Lecture fys4480, September 1, 2023

ansatz

$$\Phi_0(\vec{x}_1, \vec{x}_2, \ldots \vec{x}_N; \alpha_0 \ldots \alpha_{N-1})$$

$$= \frac{1}{\sqrt{N!}} \begin{vmatrix} \varphi_{\alpha_0}(\vec{x}_1) & \varphi_{\alpha_0}(\vec{x}_2) & \cdots & \varphi_{\alpha_0}(\vec{x}_N) \\ \varphi_{\alpha_1}(\vec{x}_1) & \vdots & & \\ \vdots & \vdots & & \\ \varphi_{\alpha_{N-1}}(\vec{x}_1) & \vdots & & \varphi_{\alpha_{N-1}}(\vec{x}_N) \end{vmatrix}$$

$$= \frac{1}{\sqrt{N!}} \sum_{P} (-1)^P \hat{P} \underbrace{\varphi_{\alpha_0}(\vec{x}_1) \varphi_{\alpha_1}(\vec{x}_2) \ldots \varphi_{\alpha_{N-1}}(\vec{x}_N)}_{\Phi_H}$$

$$\hat{A} = \frac{1}{N!} \sum_{P} (-1)^{P} \hat{P}$$

$N = 2$ $\qquad$ $$\hat{A}_2 = \frac{1}{2}\left(1 - \hat{P}_{12}\right)$$

$$\langle \Phi_0 | H_0 | \Phi_0 \rangle = \sum_{\alpha_i = 0}^{N-1} \varepsilon_{\alpha_i}$$

$$\hat{h}_0(\vec{x}_1)\, \varphi_\alpha(\vec{x}_1) = \varepsilon_\alpha \varphi_\alpha(\vec{x}_i)$$

$\downarrow$

$\hat{O}_1$ $\qquad$ $\varepsilon_{\alpha_i} \longrightarrow \langle \varphi_{\alpha_j} | \hat{O}_1 | \varphi_{\alpha_i} \rangle$

$\langle \Phi_i | H_0 | \Phi_0 \rangle$ $\qquad$ Φ_i differs by one sp-state

$$\langle \Phi_0 | H_1 | \Phi_0 \rangle$$

$$= \sum_{i<j} \int d\vec{x}_1 d\vec{x}_2 \ldots d\vec{x}_i \ldots d\vec{x}_j \ldots d\vec{x}_N$$

$$\times \quad \varphi^*_{\alpha_0}(\vec{x}_1) \ldots \varphi^*_{\alpha_{N-1}}(\vec{x}_N) \, v(x_i, x_j)$$

$$\sum_P (-1)^P \hat{P} \quad \varphi_{\alpha_a}(\vec{x}_1) \ldots \varphi^*_{\alpha_{N-1}}(\vec{x}_N)$$

$P = 0$

$k \neq i$ and j $\quad \int dx_k \, \varphi^*_{\alpha_k} \varphi_{\alpha_k}$

$\langle \alpha_i \alpha_j | v | \alpha_i \alpha_j \rangle$

$p = 1$

$$\sum_{\alpha j} \langle \alpha_1' \alpha_j | v | \alpha_j \alpha_1' \rangle$$

$p \geq 2$ $\qquad P_{12} P_{34}$

$i = 1 \quad j = 2$

$$- \int dx_1 dx_2 \, \varphi^*_{\alpha_0}(\vec{x}_1) \varphi^*_{\alpha_1}(\vec{x}_2) v(x_1 x_2)$$

$$\times \varphi_{\alpha_0}(\vec{x}_2) \varphi_{\alpha_1}(\vec{x}_1) \int dx_3 dx_4$$

$$\varphi^*_{\alpha_2}(\vec{x}_3) \varphi^*_{\alpha_3}(\vec{x}_4) \varphi_{\alpha_2}(\vec{x}_4) \varphi_{\alpha_3}(\vec{x}_3)$$

$$= 0$$

$$\langle \Phi_0 | H_1 | \Phi_0 \rangle =$$

$$\sum_{i<j} \left\{ \langle \alpha_i \alpha_j | v | \alpha_i \alpha_j \rangle - \langle \alpha_i \alpha_j | v | \alpha_j \alpha_i \rangle \right\}$$

$$= \frac{1}{2} \sum_{i,j} \left\{ \text{———} \quad , \quad \text{———} \right\}$$

$$= \frac{1}{2} \sum_{i,j} \langle \alpha_i \alpha_j | v | \alpha_i \alpha_j \rangle_{AS}$$

$$\hat{H} \Phi_0 \neq E_{exact} \Phi_0$$

$$E_0 = \sum_{i=0}^{N-1} \varepsilon_{\alpha_i} + \frac{1}{2} \sum_{i,j} \langle \alpha_i \alpha_j | v | \alpha_i \alpha_j \rangle_{AS}$$

$$\langle \Phi_0 | H_I | \Phi_i \rangle \propto \sum_k \langle \alpha_\ell \alpha_k | v | \alpha_a \alpha_b \rangle_{AS}$$

differs by one single-particle state only,

$\varphi_{\alpha_\ell}(x_i) \neq \varphi_{\alpha_k}(x_j)$

$$\langle \Phi_0 | H_1 | \Phi_i \rangle$$

differs by two single particle states

$$\underbrace{\varphi_{\alpha_k}(x_i) \wedge \varphi_{\alpha_l}(x_j)}_{\text{ket side}}$$

Bra-side

$$\varphi_{\alpha_i'}(x_i) \wedge \varphi_{\alpha_j'}(x_j)$$

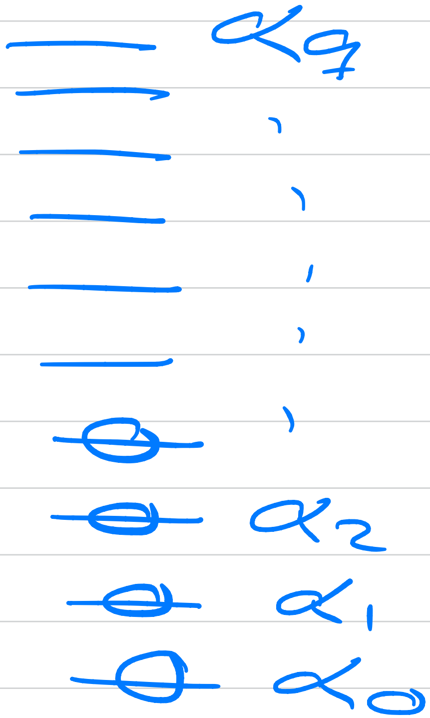
$$\langle \Phi_0 | H_I | \Phi_1 \rangle = \langle \alpha_i' \alpha_j' | v | \alpha_k \alpha_l \rangle_{AS}$$

Condon-Slater rules

if we have more than two sp-states which differ and if we have at most a twobody interaction

$$\langle \Phi_0 | H_I | \Phi_i \rangle = 0$$

Encode SD as bit strings



$N = 4$

$$|1\ 1\ 1\ 1\ 0 \cdots 0\rangle$$
$$\alpha_0\ \alpha_1\ \alpha_2\ \alpha_3 \cdots \alpha_q$$

1111000000

α_9

α_8

α_7

α_6

α_5

α_4

α_3

α_2

α_1

α_0

$$|0000111100\rangle$$

$$= \Phi_1$$

$$\langle \Phi_0 | H_1 | \Phi_1 \rangle = 0$$

compare

$|\phi_0\rangle$ and $|\Phi_1\rangle$

Second quantization, Basic definitions

$N = 4, \quad \alpha_0 \alpha_1, \ldots \alpha_9$

$|\Phi_0\rangle = |\alpha_0 \alpha_1 \alpha_2 \alpha_3\rangle$ compact representation of a SD.

we define a creation operator

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

↑ vacuum

2 particles $\quad |\alpha\beta\rangle = a_\alpha^\dagger a_\beta^\dagger |0\rangle$

$|\Phi_0\rangle = a_{\alpha_0}^\dagger a_{\alpha_1}^\dagger a_{\alpha_2}^\dagger a_{\alpha_3}^\dagger |0\rangle$

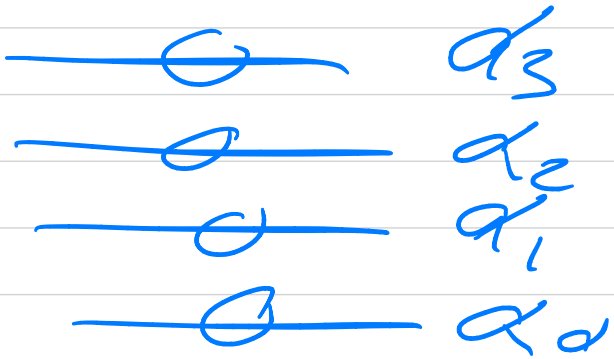
$$\underbrace{|\alpha_0\alpha_1\alpha_2\alpha_3\rangle}_{\text{standard ordering}} = -|\alpha_0\alpha_2\alpha_1\alpha_3\rangle$$

4-particle state

$$|\alpha_0\alpha_1\alpha_2\alpha_3\rangle = a^\dagger_{\alpha_0}a^\dagger_{\alpha_1}a^\dagger_{\alpha_2}a^\dagger_{\alpha_3}|0\rangle$$

$$a^\dagger_{\alpha}|\alpha_0\alpha_1\alpha_2\alpha_3\rangle = a^\dagger_{\alpha}a^\dagger_{\alpha_0}a^\dagger_{\alpha_1}a^\dagger_{\alpha_2}a^\dagger_{\alpha_3}|0\rangle$$

$$\alpha = \{\alpha_0\alpha_1\alpha_2\alpha_3\}$$



$$a^\dagger_{\alpha_0}a^\dagger_{\alpha_0}|0\rangle = 0$$

$$\alpha \neq \{\alpha_0\, \alpha_1\, \alpha_2\, \alpha_3\}$$

$$|\alpha\, \alpha_0\, \alpha_1\, \alpha_2\, \alpha_3\rangle$$

$$\alpha_0 < \alpha_1 < \alpha_2 < \alpha_3 \;\ldots\; < \alpha_{d-1}$$

$$\alpha = \alpha_5$$

$$|\alpha_0\, \alpha_1\, \alpha_2\, \alpha_3\, \alpha_5\rangle$$

— 5-particle

$$|\alpha\, \alpha_0\, \alpha_1\, \alpha_2\, \alpha_3\rangle = a^\dagger_\alpha a^\dagger_{\alpha_0} a^\dagger_{\alpha_1} a^\dagger_{\alpha_2} a^\dagger_{\alpha_3} |0\rangle$$

$$= -|\alpha_0\, \alpha\, \alpha_1\, \alpha_2\, \alpha_3\rangle = -a^\dagger_{\alpha_0} a^\dagger_\alpha a^\dagger_{\alpha_1} a^\dagger_{\alpha_2} a^\dagger_{\alpha_3}$$

$$a^\dagger_\alpha a^\dagger_{\alpha_0} + a^\dagger_{\alpha_0} a^\dagger_\alpha = 0$$

$$\Rightarrow \quad [a^\dagger_\alpha, a^\dagger_{\alpha_0}]_+ = \{a^\dagger_\alpha, a^\dagger_{\alpha_0}\}$$

$$= 0 \quad \Rightarrow \{a^\dagger_\alpha, a^\dagger_\beta\} = 0$$

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

Define annihilation operator

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

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

$$a_\alpha \,|\alpha_0\, \alpha_1\, \alpha_2\, \alpha_3\rangle = ?$$

$$\alpha \in \{\alpha_0\, \alpha_1\, \alpha_2\, \alpha_3\}$$

$$\alpha = \alpha_0$$

$$\underset{N=4}{a_\alpha \,|\alpha_0\, \alpha_1\, \alpha_2\, \alpha_3\rangle} = \underset{N=3}{|\alpha_1\, \alpha_2\, \alpha_5\rangle}$$

$$a_\alpha = \left(a^\dagger_\alpha\right)^\dagger$$ hermitian conjugate of $a^\dagger_\alpha$

$$\Rightarrow \{a_\alpha, a_\beta\} = 0$$

2 commutation relations

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

$$= 0$$

$$a_\alpha a_\beta + a_\beta a_\alpha$$

we need an additional rule

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

Example

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

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

norm

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

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

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

$$\langle 0 | a_\beta a_\alpha^\dagger | 0 \rangle = \delta_{\alpha\beta} \underbrace{\langle 0 | 0 \rangle}_{=1}$$

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

$$= \delta_{\alpha\beta}$$