FYS4480 September 23

new vacuum $|c\rangle = |\Phi_0\rangle$

$$H|c\rangle \neq \lambda|c\rangle$$

$$b_\alpha^\dagger = \begin{cases} a_\alpha^\dagger & \alpha > F \\ a_\alpha & \alpha \leq F \end{cases}$$

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$$\overbrace{b_\alpha b_\beta^\dagger} = 0$$

$$\hat{H}_0 = \sum_{\alpha\beta > F} \langle\alpha|\hat{h}_0|\beta\rangle b_\alpha^\dagger b_\beta$$

$$+ \sum_{\substack{\alpha > F \\ \beta \leq F}} \left[\langle\alpha|\hat{h}_0|\beta\rangle b_\alpha^\dagger b_\beta^\dagger + \langle\beta|\hat{h}_0|\alpha\rangle b_\beta b_\alpha\right]$$

$$- \sum_{\alpha\beta \leq F} \langle\beta|\hat{h}_0|\alpha\rangle b_\alpha^\dagger b_\beta$$

$$+ \sum_{\alpha \leq F} \langle\alpha|\hat{h}_0|\alpha\rangle$$

$$\hat{h}_0 |\alpha\rangle = \varepsilon_\alpha |\alpha\rangle$$

$ijkl\ldots \le F$

$abcd\ldots > F$

$pqrs\ldots$ general single-particle state

$$a_i^\dagger a_j = \delta_{ij}$$

$$a_p^\dagger a_q = \delta_{pq} \quad \text{if } p,q \le F$$

$$a_p a_q^\dagger = \delta_{pq} \quad \text{if } p,q > F$$

$$|\Phi_i\rangle = a_i |\Phi_0\rangle \neq 0$$

if $i \in |\Phi_0\rangle$

$$|\Phi^a\rangle = a_a^\dagger |\Phi_0\rangle$$

$a \notin |\Phi_0\rangle$

1p1h $\quad |\Phi_i^a\rangle = a_a^\dagger a_i |\Phi_0\rangle$

2p2h $\quad |\Phi_{ij}^{ab}\rangle = a_a^\dagger a_b^\dagger a_j a_i |\Phi_0\rangle$

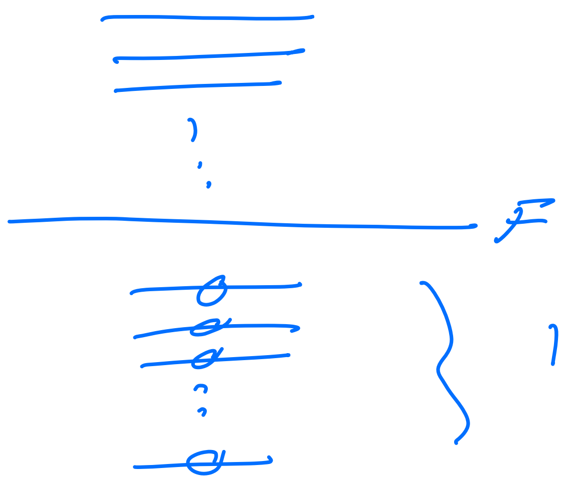
$b_a^\dagger b_b^\dagger b_j^\dagger b_i^\dagger$

NpNh $|\Phi^{a_1 a_2 \ldots a_N}_{i_1 i_2 \ldots i_N}\rangle$

$$a^{\dagger}_{a_1} a^{\dagger}_{a_2} \ldots a^{\dagger}_{a_N} a_{i_N} \ldots a_{i_1} |\Phi_0\rangle$$

general notation for a general p-H state

$$|\Phi^{P}_{H}\rangle$$



$|c\rangle = |\Phi_0\rangle$

N-particles and n slots

configurations $= \binom{n}{N}$

$$= \frac{n!}{(n-N)!\,N!} \qquad n \geq N$$

order configurations in terms of PH-excitations

0p-0h : $|\Phi_0\rangle$

1p-1h : $|\Phi_i^a\rangle$

2p-2h . . .

$$\langle \Phi_{H'}^{P'} | \Phi_H^P \rangle = \delta_{PP'} \delta_{HH'}$$

$$|\Psi_0\rangle = \sum_J U_{J0} |\Phi_J\rangle$$

$$= \sum_{\underbrace{PH}_{J}} C_H^P |\Phi_H^P\rangle$$

$\langle \Phi_{H'}^{P'} | \hat{H} | \Phi_H^P \rangle$ needed

Two-body Hamiltonian

$$\hat{H} = \underbrace{E_0^{Ref}}_{\langle \Phi_0 | H | \Phi_0 \rangle} + \hat{F} + \hat{V}$$

$$\hat{F} = \sum_{pq} \langle p | \hat{f} | q \rangle \{ a_p^\dagger a_q \}$$

$$\langle p|\hat{f}|q\rangle = \langle p|\hat{h}_0|q\rangle + \sum_j \langle pj|\hat{v}|qj\rangle_{AS}$$

$$\langle pj|\hat{v}|qj\rangle_{AS} = \langle pj|\hat{v}|qj\rangle - \langle pj|\hat{v}|jq\rangle$$

$$= \langle jp|\hat{v}|jq\rangle_{AS} = -\langle pj|\hat{v}|jq\rangle_{AS}$$

$$\hat{V} = \frac{1}{4}\sum_{pqrs} \langle pq|\hat{v}|rs\rangle_{AS} \times \{a_p^\dagger a_q^\dagger a_s a_r\}$$

$$\langle \Phi_i^a|H|\Phi_r^a\rangle =$$

$$\langle c|a_r^\dagger a_a \Big(E_0^{Ref} + \sum_{pq} \langle p|\hat{f}|q\rangle a_p^\dagger a_q + \frac{1}{4}\sum_{pqrs} \langle pq|\hat{v}|rs\rangle a_p^\dagger a_q^\dagger a_s a_r\Big) |a_a^\dagger a_i|c\rangle$$

$$= \langle c|a_r^\dagger a_a\, a_a^\dagger a_{i'}|c\rangle E_0^{Ref}$$

$$\left(\begin{array}{l} \langle c | a_i^\dagger a_i | c \rangle \quad i \in |c\rangle \\ \underbrace{\quad}\\ \langle \Phi_i | \Phi_i \rangle = 1 \end{array} \right)$$

$$+ \sum_{pq} \langle p | \hat{f} | q \rangle$$

$$\times \langle c | a_i^\dagger a_a \, a_p^\dagger a_q \, a_a^\dagger a_i | c \rangle$$

$$\delta_{pa} \qquad \delta_{qa}$$

$$\delta_{iq} \qquad \delta_{ip}$$

$$\left(\delta_{ii} \langle a | \hat{f} | a \rangle - \langle i | \hat{f} | i \rangle \delta_{aa} \right)$$

$$= \underbrace{\langle a | h_0 | a \rangle}_{\varepsilon_a} + \sum_j \langle aj | \hat{v} | aj \rangle_{AS}$$

$$- \langle i | h_0 | i \rangle - \sum_j \langle ij | v | ij \rangle_{AS})$$

$$+ \frac{1}{4} \sum_{pqrs} \langle pq | \hat{v} | rs \rangle \langle c | a_i^\dagger a_a a_p^\dagger a_q^\dagger a_s a_r$$

$$\times a_a^\dagger a_i | c \rangle \quad \approx 0$$

$$\langle c | a_i^\dagger a_a \, a_p^\dagger a_q^\dagger \, a_s a_r \, a_a^\dagger a_i | c \rangle$$

$$= E_0^{Ref} + \langle a|\hat f|a\rangle - \langle i|\hat f|i\rangle$$

$$\langle \Phi_0 | H | \Phi_i^a \rangle =$$

$$E_0^{Ref} \langle \Phi_0 | \overbrace{a_a^\dagger a_i}^{=0} | \Phi_0 \rangle$$

$$+ \sum_{pq} \langle p|\hat f|q\rangle \langle c| \overbrace{a_p^\dagger \underbrace{a_q \, a_a^\dagger}_{\delta_{qa}} a_i}^{\delta_{pi}} |c\rangle$$

$$\Big(\langle i|f|a\rangle = \langle i|h_0|a\rangle + \sum_j \langle ij|v|aj\rangle_{AS}$$

$$+ \frac{1}{4} \sum_{pqrs} \langle pq|v|rs\rangle \langle c| a_p^\dagger \underbrace{a_q^\dagger a_s}_{=0} \underbrace{a_r \, a_a^\dagger}_{} a_i |c\rangle$$

$$= \langle i|f|a\rangle$$

$$\langle \Phi_0 | H | \Phi_{ij}^{ab} \rangle = \qquad \delta_{aj} \, \delta_{bj}$$

$$E_0^{Ref} \underbrace{\langle c| a_a^\dagger a_b^\dagger a_j a_i |c\rangle}_{=0}$$

δ_{pj}

$$+ \sum_{pq} \langle p|\hat{f}|q\rangle \langle c|a_p^+ \underbrace{a_q\, a_a^+}_{\delta_{qa}} a_r^+ \underbrace{a_j\, a_i}_{\delta_{ri}} |c\rangle \approx 0$$

$$+\frac{1}{4}\sum_{pqrs} \langle pq|\hat{v}|rs\rangle_{AS}$$

$$\langle c|a_p^+ a_q^+ a_s a_r \; a_a^+ a_b^+ a_j a_i \;|c\rangle$$

$$\langle ij|\hat{v}|ab\rangle_{AS}$$

δ_{pi} δ_{qj} δ_{ra} δ_{sb}

$$-\langle ji|\hat{v}|ab\rangle_{AS}$$
$$= \langle ij|\hat{v}|ab\rangle_{AS}$$

δ_{pi} δ_{qj} δ_{rb} δ_{sa}

$$+\langle ji|\hat{v}|ba\rangle_{AS}$$
$$= \langle ij|\hat{v}|ab\rangle_{AS}$$

δ_{pi} δ_{qj} δ_{ra} δ_{sb}

δ_{ra} δ_{sb}

δ_{pi} δ_{qj}

$$-\langle ij|\hat{v}|ba\rangle_{AS}$$

$$= \langle ij | \hat{v} | ab \rangle_{AS}$$

$$\Rightarrow$$

$$\langle \Phi_0 | H | \Phi_{ij}^{ab} \rangle = \langle ij | \hat{v} | ab \rangle_{AS}$$

$$\langle \Phi_0 | H | \Phi_{ijk}^{abc} \rangle$$

$$= \underbrace{\langle \Phi_0 | a_a^\dagger a_b^\dagger a_c^\dagger a_k a_j a_i | \Phi_0 \rangle}_{} \overset{=0}{} E_0^{Ref}$$

$$+ \langle \Phi_0 | a_p^\dagger a_q \, a_a^\dagger a_b^\dagger a_c^\dagger a_k a_j a_i | \Phi_0 \rangle \overset{=0}{}$$

$$+ \langle \Phi_0 | a_p^\dagger a_q^\dagger a_s a_r \, a_a^\dagger a_b^\dagger a_c^\dagger a_k a_j a_i | \Phi_0 \rangle$$

$$\langle \Phi_i^a | \qquad \langle \Phi_0 | a_i^\dagger a_a \overset{=0}{}$$

$$\langle \Phi_i^a | H | \Phi_j^b \rangle = \qquad \boxed{\begin{matrix} a \neq b \\ i \neq j \end{matrix}}$$

$$E_0^{Ref} \langle \Phi_0 | a_i^\dagger a_a \, a_b^\dagger a_j | \Phi_0 \rangle \overset{=0}{}$$

$$+ \langle \Phi_0 | a_i^\dagger a_a \, a_p^\dagger a_q \, a_b^\dagger a_j | \Phi_0 \rangle \overset{=0}{}$$

$$=0 \, .$$

δ_{ab}

$$+ \langle \Phi_c | a_i^\dagger a_a \, a_p^\dagger a_q^\dagger a_s \, a_r \, a_b^\dagger a_j | \Phi_c \rangle$$

$$\delta_{is} \, \delta_{ap} \, \delta_{qj} \, \delta_{rb} \; - \langle aj | v | bi \rangle_{AS}$$

$+ \; 3$ more contractions (show)

$$= \langle aj | v | ib \rangle_{AS}$$

$$\langle \Phi_i^a | H | \Phi_{jk}^{bc} \rangle = ?$$

(Shavitt + Bartlett, chap 3.8)