PH 451/551 Lecture # 22 ①

QM

Two identical particles in 1D

Recall: bosons $\Rightarrow |\psi_S\rangle$ $\quad P_{ij}|\psi_S\rangle = |\psi_S\rangle$

integer

fermions $\Rightarrow |\psi_A\rangle$ $\quad P_{ij}|\psi_A\rangle = -|\psi_A\rangle$

spin half-integer

exchange (permutation) operator

Ex. two particles, two available states

$|a\rangle, |b\rangle$ for each particle

$\frac{1}{\sqrt{2}}(|ab\rangle \pm |ba\rangle)$ ← state of the two-particle system if particles are bosons

if fermions

If we are talking about spin states $\Rightarrow$ e.g. $|a\rangle = |+\rangle$ m_s

$|b\rangle = |-\rangle$

$|\psi^{spin}_{S,A}\rangle = \frac{1}{\sqrt{2}}(|+-\rangle \pm |-+\rangle)$

Note: $|\psi\rangle_{total,\ S\ or\ A} = |\psi_{spatial}\rangle |\psi_{spin}\rangle$

e.g. $|n\ell m_\ell\rangle$ $\quad |s m_s\rangle$

but need to symmetrize or anti-symm!

$|\psi_{S}\rangle_{total} = |\psi_{spatial}\rangle |\psi_{spin}\rangle$
$\quad$ S S
$\quad$ A A

$|\psi_{A}\rangle_{total} = |\psi_{spatial}\rangle |\psi_{spin}\rangle$
$\quad$ A S
$\quad$ S A

2

Also: how do we symmetrize or anti-symmetrize functions for more than 2 particles?

S : $\frac{1}{\sqrt{2}}(|ab\rangle + |ba\rangle)$ $\Rightarrow$ what if there are 3 particles?

1	2	3	← particles
•	•	•	
$\boxed{a}$	$\boxed{b}$	$\boxed{c}$	← states
a	c	b	
b	a	c	
b	c	a	
c	a	b	
c	b	a	

6

$6 = 3 \cdot 2 \cdot 1 = 3!$

3 choices to fill 1st box, 2 choices to fill 2nd box, 1 choice to fill the last box

$\frac{1}{\sqrt{N!}} \sum P(|abc\ldots\rangle)$

sum over all possible permutations (generalize to N particles)

$\Downarrow$

add all these together to get a symmetric $\psi \Rightarrow |\psi_s\rangle = \frac{1}{\sqrt{N!}} \sum P(|abc..\rangle)$

A : $\frac{1}{\sqrt{2}}(|ab\rangle - |ba\rangle)$ $\Rightarrow$ can be rewritten as a determinant

$\parallel$

$$\frac{1}{\sqrt{2}} \begin{vmatrix} |a\rangle & |a\rangle \\ |b\rangle & |b\rangle \end{vmatrix}$$

particle 1 particle 2

(both can be in a state $|a\rangle$ or $|b\rangle$)

$\Leftarrow$ note if $|a\rangle = |b\rangle$ the determinant $= 0$

Pauli exclusion is satisfied

Generalize to N particles:

$$|\psi_A\rangle = \frac{1}{\sqrt{N!}} \begin{vmatrix} |a\rangle & |a\rangle & \cdots & |a\rangle \\ |b\rangle & |b\rangle & \cdots & |b\rangle \\ \vdots & & \cdots & \vdots \end{vmatrix} \begin{array}{l} \leftarrow \text{state } |a\rangle \\ \leftarrow \text{state } |b\rangle \\ \quad \vdots \\ (N \text{ states}) \end{array}$$

$$\underbrace{\quad}_{\text{particle } 1} \quad \underbrace{\quad}_{2} \quad \cdots \quad \underbrace{\quad}_{N}$$

N × N determinant Slater's determinant

↑ particles, ↑ states

⇓ from math

⇓

- if any two rows or colums are same ⇒ det = 0
- if we swap any two rows or colums

⇓ the determinant changes the sign

Pauli excl. principle is satisfied! ⇐

⇙ requirement for antisymmetry w.r.t. any permutation of two particles satisfied!

Now back to two particles! ⇒

$$H = \underbrace{\frac{p_1^2}{2m} + V(x_1)}_{H_1} + \underbrace{\frac{p_2^2}{2m} + V(x_2)}_{H_2''}$$

If we know that $H_{1,2}\varphi_n(x_{1,2}) = E_n \varphi_n(x_{1,2})$ 4

$$H\Psi(x_1,x_2) = \underline{E}\,\Psi(x_1,x_2)$$

total energy ? ? ← two-particle wave function

how do we construct this from $\varphi_n(x_1)$ & $\varphi_n(x_2)$

Note:

$$H_1 \varphi_{n_a}(x_1)\varphi_{n_b}(x_2) = E_{n_a}\varphi_{n_a}(x_1)\varphi_{n_b}(x_2)$$

acts on this but not on this

$$H_2 \varphi_{n_a}(x_1)\varphi_{n_b}(x_2) = E_{n_b}\varphi_{n_a}(x_1)\varphi_{n_b}(x_2)$$

Now add these !

$$\underbrace{(H_1+H_2)}_{"H}\underbrace{\varphi_{n_a}(x_1)\varphi_{n_b}(x_2)}_{\Psi(x_1,x_2)} = \underbrace{(E_{n_a}+E_{n_b})}_{E}\underbrace{\varphi_{n_a}(x_1)\varphi_{n_b}(x_2)}_{\Psi(x_1,x_2)}$$

two-particle wave function

two-particle energy

If particles 1 & 2 are distinguishable, we are done !

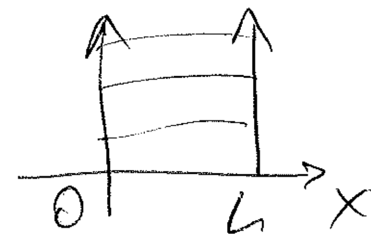
But: $\Psi(x_1, x_2) = \varphi_{n_a}(x_1)\,\varphi_{n_b}(x_2)$ S

is not S or A for arbitrary n_a & n_b

(S if $n_a = n_b$)

normalis. const

So need: $\Psi_{\substack{S\\A}}(x_1, x_2) = N_{\substack{S\\A}}\left(\varphi_{n_a}(x_1)\,\varphi_{n_b}(x_2) \pm \varphi_{n_a}(x_2)\,\varphi_{n_b}(x_1)\right)$



Ex. Two particles in a box

$$\varphi_n(x) = \sqrt{\frac{2}{L}}\sin\frac{\pi n x}{L} \text{ for each particle} \qquad E_n = \frac{\pi^2 n^2 \hbar^2}{2mL^2}$$

(a) distinguishable particles ⇒

$$\Psi(x_1, x_2) = \frac{2}{L}\sin\frac{\pi n_a x_1}{L}\sin\frac{\pi n_b x_2}{L}$$

Ground state: $n_a = n_b = 1$

$$\Psi(x_1, x_2) = \frac{2}{L}\sin\frac{\pi x_1}{L}\sin\frac{\pi x_2}{L}; \quad E = E_1 \cdot 2$$

First excited state: $n_a = 1,\ n_b = 2$

$$\Psi(x_1, x_2) = \frac{2}{L}\sin\frac{\pi x_1}{L}\sin\frac{2\pi x_2}{L}; \quad E = E_1 + E_2$$

(b) identical fermions

$$\Psi_A(x_1, x_2) = \frac{2}{L}\frac{1}{\sqrt{2}}\left(\sin\frac{\pi n_a x_1}{L}\sin\frac{\pi n_b x_2}{L} - \sin\frac{\pi n_a x_2}{L}\cdot\sin\frac{\pi n_b x_1}{L}\right.$$

If $n_a = n_b \Rightarrow \psi_{A}(x_1, x_2) = 0$

Pauli exclusion: can't have both particles in the same state!

If $n_a = 1,\ n_b = 2 \Rightarrow$

$$\psi_{A}(x_1, x_2) = \frac{2}{L}\frac{1}{\sqrt{2}}\left(\sin\frac{\pi x_1}{L}\sin\frac{2\pi x_2}{L} - \sin\frac{\pi x_2}{L}\sin\frac{2\pi x_1}{L}\right)$$

(c) identical Bosons

$$\psi_{S}(x_1, x_2) = \frac{2}{L}\frac{1}{\sqrt{2}}\left(\sin\frac{\pi n_a x_1}{L}\sin\frac{\pi n_b x_2}{L} + \sin\frac{\pi n_a x_2}{L}\cdot\sin\frac{\pi n_b x_1}{L}\right).$$

If $n_a = n_b = 1 \Rightarrow$

$$\psi_{S}(x_1, x_2) = \frac{2}{L}\sin\frac{\pi x_1}{L}\sin\frac{\pi x_2}{L}$$

If $n_a = 1,\ n_b = 2 \Rightarrow$

$$\psi_{S}(x_1, x_2) = \frac{2}{L}\frac{1}{\sqrt{2}}\left(\sin\frac{\pi x_1}{L}\sin\frac{2\pi x_2}{L} + \sin\frac{\pi x_2}{L}\cdot\sin\frac{2\pi x_1}{L}\right)$$

All this was for constructing S or A <u>spatial</u> wavefunction!

If we have a spin degree of freedom $\Rightarrow$ need S or A <u>total</u> $|\psi\rangle = |\psi_{spatial}\rangle|\psi_{spin}\rangle$

Ex, two identical spin-1/2 particles in a box $\Rightarrow$

need total $|\Psi_{A}\rangle = |\Psi_{spatial}\rangle \, |\Psi_{spin}\rangle$

$$\begin{array}{ccc} \downarrow & A & S \\ ? & S & A \end{array}$$

for $n_a = n_b = 1$

$\downarrow$

1) can't construct $|\Psi_{spatial}\rangle_{A}$, so only $|\Psi_{spatial}\rangle_{S}$ is possible

see p. 6

$$|\Psi_{spatial}\rangle_{S} \doteq \frac{2}{L} \sin\frac{\pi x_1}{L} \sin\frac{\pi x_2}{L}$$

2) need $|\Psi_{spin}\rangle_{A}$ $\Longrightarrow$ recall $s_1 = s_2 = 1/2 \Rightarrow$

$S = 0, 1 \Rightarrow$

$\vec{S} = \vec{S}_1 + \vec{S}_2$

$$\begin{array}{ll} & |S\ m_s\rangle = |m_{s_1} m_{s_2}\rangle \\ S & \begin{cases} |1 \pm 1\rangle = |\pm\pm\rangle \\ |1\ 0\rangle = \frac{1}{\sqrt{2}}(|+-\rangle + |-+\rangle) \end{cases} \\ A & \{ |0\ 0\rangle = \frac{1}{\sqrt{2}}(|+-\rangle - |-+\rangle) \end{array}$$

$$\text{Total } |\Psi\rangle_{A} \doteq \underbrace{\frac{2}{L} \sin\frac{\pi x_1}{L} \sin\frac{\pi x_2}{L}}_{|\Psi_{spatial}\rangle_S} \underbrace{(|+-\rangle - |-+\rangle)\frac{1}{\sqrt{2}}}_{|\Psi_{spin}\rangle_A}$$

only 1 possibility

$E = 2E_1 \leftarrow$ non-degenerate

What about $n_a = 1,\ n_b = 2$? $\Rightarrow$

Can have both $|\psi_{\underset{S}{spatial}}\rangle$ & $|\psi_{\underset{A}{spatial}}\rangle \Rightarrow$

$$|\psi_{\underset{A}{total}}\rangle \doteq \underbrace{\frac{1}{\sqrt{2}}\left(\sin\frac{\pi x_1}{L}\sin\frac{2\pi x_2}{L} + \sin\frac{\pi x_2}{L}\sin\frac{2\pi x_1}{L}\right)}_{\psi_{\underset{S}{spatial}}} \cdot$$

$$\cdot \underbrace{\frac{1}{\sqrt{2}}\left(|+-\rangle - |-+\rangle\right)}_{\psi_{\underset{A}{spin}}}$$

or

$$|\psi_{\underset{A}{total}}\rangle \doteq \underbrace{\frac{1}{\sqrt{2}}\left(\sin\frac{\pi x_1}{L}\sin\frac{2\pi x_2}{L} - \sin\frac{\pi x_2}{L}\sin\frac{2\pi x_2}{L}\right)}_{\psi_{\underset{A}{spatial}}} \cdot$$

$$\cdot \underbrace{\begin{cases} |++\rangle \\ |--\rangle \\ \frac{1}{\sqrt{2}}\left(|+-\rangle + |-+\rangle\right) \end{cases}}$$ $\leftarrow$ 3 choices of $\psi_{\underset{S}{spin}}$

So $E = E_1 + E_2$ is 4-fold degenerate !