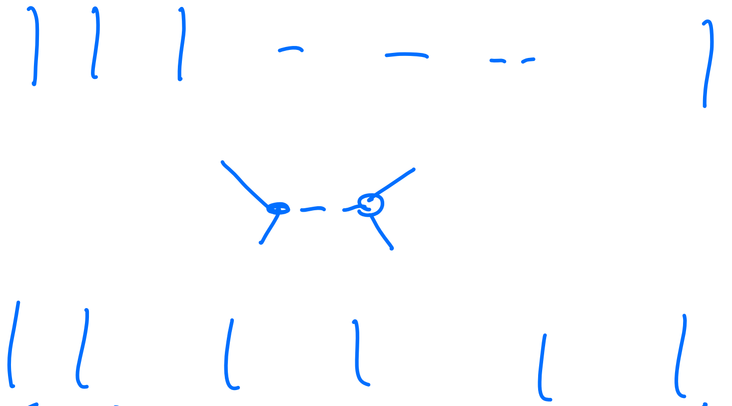
FYS4480 September 22

particle-hole formalism
using Wick's theorem

$\alpha_1\ \alpha_2\ \alpha_3 \qquad\qquad \alpha_n$



$\alpha_1\ \alpha_2\ \alpha_3 \qquad\qquad \alpha_n$

$$a^\dagger_{\alpha_1} a^\dagger_{\alpha_2} a^\dagger_{\alpha_3} \cdots a^\dagger_{\alpha_n} |0\rangle$$

n-particle state

add one particle

$$a^\dagger_{\alpha_{n+1}} |\alpha_1 \alpha_2 \ldots \alpha_n\rangle$$

$$(\alpha_1 < \alpha_2 < \alpha_3 \ldots < \alpha_n)$$

$$= (-)^n |\alpha_1 \alpha_2 \ldots \alpha_n \alpha_{n+1}\rangle$$

n+1 - particle state

$$= a^\dagger_{\alpha_1} a^\dagger_{\alpha_2} \cdots a^\dagger_{\alpha_n} a^\dagger_{\alpha_{n+1}} |0\rangle$$

$$\times \ (-)^n$$

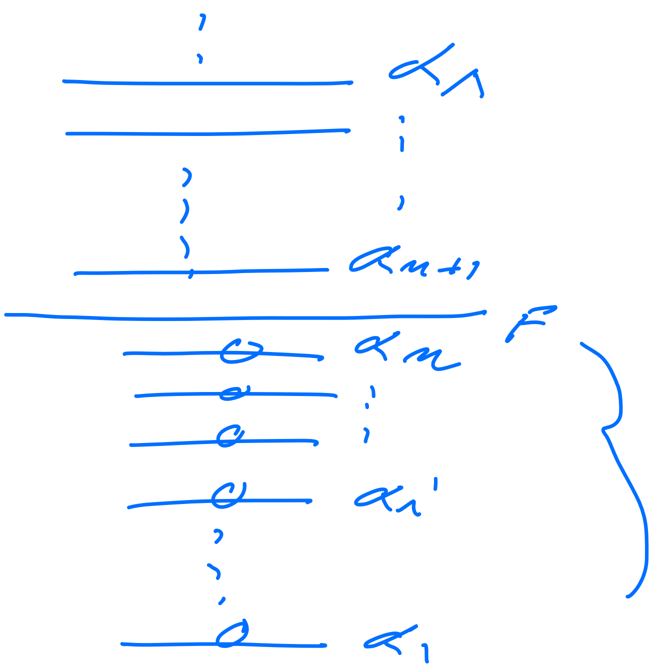
$$a_\alpha |\alpha_1, \alpha_2 \ldots \alpha_n\rangle \qquad \alpha = n$$

$$= (-)^{n-1} a^\dagger_{\alpha_1} a^\dagger_{\alpha_2} \ldots a^\dagger_{\alpha_{n-1}} |0\rangle$$

$n-1$-particle state.

if $\alpha \in \{\alpha_1 \alpha_2 \ldots \alpha_n\}$

$$|\alpha_1 \alpha_2 \ldots \alpha_n\rangle = |c\rangle = |\Phi_0\rangle$$



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

if $\alpha \notin \{\alpha_1 \alpha_2 \ldots \alpha_n\}$

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

else $a_\alpha |c\rangle \neq 0$

$$a^\dagger_\alpha |c\rangle = 0 \quad \text{if } \alpha \in \{\alpha_1 \alpha_2 .. \alpha_n\}$$

else $|\alpha \alpha_1 \alpha_2 \ldots \alpha_n\rangle$

$$= (-)^n a^\dagger_{\alpha_1} a^\dagger_{\alpha_2} \ldots a^\dagger_{\alpha_n} a_\alpha |0\rangle$$

$$a^\dagger_\alpha |c\rangle \neq 0$$

Define new operator

$$b_\alpha |c\rangle = 0 \quad (a_\alpha |0\rangle = 0)$$

$$\{b^\dagger_\alpha, b^\dagger_\beta\} = \{b_\alpha, b_\beta\} = 0$$

$$\{b_\alpha, b^\dagger_\beta\} = \delta_{\alpha\beta}$$

$$\overbrace{b_\alpha b^\dagger_\beta} = \delta_{\alpha\beta}$$

$$\overbrace{b^\dagger_\alpha b_\beta} = b^\dagger_\alpha b^\dagger_\beta = \overbrace{b_\alpha b_\beta} = 0$$

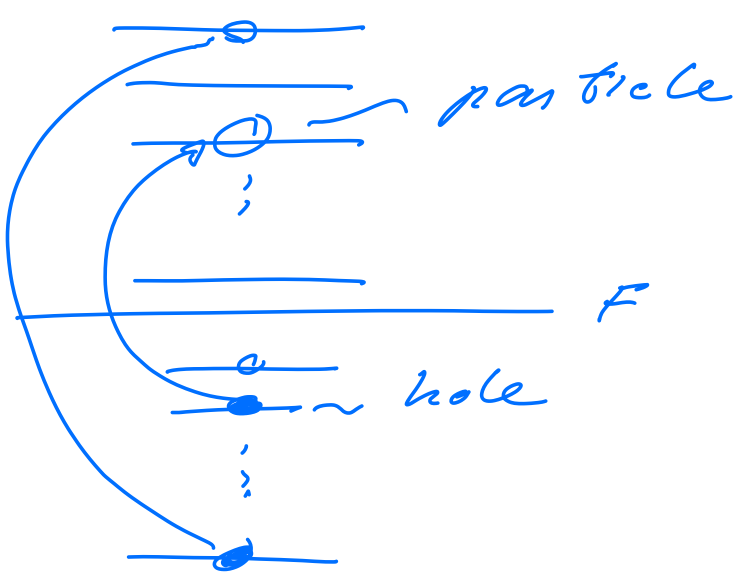
$$b^\dagger_\alpha |c\rangle = \begin{cases} a^\dagger_\alpha |c\rangle & \alpha > F \\ a_\alpha |c\rangle & \alpha \leqq F \end{cases}$$

$$\langle c|c\rangle = \langle \Phi_0|\Phi_0\rangle = 1$$

$$b_\alpha = \left(b_\alpha^\dagger\right)^\dagger$$

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

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



$$\hat{N} = \sum_{\alpha=0}^{\infty} a_\alpha^\dagger a_\alpha$$

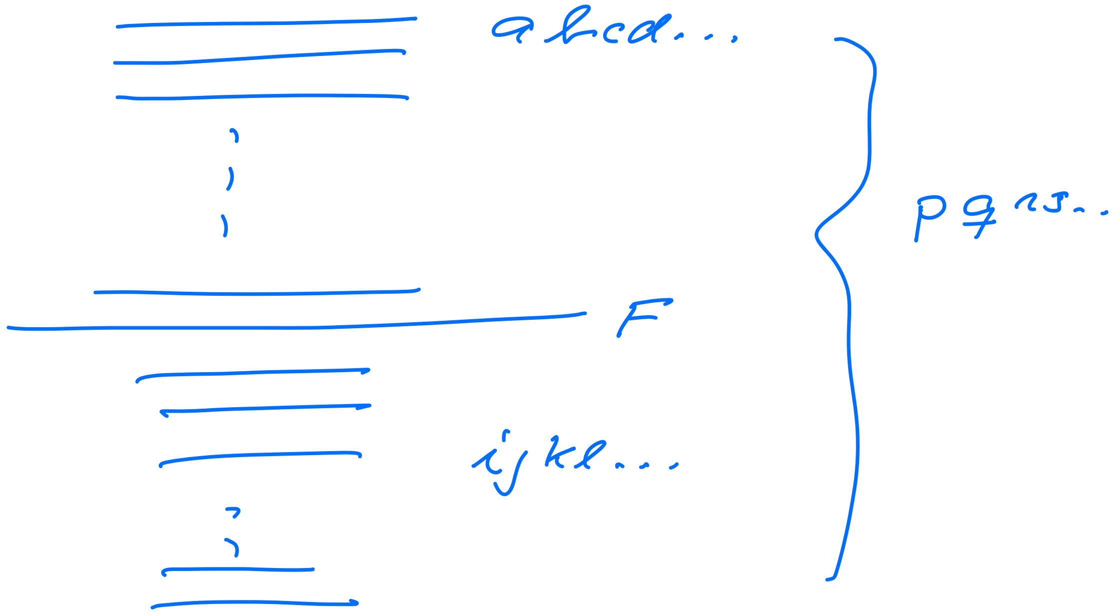
$$= \sum_{\alpha > F} a_\alpha^\dagger a_\alpha + \sum_{\alpha \le F} a_\alpha^\dagger a_\alpha$$

$$= \sum_{\alpha > F} b_\alpha^\dagger b_\alpha + \sum_{\alpha \le F} \underbrace{b_\alpha b_\alpha^\dagger}_{\delta_{\alpha\alpha} - b_\alpha^\dagger b_\alpha}$$

$$\sum_{\alpha \le F} \delta_{\alpha\alpha} = n$$

$$\sum_{\alpha > F} b_\alpha^\dagger b_\alpha + n - \sum_{\alpha \le F} b_\alpha^\dagger b_\alpha$$

Definition (labeling) of sp-states



$$\hat{N} = \sum_a b_a^\dagger b_a - \sum_i b_i^\dagger b_i$$

$$+ n$$

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

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

$n+1$ state

$$b_i^\dagger |\Phi_0\rangle = a_i |\Phi_0\rangle = |\Phi_i\rangle$$

$n-1$ state

$$b_a^\dagger b_i^\dagger |\Phi_0\rangle = a_a^\dagger a_i |\Phi_0\rangle$$

$$= |\Phi_i^a\rangle \quad \text{1p 1h excitation}$$

$$b_a^\dagger b_b^\dagger b_j^\dagger b_i^\dagger |\Phi_0\rangle = a_a^\dagger a_b^\dagger a_j a_i |\Phi_0\rangle$$

$$= |\Phi_{ij}^{ab}\rangle \quad \text{2p2h excitation}$$

<u>Example</u>

n-particle

$$\langle \Phi_i^a | \hat{N} | \Phi_i^a \rangle \qquad \sum_{ai} |\Phi_i^a\rangle$$

$$\langle c|\, b_i b_a \Big(\sum_b b_b^{\dagger} b_b - \sum_j b_j^{\dagger} b_j + n \Big) \times b_a^{\dagger} b_i^{\dagger} \,|c\rangle$$

$$\sum_b \{b_i b_a\}\{b_b^{\dagger} b_b\}\{b_a^{\dagger} b_i^{\dagger}\}\ \delta_{ab}$$

$> F$

$$- \sum_j b_i b_a\, b_j^{\dagger} b_j\, b_a^{\dagger} b_i^{\dagger} \quad - \delta_{ij}$$

$$+ n \left(b_i b_a b_a^{\dagger} b_i^{\dagger} \right) = n$$

only different from zero contraction is $b_p b_q^{\dagger}$
$= \delta_{pq}$

$$\sum_a b_a^{\dagger} b_a - \sum_j b_j^{\dagger} b_j$$

$$\langle c|\, a_a^{\dagger} a \,|c\rangle = a_a^{\dagger} a_a = 0$$

$a \notin |c\rangle$

$$\langle 0 | a_a a_b^\dagger | 0 \rangle = \overbrace{a_a a_b^\dagger} = \delta_{ab}$$

$$\langle 0 | a_a^\dagger a_b | 0 \rangle = \overbrace{a_a^\dagger a_b} = 0$$

$$\langle c | a_b a_a^\dagger | c \rangle = \overbrace{a_b a_a^\dagger}$$

$$= \delta_{ab}$$

$$\langle c | b_a b_b^\dagger | c \rangle = \overbrace{b_a b_b^\dagger}$$

$$= \delta_{ab}$$

$$- \langle c | b_i b_j^\dagger | c \rangle = - \overbrace{b_i b_j^\dagger} =$$

$$- \delta_{ij}$$

$$- \langle c | a_i^\dagger a_j | c \rangle = - \overbrace{a_i^\dagger a_j}$$

$$= - \delta_{ij}$$

$$\overbrace{a_i^\dagger a_j} = \delta_{ij} \quad \text{if} \quad i,j \leq F$$

$$\overbrace{a_a a_b^\dagger} = \delta_{ab} \quad \text{if} \quad a,b > F$$

$$\sum_a b_a^+ b_a - \sum_i b_i^+ b_i + n$$

$$= \sum_p \{a_p^+ a_q\} + n$$

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

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

$$|\Phi_i^a\rangle = a_a^+ a_i |c\rangle = a_a^+ a_i |\Phi_c\rangle$$

$$\langle \Phi_i^a | \hat{N} | \Phi_i^a \rangle =$$

$$\langle c | a_i^+ a_a \left(\sum_p \{a_p^+ a_p\} + n \right) a_a^+ a_i |0\rangle$$

$$a_i^+ a_a a_p^+ a_p a_a^+ a_i \qquad \delta_{pa}\delta_{ii}$$

$$a_i^+ a_a a_p^+ a_p a_a^+ a_i \qquad -\delta_{pi}\delta_{aa}$$

$$n\,(a_i^\dagger a_a\, a_a^\dagger a_i) = n$$

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

$$= \sum_{\alpha\beta > F} \langle \alpha | h_0 | \beta \rangle\, b_\alpha^\dagger b_\beta$$

$$+ \sum_{\substack{\alpha > F \\ \beta \le F}} \langle \alpha | h_0 | \beta \rangle\, b_\alpha^\dagger b_\beta^\dagger$$

$$+ \sum_{\substack{\alpha \le F \\ \beta > F}} \langle \alpha | h_0 | \beta \rangle\, b_\alpha b_\beta$$

$$\alpha \longleftrightarrow \beta$$

$$\left(\sum_{\substack{\alpha > F \\ \beta \le F}} \langle \beta | h_0 | \alpha \rangle\, b_\beta b_\alpha \right)$$

$$+ \sum_{\alpha\beta \le F} \langle \alpha | h_0 | \beta \rangle\, \underbrace{b_\alpha b_\beta^\dagger}_{\delta_{\alpha\beta} - b_\beta^\dagger b_\alpha}$$

$$= \sum_{\alpha\beta > F} \langle \alpha | h_0 | \beta \rangle\, b_\alpha^\dagger b_\beta$$

$$+ \sum_{\substack{\alpha > F \\ \beta \leq F}} \left[\langle \alpha | h_0 | \beta \rangle b_\alpha^\dagger b_\beta^\dagger + \langle \beta | h_0 | \alpha \rangle b_\beta b_\alpha \right]$$

$$+ \sum_{\alpha \leq F} \underbrace{\langle \alpha | h_0 | \alpha \rangle}_{\varepsilon_\alpha} \quad \varepsilon_0$$

$$- \sum_{\alpha\beta \leq F} \langle \beta | h_0 | \alpha \rangle b_\alpha^\dagger b_\beta$$

Example

$$\langle \Phi_c | H_0 | \Phi_c \rangle$$

$$\sum_{\alpha\beta > F} \langle c | b_\alpha^\dagger b_\beta | c \rangle = 0$$

$$+ 0 + 0 \ldots + \sum_\alpha \varepsilon_\alpha$$

$$h_0 | \alpha \rangle = \varepsilon_a | \alpha \rangle$$

Example

$$\langle \Phi_i^a | H_0 | \Phi_i^a \rangle \quad \alpha$$

$$| \Phi_k^c \rangle = b_c^\dagger b_k^\dagger | c \rangle$$

$$\langle 0 | \; b_k b_c \underbrace{b_\alpha^\dagger b_\beta}_{\alpha\beta > F} b_c^\dagger b_k^\dagger | 0 \rangle$$

$$\delta_{kk}\, \delta_{c\alpha}\, \delta_{\beta c} \longrightarrow \varepsilon_c$$

$$\langle c | \; b_k b_c \, b_\alpha^\dagger b_\beta^\dagger \, b_c^\dagger b_k^\dagger | c \rangle$$

$$\alpha > F \quad \beta \leq F$$

$$- \langle c | \, b_k b_c \, b_\alpha^\dagger b_\beta \, b_c^\dagger b_k^\dagger \, | c \rangle$$

$$\alpha, \beta < F$$

$$\delta_{k\alpha}\, \delta_{k\beta}\, \delta_{cc} \longrightarrow -\varepsilon_k$$

$$\langle \Phi_k^c | H_0 | \Phi_k^c \rangle = \varepsilon_0 + \varepsilon_c - \varepsilon_k$$

$$\langle \Phi_{ke}^{cd} | H_0 | \Phi_{ke}^{cd} \rangle =$$

$$\varepsilon_0 + \varepsilon_c + \varepsilon_d - \varepsilon_k - \varepsilon_e$$

$$\hat{H}_0 = \sum_{pq} \langle p | h_0 | q \rangle \{ a_p^\dagger a_q \} + E_0$$

$$\hat{N} = \sum_{pq} \{ a_p^\dagger a_q \} + n$$

Example

$$\langle \Phi_i^a | \hat{H}_0 | \Phi_i^a \rangle$$

$$= \sum_{pq} \langle c | a_i^\dagger a_a \, a_p^\dagger a_q \, a_a^\dagger a_i | c \rangle \times \langle p | h_0 | q \rangle$$

$$+ \; E_0 \langle c | a_i^\dagger a_a a_a^\dagger a_i | c \rangle$$

$$\delta_{i'i} \; \delta_{aa}$$

$$\delta_{ii'}$$

$$a_i^\dagger a_a \; a_p^\dagger a_q \; a_a^\dagger a_{i'} \rightarrow \varepsilon_a$$

$$\delta_{ap} \qquad \delta_{qa}$$

$$a_i^{+} a_a a_p^{+} a_q a_a^{+} a_i \rightarrow -\varepsilon_i$$

$$\langle \Phi_i^a | \hat{H}_0 | \Phi_i^a \rangle = \varepsilon_0 + \varepsilon_a - \varepsilon_i$$

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

$$+ \sum_{pqi} \langle pi | v | qi \rangle \{ a_p^{+} a_q \}$$

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

$$\hat{H}_0 + \hat{H}_1 = \hat{H}$$

$$E_0^{REF} = \langle \Phi_c | H | \Phi_c \rangle =$$

$$\varepsilon_0 + \frac{1}{2} \sum_{ij} \langle ij | v | ij \rangle_{AS}$$

$$\langle p | \hat{f} | q \rangle = \sum_i \langle pi | v | qi \rangle + \langle p | h_0 | q \rangle$$

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

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

$$+ \quad E_0^{Ref}.$$

Example

$$\langle \Phi_i^a | \hat{H} | \Phi_i^a \rangle :$$

$$=0$$

$$\frac{1}{4}\sum_{pqrs} \langle c | a_i^\dagger a_a \, a_p^\dagger a_q^\dagger a_s a_r \, a_a^\dagger a_i | c\rangle$$

$$\times \langle pq||rs\rangle_{AS}$$

$$+ \sum_{pq} \langle p|f|q\rangle \langle c| a_i^\dagger a_a \, a_p^\dagger a_q \, a_a^\dagger a_i | c\rangle$$

$$+ \quad E_0^{Ref}$$

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

$$+ E_0^{Ref}.$$

Example

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