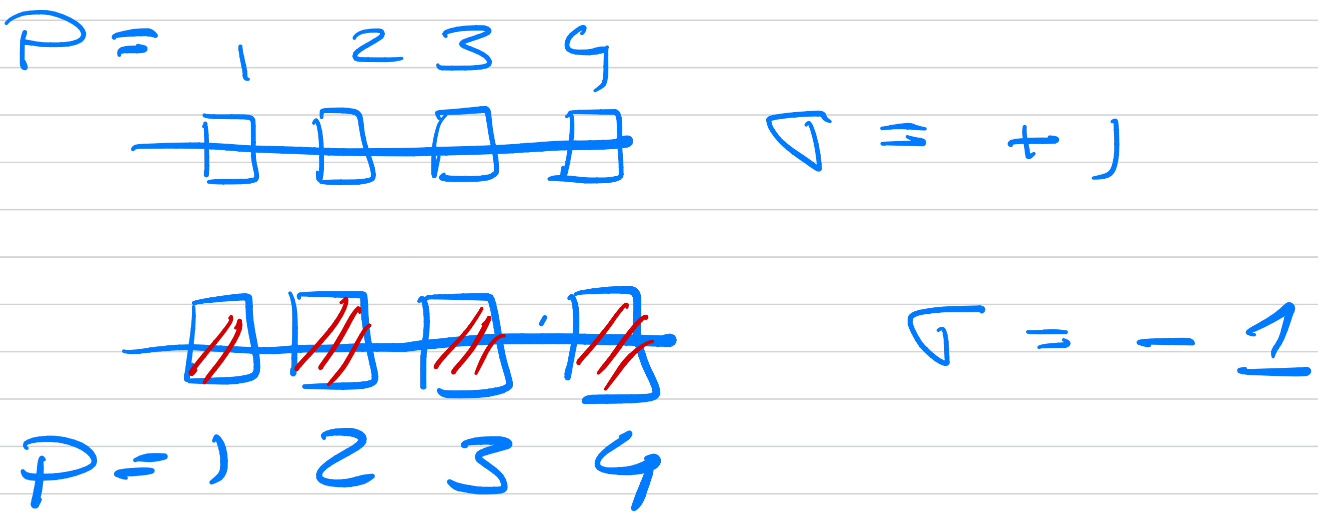
Lecture
FY4480/9480
September 13, 2024

FYS4480/9480, Sept 13

Particle-hole formalism.

Example: Lipkin with $N=4$



$$|\Phi_c\rangle = a^{+}_{1-}\, a^{+}_{2-}\, a^{+}_{3-}\, a^{+}_{4-}\, |0\rangle$$

σ

$$a^{+}_{p\sigma}|0\rangle$$

$$\hat{H}_0 = \frac{1}{2}\varepsilon \sum_{p\sigma} \sigma\, a^+_{p\sigma} a_{p\sigma}$$

$$\langle \Phi_0 | \hat{H}_0 | \Phi_0 \rangle =$$

$$\frac{1}{2}\varepsilon \sum_{p\sigma} \sigma \langle 0 | a_{4-} a_{3-} a_{2-} a_{1-}\, a^+_{p\sigma} a_{p\sigma}$$

$$\times\, a^+_{1-} a^+_{2-} a^+_{3-} a^+_{4-}$$

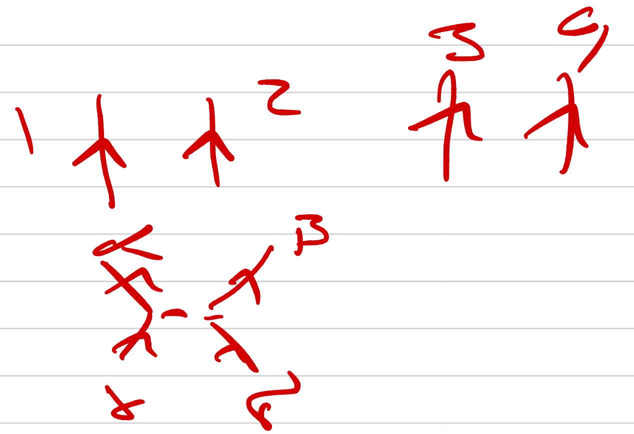
$$= -\frac{1}{2}\varepsilon \sum_{p} \langle 0 | a_4 a_3 a_2 a_1 a^+_p \underbrace{a_p a^+_1}_{\delta_{p1}} a_2 a^+_3 a^+_4 | 0 \rangle$$

$$= -2\varepsilon$$

Expectation value of H_I

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

(1, 2) $\quad \langle 12|v|12\rangle_{AS}\, \delta_{33}\, \delta_{44}$

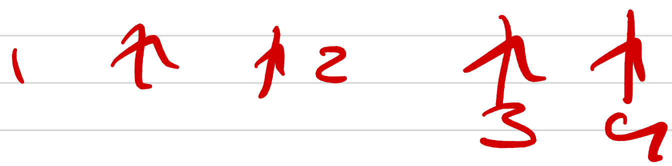


(1, 3) $\quad \langle 13|v|13\rangle_{AS}\, \delta_{22}$

$\times\, \delta_{44}$

(1, 4) $\quad \langle 14|v|14\rangle_{AS}$

$\times\, \delta_{22}\, \delta_{33}$



$(2,3)\; : \quad \langle 23|v|23\rangle_{AS}\, \delta_{11}\, \delta_{44}$

$$a_4\, a_3\, a_2\, a_1\, a_\alpha^\dagger a_\beta^\dagger a_\delta a_\gamma a_1^\dagger a_2^\dagger a_3^\dagger a_4^\dagger$$

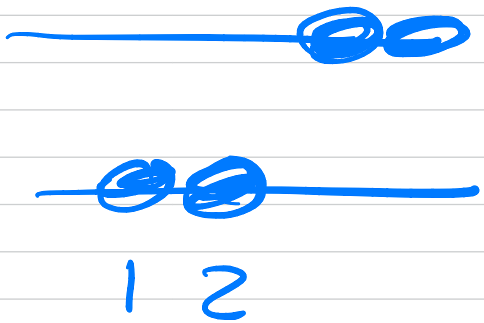
+ 3 other ones

$(2,4)\; : \quad \langle 24|v|24\rangle_{AS}\, \delta_{11}\, \delta_{33}$

$(3,4)\; : \quad \langle 34|v|34\rangle_{AS}\, \delta_{11}\, \delta_{22}$

$$\langle \Phi_0 | H | \Phi_0 \rangle = -2\varepsilon + \frac{1}{2} \sum_{i,j \leq 1}^{4} \langle ij|v|ij\rangle_{AS}$$

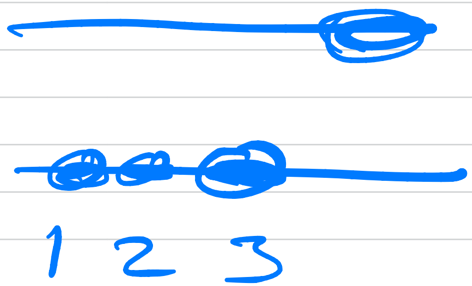
H_1



$\sigma = +1$

$\sigma = -1$

H_2



$\sigma = +1$

$\sigma = -1$

$$\langle \Phi_0 | \hat{H} | \Phi_0 \rangle = -2\varepsilon$$

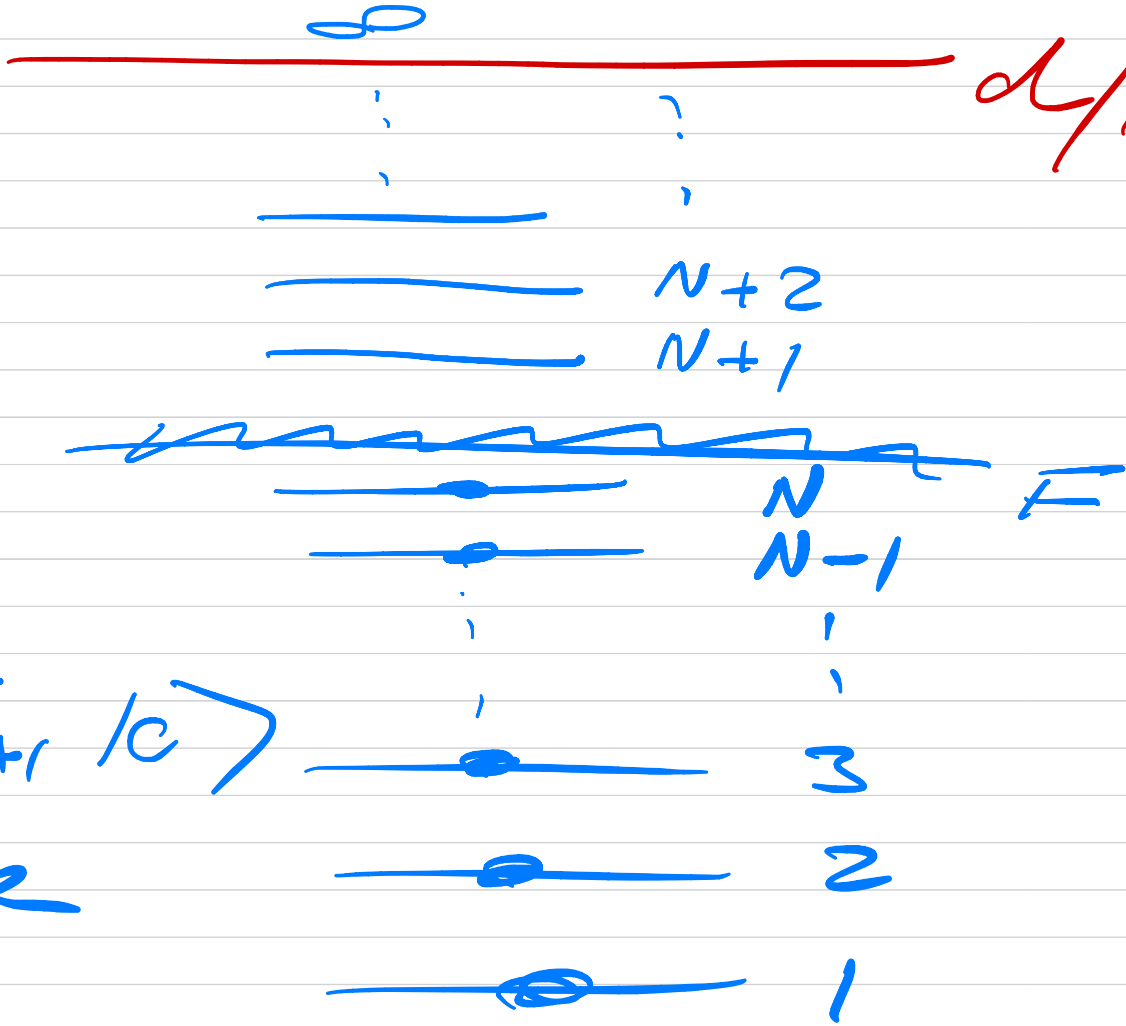
$$|\Phi_1\rangle = a^\dagger_{1-} a^\dagger_{2-} a^\dagger_{3-} a^\dagger_{1+} |0\rangle$$

Particle-hole formalism

$$|\Phi_0\rangle = a_1^\dagger a_2^\dagger \cdots a_N^\dagger |0\rangle$$

$$a_{N+1}^\dagger |\Phi_0\rangle = (-)^N a_1^\dagger a_2^\dagger \cdots a_N^\dagger a_{N+1}^\dagger |0\rangle$$

N+1 particle state



d/n

$$a_\alpha |123\ldots N\rangle$$

$$= a_\alpha a_1^\dagger a_2^\dagger \ldots a_{\alpha-1}^\dagger a_\alpha^\dagger a_{\alpha+1}^\dagger \ldots a_N^\dagger |0\rangle$$

$$(\alpha \in \{1,2,3\ldots N\})$$

$$= (-1)^{\alpha-1} \underbrace{a_1^\dagger a_2^\dagger \ldots a_{\alpha-1}^\dagger a_{\alpha+1}^\dagger \ldots a_N^\dagger |0\rangle}_{N-1 \text{ state}}$$

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

$$\hat{H}_0 |\Phi_0\rangle = \mathcal{E}_0 |\Phi_0\rangle$$

$$\mathcal{E}_0 = \sum_{i \le F} \varepsilon_i$$

intermediate step

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

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

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

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

$$b_\alpha^\dagger |\Phi_0\rangle = a_\alpha^\dagger |\Phi_0\rangle$$

if $\alpha \notin |\Phi_0\rangle$

$= a_\alpha |\Phi_0\rangle$ if α is included in $|\Phi_0\rangle$

$$\hat{N} = \sum_{\alpha} a_{\alpha}^{+} a_{\alpha}$$

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

$$= \sum_{\alpha > F} b_{\alpha}^{+} b_{\alpha} + \sum_{\alpha \leq F} b_{\alpha} b_{\alpha}^{+}$$

$$b_{\alpha} b_{\alpha}^{+} + b_{\alpha}^{+} b_{\alpha} = \delta_{\alpha\alpha}$$

$$= \sum_{\alpha > F} b_{\alpha}^{+} b_{\alpha} - \sum_{\alpha \leq F} b_{\alpha}^{+} b_{\alpha} + \underbrace{N}_{\text{Reference value}}$$

Reference value $\langle \Phi_0 | \underbrace{\hat{N}}_{\displaystyle N} | \Phi_0 \rangle$

$$\prod_{\alpha \le F} a_\alpha^\dagger |0\rangle$$

$$\boxed{\langle \Phi_0 | \Phi_0 \rangle = 1}$$

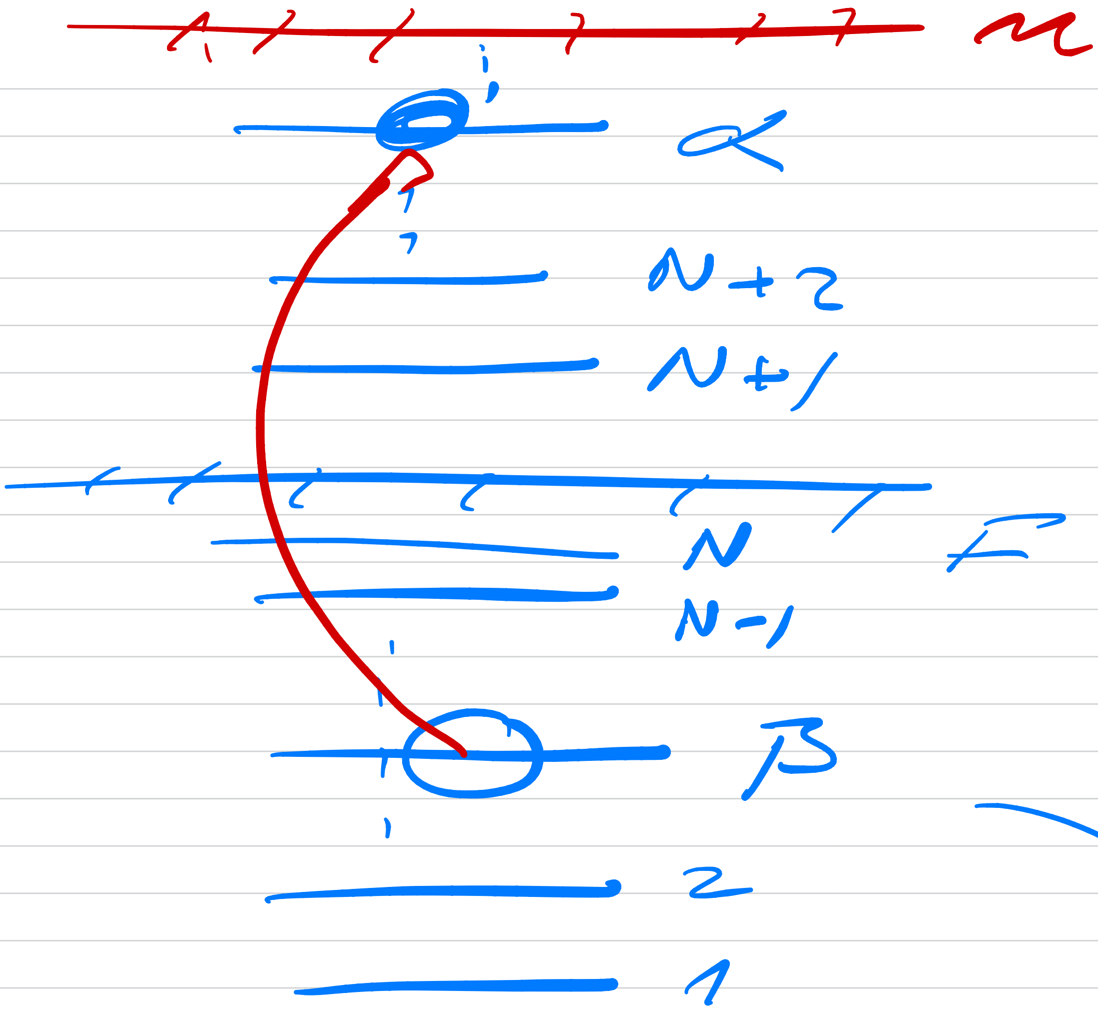
$$\langle \Phi_0 | N[x \cdots] | \Phi_0 \rangle = 0$$

Define new states

$$b_\alpha^\dagger b_\beta^\dagger | \Phi_0 \rangle \qquad \alpha > F$$

$$\beta \le F$$

$$a_\alpha^\dagger a_\beta | \Phi_0 \rangle$$



$\#$ configs $= \binom{n}{N}$

1 particle-1 hole state

1p1h

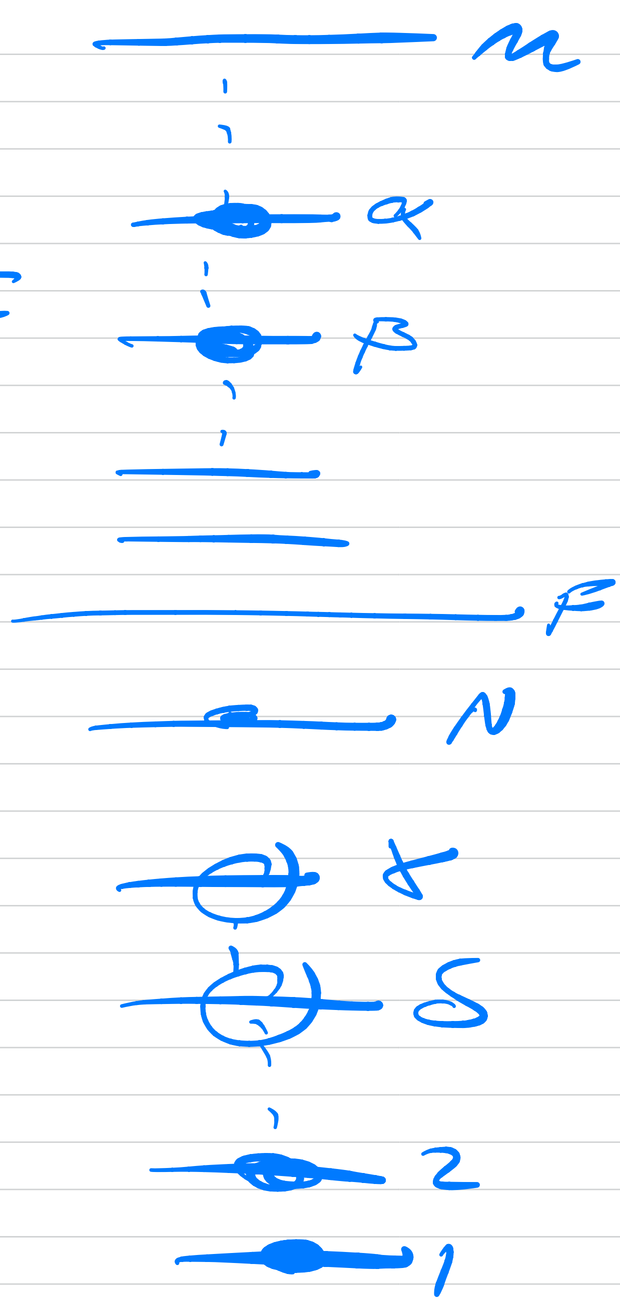
$$|\Phi_\beta^\alpha\rangle = a_\alpha^\dagger a_\beta |\Phi_0\rangle$$

$$b^\dagger_\alpha b^\dagger_\beta b^\dagger_\delta b^\dagger_\gamma |\Phi_0\rangle$$

$$\alpha, \beta > F \qquad \delta, \gamma \le F$$

$$a^\dagger_\alpha a^\dagger_\beta a_\delta a_\gamma |\Phi_0\rangle$$

2p-2h state



$$\hat{H}_0 = \sum_{\alpha\beta} \langle \alpha | h_0 | \beta \rangle a_\alpha^\dagger a_\beta$$

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

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

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

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

$$\left(b_\alpha b_\beta^\dagger = \delta_{\alpha\beta} - b_\beta^\dagger b_\alpha \right)$$

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

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

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

$$\langle \Phi_0 | H_0 | \Phi_0 \rangle = \sum_{\alpha \leq F} \varepsilon_\alpha = \mathcal{E}_0$$

Reference energy for H_0

$$|\Phi_\gamma^\delta\rangle = b_\delta^\dagger b_\gamma^\dagger |\Phi_0\rangle$$

$$\langle \Phi_\gamma^\delta | \hat{H}_0 | \Phi_\gamma^\delta \rangle$$

$$\langle \Phi_0 | b_\gamma b_\delta \; H_0 \; b_\delta^\dagger b_\gamma^\dagger | \Phi_0 \rangle$$

$$b_\gamma b_\delta b_\alpha^\dagger b_\beta b_\delta^\dagger b_\gamma^\dagger$$

$\alpha,\beta > F$

$\delta > F$

$$\delta_{\gamma\gamma}\,\delta_{\alpha\delta}\,\delta_{\beta\delta} \qquad \langle\alpha|h_0|\beta\rangle = \varepsilon_\delta$$

$\alpha > F \wedge \beta \le F$ $\qquad b_\gamma b_\delta b_\alpha^\dagger b_\beta^\dagger b_\delta^\dagger b_\gamma^\dagger$

$\beta > F \wedge \alpha \le F$ $\qquad$ — " — $\; b_\beta b_\alpha b_\delta^\dagger b_\gamma^\dagger$

$$-\sum_{\substack{\alpha\beta\le F\\ \gamma\le F}} \langle\Phi_0| b_\gamma b_\delta b_\beta^\dagger b_\alpha b_\delta^\dagger b_\gamma^\dagger |0\rangle$$

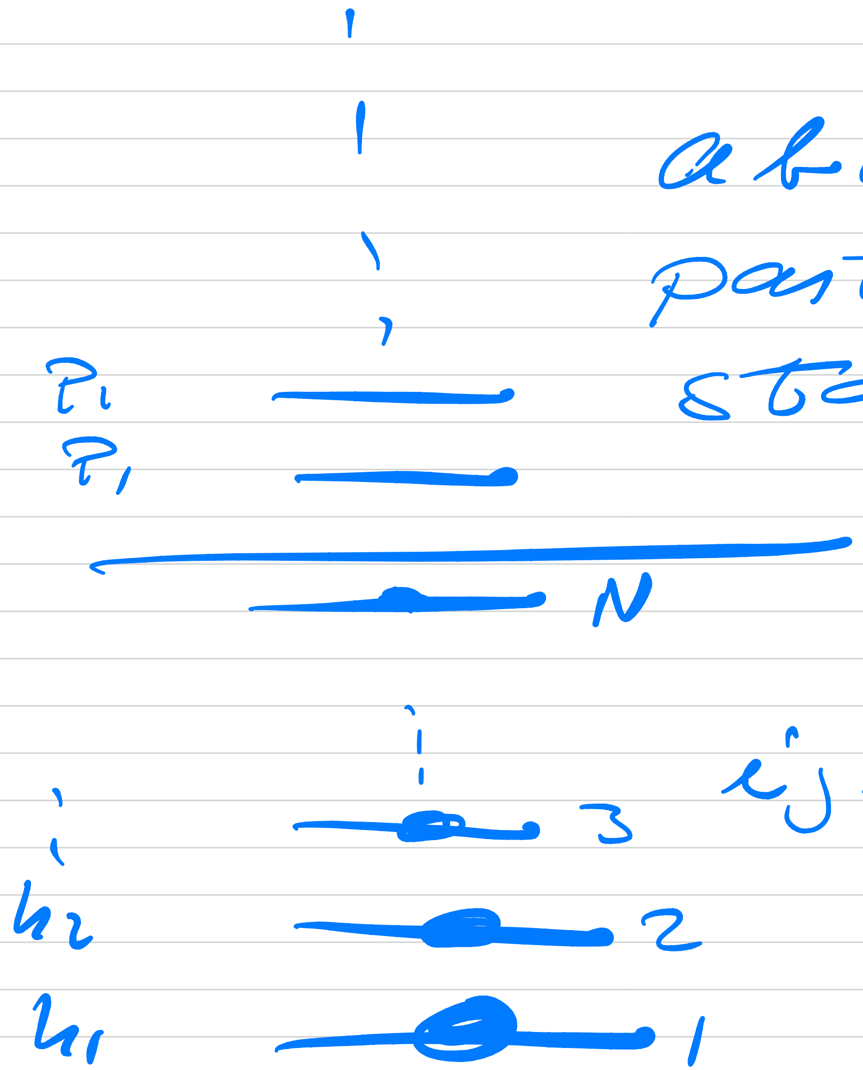
$$\delta_{\gamma\beta}\,\delta_{\delta\delta}\,\delta_{\alpha\gamma}$$

$$-\varepsilon_\alpha$$

$$= \underbrace{\sum \delta}_{\delta > F} - \underbrace{\sum \gamma}_{\gamma \leq F} + \sum_{\alpha \leq F} \varepsilon \alpha$$

$$= \sum \delta + \sum_{\alpha \neq \gamma} \varepsilon \alpha$$

New labels



abcd.. particle states

ijkl.. hole states

all sp states — n — pqrs..

$$|\Phi_\gamma^\delta\rangle \Rightarrow |\Phi_i^a\rangle$$

$$= b_a^\dagger b_i^\dagger |\Phi_c\rangle$$

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

$$|\Phi_{ij}^{ab}\rangle = a_a^\dagger a_b^\dagger a_j a_i |\Phi_c\rangle$$

$$2p2h$$

$$|\Phi_{ijk}^{abc}\rangle \; : \; 3p3h \; \ldots \; NpNh$$

Back to $a^\dagger$ and a

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

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

$$\langle \Phi_0 | a_p^\dagger a_q | \Phi_0 \rangle = \langle \Phi_0 | \Phi_0 \rangle$$

$$= \underline{1}$$

$$\hat{N} = \sum_{\alpha > F} b_\alpha^\dagger b_\alpha - \sum_{\alpha \leq F} b_\alpha^\dagger b_\alpha$$

$$+ N$$

$$= \sum_p \underbrace{\{ a_p^\dagger a_p \}}_{\substack{\text{Normal} \\ \text{ordering} \\ \text{wrt to} \\ \text{new} \\ \text{reference state}}} + N$$

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

$$+ \; E_0$$

$$\langle \Phi_0 | H_0 | \Phi_0 \rangle$$

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

$$= \sum_{pq} \langle \Phi_0 | a_i^\dagger a_a \, a_p^\dagger a_q \, a_a^\dagger a_i | \Phi_0 \rangle$$

$$\times \langle p | h_0 | q \rangle$$

$$= \varepsilon_a - \varepsilon_i + \varepsilon_0$$