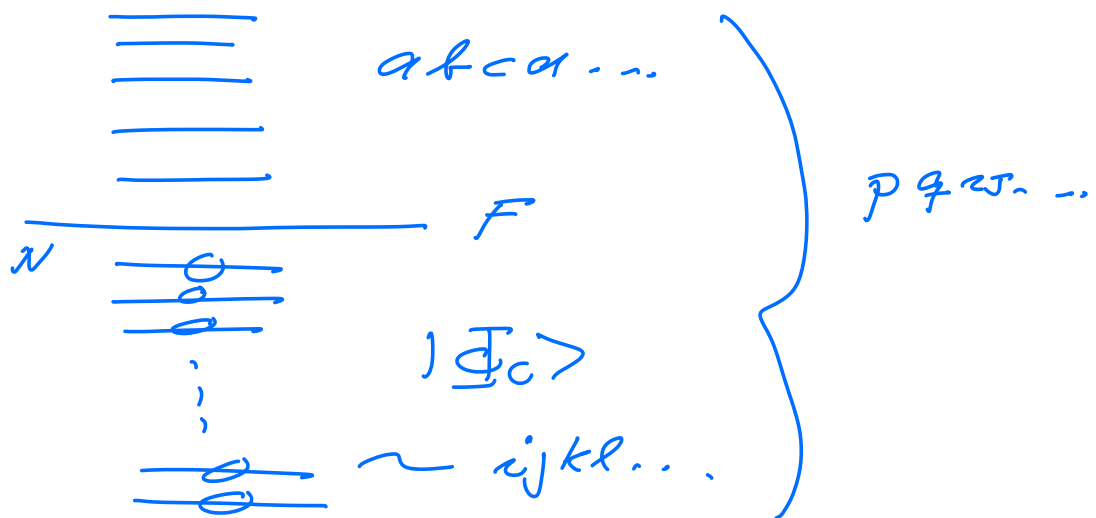


FYS4480 Sept 29, 2022

New vacuum state

$|c\rangle = |\Phi_0\rangle$ N-body state



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

$$+ \frac{1}{4} \sum_{p,q,r,s} \langle p q | \hat{v} | r s \rangle_{AS} \times \{a_p^\dagger a_q^\dagger a_s a_r\}$$

$$+ E_0^{ref}$$

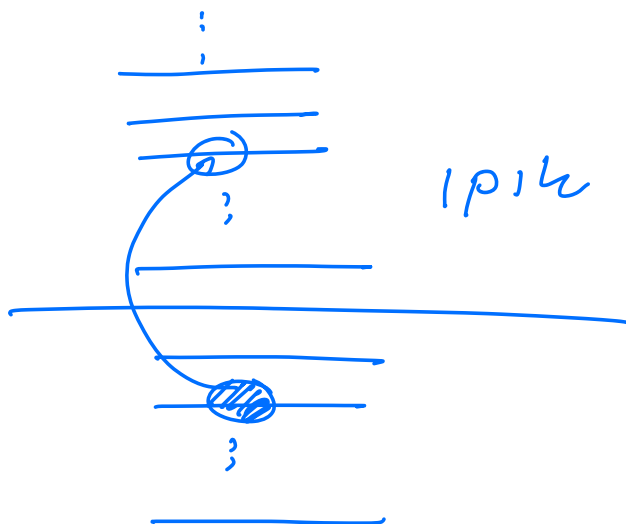
$$= \hat{F}_N + \hat{V}_N + E_0^{ref},$$

$$E_0^{ref} = \sum_i \langle i | \hat{h}_0 | i \rangle + \frac{1}{2} \sum_{ij} \langle ij | \hat{v} | ij \rangle_{AS}$$

$$= \langle \Phi_0 | H | \Phi_0 \rangle$$

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

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



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

⋮

$$|\Phi_{i_1, i_2, \dots, i_N}^{a_1, a_2, \dots, a_N}\rangle = a_{a_1}^\dagger a_{a_2}^\dagger \dots a_{a_N}^\dagger a_{i_N} a_{i_{N-1}} \dots a_{i_1} \times |\Phi_0\rangle$$

NPNH

Ground state :

$$|\psi_0\rangle = \sum_j c_{j0} |\Phi_j\rangle$$

$$c_{j0} = \langle \psi_0 | \Phi_j \rangle$$

$$\langle \Phi_0 | H | \Phi_n^a \rangle = \langle i | \hat{f} | a \rangle$$

$$\begin{aligned} \langle \Phi_n^a | H | \Phi_n^a \rangle &= \langle a | \hat{f} | a \rangle \\ &\quad - \langle i | \hat{f} | i \rangle \\ &\quad + E_0^{\text{Ref}}. \end{aligned}$$

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

Diagrammatic representation

vacuum $|0\rangle$

$$\overbrace{a_p a_q^\dagger}^+ = \delta_{pq} \quad \text{only non-zero}$$

$$\begin{array}{|c|} \hline p \\ \hline \\ \hline q \\ \hline \end{array} = \begin{array}{|c|} \hline \Delta \\ \hline \end{array} \Rightarrow \sqrt{p q}^+$$

$$\hat{h}_0 \rightarrow \begin{array}{|c|} \hline p \\ \hline \\ \hline q \\ \hline \end{array} \cdots x$$

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

$$\begin{array}{|c|} \hline a_1 \\ \hline \\ \hline p \\ \hline \\ \hline q \\ \hline \\ \hline a_1 \\ \hline \end{array} \begin{array}{|c|} \hline a_2 \\ \hline \\ \hline \\ \hline \\ \hline q_2 \\ \hline \end{array} \cdots x \rightarrow \begin{array}{|c|} \hline a_1 \\ \hline \\ \hline \\ \hline a_1 \\ \hline \end{array} \cdots x$$

$$\langle a_1 | \hat{h}_0 | a_1 \rangle$$

$$H_I = \frac{1}{g} \sum_{a_1 a_2} a_p^\dagger a_q^\dagger a_s a_r \langle pq | \hat{V} | rs \rangle_{AS}$$

$$\begin{array}{|c|} \hline a_1 \\ \hline \\ \hline p \\ \hline \\ \hline r_2 \\ \hline \\ \hline a_1 \\ \hline \end{array} \begin{array}{|c|} \hline a_2 \\ \hline \\ \hline q \\ \hline \\ \hline s \\ \hline \\ \hline a_2 \\ \hline \end{array} \cdots x + \begin{array}{|c|} \hline \\ \hline \\ \hline \\ \hline \end{array}$$

$$= \begin{array}{c} q_1 \quad q_2 \\ \diagdown \quad \diagup \\ \circ \quad \circ \\ \diagup \quad \diagdown \\ q_1 \quad q_2 \end{array} + \begin{array}{c} q_1 \quad q_2 \\ \diagdown \quad \diagup \\ \circ \quad \circ \\ \diagup \quad \diagdown \\ q_2 \quad q_1 \end{array}$$

$$\langle q_1, q_2 | \hat{r} | q_1, q_2 \rangle - \langle q_2, q_1 | \hat{r} | q_1, q_2 \rangle$$

Now

$$\overbrace{a_b a_a}^+ = \begin{array}{c} \uparrow b \\ \downarrow a \end{array} = \begin{array}{c} a \\ \uparrow \\ a \end{array} = \delta_{ab}$$

$$\overbrace{a_i a_j}^+ = \begin{array}{c} \uparrow j \\ \downarrow i \end{array} = \begin{array}{c} i \\ \uparrow \\ i \end{array} = \delta_{i,j}$$

$$\langle \Phi_0 | H | \Phi_n^q \rangle = 0$$

$$\langle \Phi_0 | \overbrace{a_p^\dagger a_q^\dagger a_a^\dagger a_i} | \Phi_0 \rangle$$

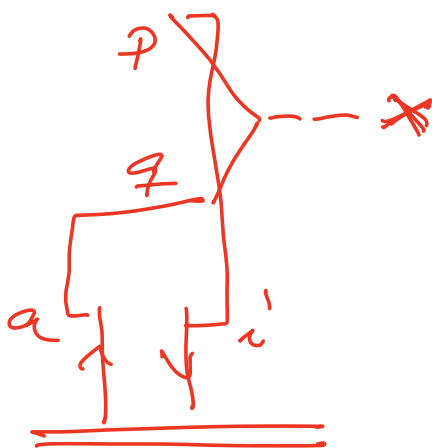
$$+ \langle \Phi_0 | \underbrace{a_p^\dagger a_q^\dagger}_{=0} \overbrace{a_j a_2 a_a^\dagger a_i} | \Phi_0 \rangle$$

$$\langle \Phi_0 |$$



$$a \uparrow \downarrow | \Phi_0 \rangle$$

(Shavitt & Bartlett)



$$= \langle i | \hat{g} | a \rangle$$

$$= i \uparrow \downarrow a$$

$$\left(\begin{matrix} x i \\ a \end{matrix} \right) \text{---} x$$

$$\hat{F} = \sum_{pq} \langle p | h_0 | q \rangle \hat{a}_p^\dagger \hat{a}_q$$

$$\begin{aligned}
 & + \sum_{p q i} \langle p i | \vec{U} | q i \rangle_{AS} q_p^\dagger q_q \\
 & \sum_{p q} \text{diagram} \equiv \text{diagram} \\
 & \sum_i \text{diagram} = \text{diagram} \\
 & \sum_{i q} \text{diagram} = \text{diagram}
 \end{aligned}$$

The diagrams are Feynman diagrams representing various terms in a quantum field theory calculation. They involve fermion lines (solid), boson lines (dashed), and interaction vertices (crosses or loops).

$$\langle \Phi_0 | \equiv \equiv$$

$$\begin{aligned}
 & \text{diagram} = \text{diagram} \\
 & \text{diagram} \quad | \Phi_0
 \end{aligned}$$

$$\langle i | f^\dagger | a \rangle = \text{diagram}$$

$$+ i' \nearrow \overline{a} \circ j' + i' \nearrow \overline{a} \circ j'$$

$$i' \nearrow \overline{a} \circ j' \quad \text{and} \quad \text{red diagram}$$

$$\langle \Phi_0 | H | \Phi_y^{av} \rangle = \langle i' j' | \sigma | ab \rangle_{AS}$$

$$\text{Diagram with labels } p, q, r, s, a, i', j'$$

$$\text{2pe4} \\ = \overline{i'} \nearrow \overline{a} \circ \overline{j'} \nearrow \overline{a} \\ = \langle i' j' | \sigma | ab \rangle$$

$$\langle \Phi_0 | H | \Phi_0 \rangle = E_0^{Ref}$$

$$= \sum_i \langle i' | G_0 | i \rangle$$

$$+ \frac{1}{2} \sum_{i' j'} \{ \langle i' j' | \sigma | i j \rangle - \langle j i | \sigma | i' j' \rangle \}$$

$$\begin{aligned}
& \sum_i \left[\begin{array}{c} i' \downarrow \\ \uparrow i \end{array} \right] \text{---} x \quad \left(\begin{array}{c} i' \downarrow \\ \uparrow i \end{array} \right) \text{---} x \\
& = i' \bigcirc \text{---} x \\
& \sum_{i'j'} \left[\begin{array}{c} i' \downarrow \\ \uparrow i' \end{array} \text{---} \begin{array}{c} \downarrow j \\ \uparrow j' \end{array} + \begin{array}{c} i' \downarrow \\ \uparrow i' \end{array} \text{---} \begin{array}{c} \downarrow j' \\ \uparrow j \end{array} \right] \\
& i' \bigcirc \text{---} \bigcirc j' + \begin{array}{c} \text{---} j' \\ \text{---} j \end{array} \\
& = i' \bigcirc \bullet \bigcirc j' \\
& \quad m_2 + m_2 \\
& (-1) \\
& \bigcirc \text{---} \bigcirc
\end{aligned}$$

FCI = Full configuration interaction theory.

$$|\Phi_c\rangle = \prod_{i=1}^N a_i^\dagger |0\rangle$$

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

$$\langle \Phi_i^a | \Phi_j^b \rangle = \delta_{ab} \delta_{i,j}$$

General states $|\Phi_\alpha\rangle, |\Phi_\lambda\rangle$

$$\langle \Phi_\lambda | \Phi_\alpha \rangle = \delta_{\lambda\alpha}$$

$$|\psi_0\rangle = \sum_\lambda C_{\lambda 0} |\Phi_\lambda\rangle$$

$$= \underbrace{C_{00}}_{C_0} |\Phi_0\rangle + \sum_{a,i} C_i^a |\Phi_i^a\rangle$$

$$+ \sum_{\substack{a,b \\ i,j}} C_{ij}^{ab} |\Phi_{ij}^{ab}\rangle + \dots$$

$$\sum_{\substack{a_1, a_2, \dots, a_N \\ i_1, i_2, \dots, i_N}} C_{i_1, i_2, \dots, i_N}^{a_1, a_2, \dots, a_N} |\Phi_{i_1, \dots, i_N}^{a_1, \dots, a_N}\rangle$$

$$= (C_0 + \hat{C}) |\Phi_0\rangle$$

$$\sum_{a,i} C_i^a |\Phi_i^a\rangle = \sum_{a,i} C_i^a a_a^\dagger a_i |\Phi_0\rangle$$

\hat{C} = correlation operator,

$$|\psi_0\rangle = \sum_{PH} c_H^P |\Phi_H^P\rangle$$

$$E = \langle \psi_0 | \hat{H} | \psi_0 \rangle$$

$$= \sum_{\substack{PH \\ P'H'}} (c_H^P)^* c_{H'}^{P'} \langle \Phi_H^P | \hat{H} | \Phi_{H'}^{P'} \rangle$$

$$E = \frac{\langle \psi_0 | \hat{H} | \psi_0 \rangle}{\langle \psi_0 | \psi_0 \rangle}$$

$$\frac{\partial E}{\partial (c_H^P)^*} = 0$$

$$\sum_{P'H'} \left[\langle \Phi_H^P | \hat{H} | \Phi_{H'}^{P'} \rangle c_{H'}^{P'} - E c_{H'}^{P'} \langle \Phi_H^P | \Phi_{H'}^{P'} \rangle \right] = 0$$

$$(PH) \rightarrow i \quad (P'H') \rightarrow j$$

$$\langle \Phi_H^P | \hat{H} | \Phi_{H'}^{P'} \rangle = H_{ij'}$$

$$C_{H'}^{P'} \rightarrow C_j$$

$$\langle \Phi_{H'}^{P'} | \Phi_H^P \rangle = S_{ij'}$$

$$\frac{\partial E}{\partial C_i^*} = \sum_{j'} C_j (H_{ij'} - E S_{ij'}) = 0$$

$$S_{ij'} = S_{i'j'}$$

$$\sum_j C_j H_{ij'} = C_i E$$

$$HC = EC$$

$$\begin{array}{ccccccc} \text{0p1h} & \text{1p1h} & \text{2p2h} & & \text{npnh} \\ |\Phi_0\rangle & |\Phi_n^a\rangle & |\Phi_{ij}^{ab}\rangle & \dots & |\Phi_{i'j'}^{ab\dots}\rangle \end{array}$$

$$\begin{array}{l} \langle \Phi_0 | \\ \langle \Phi_n^a | \\ \langle \Phi_{ij}^{ab} | \\ \text{3p3h} \end{array} \left[\begin{array}{c} \text{---} \end{array} \right]$$

$$\begin{array}{c}
 4p44 \\
 \vdots \\
 NpNH
 \end{array}
 \left| \right.
 \begin{array}{c}
 C_0 \\
 C(1p14) \\
 C(2p24) \\
 \vdots \\
 C(NpNH)
 \end{array}
 \begin{array}{c}
 \\
 \\
 \\
 \\
 \\
 \end{array}
 = E
 \begin{array}{c}
 C_0 \\
 C(1p14) \\
 \vdots \\
 C(NpNH)
 \end{array}$$

$$\det(H - ES) = 0$$

$$\begin{array}{c}
 H \\
 = 0p44 \\
 1p14 \\
 2p24 \\
 3p34 \\
 \vdots \\
 \vdots \\
 \vdots \\
 NpNH
 \end{array}
 \begin{array}{c}
 0p44 \quad 1p14 \quad 2p24 \quad 3p34 \quad \dots
 \end{array}
 \begin{array}{|cccc|}
 \hline
 x & x & x & 0 \dots 0 \\
 x & x & x & x \quad 0 \dots \\
 x & x & x & x \quad x \quad 0 \dots \\
 0 & x & x & \\
 0 & 0 & x & \\
 \vdots & \vdots & 0 & \\
 0 & 0 & 0 & \\
 \hline
 \end{array}$$

two-body operator

$$\langle \Phi_0 | H | \Phi_{ijk}^{abc} \rangle = 0$$

$$\langle \Phi_0 | H | \Phi_0 \rangle = E_0^{\text{ref}}$$

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

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