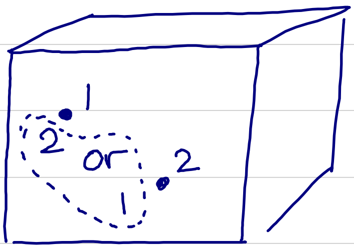
LECTURE 3: Many-body wavefunction of identical and indistinguishable quantum particles

1° Eigenstates of two NONINTERACTING or FREE fermions (f) or bosons (b) in a box



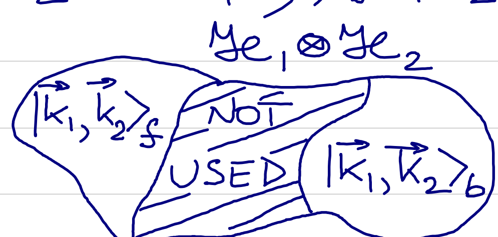
$$\hat{H}_{N=2} = -\frac{\hbar^2}{2m}\nabla_1^2 \otimes \hat{I}_2 - \hat{I}_1 \otimes \frac{\hbar^2}{2m}\nabla_2^2 \quad \text{in } \mathcal{H}_1 \otimes \mathcal{H}_2$$

$$\hat{H}_{N=2} |\vec{k}_1\rangle \otimes |\vec{k}_2\rangle = \left(\frac{\hbar^2 \vec{k}_1^2}{2m} + \frac{\hbar^2 \vec{k}_2^2}{2m}\right) \underbrace{|\vec{k}_1\rangle \otimes |\vec{k}_2\rangle}_{\text{NOT realized in nature}}$$

$$|\vec{k}_1, \vec{k}_2\rangle_f = \frac{1}{\sqrt{2}} \left(|\vec{k}_1\rangle \otimes |\vec{k}_2\rangle - |\vec{k}_2\rangle \otimes |\vec{k}_1\rangle \right)$$

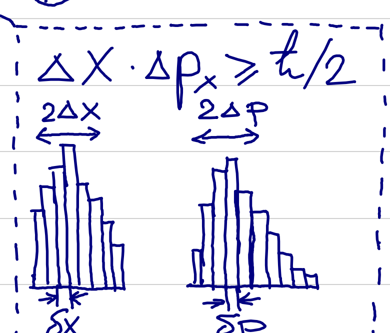
$= 0$ if $\vec{k}_1 = \vec{k}_2$ as manifestation of the Pauli principle

$$|\vec{k}_1, \vec{k}_2\rangle_b = \begin{cases} \frac{1}{\sqrt{2}} \left(|\vec{k}_1\rangle \otimes |\vec{k}_2\rangle + |\vec{k}_2\rangle \otimes |\vec{k}_1\rangle \right), & \text{if } \vec{k}_1 \neq \vec{k}_2 \\ |\vec{k}\rangle \otimes |\vec{k}\rangle, & \text{if } \vec{k}_1 = \vec{k}_2 \end{cases}$$



- elementary or older QM textbooks say:

NO classical trajectories, so we cannot label and follow quantum particles



$$|\Psi(\vec{r}_1, \vec{r}_2)|^2 = |\Psi(\vec{r}_2, \vec{r}_1)|^2$$

$$\begin{cases} \Psi(\vec{r}_1, \vec{r}_2) = e^{i\varphi} \Psi(\vec{r}_2, \vec{r}_1) \\ \Psi(\vec{r}_2, \vec{r}_1) = e^{i2\varphi} \Psi(\vec{r}_1, \vec{r}_2) \end{cases}$$

$\varphi = 1$
$\varphi = -1$ $\quad e^{i2\varphi} = 1$

what about more than two particles or different representations?

2° Symmetrization postulate of Quantum Mechanics

i) permutation symmetry of Hamiltonian gives degeneracies and selection rules

ii) permutation symmetry of all observables gives superselection rules

iii) SYMMETRIZATION POSTULATE restricts quantum states of particle species to be of a single symmetry type

$\Downarrow$

we cannot attach labels in equations to distinguish individual electrons (or protons or neutrons ...) which are all identical

i) Hilbert space of 2 particles $\mathcal{H}_1 \otimes \mathcal{H}_2$

$$\underbrace{|\alpha\rangle_1 \otimes |\beta\rangle_2 \equiv |\alpha\rangle_1 |\beta\rangle_2}_{\text{equivalent notation}} \equiv |\alpha,\beta\rangle \longrightarrow \text{basis in } \mathcal{H}_1 \otimes \mathcal{H}_2$$

$|\alpha\rangle_1$: basis in $\mathcal{H}_1$; $|\beta\rangle_2$: basis in $\mathcal{H}_2$

α, β: eigenvalues of same observable

$$|\psi\rangle = \sum_{\alpha,\beta}' c_{\alpha,\beta} |\alpha\rangle|\beta\rangle$$

$$\psi(\vec{r}_1,\vec{r}_2) = \left(\langle\vec{r}_1|\langle\vec{r}_2|\right)|\psi\rangle = \sum_{\alpha,\beta} c_{\alpha,\beta} \langle\vec{r}_1|\alpha\rangle\langle\vec{r}_2|\beta\rangle$$

permutation operator as representation of permutation in $\mathcal{H}_1 \otimes \mathcal{H}_2$

$$\hat{P}_{12}|\alpha\rangle|\beta\rangle = |\beta\rangle|\alpha\rangle \quad , \quad \underbrace{\hat{P}_{12}^{+} = \hat{P}_{12} \;,\; \hat{P}_{12}^{-1} = \hat{P}_{12}}_{\hat{P}_{12}^{+} = \hat{P}_{12}^{-1} \Leftrightarrow (\hat{P}_{12})^2 = \hat{I}}$$

$$\hat{P}_{12}\psi(\vec{r}_1,\vec{r}_2) = \psi(\vec{r}_2,\vec{r}_1)$$

$$\langle\Psi|\hat{H}|\Psi\rangle = \langle\Psi|(\hat{P}_{12}^{+})\hat{H}\hat{P}_{12}|\Psi\rangle$$

$$\hat{H} = \hat{P}_{12}^{+}\hat{H}\hat{P}_{12} \Leftrightarrow \hat{P}_{12}\hat{H} = \hat{H}\hat{P}_{12} \Leftrightarrow \underbrace{[\hat{H},\hat{P}_{12}]=0}$$

$\Downarrow$ complete set of common eigenvectors can be chosen

$\underbrace{\hat{P}_{12}^{2} = \hat{I} \Rightarrow \text{its eigenvalues are } +1 \text{ or } -1}$

$\Downarrow$

$$\left.\begin{array}{c} \Psi(\vec{r}_1,\vec{r}_2) = \Psi(\vec{r}_2,\vec{r}_1) \\ \text{or} \\ \Psi(\vec{r}_1,\vec{r}_2) = -\Psi(\vec{r}_2,\vec{r}_1) \end{array}\right\}$$

eigenvectors of $\hat{P}_{12}$ can be also eigenvectors of $\hat{H}$ which are symmetric or antisymmetric under exchange of particles

- Hilbert space of 3 particles $\mathcal{H}_1 \otimes \mathcal{H}_2 \otimes \mathcal{H}_3$

$|\alpha\rangle_1|\beta\rangle_2|\gamma\rangle_3$ basis in $\mathcal{H}_1 \otimes \mathcal{H}_2 \otimes \mathcal{H}_3$

$\Rightarrow$ permutation operators: $\underbrace{\hat{I}, \hat{P}_{12}, \hat{P}_{23}, \hat{P}_{31}, \hat{P}_{123}, \hat{P}_{123}^{2}}$

$\hat{H}$ commutes with all of them

$$\hat{P}_{12}|\alpha\rangle|\beta\rangle|\gamma\rangle = |\beta\rangle|\alpha\rangle|\gamma\rangle$$
$$\hat{P}_{23}|\alpha\rangle|\beta\rangle|\gamma\rangle = |\alpha\rangle|\gamma\rangle|\beta\rangle$$
$$\hat{P}_{31}|\alpha\rangle|\beta\rangle|\gamma\rangle = |\gamma\rangle|\beta\rangle|\alpha\rangle$$
$$\hat{P}_{123}|\alpha\rangle|\beta\rangle|\gamma\rangle = |\gamma\rangle|\alpha\rangle|\beta\rangle \Rightarrow \hat{P}_{123}^{2}|\alpha\rangle|\beta\rangle|\gamma\rangle = |\beta\rangle|\alpha\rangle|\gamma\rangle$$

$\hat{P}_{12}\cdot\hat{P}_{23} \neq \hat{P}_{23}\cdot\hat{P}_{12} \Rightarrow$ there is no common set of eigenvectors for $\hat{H}, \hat{P}_{12}, \hat{P}_{23}, \hat{P}_{31}, \hat{P}_{123}, \hat{P}_{123}^{2}$

$\Rightarrow$ Since IT IS IMOSSIBLE for every eigenstate of $\hat{H}$ to be SYMMETRIC or ANTISYMMETRIC under pair exchange, we should divide $\mathcal{H}_1 \otimes \mathcal{H}_2 \otimes \mathcal{H}_3$ into INVARIANT SUBSPACES whose vectors are transformed by permutation operators into another vector in the same SUBSPACE

■ SYMMETRIC subspace:

$$\frac{1}{\sqrt{6}}\Big(|\alpha\rangle|\beta\rangle|\gamma\rangle + |\beta\rangle|\alpha\rangle|\gamma\rangle + |\alpha\rangle|\gamma\rangle|\beta\rangle + |\gamma\rangle|\beta\rangle|\alpha\rangle + |\gamma\rangle|\alpha\rangle|\beta\rangle + |\beta\rangle|\gamma\rangle|\alpha\rangle\Big)$$

$\rightarrow$ this vector is invariant under all permutations

■ ANTISYMMETRIC subspace

$$\frac{1}{\sqrt{6}}\Big(|\alpha\rangle|\beta\rangle|\gamma\rangle - |\beta\rangle|\alpha\rangle|\gamma\rangle - |\alpha\rangle|\gamma\rangle|\beta\rangle - |\gamma\rangle|\beta\rangle|\alpha\rangle + |\gamma\rangle|\alpha\rangle|\beta\rangle + |\beta\rangle|\gamma\rangle|\alpha\rangle\Big)$$

$\rightarrow$ this vector changes sign under $\hat{P}_{12}$, $\hat{P}_{23}$ and $\hat{P}_{31}$ while remaining unchanged under other permutations

■ PARTIALLY SYMMETRIC subspaces:

a) $$\frac{1}{\sqrt{12}}\Big(2|\alpha\rangle|\beta\rangle|\gamma\rangle + 2|\beta\rangle|\alpha\rangle|\gamma\rangle - |\alpha\rangle|\gamma\rangle|\beta\rangle - |\gamma\rangle|\alpha\rangle|\beta\rangle - |\gamma\rangle|\alpha\rangle|\beta\rangle - |\beta\rangle|\gamma\rangle|\alpha\rangle\Big)$$

$$\frac{1}{2}\Big(0 + 0 - |\alpha\rangle|\gamma\rangle|\beta\rangle + |\gamma\rangle|\alpha\rangle|\beta\rangle + |\gamma\rangle|\alpha\rangle|\beta\rangle - |\beta\rangle|\alpha\rangle|\gamma\rangle\Big)$$

$\hat{P}_{12}$ acting on first (second) vector gives $+$ $(-)$ times that vector

b) $1/2\,(0 + 0 - |\alpha\rangle|\gamma\rangle|\beta\rangle$
$+ |\gamma\rangle|\beta\rangle|\alpha\rangle - |\gamma\rangle|\alpha\rangle|\beta\rangle + |\beta\rangle|\gamma\rangle|\alpha\rangle)$

$1/\sqrt{12}\,(2|\alpha\rangle|\beta\rangle|\gamma\rangle - 2|\beta\rangle|\alpha\rangle|\gamma\rangle + |\alpha\rangle|\gamma\rangle|\beta\rangle$
$+ |\gamma\rangle|\beta\rangle|\alpha\rangle - |\gamma\rangle|\alpha\rangle|\beta\rangle - |\beta\rangle|\alpha\rangle|\gamma\rangle)$

$\hat{P}_{12}$ acting on first (second) vector gives + (−) times that vector

→ eigenstates of $\hat{H}$ can be chosen to belong to one of these subspaces ⇒ since $\hat{H}|\psi\rangle$ and $|\psi\rangle$ belong to the same subspace, time evolution $i\hbar\,\partial|\psi\rangle/\partial t = H|\psi\rangle$ keeps $|\psi(t)\rangle$ in the same subspace

ii) Dynamical states which differ only by a permutation of identical particles CANNOT BE DISTINGUISHED by any measurement whatsoever

→ EXAMPLE: $\hat{H} = \hat{p}_{e^-}^2/2m + \hat{p}_{e^+}^2/2m - \dfrac{e^2}{4\pi\varepsilon_0|\vec{r}_{e^-} - \vec{r}_{e^+}|}$
of positronium atom is invariant under exchange of particles, but e^- and e^+ are not identical particles and they can be distinguished by applying an electric or a magnetic field

$$\Rightarrow \langle\Psi|\hat{A}|\Psi\rangle = \langle\Psi|\hat{P}_{ij}^{+}\hat{A}\hat{P}_{ij}|\Psi\rangle$$

$$\hat{A} = P_{ij}^{+}\hat{A}P_{ij} \Leftrightarrow \hat{P}_{ij}\hat{A} = \hat{A}\hat{P}_{ij}$$

$$\hookrightarrow \hat{P}_{ij}^{+} = \hat{P}_{ij} = \hat{P}_{ij}^{-1}$$

all physical observables must be permutation invariant

$\Rightarrow$ EXAMPLE: $\hat{S}_x = \sum_i \hat{S}_x^{(i)}$ is permutation invariant, but $\hat{S}_x^{(1)}$ is not and, therefore, not observable; if particles are localized around $\vec{r}_1, \vec{r}_2, \dots \vec{r}_N$ then "spin of the particle located at $\vec{r}_1$" would be permutation-invariant observable, but attachment of labels to distinguish the individual particles themselves is forbidden by the PRINCIPLE OF INDISTINGUISHABILITY

■ SUPERSELECTION RULE: interference between states of different symmetry is not observable

$$\hat{P}_{ij}|s\rangle = |s\rangle \quad , \quad \hat{P}_{ij}|a\rangle = -|a\rangle$$

$$\langle s|\hat{A}|a\rangle = \langle s|\hat{P}_{ij}\hat{A}|a\rangle = \langle s|\hat{A}\hat{P}_{ij}|a\rangle$$

$$\langle s|\hat{A}|a\rangle = -\langle s|\hat{A}|a\rangle \equiv 0$$

$$|\Psi\rangle = |s\rangle + c|a\rangle \quad , \quad c = e^{i\varphi}$$

$$\langle\Psi|\hat{A}|\Psi\rangle = \langle s|\hat{A}|s\rangle + \langle a|\hat{A}|a\rangle$$ is independent of phase φ

iii) SYMMETRIZATION POSTULATE:

a) BOSONS: particles whose spin is INTEGER multiple of $\hbar$ have only SYMMETRIC states

b) FERMIONS: particles whose spin HALF ODD-INTEGER multiple of $\hbar$ have only ANTISYMMETRIC states

c) partially symmetric states are unphysical

starting state $|\alpha\beta\gamma\rangle$ is not antisymmetrized

■ EXAMPLES: $|\alpha\beta\gamma\rangle_f = \frac{1}{\sqrt{6}}\Big(\underbrace{|\alpha\rangle|\beta\rangle|\gamma\rangle} - |\beta\rangle|\alpha\rangle|\gamma\rangle$

$- |\alpha\rangle|\gamma\rangle|\beta\rangle - |\gamma\rangle|\beta\rangle|\alpha\rangle +$

$|\gamma\rangle|\alpha\rangle|\beta\rangle + |\beta\rangle|\gamma\rangle|\alpha\rangle\Big)$

if $\alpha=\beta$
$|\psi\rangle \equiv 0$

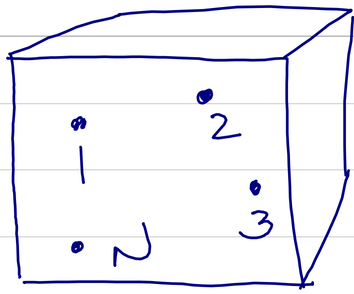
→ Pauli exclusion principle: in a system of identical fermions NO more than ONE particle can have exactly the same single particle quantum numbers

starting state $|\alpha\alpha\gamma\rangle$ is not symmetrized

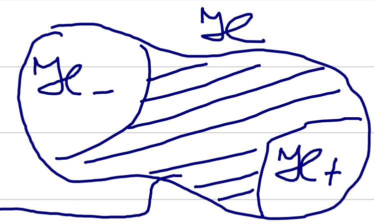
$$|\alpha\alpha\gamma\rangle_b = \frac{1}{\sqrt{3!\,2!\,1!}}\Big(\underbrace{|\alpha\rangle|\alpha\rangle|\gamma\rangle} + |\alpha\rangle|\gamma\rangle|\alpha\rangle + |\gamma\rangle|\alpha\rangle|\alpha\rangle + |\alpha\rangle|\alpha\rangle|\gamma\rangle + |\gamma\rangle|\alpha\rangle|\alpha\rangle + |\alpha\rangle|\gamma\rangle|\alpha\rangle\Big)$$

$$= \frac{1}{\sqrt{3}}\Big(|\alpha\rangle|\alpha\rangle|\gamma\rangle + |\alpha\rangle|\gamma\rangle|\alpha\rangle + |\gamma\rangle|\alpha\rangle|\alpha\rangle\Big)$$

3° System of N free bosons or fermions in a box



$$\hat{H}_N = \sum_{i=1}^{N}{}' - \frac{\hbar^2}{2m}\nabla_i^2$$



UNPHYSICAL

$$|\vec{k}_1, \dots, \vec{k}_N\rangle_f = \frac{1}{\sqrt{N!}} \sum_P (-1)^P |\vec{k}_1\rangle \otimes \dots \otimes |\vec{k}_N\rangle \in \mathcal{H}_-$$

$$|\vec{k}_1, \dots, \vec{k}_N\rangle_b = \frac{1}{\sqrt{N! \prod_j n_j!}} \sum_P |\vec{k}_1\rangle \otimes \dots \otimes |\vec{k}_N\rangle \in \mathcal{H}_+$$

$\Rightarrow$ any trace in quantum statistical mechanics MUST be performed using basis in EITHER $\mathcal{H}_-$ or $\mathcal{H}_+$ subspace of $\mathcal{H}$

$$\mathrm{Tr}(\hat{\rho}\cdot\hat{A})$$

fermions

$$\sum_{\vec{k}_1,\dots,\vec{k}_N} {}_f\langle \vec{k}_1, \dots, \vec{k}_N | \hat{\rho}\cdot\hat{A} | \vec{k}_1, \dots, \vec{k}_N\rangle_f$$

bosons

$$\sum_{\vec{k}_1,\dots,\vec{k}_N} {}_b\langle \vec{k}_1, \dots, \vec{k}_N | \hat{\rho}\cdot\hat{A} | \vec{k}_1, \dots, \vec{k}_N\rangle_b$$

this is because quantum states realized in nature reside in either $\mathcal{H}_-$ (for fermions) or $\mathcal{H}_+$ (for bosons), while states in $\mathcal{H} \setminus \mathcal{H}_- \cup \mathcal{H}_+$ are matematically correct but UNPHYSICAL