. bound state of H^-

- subtle; pert thy. $\Rightarrow -0.4726 \frac{e^2}{a_0} > (-0.5 + 0)\left(\frac{e^2}{a_0}\right)$

but var. calc $\Rightarrow -0.528 \frac{e^2}{a_0}$.

Central field approximation

No analytic solutions known for atomic systems with $N \geq 2$ electrons.

Can go beyond pert. theory using Central field approximation

Assume effective potential for each e^- comes from nucleus + charge distribution of other e^-'s.

Simplest version:

Hartree self-consistent field approximation

For an N-electron system,

assume potential for electron i arises from

a) nuclear potential $-Ze^2/r$

b) charge distribution of other electrons $\sum_{k \neq i} -e|\phi_k|^2$

Take wavefunction to be product form

$$\psi(x_1, \ldots, x_N) = \phi_1(x_1)\phi_2(x_2) \cdots \phi_N(x_N)$$

Hartree equations:

$$H_i\phi_i = -\frac{1}{2}\nabla_i^2\phi_i - \frac{Ze^2}{r_i}\phi_i + \sum_{k\neq i}\left(\int dx_k \frac{|\phi_k(x_k)|^2 e^2}{r_{ki}}\right)\phi_i$$

$$= \varepsilon_i\phi_i$$

[meaning of ε_i ?]

Assume $\int \phi_i^*(x_i)\,\phi_i(x_i)\,dx_i = 1$

$$\langle\psi|H_i|\psi\rangle = \varepsilon_i$$

and

count each pair once

$$\langle\psi|H|\psi\rangle = \langle\psi|\sum_i\left(-\frac{1}{2}\nabla_i^2 - \frac{Ze^2}{r_i}\right) + \sum_{i<j}\frac{e^2}{r_{ij}}|\psi\rangle$$

$$= \sum\varepsilon_i - \sum_{i<j}\langle\frac{e^2}{r_{ij}}\rangle$$

So $\langle H\rangle_{\text{Hartree}}$ follows once solve Hartree eqns.

Ex. ground state of helium

$$\psi(\vec{x}_1,\vec{x}_2) = \phi(\vec{x}_1)\,\phi(\vec{x}_2)$$ (assume symmetric state)

Hartree eqn

$$-\frac{1}{2}\nabla^2\phi(\vec{x}) - \frac{Ze^2}{|x|}\phi(\vec{x}) + \int d^3\vec{y}\,\frac{e^2}{|\vec{x}-\vec{y}|}\,\phi(\vec{y})^2\,\phi(\vec{x}) = \varepsilon\,\phi(\vec{x})$$

Tricky integro-differential equation.

Can solve recursively:

Start with trial function $\phi_0(\vec{x})$.
Use to compute $V(\vec{x}) = \int d^3\vec{y}\,\frac{e^2}{|\vec{x}-\vec{y}|}\,\phi(\vec{y})^2$
Plug into Schrödinger - solve for $\phi_1(\vec{x})$ . . .

$\langle H\rangle = 2\varepsilon - \langle\frac{e^2}{|\vec{x}_1-\vec{x}_2|}\rangle$. Can solve 1D analogue exactly [HW]

7.6 N>2 identical particles & the symmetric group

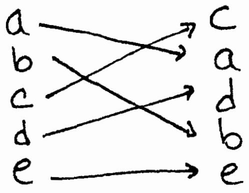
For understanding systems of many identical particles, symmetric group S_N of permutations on N elements is an essential tool.

Permutation group S_N

Given N ordered objects $a, b, c, \ldots$ a permutation is a general rearrangement of the objects' ordering

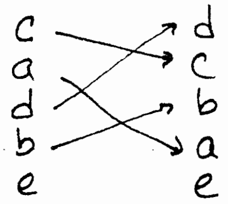
ex.

P :



action of P depends on positions of objects, not labels

P :



Can describe any permutation by cycle structure

$$\begin{tikzcd}(1 & 3 \arrow[l] & 4 \arrow[l] & 2) \arrow[l] \arrow[lll, phantom] & (5 \arrow[loop above]) \end{tikzcd}$$

write $(1342)(5)$

[often drop cycles of length 1 $\Rightarrow$ (1342)]

N! permutations on N objects form group S_N

S_N is a nonabelian group, $P_1 P_2 \neq P_2 P_1$ in general

ex. $P_1 = (1\,2\,3)$ $\quad P_2 = (1\,2)$

Transpositions $P_{(ij)}$ switch i, j $\quad (i\,j)$.

All permutations can be written as a product of $P_{(ij)}$'s.

<u>Parity</u> of a permutation $\delta_P = (-1)^k$ where k = # of transpositions needed to make P.

<u>Representation theory of S_N</u>

Consider $N!$ - dimensional vector space spanned by all permutations of $\{1, \ldots, N\}$

ex. for $N=3$, $|123\rangle$, $|132\rangle$, $|231\rangle$, $|213\rangle$, $|312\rangle$, $|321\rangle$

Any permutation acts on this basis as perm. matrix (one 1 in each row, column, other entries = 0)

$$\text{ex.} \quad P_{(23)} \to \left(\begin{array}{cccccc} 0 & 1 & & & & \\ 1 & 0 & & & & \\ & & 0 & 1 & & \\ & & 1 & 0 & & \\ & & & & 0 & 1 \\ & & & & 1 & 0 \end{array}\right) \begin{array}{l} |123\rangle \\ |132\rangle \\ |231\rangle \\ |213\rangle \\ |312\rangle \\ |321\rangle \end{array}$$

This is <u>regular representation</u>. Contains all irreps.

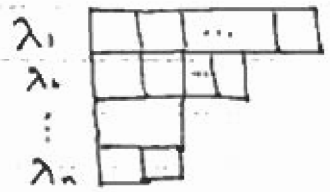
Young diagrams

Partition of N : $\lambda_1 + \dots + \lambda_n = N$

$\lambda_1 \geq \lambda_2 \geq \dots \geq \lambda_n$

partitions of N $\xleftrightarrow{1-1}$ conjugacy classes $g \sim h^{-1} g h$ in S_N
(cycle lengths)

For each partition of N, $\exists$ Young diagram Y_λ



Ex. N = 2 $\lambda = (2)$ $\begin{array}{|c|c|}\hline \ & \ \\ \hline\end{array}$

$\lambda = (1,1)$ $\begin{array}{|c|}\hline \ \\ \hline \ \\ \hline\end{array}$

N = 3 $\lambda = (3)$ $\begin{array}{|c|c|c|}\hline \ & \ & \ \\ \hline\end{array}$

$\lambda = (2,1)$ $\begin{array}{|c|c|}\hline \ & \ \\ \hline \ \\ \cline{1-1}\end{array}$

$\lambda = (1,1,1)$ $\begin{array}{|c|}\hline \ \\ \hline \ \\ \hline \ \\ \hline\end{array}$

Young tableaux

Given a Young diagram, label with integers 1, 2, ... N
"standard tableau" : rows & columns increase right & down.

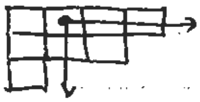
Ex. $\begin{array}{|c|c|c|}\hline \ & \ & \ \\ \hline\end{array} \longrightarrow \begin{array}{|c|c|c|}\hline 1 & 2 & 3 \\ \hline\end{array}$

$\begin{array}{|c|c|}\hline \ & \ \\ \hline \ \\ \cline{1-1}\end{array} \longrightarrow \begin{array}{|c|c|}\hline 1 & 2 \\ \hline 3 \\ \cline{1-1}\end{array}$ & $\begin{array}{|c|c|}\hline 1 & 3 \\ \hline 2 \\ \cline{1-1}\end{array}$

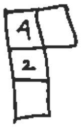
# of standard tableaux for a diagram:

$$D_\lambda = \frac{N!}{\prod_{\text{boxes}} h(i,j)}$$

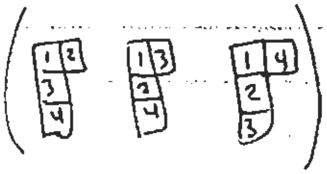
$h(i,j)$ = "hook length" = # of boxes intercepted by lines right & down

e.g.  $h(1,2) = 4$

Ex. $\lambda = (2,1^2)$



$$D_\lambda = \frac{4!}{4 \cdot 2} = 3$$



Irreps of S_N:

Each irrep. of S_N corresponds to a Young diagram.

D_λ = dimensionality of rep.

also = # of times rep. appears in regular rep.

$$\Rightarrow N! = \sum_{\substack{\lambda \\ (N \text{ boxes})}} D_\lambda^2 \qquad \text{(theorem)}$$

Constructing S_N irreps explicitly

Given a diagram $Y\lambda$, construct a rep. as follows:

for each "standard tableau."

take linear combination of states — symmetrize on rows,
then antisymmetrize on columns
(using positions)
(can also do consistently w/ labels)

Ex. $N=3$ $\lambda=(2,1)$ $\begin{array}{|c|c|}\hline \; & \; \\ \hline \; \\ \cline{1-1}\end{array}$

$\begin{array}{|c|c|}\hline 1 & 2 \\ \hline 3 \\ \cline{1-1}\end{array} \Rightarrow |123\rangle + |213\rangle - |321\rangle - |312\rangle$ (A)

$\begin{array}{|c|c|}\hline 1 & 3 \\ \hline 2 \\ \cline{1-1}\end{array} \Rightarrow |132\rangle + |231\rangle - |312\rangle - |321\rangle$ (B)

form a basis for a 2D rep. of S_3

Check:

$(123)\,A = |231\rangle + |132\rangle - |213\rangle - |123\rangle = B - A$

$(12)\,A = |213\rangle + |123\rangle - |231\rangle - |132\rangle = A - B$

$\vdots$

Irreps of S_3

$\begin{array}{|c|c|c|}\hline \; & \; & \; \\ \hline\end{array}$	symmetric	$D=1$	$(\times 1)$	1
$\begin{array}{|c|c|}\hline \; & \; \\ \hline \; \\ \cline{1-1}\end{array}$	mixed	$D=2$	$(\times 2)$	4
$\begin{array}{|c|}\hline \; \\ \hline \; \\ \hline \; \\ \hline\end{array}$	antisymmetric	$D=1$	$(\times 1)$	1
				6 = 3!

Bases for reps

$$\begin{array}{cllllllll} & & |123\rangle & |132\rangle & |231\rangle & |213\rangle & |312\rangle & |321\rangle & \\ & \psi_S = \frac{1}{\sqrt{6}}[& 1 & 1 & 1 & 1 & 1 & 1 &] \\ & \psi_A = \frac{1}{\sqrt{6}}[& 1 & -1 & 1 & -1 & 1 & -1 &] \\ 1\{ & \psi_{M1,1} = \frac{1}{2}[& 1 & 0 & 0 & 1 & -1 & -1 &] \\ & \psi_{M1,2} = \frac{1}{2\sqrt{3}}[& -1 & 2 & 2 & -1 & -1 & -1 &] \\ 2\{ & \psi_{M2,1} = \frac{1}{2}[& 1 & 0 & 0 & -1 & -1 & 1 &] \\ & \psi_{M2,2} = \frac{1}{2\sqrt{3}}[& 1 & 2 & \underline{-2} & -1 & 1 & -1 &] \end{array}$$

Can similarly construct reps of any S_N.

Note: ψ_{M1} symm. under exchanging 1,2 labels
ψ_{M2} antisymm. " " " "

So — Young diagrams label irreps of S_N.
standard tableaux give basis for irreps

Applications of Young diagrams:

A) characterizing & constructing irreps of S_N
B) characterizing multi-particle states in $(\mathcal{H}_k)^N$ under S_N
C) characterizing irreps of $SU(k)$ & constructing on $(\mathcal{H}_k)^N$.

(these 3 conflated in book)

B) Multi-particle states under S_N

Consider N particles each with Hilbert space $\mathcal{H}_k$ of dimension k.

Total Hilbert space $\mathcal{H} = (\mathcal{H}_k)^N$, $\dim \mathcal{H} = k^N$.

(e.g. $k=2$, spin-1/2 particles; basis $|\pm \pm \cdots \pm\rangle$)

How does $(\mathcal{H}_k)^N$ decompose into S_N irreps?

Answer: for each Young diagram, get 1 copy of irrep for each "standard k-tableau" (nonstandard notation - often "standard" used for this also) satisfying:

- entries $\leq k$
- rows are nondecreasing
- columns are increasing

dim of irrep is still D_λ, of course.

Denote D^k_λ = # of standard k-tableaux for Y.D. λ

Formulae for D^k_λ

writing $\delta_i = \lambda_i - \lambda_{i+1}$ $\quad i = 1, \cdots, k-1$

$$\begin{aligned} D^k_\lambda = & (1+\delta_1)(1+\delta_2)\cdots(1+\delta_{k-1}) \\ & \times\left(1+\frac{\delta_1+\delta_2}{2}\right)\left(1+\frac{\delta_2+\delta_3}{2}\right)\cdots\left(1+\frac{\delta_{k-2}+\delta_{k-1}}{2}\right) \\ & \times\left(1+\frac{\delta_1+\delta_2+\delta_3}{3}\right)\cdots\left(1+\frac{\delta_{k-3}+\delta_{k-2}+\delta_{k-1}}{3}\right) \\ & \times\cdots \\ & \times\left(1+\frac{\delta_1+\cdots+\delta_{k-1}}{r-1}\right) \end{aligned}$$

Alternative expression:

recall "hook length" $h(i,j)$

also define $D(i,j) = j - i$ = (column #) − (row #)

0	1	2	...
-1	0	1	
-2	-1	0	
⋮			

$$D^k_\lambda = \prod_{\text{boxes}} \frac{(k + D(i,j))}{h(i,j)}$$ equivalent to above.

Theorem: $\sum D^k_\lambda D_\lambda = k^N$

Ex. 3 spin-1/2 particles : 8D Hilbert space

irreps: $\left.\begin{array}{l} \begin{array}{|c|c|c|}\hline - & - & - \\ \hline\end{array} \\ \begin{array}{|c|c|c|}\hline - & - & + \\ \hline\end{array} \\ \begin{array}{|c|c|c|}\hline - & + & + \\ \hline\end{array} \\ \begin{array}{|c|c|c|}\hline + & + & + \\ \hline\end{array} \end{array}\right\}$ $D_\lambda = 1$ symmetric states

$$\left(D^2_\lambda = \overset{(1+3)}{\frac{2}{3}} \cdot \frac{3}{2} \cdot \frac{4}{1} = 4 \qquad \begin{array}{l} [\delta_1 = 3] \\ \left[\begin{array}{l} h = \begin{array}{|c|c|c|}\hline 3 & 2 & 1 \\ \hline\end{array} \\ D = \begin{array}{|c|c|c|}\hline 0 & 1 & 2 \\ \hline\end{array} \end{array}\right. \end{array} \right)$$

$\cancel{\begin{array}{|c|}\hline \\ \hline \\ \hline \\ \hline\end{array}}$

$\left.\begin{array}{l} \begin{array}{|c|c|}\hline - & - \\ \hline + & \\ \cline{1-1}\end{array} \\ \begin{array}{|c|c|}\hline - & + \\ \hline + & \\ \cline{1-1}\end{array} \end{array}\right\}$ $D_\lambda = 2$ mixed states

$$D^2_\lambda = (1+1) = 2 \qquad [\delta_1 = 1]$$

$$1 \times 4 + 2 \times 2 = 8$$

To get states, plug into states for standard tableaux
– get redundancy ; linear dependencies or vanishing

explicitly, : $\begin{array}{|c|c|}\hline - & - \\ \hline + & \\ \cline{1-1}\end{array}$

$$\psi_{M_1,1} = \frac{1}{\sqrt{2}}\left(|--+\rangle - |+--\rangle\right)$$

$$\psi_{M_1,2} = \frac{1}{\sqrt{6}}\left(|--+\rangle + |+--\rangle - 2|-+-\rangle\right)$$

$$\psi_{M_2,i} = 0 .$$

We now understand: • irreps of S_N, dim D_λ
• how to decompose regular rep & $(\mathcal{H}_k)^N$ into S_N irreps.
(including multiplicities D_λ, D^k_λ & explicit wt's)

c) Classify irreps of $SU(k)$

Last semester, classified irreps of $SU(2)$:
for each $j \in \mathbb{Z}/2$, $\{|j,m\rangle,\ m = -j, \ldots, j\}$

Fundamental rep. of $SU(k)$: k-dimensional defining rep. on $\mathcal{H}_k$.
Denote by □

Irreps found by considering action on $(\mathcal{H}_k)^N$, decomposing.
irreps determined by S_N symmetries – action of $su(k)$ leaves symmetry structure fixed since $[SU(k), S_N] = 0$.

Theorem: irreps of $SU(k)$ $\xleftrightarrow{1-1}$ Young diagrams with $<$ k rows

$$\text{Dim of irrep } \lambda = D^k_\lambda$$

$$\#\text{ of times } \lambda \text{ appears in } (\mathcal{H}_k)^N = D_\lambda$$

(proof later) [include k rows; Y_λ w/ k rows ~ Y_λ w/<k]

Comments:

- Fits with $\sum_\lambda D^k_\lambda D_\lambda = k^N$
- Explicit rep. found by action of $SU(k)$ on states associated with standard k-tableaux.
- Columns w/ k boxes → totally antisymmetric, act as singlet & can be dropped.

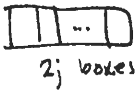
Ex. $SU(2)$ reps

□ Fundamental $(j = 1/2)$ $D^2_\lambda = 2$

□□ $(j = 1)$ $D^2_\lambda = 3$

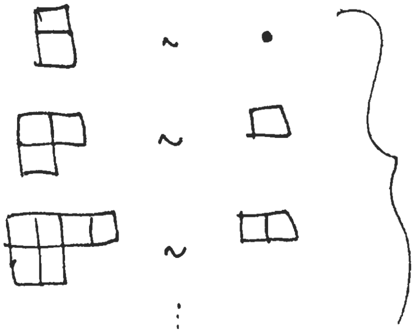
 (j = 3/2) $D^2_\lambda = 4$

⋮



(j = anything) $D^2_\lambda = 2j+1$

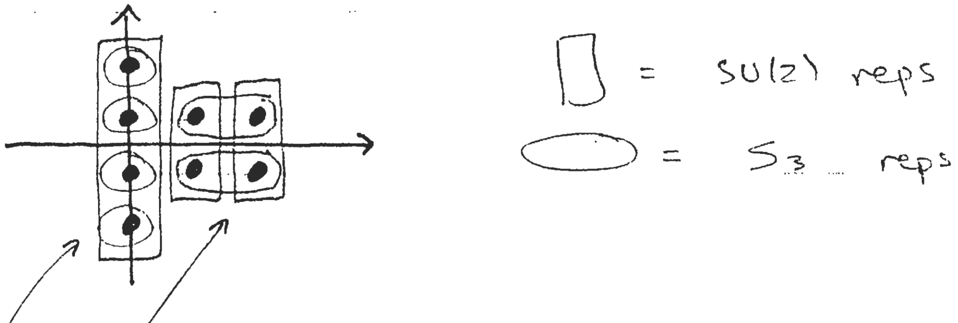
also:



appear in $(\mathcal{H}_2)^N$, needed for countings but D^k_λ same for different equivalent diagram.

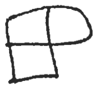
Example: Decomposition of $(\mathcal{H}_2)^3$ = 8d space under SU(2), S_3

(3 spin-1/2 particles ⇒ (j = 3/2) × 1, (j = 1/2) × 2



 $D_\lambda = 1$ $D^2_\lambda = 4$

(4 D=1 reps of S_3,
1 D=4 rep of SU(2))

 $D_\lambda = D^2_\lambda = 2$

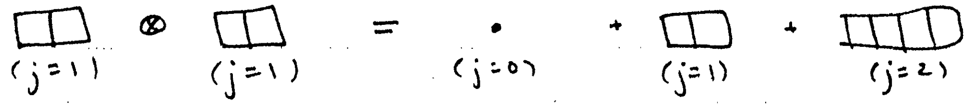
(2 D=2 reps. of S_3, SU(2))

Tensor product reps

First do SU(N)

Want decomposition of tensor product in irreps

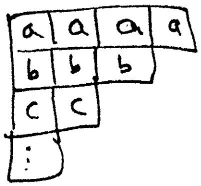
Ex. (for SU(2))



3 × 3 = 1 + 3 + 5

General rule

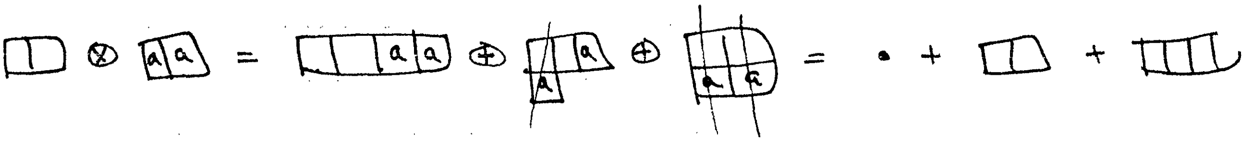
1) label second diagram w/ a, b, c ... in 1st, 2nd, 3rd rows...



2) attach a's to the 1st diagram in all ways such that
  a) no 2 a's in same column
  b) still a Young diagram (row lengths nonincreasing, etc...)
repeat with b's, c's, ...

3) read letters in right - left order, rows from top down to get string aaba...
reject if to left of any symbol more b's than a's, c's than b's, etc...

Ex. for SU(2)



Note that decomposition of $(\mathcal{H}_k)^N$ is just $\underbrace{\square \otimes \square \otimes \cdots \otimes \square}_{N}$

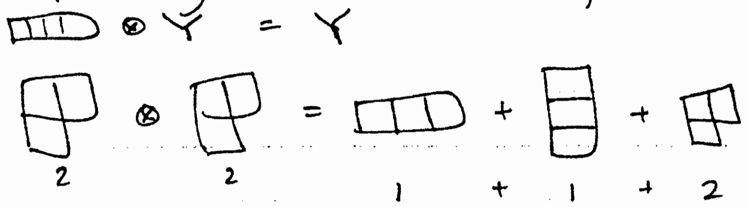
repeating rule, adding 1 box @ a time gives all
Standard Young tableaux with $\leq k$ rows
(labeling = order of placement of boxes)

$\Rightarrow$ proves $D_\lambda = \underline{\#\text{ of}}$ times Y_λ appears in $(\mathcal{H}_k)^N$

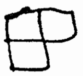
Would like analogous formula for tensor product of S_N representations, giving decomp. of $Y_\lambda \otimes Y_{\lambda'}$ in S_N irreps.

No simple algorithm known for general case!

Special cases:



Can show from following argument:

		# SU(2) reps (D_λ)	# S_3 reps (D^2_λ)	
$(\mathcal{H}_2)^3 \Rightarrow$		1	4	$(1\cdot4+2\cdot2=8)$
		2	2	
$(\mathcal{H}_4)^3 \Rightarrow$		1	20	$(1\cdot20+2\cdot20+1\cdot4)=64)$
		2	20	
		1	4	

Since $\mathcal{H}_4 = \mathcal{H}_2 \otimes \mathcal{H}_2$, we must have for S_3 reps:

$$\left(4\,\ydiagram{3} + 2\,\ydiagram{2,1}\right) \otimes \left(4\,\ydiagram{3} + 2\,\ydiagram{2,1}\right)$$

$$= 16\,\ydiagram{3} \oplus 16\,\ydiagram{2,1} \oplus 4\left(\ydiagram{2,1} \otimes \ydiagram{2,1}\right)$$

$$= 20\,\ydiagram{3} \oplus 20\,\ydiagram{2,1} \oplus 4\,\ydiagram{1,1,1}$$

$$\Rightarrow \ydiagram{2,1} \otimes \ydiagram{2,1} = \ydiagram{3} \oplus \ydiagram{1,1,1} \oplus \ydiagram{2,1}.$$

Can do more explicitly with states $-\ \psi_S = \psi_m \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \tilde{\psi}_m$

$\psi_A = \psi_m \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} \tilde{\psi}_m$

$$\psi_S(r_1, r_2, r_3; s_1, s_2, s_3) = \psi_{M,1}(r_1, r_2, r_3)\,\psi_{M,1}(s_1, s_2, s_3) + \psi_{M,2}(r_1, r_2, r_3)\,\psi_{M,2}(s_1, s_2, s_3)$$

$$\psi_A(r_1, r_2, r_3; s_1, s_2, s_3) = \psi_{M,1}(r_1, r_2, r_3)\,\psi_{M,2}(s_1, s_2, s_3) - \underline{\psi_{M,2}}(r_1, r_2, r_3)\,\psi_{M,1}(s_1, s_2, s_3)$$

__General result__: Antisymmetric rep only appears in $Y \otimes \tilde{Y}$, $\tilde{Y} = \text{transpose}(Y)$ Natural: $(\underset{1}{A})(\underset{1}{S})(\underset{2\,1}{AS})$

ex. $\ydiagram{3,1} \otimes \ydiagram{2,1,1} = \ydiagram{1,1,1,1} + \ydiagram{2,2} + \ydiagram{2,1,1} + \ydiagram{3,1}$

__Example applications__:

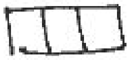
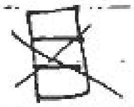
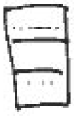
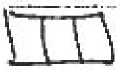
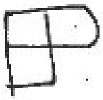
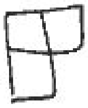
1) $(2p)^3$ states in Nitrogen (see also Sakurai)

total # of states: $\binom{6}{3} = \frac{6!}{3!3!} = \frac{6 \cdot 5 \cdot 4}{3 \cdot 2 \cdot 1} = 20$

Combined space-spin wavefunction must be antisymmetric.
write in basis of $\Psi_{\text{space}} \otimes \Psi_{\text{spin}}$ space: $j=1$ ($\mathcal{H}_3$)
spin: $j=1/2$ ($\mathcal{H}_2$)

Need to get  in tensor product of $Y_{space} \otimes Y_{spin}$

Possibilities:

space	spin	
	 $D^2_\lambda = 0$	
 $D^3_\lambda = 1$	 $D^2_\lambda = 4$	(4 states) $l=0,\ s = 3/2 \Rightarrow {}^4S_{3/2}$
 $D^3_\lambda = 8$	 $D^2_\lambda = 2$	(16 states) $l = 2, 1,\ s = 1/2$ $\Rightarrow {}^2D_{5/2},\ {}^2D_{3/2},\ {}^2P_{3/2},\ {}^2P_{1/2}$

(Note: (8) of SU(3) contains (4) + 2×(2) of SU(2)

)

Example: construct ${}^2D_{5/2}$ $m = 5/2$ state

must have $\psi_M(++0)$ space
$\psi_M(\uparrow\uparrow\downarrow)$ spin

$$\psi_A(++0;\uparrow\uparrow\downarrow) = \psi_{M,1}(++0)\,\psi_{M,2}(\uparrow\uparrow\downarrow) - \psi_{M,2}(++0)\,\psi_{M,1}(\uparrow\uparrow\downarrow)$$

$$= \frac{1}{\sqrt{6}}\Big[\,|+^\uparrow +^\downarrow 0^\uparrow\rangle - |+^\downarrow +^\uparrow 0^\uparrow\rangle + |+^\downarrow 0^\uparrow +^\uparrow\rangle - |+^\uparrow 0^\uparrow +^\downarrow\rangle + |0^\uparrow +^\uparrow +^\downarrow\rangle - |0^\uparrow +^\downarrow +^\uparrow\rangle\Big)$$

Note: can write any antisymmetric state in Slater determinant form

$$\psi_A = \frac{1}{\sqrt{N!}} \begin{vmatrix} \phi_1(x_1) & \phi_1(x_2) & \cdots & \phi_1(x_N) \\ \phi_2(x_1) & \phi_2(x_2) & \cdots & \phi_2(x_N) \\ \vdots & \vdots & & \vdots \\ \phi_N(x_1) & \phi_N(x_2) & \cdots & \phi_N(x_N) \end{vmatrix}$$

[obvious generalization to include spin, etc...)

State $\psi_A(++0;\uparrow\uparrow\downarrow)$ uniquely determined by this form.

- Not true for other states (e.g. $^2P_{3/2}$, $m = 3/2^{*}$, [HW])
  [can fix either by using tensor product formalism or operator manipulations]

---

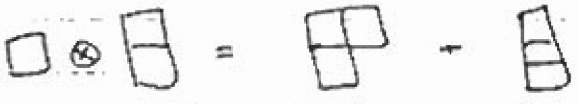
2) Quarks in a baryon

quarks have wavefunction in $\mathcal{H}_{space} \otimes \mathcal{H}_{spin} \otimes \mathcal{H}_{flow} \otimes \mathcal{H}_{\substack{color \\ (SU(3))}}$

consider 3 light quarks: u, d, s

Live in SU(3) flavor multplets: q in $\underset{(3)}{\square}$ $\bar{q}$ in $\underset{(\bar{3})}{\begin{smallmatrix}\square\\\square\end{smallmatrix}}$

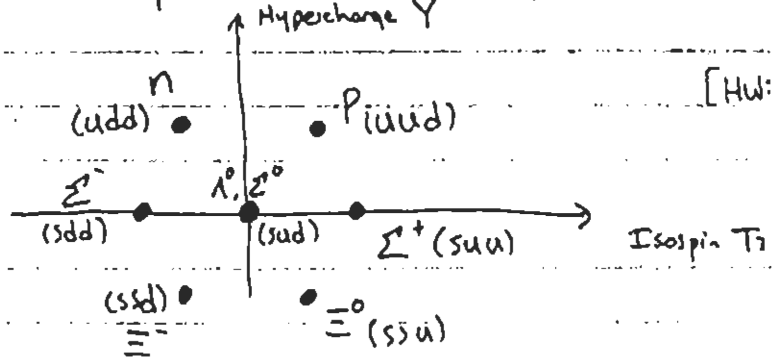
mesons:
$(q\bar{q})$



(as SU(3) reps) $3 \times \bar{3}$ = $D^3_\lambda = 8$ (octets) + $D^3_\lambda = 1$ (singlets)

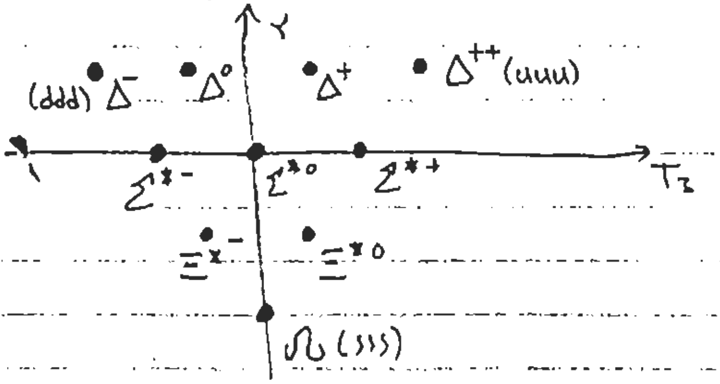
baryons: $\yng(1) \otimes \yng(1) \otimes \yng(1) = \underset{D^3_\lambda = 10}{\yng(3)} \oplus \underset{8}{\yng(2,1)} \oplus \underset{8}{\yng(2,1)} \oplus \underset{1}{\yng(1,1,1)}$
(qqq)

spin $1/2^+$ baryon octet ($\yng(2,1)$)



[HW: wfunction of proton]

spin $3/2^+$ decuplet ($\yng(3)$)



early puzzle:

baryon decuplet $\Delta^{++}, \ldots$ $\yng(3)$ flavor
have $S = 3/2$ ($\yng(3)$ spin)
in ground state of spatial wf $\Rightarrow$ $\yng(3)$ space
where is antisymmetry?

answer: $\yng(1,1,1)$ in color $\psi_{color} = \frac{1}{\sqrt{6}}\left(|RBY\rangle - |RYB\rangle + \ldots \right)$

Refs. on group theory & Applications to QM:
"A course on the Application of group theory to QM", Irene V. Shensted
"Group theory", M. Hamermesh