# FYS 4480 Sept 2

$\hat{O}_1$ examples $H_0$

$\hat{O}_2$ — " — $H_I = \sum_{i<j}^{N} v(x_{ij})$

$N = 4$

$\langle \Phi | \hat{O}_2 | \Phi_{\alpha_3}^{\alpha_3'} \rangle$ $\langle \Phi | \hat{O}_2 | \Phi_{\alpha_3 \alpha_4}^{\alpha_3' \alpha_4'} \rangle$

$$\int dx_1 dx_2 dx_3 dx_4 \, \varphi_{\alpha_1}^*(x_1) \varphi_{\alpha_2}^*(x_2) \varphi_{\alpha_3}^*(x_3)$$

$$\times \varphi_{\alpha_4}^*(x_4) \big( \cancel{v(x_{12})} + v(x_{13}) + \cancel{v(x_{14})} + v(x_{23}) + \cancel{v(x_{24})} + v(x_{34}) \big)$$

$$\times \Big( \sum_P (-1)^P \hat{P} \Big) \varphi_{\alpha_1'}(x_1) \varphi_{\alpha_2}(x_2) \varphi_{\alpha_3'}(x_3)$$

$$\varphi_{\alpha_4}(x_4)$$

$$(1 - P_{12} - P_{13} - \cdots)$$

$$= \sum \big( \langle \alpha_1' \alpha_3 | v | \alpha_1' \alpha_3' \rangle$$

$$- \sum_{\alpha_1' \neq \alpha_3'} \quad - \langle \alpha_1' \alpha_3 | v | \alpha_3' \alpha_1' \rangle \Big)$$

$$\langle \Phi | H_1 | \Phi^{\alpha_3 \alpha_4}_{\alpha_3' \alpha_4'} \rangle$$

$$\propto \int dx_1\, dx_2\, dx_3\, dx_4$$

$$\times \left( \varphi^*_{\alpha_1}(x_1)\, \varphi^*_{\alpha_2}(x_2)\, \varphi^*_{\alpha_3}(x_3)\, \varphi^*_{\alpha_4}(x_4) \right)$$

$$\times \big( v(x_{12}) + v(x_{13}) + v(x_{14}) + v(x_{23}) + v(x_{24}) + v(x_{34}) \big)$$

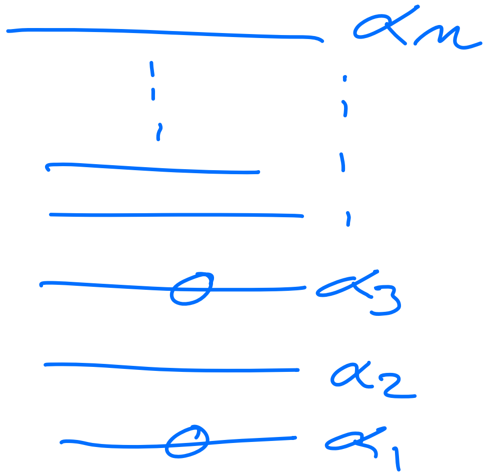
$$\times \Big( \sum_P (-)^P \hat{P} \Big)\, \varphi_{\alpha_1}(x_1)\, \varphi_{\alpha_2'}(x_2)\, \varphi_{\alpha_3'}(x_3) \times \varphi_{\alpha_4'}(x_4) \Big)$$

$$= \langle \alpha_3 \alpha_4 | v | \alpha_3' \alpha_4' \rangle - \langle \alpha_3 \alpha_4 | v | \alpha_4' \alpha_3' \rangle$$

$$\langle \Phi | v | \Phi^{\alpha_2 \alpha_3 \alpha_4}_{\alpha_2' \alpha_3' \alpha_4'} \rangle = 0$$

if $v$ is a 2-body int

# Second quantization




$N \Rightarrow$

$$\# \text{configs} = \binom{n}{N}$$

$$N \le n$$

$$\underset{\alpha_1}{\boxed{1}}\;\underset{\alpha_2}{\boxed{0}}\;\underset{\alpha_3}{\boxed{1}}\; - \;-\; - \;\underset{\alpha_n}{\boxed{\phantom{0}}}$$

$n, l, m_l, s, \ldots$

Define a vacuum state

$$|0\rangle$$

Define a creation operator

$$a^\dagger_\alpha |0\rangle = |\alpha\rangle$$

Two-body state

$$a^\dagger_{\alpha_1} a^\dagger_{\alpha_2} |0\rangle = |\alpha_1 \alpha_2\rangle$$

Slater det is now given

by $|\alpha_1 \alpha_2\rangle$ , for many

$$a^\dagger_{\alpha_1} a^\dagger_{\alpha_2} \dots a^\dagger_{\alpha_N} |0\rangle =$$

$$\prod_{\alpha_i=1}^{N} a^\dagger_{\alpha_i} |0\rangle$$

<u>$N=2$</u>

$$a^\dagger_{\alpha_1} a^\dagger_{\alpha_2} |0\rangle = - a^\dagger_{\alpha_2} a^\dagger_{\alpha_1} |0\rangle$$

$$|\alpha_1\rangle = a^\dagger_{\alpha_1} |0\rangle$$

$$a^\dagger_{\alpha_1} a^\dagger_{\alpha_1} |0\rangle = 0$$

$$\left( a^\dagger_{\alpha_1} a^\dagger_{\alpha_2} + a^\dagger_{\alpha_2} a^\dagger_{\alpha_1} \right) |0\rangle = 0$$

$$\Rightarrow \quad \left\{ a^\dagger_{\alpha_1}, a^\dagger_{\alpha_2} \right\} = 0$$

Define annihilation/destruction operator : Hermitian conjugate of $a^\dagger$

$$a = (a^\dagger)^\dagger$$

$$a|0\rangle = 0$$

$$a_\alpha|\alpha\rangle = a_\alpha a_\alpha^\dagger|0\rangle = |0\rangle$$

$$\{a_{\alpha_1}, a_{\alpha_2}\} = 0$$

if we have

$|\alpha_1 \alpha_2 \dots \alpha_N\rangle$ N-particle state

if

$$\alpha \in \{\alpha_1 \alpha_2, \dots, \alpha_N\}$$

$$a_\alpha a_{\alpha_1}^\dagger a_{\alpha_2}^\dagger \dots a_{\alpha_k}^\dagger a_\alpha^\dagger a_{\alpha_{k+1}}^\dagger \dots a_{\alpha_N}^\dagger|0\rangle$$

will remove a particle in the state $\alpha$ $\Rightarrow$

N-1 particle state

$$\langle \underbrace{\alpha_1 \alpha_2 \dots \alpha_N}_{N} | a_\alpha | \underbrace{\alpha_1 \alpha_2 \dots \alpha \dots \alpha_N}_{N-1} \rangle$$

$$= 0$$

$$\alpha \notin \{\alpha_1 \alpha_2 \dots \alpha_N\}$$

Then $\quad a_\alpha |\alpha_1 \alpha_2 \ldots \alpha_N\rangle = 0$

$$\left.\begin{array}{ll} a_\alpha^\dagger a_\alpha & a_\alpha^\dagger a_\beta \\ a_\alpha a_\alpha^\dagger & a_\beta a_\alpha^\dagger \end{array}\right\} \quad \{a_\alpha, a_\beta^\dagger\} = \delta_{\alpha\beta}$$

$$a_\alpha^\dagger a_\alpha |\alpha_1 \alpha_2 \ldots \alpha_N\rangle = 0$$

$$\alpha \notin \{\alpha_1 \alpha_2, \ldots \alpha_N\}$$

$$a_\alpha a_\alpha^\dagger |\alpha_1 \alpha_2 \ldots \alpha_N\rangle$$

$$\alpha \notin \{\alpha_1 \alpha_2 \ldots \alpha_N\}$$

$$= a_\alpha |\alpha \alpha_1 \ldots \alpha_N\rangle$$

$$= |\alpha_1 \alpha_2 \ldots \alpha_N\rangle$$

$$\alpha \in \{\alpha_1 \alpha_2 \ldots \alpha_N\}$$

$$a_\alpha^\dagger a_\alpha |\alpha_1 \alpha_2 \ldots \alpha_N\rangle$$

$$a_\alpha^\dagger a_\alpha |\alpha_1 \alpha_2 \ldots \alpha_k \underline{\alpha} \alpha_{k+1} \ldots \alpha_N\rangle$$

$$\left( |\alpha_1\rangle \otimes |\alpha_2\rangle \cdots \overset{a_\alpha'}{\cdot} \otimes |\alpha_N\rangle \right)$$

$$a_\alpha a_\alpha^\dagger |0\rangle$$

$$\underbrace{\{a_\alpha^\dagger, a_\beta^\dagger\}}_{|0\rangle} = 0 \qquad a_\alpha^\dagger a_\beta^\dagger = - a_\beta^\dagger a_\alpha^\dagger$$

$$a_\alpha^\dagger a_\alpha \left( a_{\alpha_1}^\dagger a_{\alpha_2}^\dagger \cdots a_{\alpha_k}^\dagger a_\alpha^\dagger a_{\alpha_{k+1}}^\dagger \cdots \right)|0\rangle$$

$$= a_\alpha^\dagger a_\alpha (-)^k a_\alpha^\dagger a_{\alpha_1}^\dagger \cdots a_{\alpha_k}^\dagger a_{\alpha_{k+1}}^\dagger \cdots a_{\alpha_N}^\dagger |0\rangle$$

$$= a_\alpha^\dagger (-)^k \underbrace{|\alpha_1 \alpha_2 \cdots \alpha_k \alpha_{k+1} \cdots \alpha_N\rangle}_{N-1 \text{ particle state}}$$

$$= (-)^k |\alpha \alpha_1 \alpha_2 \cdots \cdots \alpha_N\rangle$$

$$= |\alpha_1 \alpha_2 \cdots \alpha_k \alpha \alpha_{k+1} \cdots \alpha_N\rangle$$

$$a_\alpha a_\alpha^\dagger |\alpha_1 \alpha_2 \cdots \alpha \cdots \alpha_N\rangle = 0$$

$$\left( a_\alpha a_\alpha^\dagger + a_\alpha^\dagger a_\alpha \right) |\alpha_1 \alpha_2 \ldots \alpha_N\rangle$$

$$= |\alpha_1 \alpha_2 \ldots \alpha_N\rangle \Rightarrow$$

$$\{ a_\alpha , a_\alpha^\dagger \} = a_\alpha a_\alpha^\dagger + a_\alpha^\dagger a_\alpha$$

$$= \underline{\mathbb{1}}$$

$$a_\alpha^\dagger a_\beta \qquad a_\beta a_\alpha^\dagger$$

$$|\alpha_1 \alpha_2 \ldots \alpha_N\rangle$$

(i) $\alpha , \beta \notin |\alpha_1 \alpha_2 \ldots \alpha_N\rangle$

(ii) $\alpha , \beta \in |\alpha_1 \alpha_2 \ldots \alpha_N\rangle$

(iii) $\alpha \vee \beta \in |\alpha_1 \ldots \alpha_N\rangle$

$$\Rightarrow \quad \{ a_\alpha^\dagger , a_\beta \} = a_\alpha^\dagger a_\beta + a_\beta a_\alpha^\dagger = \delta_{\alpha\beta}$$

summarize

$a^\dagger |\ \rangle \qquad |\alpha\rangle$

$$a_\alpha |0\rangle = |\alpha\rangle$$

$$a_\alpha^\dagger |\alpha\rangle = 0$$

$$a_\alpha |0\rangle = 0$$

$$a_\alpha |\alpha\rangle = |0\rangle$$

$$\{a_\alpha, a_\beta\} = \{a_\alpha^\dagger, a_\beta^\dagger\} = 0$$

$$\{a_\alpha^\dagger, a_\beta\} = \delta_{\alpha\beta}$$

## <u>Example 1</u>

$$|\alpha_1 \alpha_2\rangle = a_{\alpha_1}^\dagger a_{\alpha_2}^\dagger |0\rangle$$

$$\langle \alpha_1' \alpha_2' | \alpha_1 \alpha_2 \rangle$$

$$\langle \alpha | \beta \rangle = \delta_{\alpha\beta}$$

$$\langle 0 | a_\alpha a_\beta^\dagger | 0 \rangle$$

$$\langle 0 | a_\beta^\dagger a_\alpha | 0 \rangle = 0$$

$$\langle 0 | a_{\alpha_2'} a_{\alpha_1'} a_{\alpha_1}^\dagger a_{\alpha_2}^\dagger | 0 \rangle$$

$$a_{\alpha_2'}\left(\delta_{\alpha_1'\alpha_1} - a^\dagger_{\alpha_1} \underline{a_{\alpha_1'}}\right) \underline{a^\dagger_{\alpha_2}}$$

$$a_{\alpha_2'} a^\dagger_{\alpha_2} \delta_{\alpha_1'\alpha_1} - a_{\alpha_2'} a^\dagger_{\alpha_1}\left(\delta_{\alpha_1'\alpha_2} - \cancel{a^\dagger_{\alpha_2} a_{\alpha_1'}}\right)$$

$$\left(\delta_{\alpha_2'\alpha_2} - \cancel{a^\dagger_{\alpha_2} a_{\alpha_2'}}\right) \delta_{\alpha_1'\alpha_1}$$

$$-\left(\delta_{\alpha_1\alpha_2'} - \cancel{a^\dagger_{\alpha_1} a_{\alpha_2'}}\right) \delta_{\alpha_1'\alpha_2}$$

$$\delta_{\alpha_2'\alpha_2} \delta_{\alpha_1'\alpha_1} - \delta_{\alpha_1\alpha_2'} \delta_{\alpha_1'\alpha_2}$$

$$\alpha_2 = \alpha_2' \wedge \alpha_1' = \alpha_1 \qquad \alpha_2 \neq \alpha_1$$

$$\langle \alpha_1 \alpha_2 | \alpha_1 \alpha_2 \rangle = \delta_{\alpha_1\alpha_1} \delta_{\alpha_2\alpha_2}$$

## Example

$$a^\dagger_\alpha a_\alpha$$

$$\hat{N} = \sum_{\alpha=1}^{N} a^\dagger_\alpha a_\alpha$$

$$|\alpha_1 \alpha_2 \ldots \alpha_N\rangle$$

$$\alpha \notin |\alpha_1, \alpha_2 \ldots \alpha_N\rangle$$

$$\hat{N} |\alpha_1 \alpha_2 \ldots \alpha_N\rangle = 0$$

$$\alpha \in |\alpha_1 \alpha_2 \ldots \alpha_N\rangle$$

$$a_\alpha^+ a_\alpha |\alpha_1 \alpha_2 \alpha_k \ldots \alpha_N\rangle$$

$$= (-)^{2k} |\alpha_1 \alpha_2 \ldots \alpha_N\rangle$$

$$\hat{N} |\alpha_1 \alpha_2 \ldots \alpha_N\rangle = N |\alpha_1 \alpha_2 \ldots \alpha_N\rangle$$

<u>Example</u>

$$\hat{h}_0(x) = -\frac{\hbar^2 \nabla_x^2}{2m} + V_{ext}(x)$$

$$\hat{h}_0 = \sum_{\alpha\beta} a_\alpha^+ a_\beta \underbrace{\langle\alpha|h_0|\beta\rangle}_{\int dx\, \varphi_\alpha^*(x)\, h_0\, \varphi_\beta(x)}$$

$$\langle a_1 a_2 | \hat{h}_0 | a_1 a_2\rangle \qquad \langle\alpha|h_0|\beta\rangle = \delta_{\alpha\beta}\, \varepsilon_\alpha$$

$$\sum_{\alpha\beta} a^{\dagger}_{\alpha} a_{\beta} \langle \alpha | u_d | \beta \rangle = \sum_{\alpha} a^{\dagger}_{\alpha} a_{\alpha} \varepsilon_{\alpha}$$

$$\sum_{\alpha} \varepsilon_{\alpha} \langle 0 | a_{\alpha_2} a_{\alpha_1} \underbrace{a^{\dagger}_{\alpha} a_{\alpha}} a^{\dagger}_{\alpha_1} a^{\dagger}_{\alpha_2} | 0 \rangle$$

$$\underbrace{a^{\dagger}_{\alpha} a_{\alpha}} | \alpha_1 \alpha_2 \rangle$$

$$\langle \alpha_1 \alpha_2 | (\varepsilon_{\alpha_1} + \varepsilon_{\alpha_2}) | \alpha_1 \alpha_2 \rangle$$

$$= \varepsilon_{\alpha_1} + \varepsilon_{\alpha_2}$$