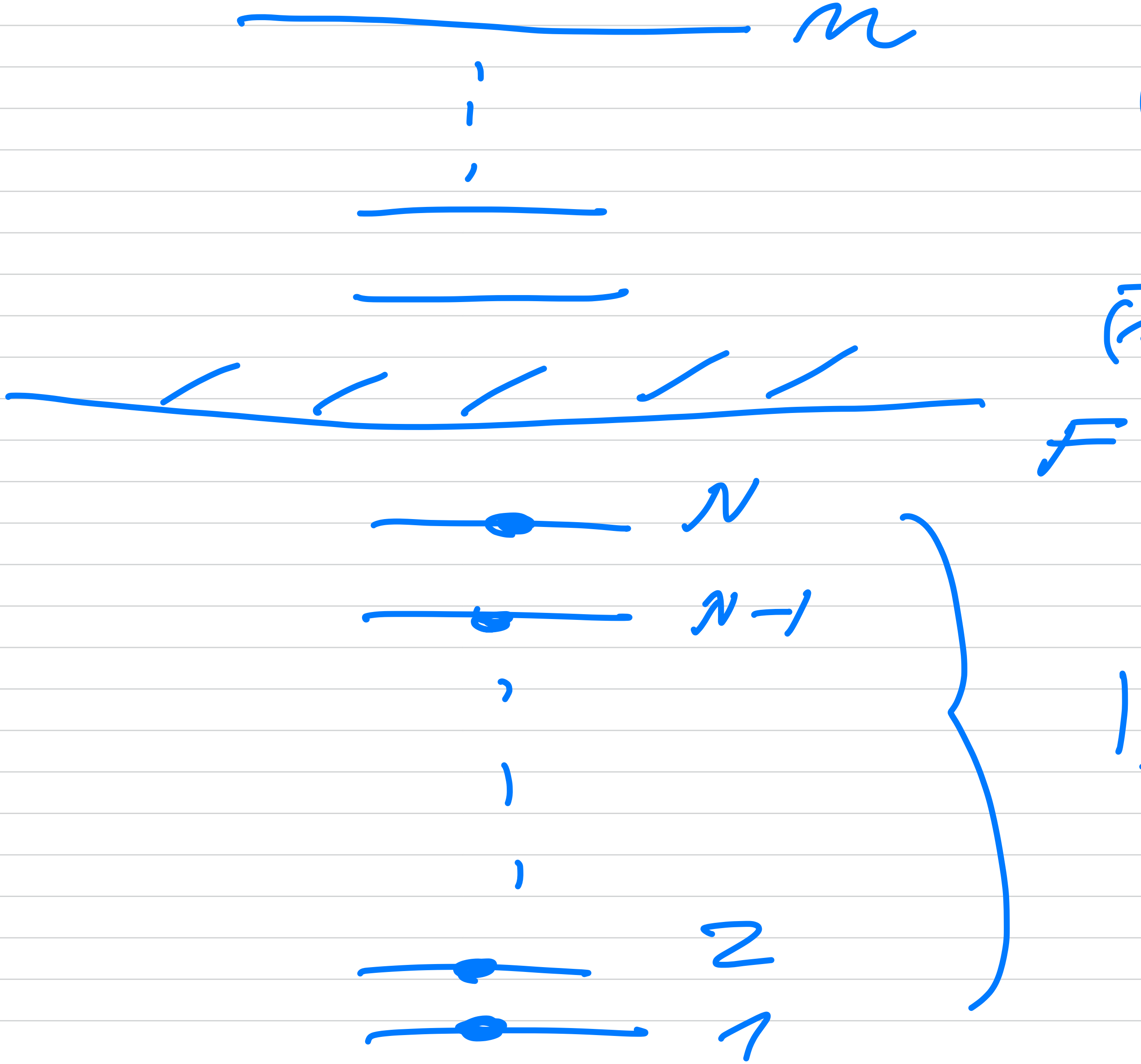
FYS4480 September 18



$|\Phi_0\rangle$

$$\binom{n}{N} = \frac{n!}{(n-N)!\,N!}$$

$$|\Phi_0\rangle = \prod_{i=1}^{N} a_i^\dagger |0\rangle$$

$$= \prod_{i \le F} a_i^\dagger |0\rangle$$

intermediate step

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

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

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

$$\overline{b_\alpha b_\beta^\dagger} = \delta_{\alpha\beta}$$

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

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

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

or $$a_\alpha |\Phi_0\rangle = |\Phi_0\rangle_{N-1}^{(-\alpha)}$$

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

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

$$b_\alpha |\Phi_0\rangle = \begin{cases} a_\alpha |\Phi_0\rangle = 0 & \alpha > F \\ a_\alpha^\dagger |\Phi_0\rangle = 0 & \alpha \le F \end{cases} \quad \text{if } \alpha \in \{|\Phi_0\rangle\}$$

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

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

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

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

$$\Rightarrow$$

$$\hat{N} = \sum_{\alpha > F} b_\alpha^+ b_\alpha - \sum_{\alpha \le F} b_\alpha^+ b_\alpha$$

$$+ \underbrace{\sum_{\alpha \le F} \delta_{\alpha\alpha}}_{N} \qquad \left(\sum_{\alpha=1}^{N} 1 = N \right)$$

$$N = \langle \Phi_0 | \hat{N} | \Phi_0 \rangle$$

$$\langle \Phi_0 | \hat{N} | \Phi_0 \rangle =$$

$$\left(|\Phi_0\rangle = \prod_{\alpha \le F} a_\alpha^\dagger |0\rangle \right)$$

$$\langle \Phi_0 | \sum_{\alpha > F} b_\alpha^\dagger b_\alpha | \Phi_0 \rangle \overset{\color{red}{=0}}{}$$

$$- \langle \Phi_0 | \sum_{\alpha \le F} b_\alpha^\dagger b_\alpha | \Phi_0 \rangle \overset{\color{red}{=0}}{}$$

$$+ \quad N \underbrace{\langle \Phi_0 | \Phi_0 \rangle}_{1}$$

$$\color{red}{= N}$$

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

$$= \sum_{\alpha\beta > F} \langle\alpha|\hat{h}_0|\beta\rangle\, b_\alpha^\dagger b_\beta$$

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

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

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

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

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

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

E_0^{Ref} + Normal-ordered operator

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

$$= \varepsilon_0^{\mathrm{ref}} \langle \Phi_0 | \Phi_0 \rangle$$

$$+ \langle \Phi_0 | \sum_{\substack{\alpha\beta \\ > F}} b_\alpha^\dagger b_\beta | \Phi_0 \rangle \quad \overset{= 0}{\alpha, \beta \notin \{ | \Phi_0 \rangle \}}$$

$$+ \langle \Phi_0 | \sum_{\substack{\alpha > F \\ \beta \leq F}} [\cdots \underset{= 0}{b_\alpha^\dagger b_\beta^\dagger} + \overset{= 0}{b_\beta b_\alpha} \quad a_\alpha \, a_\beta^\dagger \quad \times | \Phi_0 \rangle$$

$$- \langle \Phi_0 | \sum_{\alpha\beta \leq F} \cdots \underset{= 0}{b_\alpha^\dagger} b_\beta | \Phi_0 \rangle \quad \alpha, \beta \in | \Phi_0 \rangle$$

$$= \quad \varepsilon_0^{Ref} = \langle \Phi_0 | H_0 | \Phi_0 \rangle$$

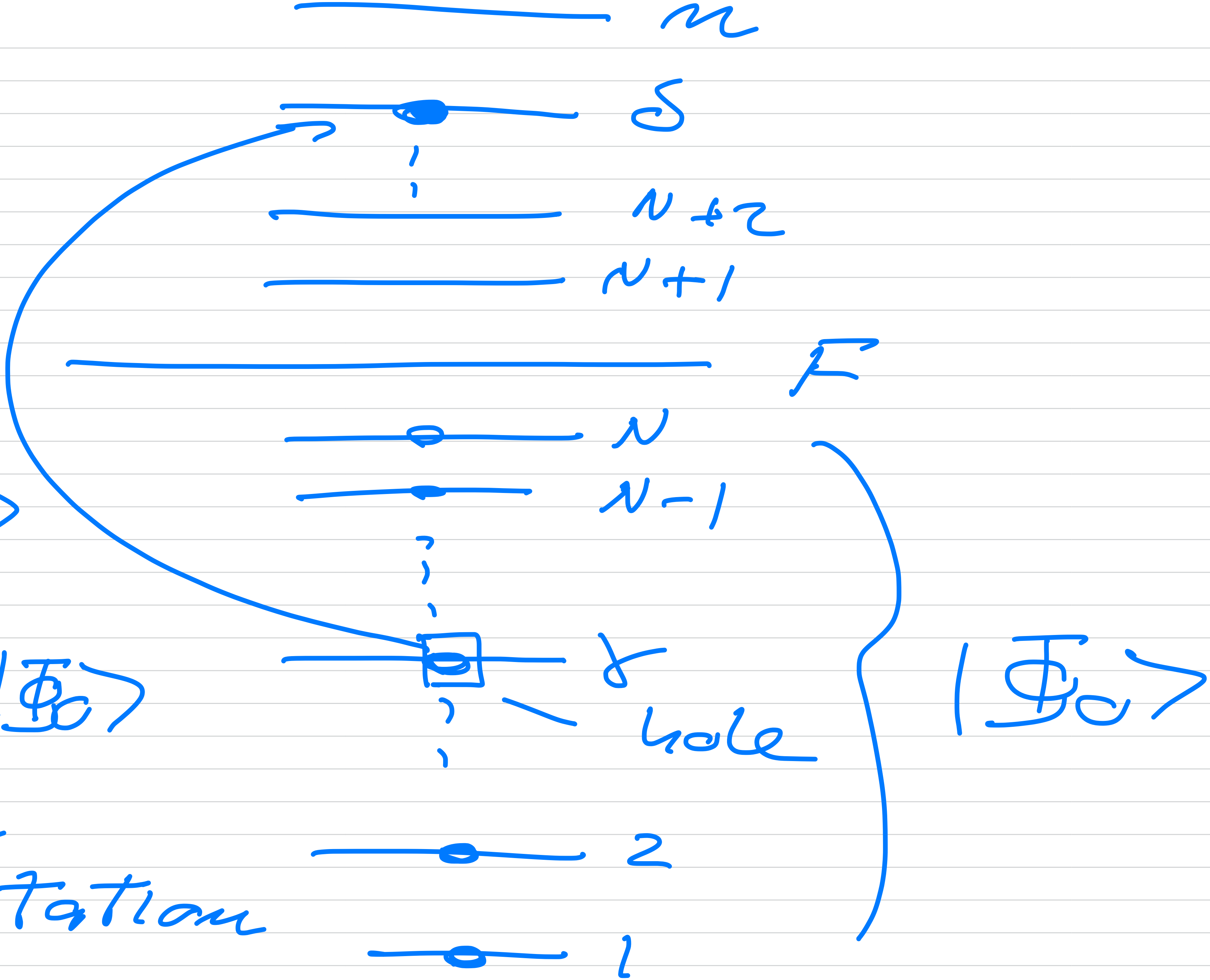
Example :

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

$$\gamma \leq F \qquad \delta > F$$

$$a_\delta^\dagger a_\gamma | \Phi_0 \rangle$$

$$= | \Phi_\gamma^\delta \rangle$$



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

1p1h excitation

$$\langle \Phi_\gamma^\delta | H_0 | \Phi_\gamma^\delta \rangle$$

$$\sum_{\alpha\beta > F} \langle \Phi_0 | \, b_\gamma b_\delta \, b_\alpha^\dagger b_\beta \, b_\delta^\dagger b_\gamma^\dagger | \Phi_0 \rangle$$

$$\delta_{\delta\alpha} \qquad \delta_{\beta\delta}$$

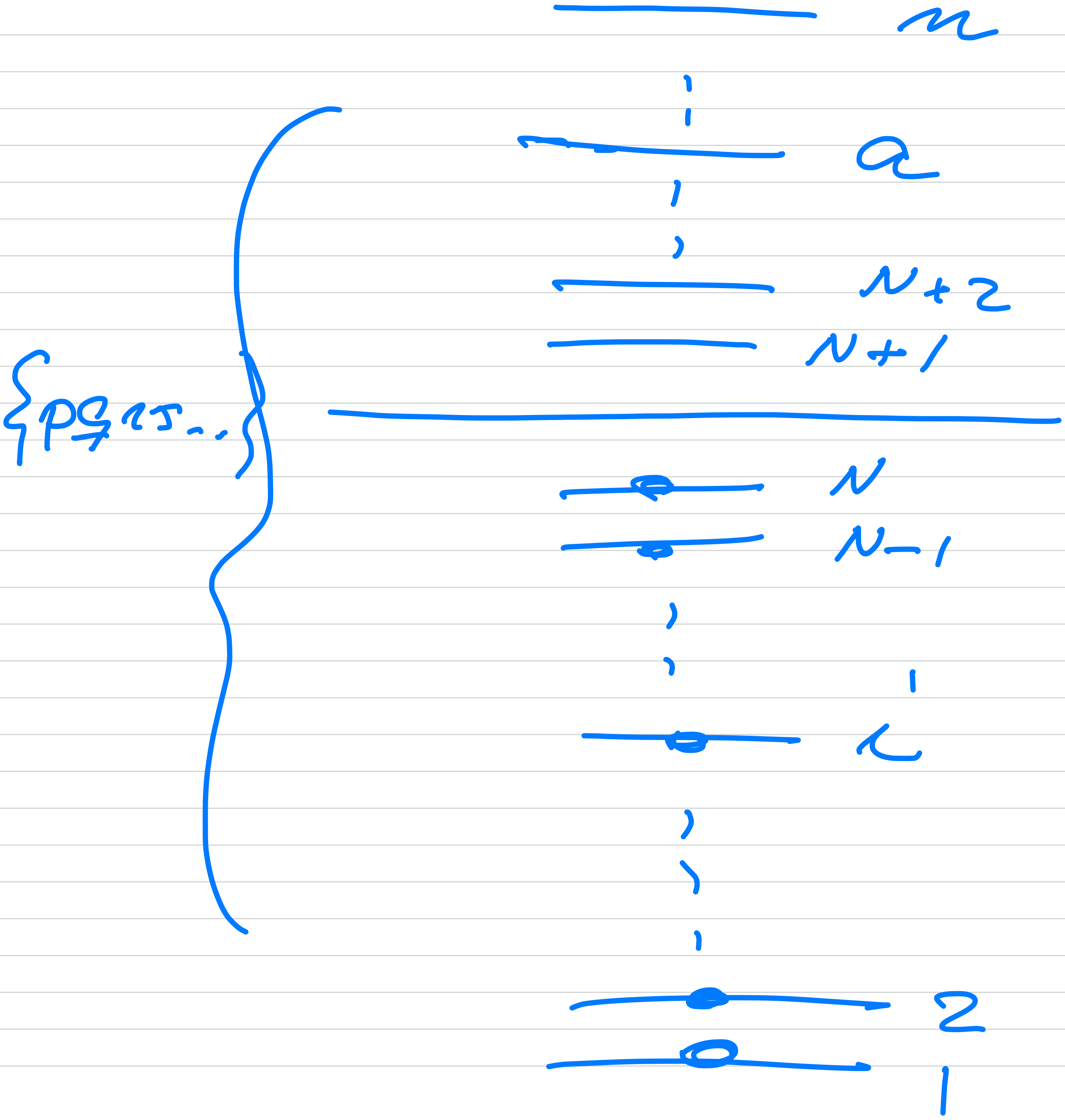
$$+ \sum_{\substack{\alpha > F \\ \beta < F}} \Big[\cdots \underbrace{b_\alpha^\dagger b_\beta^\dagger + b_\beta b_\alpha}_{=0} \cdots \Big]$$

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

$$+ \delta_{\delta\delta} \delta_{\gamma\gamma} \, E_0^{Ref}$$

$$= \underbrace{\varepsilon_{\delta} - \varepsilon_{\underline{\gamma}}}_{\text{1p1h energy difference}} + \underline{\varepsilon_0^{Ref}}.$$

$$\varepsilon_{\delta} + \sum_{\substack{\alpha \geq F \\ \alpha \neq \gamma}} \varepsilon_{\alpha}$$



$\{abcd...\} > F$

particle state

F

hole states,

$\{ijkl...\} \le F$

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

$$a_{q_1}^\dagger a_{q_2}^\dagger \cdots a_{q_N}^\dagger |0\rangle$$

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

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

$$\langle \Phi_0 | a_p^\dagger \underbrace{a_q |\Phi_0\rangle}_{q \in |\Phi_0\rangle} = \delta_{pq}$$

$$\langle 0 | a_p^\dagger a_q | 0 \rangle = 0 = \overbrace{a_p^\dagger a_q}$$

$$a_p^\dagger a_q^\dagger = a_p a_q = 0$$

$$a_a^\dagger a_i |\Phi_0\rangle \qquad a > F$$

$$i \in \{ |\Phi_0\rangle \} \qquad i \le F$$

1ph state

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

$$a_a^\dagger a_i \, a_1^\dagger a_2^\dagger \cdots a_{i-1}^\dagger a_i^\dagger a_{i+1}^\dagger \cdots a_N^\dagger |0\rangle$$

$$a_a^\dagger (-)^{i-1} a_1^\dagger a_2^\dagger \cdots a_{i-1}^\dagger a_{i+1}^\dagger \cdots a_N^\dagger |0\rangle$$

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

N-particle

$$= |\Phi_i^a\rangle$$

2p2h-state

$$a_a^+ a_b^+ a_j a_i |\Phi_0\rangle = |\Phi_{ij}^{ab}\rangle$$

$$(j\,i) \in \{|\Phi_0\rangle\}$$

$$(a\,b) \notin \{|\Phi_0\rangle\}$$

3p3h $|\Phi_{ijk}^{abc}\rangle$

Organizing basis in terms of P-H excitations

$$\left| \Phi^{P}_{H} \right\rangle$$

P: given number of particle states

H: given number of hole states

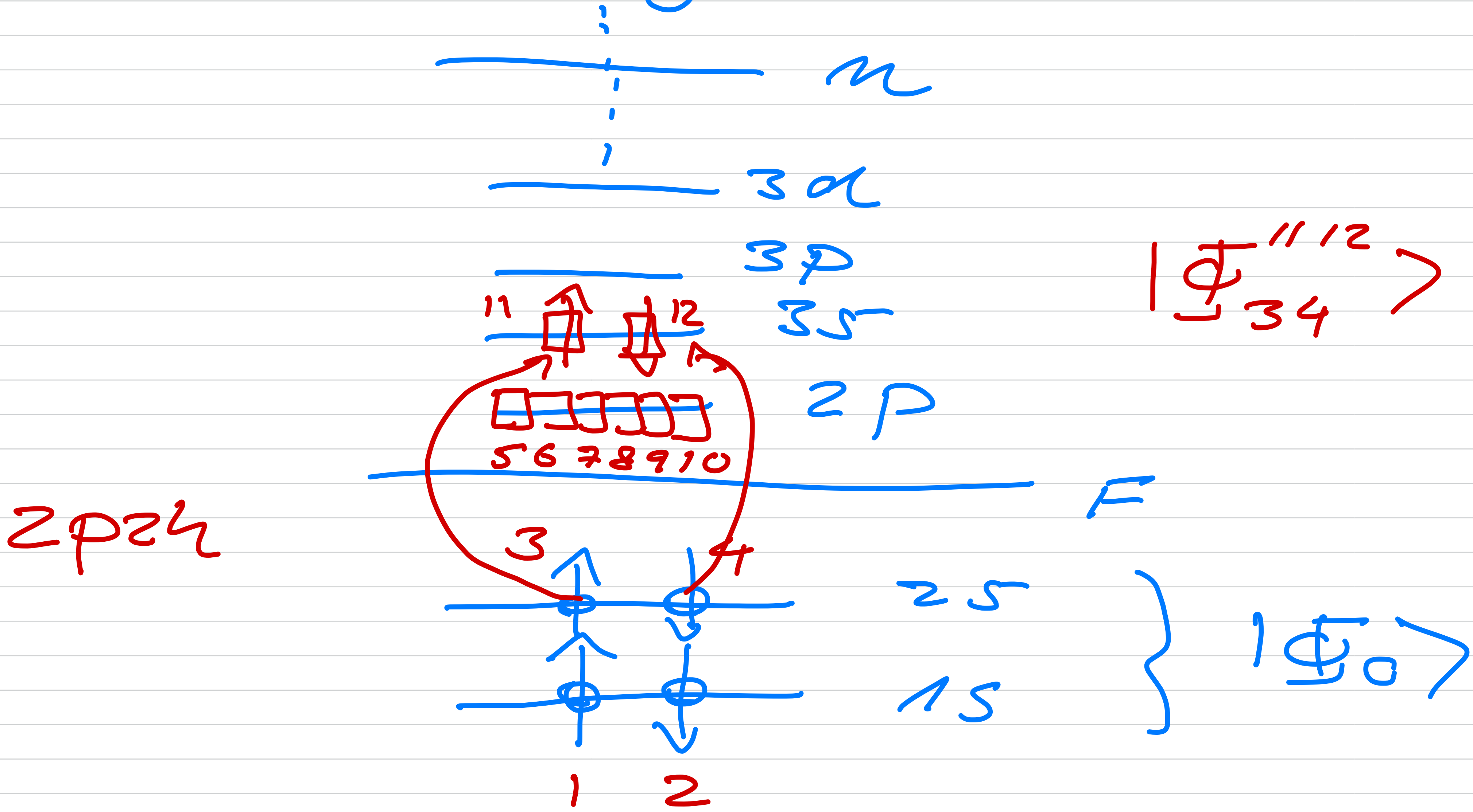
$$\{PH\} = \{0p0h,\ 1p1h,\ 2p2h,\ \ldots\ NpNh\}$$

$0p0h$: $|\Phi_0\rangle$

$$\{|\Phi_0\rangle,\ |\Phi_1\rangle,\ |\Phi_2\rangle\ \ldots\ |\Phi_\infty\rangle\}$$

Example 1

Atomic Beryllium



Suppose we have the "exact" state for the ground state

$$|\Psi_0\rangle = \sum_{PH} C_H^P \underbrace{|\Phi_H^P\rangle}_{\text{ph-basis}}$$

$$= C_0^0 |\Phi_0\rangle + \sum_{ai} C_i^a \underbrace{|\Phi_i^a\rangle}_{(1p1h)\; a_a^\dagger a_i |\Phi_0\rangle} + \sum_{\substack{ab\\ij}} C_{ij}^{ab} \underbrace{|\Phi_{ij}^{ab}\rangle}_{2p2h \;=\; a_a^\dagger a_b^\dagger a_j a_i |\Phi_0\rangle} + \cdots +$$

$$+ \sum_{\substack{a_1 a_2 \ldots a_n \\ i_1 i_2 \ldots i_N}} C_{i_1 i_2 \ldots i_N}^{a_1 a_2 \ldots a_n} \left| \Phi_{i_1 i_2 \ldots i_N}^{a_1 a_2 \ldots a_n} \right\rangle$$

$$\sum_{pq} \langle p | \hat{h}_0 | q \rangle \underbrace{a_p^\dagger a_q}_{\text{normal-ordered with respect to vacuum } |0\rangle}$$

$$a_p^\dagger a_q + a_q a_p^\dagger = \delta_{pq}$$

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

normal-ordered
w.r.t. $|\Phi_0\rangle$

$$+ \frac{\mathcal{E}_0^{Ref}}{\sum_{i=1}^{N} \langle i | \hat{h}_0 | i \rangle}$$

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

$$= \sum_{pq} \langle p | f_0 | q \rangle \Big\{$$

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

$$+ \quad E_0^{Ref} \langle \Phi_i^a | \Phi_i^a \rangle$$

$$\delta_{ii} \delta_{aa} \langle \Phi_0 | \Phi_0 \rangle$$

$$a_i^\dagger a_a a_p^\dagger a_q a_a^\dagger a_i$$

$$\delta_{ii} \, \delta_{ap} \, \delta_{qa}$$

$$a_i^\dagger a_j = \delta_{ij}$$

$$i,j \quad i,j \leq F$$

$$a_i^\dagger a_a a_p^\dagger a_q a_a^\dagger a_i$$

$$- \quad \delta_{iq} \, \delta_{pi} \, \delta_{aa}$$

$$\langle a | \underbrace{h_0 | a}_{\varepsilon_a} \rangle - \langle i | h_0 | i \rangle$$

$$\varepsilon_a - \varepsilon_i \Rightarrow$$

$$\langle \Phi_i^a | H_0 | \Phi_i^a \rangle = \varepsilon_a - \varepsilon_i + E_0^{Ref}$$