FYS4480 September 16

Wick's theorem:
chain of operators

$$XYZ\cdots W = N[XYZ\cdots W]$$

$$+ \sum_{(1)} N[XYZ\cdots W]$$

$$+ \sum_{(2)} N[XYZ\cdots W] + \cdots +$$

$$+ \sum_{(\frac{N}{2})} N[XYZ\cdots W]$$

$$= \sum_{[\frac{N}{2}]} N[XYZ\cdots W]$$

Wick's generalized theorem
an arbitrary product of
creation and annihilation
operators in which the
operators are given in terms
of strings of normal-ordered

operators is given

$$N[A_1 A_2 \ldots A_m]\, N[B_1 B_2 \ldots B_n]\, N[C_1 C_2 \ldots C_p]$$

$$= N[A_1 A_2 \ldots A_m B_1 B_2 \ldots B_n C_1 C_2 \ldots C_p]$$

$$+ \sum_{All} N[A_1 A_2 \ldots B_1 B_2 \ldots C_1 C_2 \ldots]$$

→ contractions run only over contractions between operators from different normal-ordered products

<u>Example</u>

$$\langle \alpha_1 \alpha_2 | H_0 | \alpha_1 \alpha_2 \rangle$$

$$H_0 = \sum_{\alpha\beta} \langle \alpha | h_0 | \beta \rangle a_\alpha^\dagger a_\beta$$

$$= \sum_{\alpha\beta} \langle \alpha | h_0 | \beta \rangle N[a_\alpha^\dagger a_\beta]$$

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

$$\langle \alpha_1 \alpha_2 | = \langle 0 | a_{\alpha_2} a_{\alpha_1}$$

$$\langle \alpha_1 \alpha_2 | H_0 | \alpha_1 \alpha_2 \rangle =$$

$$\sum_{\alpha\beta} \langle 0 | N[a_{\alpha_2} a_{\alpha_1}] \, N[a^\dagger_\alpha a_\beta] \, N[a^\dagger_{\alpha_1} a^\dagger_{\alpha_2}]$$

$$\times |0\rangle \quad \langle \alpha | h_0 | \beta \rangle$$

$$a_{\alpha_2} a_{\alpha_1} \; a^\dagger_\alpha a_\beta \; a^\dagger_{\alpha_1} a^\dagger_{\alpha_2}$$

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

$$a^\dagger_\alpha a_\beta = 0 = a_\alpha a_\beta = a^\dagger_\alpha a^\dagger_\beta$$

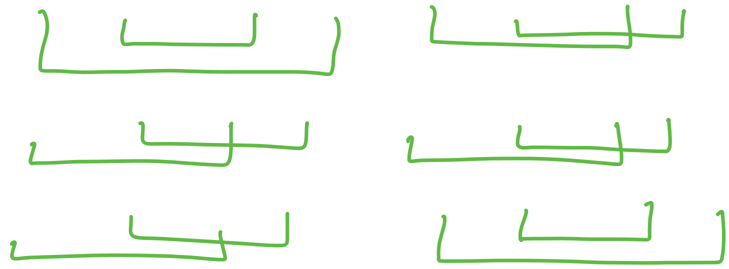
Example

$$|\Phi_0\rangle = a_1^\dagger a_2^\dagger a_3^\dagger a_4^\dagger |0\rangle$$

$$H_I = \frac{1}{2} \sum_{\alpha\beta\gamma\delta} \langle \alpha\beta | v | \gamma\delta \rangle a^\dagger_\alpha a^\dagger_\beta a_\delta a_\gamma$$

$$\langle \Phi_0 | H_1 | \Phi_0 \rangle \quad \propto$$

$$a_4 \, a_3 \, a_2 \, a_1 \; a^\dagger_\alpha a^\dagger_\beta a_\delta a_\gamma \; a^\dagger_1 a^\dagger_2 a^\dagger_3 a^\dagger_4$$



acting on $a_1^+ a_2^+$ gives –

$$\langle 12|v|12\rangle - \langle 21|v|12\rangle$$

repeat with the H_1 $a_1^+ a_3^+$

— " — — $a_1^+ a_4^+$

— " — $a_2^+ a_3^+$

— " — $a_2^+ a_4^+$

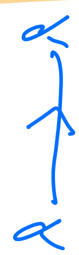
— " — $a_3^+ a_4^+$ $\Rightarrow$

$$\langle \Phi_0|H_1|\Phi_0\rangle = \sum_{i<j=1}^{4} \left[\langle ij|v|ij\rangle - \langle ij|v|ji\rangle\right]$$

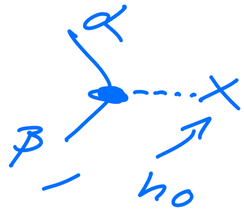
$$\langle \Phi_i|H_1|\Phi_j\rangle$$

Diagrammatic representation

(i) $\overline{a_\alpha a_\alpha^+}$ =

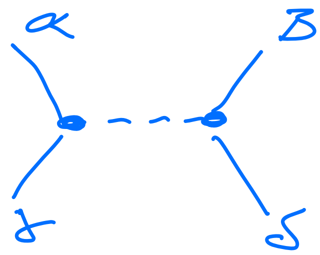


(ii) $\sum_{\alpha\beta} \langle \alpha | h_0 | \beta \rangle a_\alpha^\dagger a_\beta =$



(iii) $\sum_{\alpha\beta\gamma\delta} \langle \alpha\beta | O_2 | \gamma\delta \rangle a_\alpha^\dagger a_\beta^\dagger a_\delta a_\gamma$

$=$



(iv) "Time" upwards

$\langle \;|$ over the operator line

one-body

two-body

$| \;\rangle$ below the operator line.

Example

$$\langle \alpha_1 \alpha_2 | H_1 | \beta_1 \beta_2 \rangle =$$

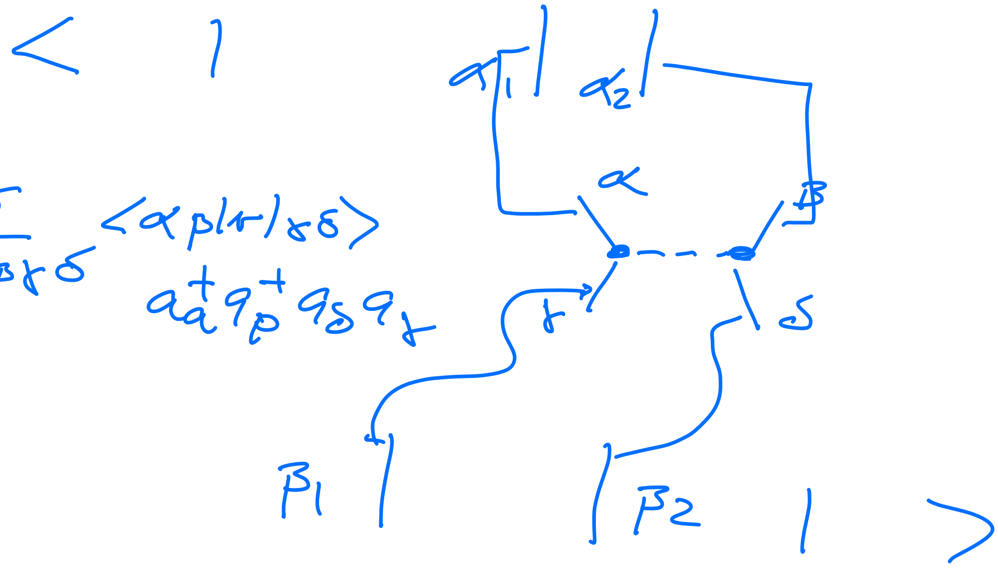
$$\frac{1}{2} \Big[\langle \alpha_1 \alpha_2 | v | \beta_1 \beta_2 \rangle - \langle \alpha_2 \alpha_1 | v | \beta_1 \beta_2 \rangle$$

$$- \langle \alpha_1 \alpha_2 | v | \beta_2 \beta_1 \rangle$$

$$+ \langle \alpha_2 \alpha_1 | v | \beta_2 \beta_1 \rangle \Big]$$

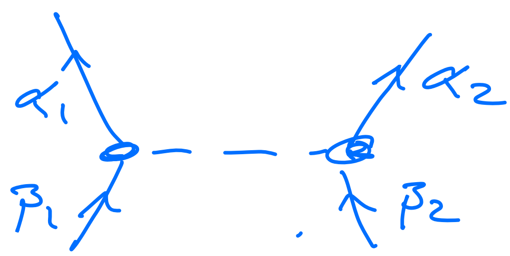
Diagrammatically

$$\sum_{\alpha\beta\gamma\delta} \langle \alpha\beta | v | \gamma\delta \rangle \, a^\dagger_\alpha a^\dagger_\beta a_\delta a_\gamma$$



$$a_{\alpha_2} a_{\alpha_1} a^\dagger_\alpha a^\dagger_\beta a_\delta a_\gamma a^\dagger_{\beta_1} a^\dagger_{\beta_2}$$

$$\overbrace{a_{\alpha_1} a^\dagger_\alpha}$$

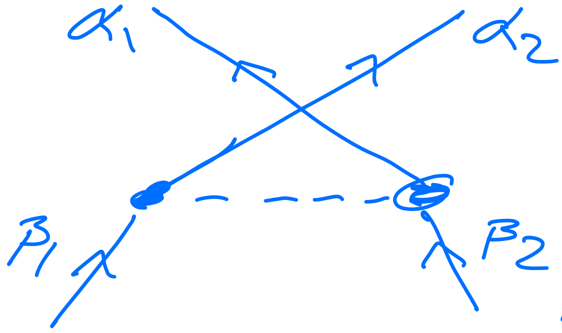


left out, right out

$$= \langle \alpha_1 \alpha_2 | v | \beta_1 \beta_2 \rangle$$

left in, right in

$$a_{\alpha_2} a_{\alpha_1} a^\dagger_\alpha a^\dagger_\beta a_\delta a_\gamma a^\dagger_{\beta_1} a^\dagger_{\beta_2}$$

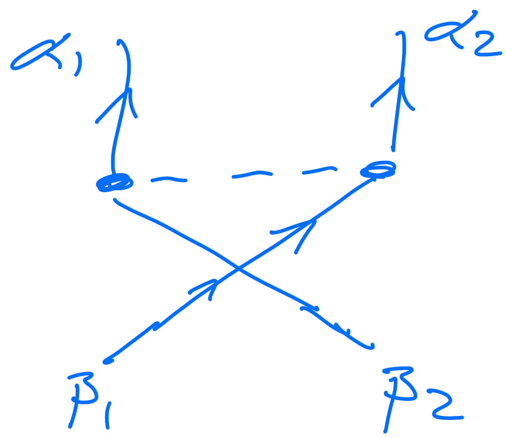


$$-\langle \alpha_2 \alpha_1 | v | \overbrace{\beta_1 \beta_2}^{\text{incoming}} \rangle$$

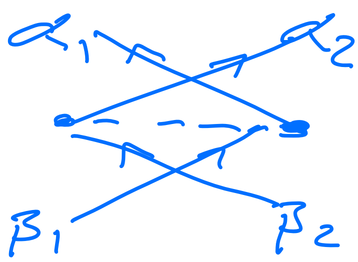
leftout left right

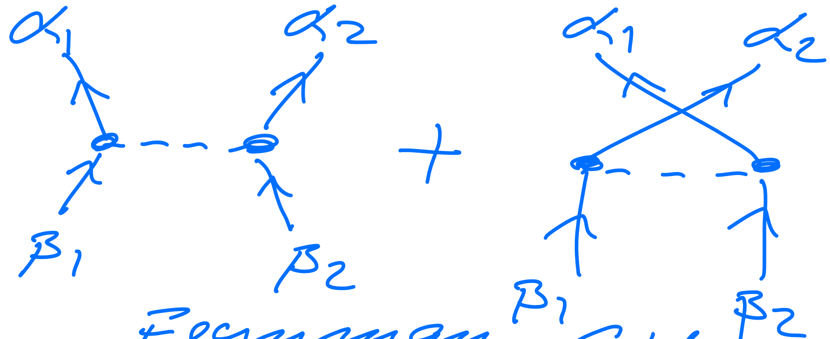
right out

$$-\langle \alpha_1 \alpha_2 | v | \beta_2 \beta_1 \rangle$$



$$\langle \alpha_2 \alpha_1 | v | \beta_2 \beta_1 \rangle$$



$$= \quad$$ 

Feynman – Goldstone

$$\langle \alpha_1 \alpha_2 | v | \beta_1 \beta_2 \rangle - \langle \alpha_2 \alpha_1 | v | \beta_1 \beta_2 \rangle$$

$$=$$ 

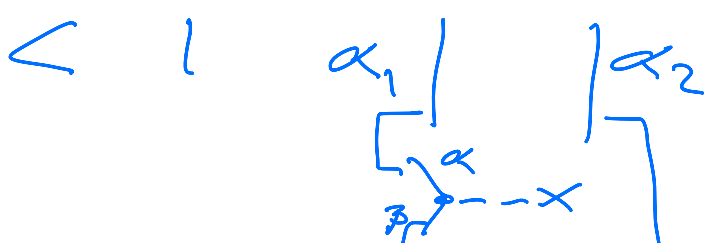
Hugenholtz diagram

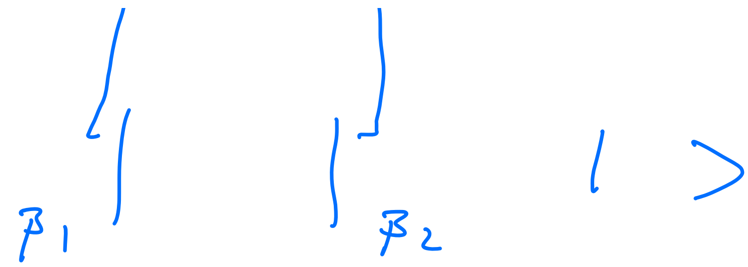
Example

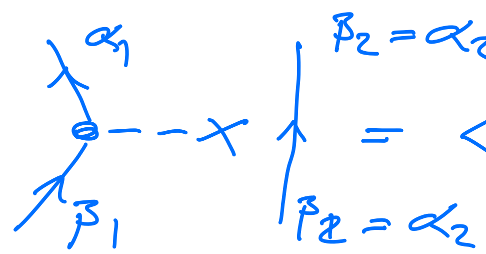
$$\hat{O}_1 = \sum_{\alpha\beta} \langle \alpha | \hat{o}_1 | \beta \rangle a^\dagger_\alpha a_\beta$$

$$\langle \alpha_1 \alpha_2 | \hat{O}_1 | \beta_1 \beta_2 \rangle$$

$$a_{\alpha_2} a_{\alpha_1} a^\dagger_\alpha a_\beta a^\dagger_{\beta_1} a^\dagger_{\beta_2} \qquad \delta_{\alpha_2 \beta_2}$$



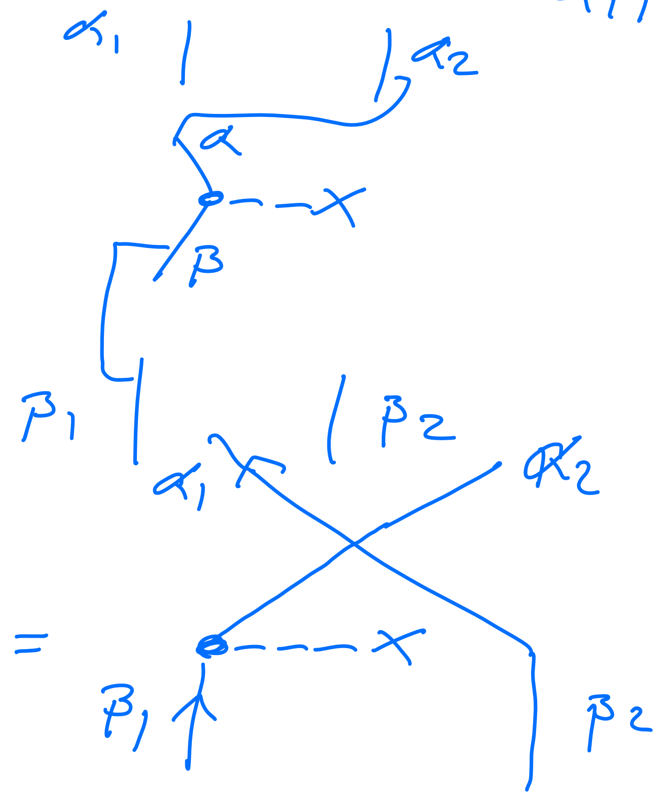


$=$ 

$= \langle \alpha_1 | O_1 | \beta_1 \rangle \, \delta_{\beta_2 \alpha_2}$

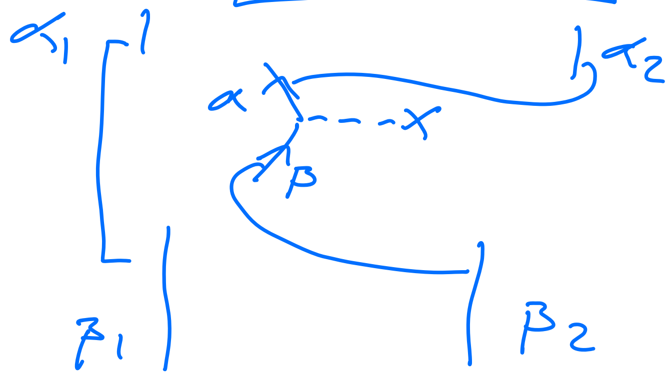
$$a_{\alpha_2} a_{\alpha_1} a^{\dagger}_{\alpha} a_{\beta} a^{\dagger}_{\beta_1} a^{\dagger}_{\beta_2}$$

$- \langle \alpha_2 | O_1 | \beta_1 \rangle \, \delta_{\alpha_1 \beta_2}$



$= - \langle \alpha_2 | O_1 | \beta_1 \rangle \, \delta_{\beta_2 \alpha_1}$

$$a_{\alpha_2} a_{\alpha_1} a_\alpha^\dagger a_\beta a_{\beta_1}^\dagger a_{\beta_2}^\dagger$$



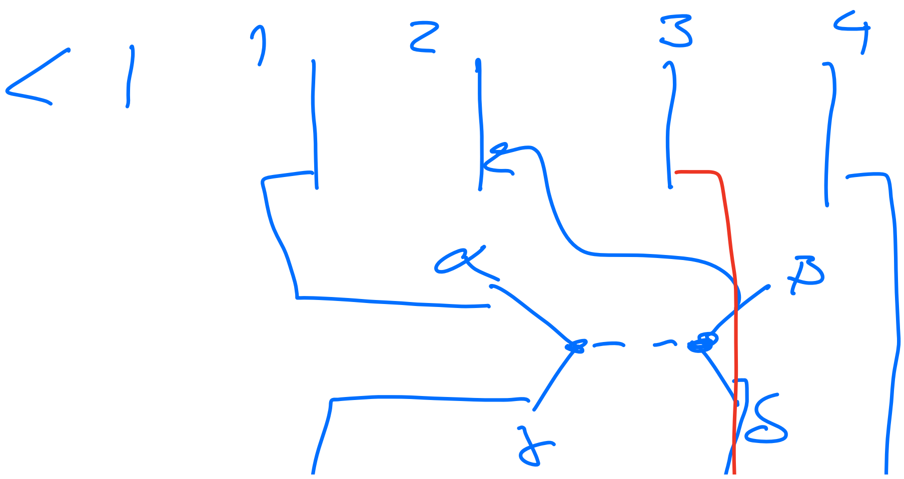
$$= \delta_{\alpha_1 \beta_1} \times \langle \alpha_2 | g | \beta_2 \rangle$$

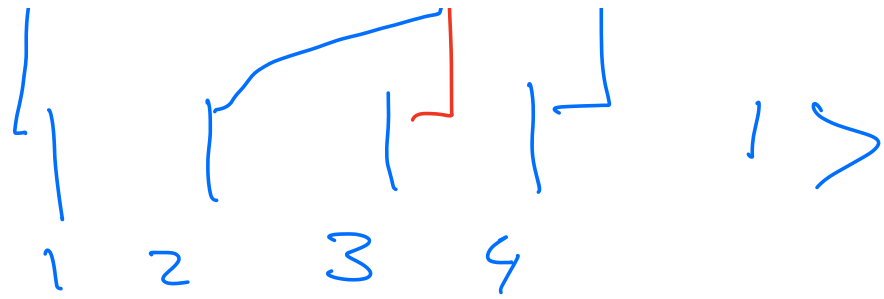
$$a_{\alpha_2} a_{\alpha_1} a_\alpha^\dagger a_\beta a_{\beta_1}^\dagger a_{\beta_2}^\dagger$$

Example

$$|\Phi_0\rangle = a_1^\dagger a_2^\dagger a_3^\dagger a_4^\dagger |0\rangle$$

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





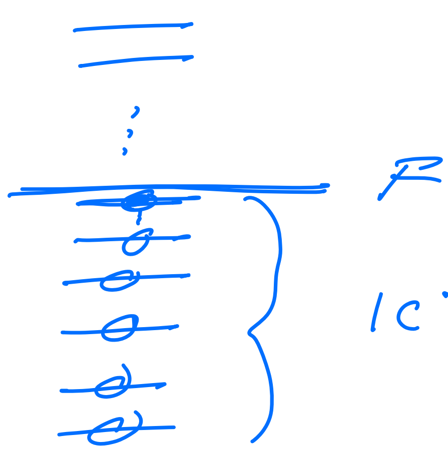
$\langle 12|v|12\rangle \, \delta_{33} \, \delta_{44}$

Can we simplify this?

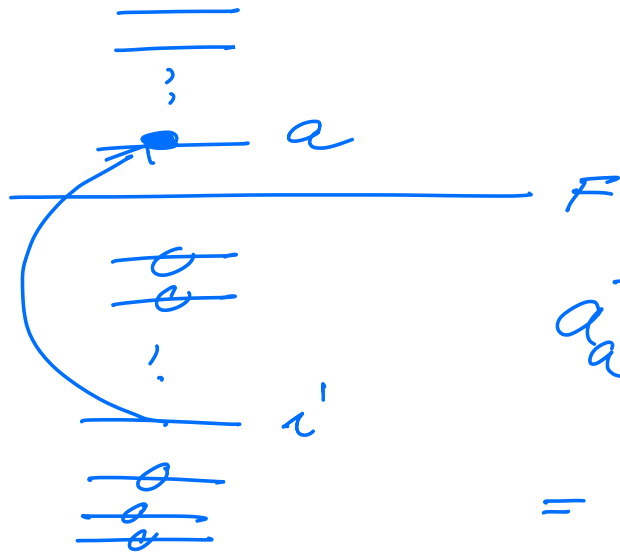
Yes $\rightarrow$ redefinition of $|0\rangle \rightarrow |c\rangle$, particle-hole formalism,

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

For Fermions we can use the Fermi level to define an ansatz for $|c\rangle$



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

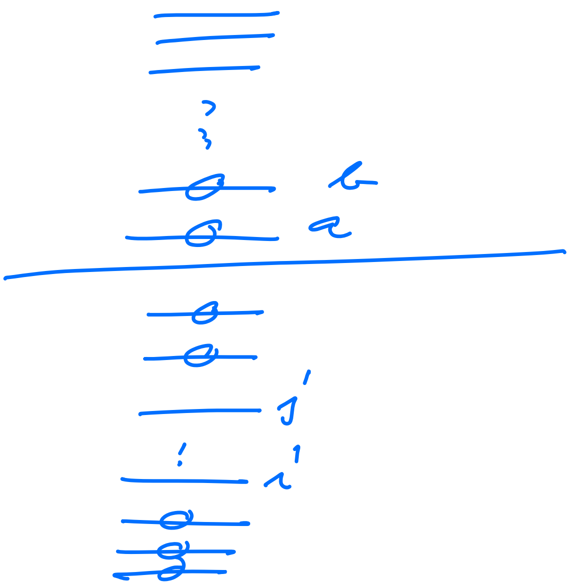


$a_a^\dagger a_i |\Phi_0\rangle$

$= |\Phi_i^a\rangle$

one-particle one-hole state

1p1h



$a_a^\dagger a_b^\dagger a_j a_i |\Phi_0\rangle$

$= |\Phi_{ij}^{ab}\rangle$

2p2h = two-particle-two-hole

with N particles, we can make up to

NpNh excitations

Redefinition of operators:

$$H_0 = \sum_{pq} \langle p | h_0 | q \rangle a_p^\dagger a_q$$

(pq are all types of single particle orbits)

$$+ \boxed{\sum_{i \le F} \langle i | h_0 | i \rangle}$$

$ijkl \ldots \le F$

$$H_I = \frac{1}{4} \sum_{pqst} \langle pq | v | st \rangle_{AS} a_p^\dagger a_q^\dagger a_t a_s$$

$$+ \sum_{pqi} a_p^\dagger a_q \langle pi | v | qi \rangle_{AS}$$

$$+ \boxed{\frac{1}{2} \sum_{ij \le F} \langle ij | v | ij \rangle_{AS}}$$

$$E_{Ref} = \langle \Phi_0 | H | \Phi_0 \rangle = \langle c | H | c \rangle$$

= Reference energy

$$= \sum_{i \le F} \langle i | h_0 | i \rangle + \frac{1}{2} \sum_{ij \le F} \langle ij | v | ij \rangle_{AS}$$