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Ex. 5

a.) $\psi_a = \sum_x C_{ax} \phi_x$

$$\langle \psi_b | \psi_a \rangle = \sum_{xv} (C_{bv})^* C_{ax} \phi_v^* \phi_x$$

Since $\langle \phi_v | \phi_x \rangle = \delta_{vx}$

$$\langle \psi_b | \psi_a \rangle = \sum_x C_{bx}^* C_{xa} = (C^* C)_{ab} = \delta_{ab} \text{ for}$$

a unitary matrix C

We can construct a slater determinant

$$\begin{pmatrix} \psi_a(x_1) & \psi_a(x_2) & \cdots & \\ \psi_b(x_1) & \psi_b(x_2) & & \vdots \\ \vdots & & \ddots & \\ & & & \psi_n(x_n) \end{pmatrix} = C \cdot \begin{pmatrix} \phi_1(x_1) & \phi_1(x_2) & \cdots \\ \phi_2(x_1) & \phi_2(x_2) & \cdots \\ \vdots & & \ddots \\ & & & \phi_n(x_n) \end{pmatrix}$$

$$\underline{\Psi} = C \underline{\Phi}$$

$$\det \Psi = \det(C \cdot \Phi) = \det[C] \cdot \det \Phi$$

for a unitary, i.e. square matrix C.

b.) $\Phi_0 = \prod_{i=1}^{n} a^\dagger_{a_i} |0\rangle$ Wick's thm says we only need to calculate all the permutations of the fully contracted term

$$\langle \Phi_0 | \Phi_0 \rangle = \langle 0 | a_{a_n} \cdots a_{a_2} a_{a_1} \cdots a^\dagger_{a_n} \cdots a^\dagger_{a_2} a^\dagger_{a_1} | 0 \rangle$$

$$= \sum_{\text{all contracted combinations}} (-)^P \text{ Product with all pairs contracted}$$

~~Ex. 5~~

$$\cancel{\psi_a = \begin{pmatrix} \psi_1(x_1) \\ \psi_2(x_2) \\ \vdots \\ \psi_a(x_1) \end{pmatrix} = \sum_x C_{ax} \phi_x}$$

Ex 5 cont.

$$\langle \phi_0 | \phi_0 \rangle = \delta_{a_n a_1} \delta_{a_{n-1} a_2} \cdots \delta_{a_{n-2} \alpha_2} \cdots \delta_{a_{(n/2)}} \delta_{a_{(n/2)}}$$

+ mixed terms

but this means only the first term survives since $\delta_{\alpha\beta} = \emptyset$ for $\alpha \neq \beta$ thus

$$\langle \phi_0 | \phi_0 \rangle = 1$$

Ex 6

$$\langle \alpha_1 \alpha_2 | \hat{F} | \alpha_1 \alpha_2 \rangle = \langle 0 | a_{\alpha_2} a_{\alpha_1} \sum_{\alpha\beta} \langle \alpha | f | \beta \rangle a_\alpha^\dagger a_\beta a_{\alpha_1}^\dagger a_{\alpha_2}^\dagger | 0 \rangle$$

$$= \sum_{\alpha\beta} \langle \alpha | f | \beta \rangle \langle 0 | a_{\alpha_2} a_{\alpha_1} a_\alpha^\dagger a_\beta a_{\alpha_1}^\dagger a_{\alpha_2}^\dagger | 0 \rangle$$

$$\delta_{\alpha_2\alpha}\, \delta_{\alpha_1}\delta_{\alpha_1}\, \delta_{\beta\alpha_2}$$

$$-\delta_{\alpha_2\alpha}\, \delta_{\alpha_1\alpha_2}\, \delta_{\alpha_1\beta}$$

$$-\delta_{\alpha_2\alpha_1}\, \delta_{\alpha_1\alpha}\, \delta_{\beta\alpha_2}$$

$$\delta_{\alpha_2\alpha_2}\, \delta_{\alpha_1\alpha}\, \delta_{\beta\alpha_1}$$

$$= \langle \alpha_2 | f | \alpha_2 \rangle \langle \alpha_1 | \alpha_1 \rangle + \langle \alpha_2 | \alpha_2 \rangle \langle \alpha_1 | f | \alpha_1 \rangle$$

$$- \cancel{\langle \alpha_1 | \alpha_2 \rangle}^{\,0} \langle \alpha_2 | f | \alpha_1 \rangle$$

$$- \cancel{\langle \alpha_2 | \alpha_1 \rangle}^{\,0} \langle \alpha_1 | f | \alpha_2 \rangle$$

$$\langle \alpha_1 \alpha_2 | \hat{G} | \alpha_1 \alpha_2 \rangle = \langle 0 | a_{\alpha_2} a_{\alpha_1} a_\alpha^\dagger a_\beta^\dagger a_\delta a_\gamma a_{\alpha_2}^\dagger a_{\alpha_1}^\dagger | 0 \rangle$$

$$\times \sum_{\alpha\beta\gamma\delta} \langle \alpha\beta | \hat{g} | \gamma\delta \rangle$$

$$a_{\alpha_2} a_{\alpha_1} a_\alpha^\dagger a_\beta^\dagger a_\delta a_\gamma a_{\alpha_2}^\dagger a_{\alpha_1}^\dagger$$

$$\delta_{\alpha_2\alpha}\, \delta_{\alpha_1\beta}\, \delta_{\delta\alpha_2}\, \delta_{\gamma\alpha_1}$$

$$-\delta_{\alpha_2\alpha}\, \delta_{\alpha_1\beta}\, \delta_{\delta\alpha_1}\, \delta_{\gamma\alpha_2}$$

$$\delta_{\alpha_2\beta}\, \delta_{\alpha_1\alpha}\, \delta_{\delta\alpha_1}\, \delta_{\gamma\alpha_2}$$

$$-\delta_{\alpha_2\beta}\, \delta_{\alpha_1\alpha}\, \delta_{\delta\alpha_2}\, \delta_{\gamma\alpha_1}$$

$$= \langle \alpha_2 \alpha_1 | \hat{g} | \alpha_1 \alpha_2 \rangle - \langle \alpha_2 \alpha_1 | \hat{g} | \alpha_2 \alpha_1 \rangle$$

$$\langle \alpha_1 \alpha_2 | \hat{g} | \alpha_2 \alpha_1 \rangle - \langle \alpha_1 \alpha_2 | \hat{g} | \alpha_1 \alpha_2 \rangle$$

I get minus signs for the direct term I think this is because $\hat{G}$ was ~~…~~ written ~~…~~ almost in anti-symmetric term

Ex. 6 cont,

I think $G = \frac{1}{2} \sum_{\alpha\beta\gamma\delta} \langle \alpha\beta | \hat{g} | \gamma\delta \rangle a_\alpha^\dagger a_\beta^\dagger a_\gamma a_\delta$

and not $G = \frac{1}{2} \sum_{\alpha\beta\gamma\delta} \langle \alpha\beta | \hat{g} | \gamma\delta \rangle a_\alpha^\dagger a_\beta^\dagger a_\delta a_\gamma$

this accounts for the minus signs.

Ex. 7

Previously $\overline{a_p a_q^\dagger} = \delta_{pq}$ $\quad \overline{a_p^\dagger a_q} = 0$ in true vacuum

Now in new ref. vacuum $\overline{a_p a_q^\dagger} = \delta_{pq}$ $\quad \overline{a_p^\dagger a_q} = \delta_{pq}$

if $p \in abc$ particle states $\quad p \in ijk$ hole states

we can represent any operator as all permutations of its contractions.

$$\hat{H}_0 = \sum_{pq} \langle p | \hat{h}_0 | q \rangle a_p^\dagger a_q$$

where

$$a_p^\dagger a_q = \{a_p^\dagger a_q\} + \{\overline{a_p^\dagger a_q}\}$$

$$= \{a_p^\dagger a_q\} + \underset{p\in i}{\delta_{pq}}.$$

thus

$$\hat{H}_0 = \sum_{pq} \langle p | \hat{h}_0 | q \rangle \left(\{a_p^\dagger a_q\} + \underset{p\in i}{\delta_{pq}} \right)$$

$$= \sum_{pq} \langle p | \hat{h}_0 | q \rangle \{a_p^\dagger a_q\} + \underset{p\in i}{\delta_{pq}} \sum_{pq} \langle p | \hat{h}_0 | q \rangle$$

$$= \sum_{pq} \langle p | \hat{h}_0 | q \rangle \{a_p^\dagger a_q\} + \sum_i \langle i | \hat{h}_0 | i \rangle$$

$\{\ \}$ - represents normal ordering

i - is a hole state

This is in the NEW ref. vacuum

Ex. 8

As in Ex 7. we can represent a string of anilhiation & creation operators as a normal ordered string and all permutations of 1, 2, 3, ... contracted pairs up to the fully contracted string.

$$\hat{H}_1 = \frac{1}{4}\sum_{pqrs} \langle pq|\hat{v}|rs\rangle_{AS} a_p^{\dagger} a_q^{\dagger} a_s a_r$$

$$a_p^{\dagger} a_q^{\dagger} a_s a_r = \{a_p^{\dagger} a_q^{\dagger} a_s a_r\} + \{a_p^{\dagger} a_q^{\dagger} a_s a_r\}$$
$$+ \{a_p^{\dagger} a_q^{\dagger} a_s a_r\} + \{a_p^{\dagger} a_q^{\dagger} a_s a_r\}$$
$$+ \{a_p^{\dagger} a_q^{\dagger} a_s a_r\}$$
$$+ \{a_p^{\dagger} a_q^{\dagger} a_s a_r\} + \{a_p^{\dagger} a_q^{\dagger} a_s a_r\}$$

$$= \{a_p^{\dagger} a_q^{\dagger} a_s a_r\} + \delta_{pr\epsilon i}\{a_q^{\dagger} a_s\} - \delta_{qr\epsilon i}\{a_p^{\dagger} a_s\}$$
$$+ \delta_{qs\epsilon i}\{a_p^{\dagger} a_r\} - \delta_{ps\epsilon i}\{a_q^{\dagger} a_r\}$$
$$+ \delta_{pr\epsilon i}\delta_{qs\epsilon i} - \delta_{ps\epsilon i}\delta_{qr\epsilon i}$$

Since pqrs are dummy variables we sum over. We can rename these. ~~begins~~ The single contractions leave just two dummy variables.

$$\langle pi|\hat{v}|ri\rangle_{AS}\{a_p^{\dagger} a_r\} - \langle pi|v|is\rangle_{AS}\{a_p^{\dagger} a_s\}$$
$$- \langle iq|v|ri\rangle_{AS}\{a_q^{\dagger} a_r\} + \langle iq|v|is\rangle\{a_q^{\dagger} a_s\}$$

$$= 4\langle pi|\hat{v}|qi\rangle\{a_p^{\dagger} a_q\}$$

~~These~~ Using the properties of the A.S. matrix elements these four terms are equal.

By similar argument the 2-contracted arguments give.

$$\langle ij|v|ij\rangle_{AS} - \langle ji|v|ij\rangle_{AS} = 2\langle ij|v|ij\rangle_{AS}$$

thus $$\hat{H}_1 = \frac{1}{4}\sum_{pqrs} \langle pq|\hat{v}|rs\rangle_{AS}\{a_p^\dagger a_q^\dagger a_s a_r\} + \frac{4}{4}\sum_{pqi} \langle pi|\hat{v}|qi\rangle_{AS}\{a_p^\dagger a_q\}$$

$$+ \frac{2}{4}\sum_{ij} \langle ij|\hat{v}|ij\rangle_{AS}$$