Lecture FYS4480, September 21, 2023

New operators

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

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

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

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

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

$$- \sum_{\alpha \leq F} b_\alpha^+ b_\alpha + N$$

$$|\Phi_\alpha\rangle = b_\alpha^+ |\Phi_0\rangle \quad \text{(1 hole state)}$$

$\alpha \leq F$

$$|\Phi_\alpha^\beta\rangle = b_\beta^+ b_\alpha^+ |\Phi_0\rangle = \text{1p1h state}$$

$\beta > F$

$\alpha \leq F$

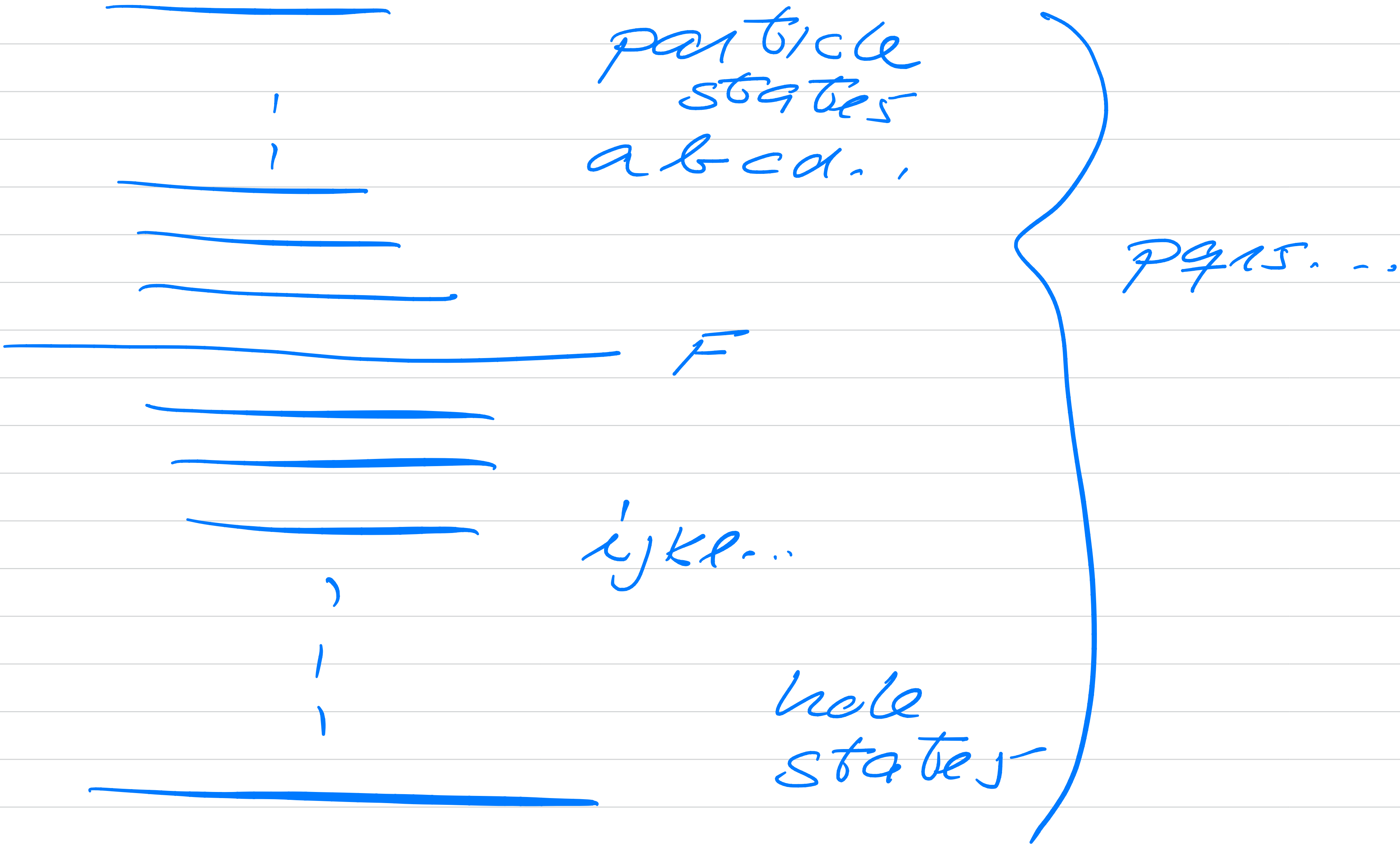
$$\hat{H}_0 = \sum_{\alpha\beta>F} \langle\alpha|\hat{h}_0|\beta\rangle b_\alpha^\dagger b_\beta$$

$$+ \sum_{\substack{\alpha>F \\ \beta\le F}} \left[\langle\alpha|\hat{h}_0|\beta\rangle b_\alpha^\dagger b_\beta^\dagger + \langle\beta|\hat{h}_0|\alpha\rangle b_\beta b_\alpha\right]$$

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

$$\underbrace{+ \sum_{\alpha\le F} \underbrace{\langle\alpha|\hat{h}_0|\alpha\rangle}_{\varepsilon_\alpha}}_{E_0}$$

New label for sp states



Back to $a^\dagger_\alpha a_\beta$

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

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

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

Normal-ordered wrt new vacuum

$$= \sum_p \{a_p^\dagger a_q\} + \underline{N}$$

reference value

$$|\Phi_\alpha^\beta\rangle \to |\Phi_i^a\rangle = \underbrace{a_a^\dagger a_i |\Phi_0\rangle}_{1p1h}$$

N

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

$$= \sum_p \langle \Phi_0 | a_i^\dagger a_a a_p^\dagger a_p a_a^\dagger a_i |\Phi_0\rangle$$

$$\delta_{ii}\,\delta_{ap}\,\delta_{pa} = 1$$

$$\langle \Phi_c | a_r^\dagger a_a a_p^\dagger a_p a_a^\dagger a_i | \Phi_c \rangle$$

$$- \underbrace{\delta_{ip} \delta_{ip} \delta_{aa}}_{1}$$

$$+ \underbrace{\langle \Phi_i^a | N | \Phi_i^a \rangle}_{= N}$$

$$= N$$

$$a_i|\Phi_c\rangle / |\Phi_i^a\rangle$$

$$\langle \Phi_i | \hat{N} | \overbrace{\Phi_i}^{} \rangle = N - 1$$

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

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

$$+ E_0$$

$$" \sum_{i \le F} \underbrace{\langle i | \hat{h}_0 | i \rangle}_{\varepsilon_i}$$

$$= \sum_{pq} \langle p | \hat{h}_0 | q \rangle \langle \Phi_0 | a_i^\dagger a_a a_p^\dagger a_q$$

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

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

$$\delta_{ap}\delta_{aq}\delta_{ii'}$$

$$\times \langle a|\hat{h}_0|a\rangle$$

$$= \varepsilon_a$$

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

$$- \delta_{ip}\delta_{i'q}\delta_{aa}$$

$$\times \langle i|\hat{h}_0|i\rangle$$

$$= \varepsilon_{i'}$$

$$\Rightarrow \quad \langle \Phi_i^a|H_0|\Phi_i^a\rangle = \varepsilon_a - \varepsilon_{i'} + \mathcal{E}_0$$

$$\langle \Phi_0 | H_0 | \Phi_i^a \rangle =$$

$$\sum_{pq} \langle \Phi_0 | a_p^\dagger a_q \, a_a^\dagger a_i | \Phi_0 \rangle \times \langle p | \hat{h}_0 | q \rangle \qquad \delta_{pi}\,\delta_{qa}$$

$$= \langle i | \hat{h}_0 | a \rangle = \delta_{ia}\, \varepsilon_a$$

$$\hat{h}_0 | a \rangle = \varepsilon_a | a \rangle$$

Two-body $\hat{v}_N$

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

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

$$\underbrace{+ \frac{1}{2} \sum_{ij} \langle ij | v | ij \rangle_{AS}}_{\langle \Phi_0 | H_I | \Phi_0 \rangle}$$

Def:

$$E_0^{Ref} = \underbrace{\mathcal{E}_0}_{\langle \Phi_0 | \hat{H}_0 | \Phi_0 \rangle} + \langle \Phi_0 | H_1 | \Phi_0 \rangle$$

$$\hat{H} = \hat{F}_N + \hat{V}_N + \underbrace{E_0^{Ref}}_{\langle \Phi_0 | H | \Phi_0 \rangle}$$

$$\hat{F}_N = \sum_{pqi} \{a_p^\dagger a_q\} \langle pi | v | qi \rangle_{AS} + \sum_{pq} \{a_p^\dagger a_q\} \langle p | \hat{h}_0 | q \rangle$$

$$\langle p | \hat{f} | q \rangle = \sum_{i \le F} \langle pi | v | qi \rangle_{AS} + \langle p | \hat{h}_0 | q \rangle$$

OP

Example

$$\langle \Phi_r^a | \hat{H} | \Phi_r^a \rangle$$

$$= \langle \Phi_r^a | \hat{V}_N + \hat{F}_N + E_0^{\text{ref}} | \Phi_r^a \rangle$$

$$\hat{F}_N = \sum_{pq} \langle p | f | q \rangle \{ a_p^\dagger a_q \}$$

$\hat{F}_N$:

$$\langle \Phi_r^a | \hat{F}_N | \Phi_r^a \rangle$$

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

$$a_i^\dagger a_a \, a_p^\dagger a_q \, a_{a'}^\dagger a_{i'}$$

$$\delta_{ii'} \delta_{pa} \delta_{qa'} \times \langle a | f | a' \rangle$$

$$- \delta_{aa'} \delta_{ip} \delta_{qi'} \times \langle i' | f | i \rangle$$

$$= \varepsilon_a + \sum_j \langle aj | v | aj \rangle_{AS}$$

$$- \varepsilon_{i'} - \sum_j \langle i'j | v | i'j \rangle_{AS}$$

$$\frac{1}{4}\sum_{pqrs}\langle pq|v|rs\rangle_{AS}$$

$$\times \langle \Phi_0 | a_i^\dagger a_a \, a_p^\dagger a_q^\dagger a_s a_r \, a_a^\dagger a_i | \Phi_0\rangle$$

$$-\frac{1}{4}\langle ai|v|ai\rangle_{AS}$$

+3 more

$$\langle ai|v|ai\rangle_{AS} = -\langle ia|v|ai\rangle_{AS}$$

$$\text{—}\;\;''\;\;\text{—} \;= \langle ia|v|ia\rangle_{AS}$$

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

$$+ \sum_j \langle aj \| v \| aj \rangle_{AS} - \sum_j \langle ij \| v \| ij \rangle_{AS}$$

$$+ \langle ai \| v \| ia \rangle_{AS} + E_0^{Ref},$$

$$\langle \Phi_i^a | H | \Phi_j^b \rangle = ?$$

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

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

2p2h

$$E_0^{Ref} \langle \Phi_{ij}^{ab} | \Phi_0 \rangle$$

$$\langle \Phi_0 | a_i^\dagger a_j^\dagger a_b a_a | \Phi_0 \rangle = 0$$

$\hat{F}_N$:

$$\sum_{pq} \langle p | \hat{f} | q \rangle \langle \Phi_0 | a_i^\dagger a_j^\dagger a_b a_a a_p^\dagger a_q \times | \Phi_0 \rangle$$

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

$$a_p^\dagger a_q | \Phi_0 \rangle \rightarrow | \Phi_0 \rangle$$

$$\langle 2p2h | \Phi_0 \rangle \text{ or } \langle 2p2 | 1p1h \rangle \rightarrow | 1p1h \rangle$$

γ_N :

$$\frac{1}{4}\sum_{pqrs} \langle pq||rs\rangle_{AS}$$

$$\times \langle \Phi_0 | a_i^{+} a_j^{+} a_b a_a \, a_p^{+} a_q^{+} a_s a_r | \Phi_0 \rangle$$

$\overline{a_p a_q^{+}} = \delta_{pq}$ $pq > F$

$\overline{a_p^{+} a_q} = \delta_{pq}$ $pq \le F$

$$\delta_{ap}\,\delta_{qb}\,\delta_{sj}\,\delta_{ir}$$

$$\times \langle ab||ij\rangle_{AS}$$

$+3$ more $\Rightarrow$ $\langle ab||ij\rangle_{AS}$

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

$$\langle \underbrace{\Phi_{ijk}^{abc}}_{3p3h} | H | \Phi_0 \rangle = 0$$

$$\langle \Phi_0 | H | \Phi_i^a \rangle$$

E_0^{Ref} :

$$E_0^{Ref} \langle \Phi_0 | \Phi_i^a \rangle = 0$$

$\hat{F}_N$:

$$\sum_{pq} \langle p|\hat{f}|q\rangle \left\{ \langle \Phi_c | a_p^\dagger a_q a_a^\dagger a_i | \Phi_c\rangle \right\}$$

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

$$= \langle i|\hat{h}|a\rangle + \sum_{j\le F} \langle ij|v|aj\rangle_{AS}$$

$\hat{V}_N$:

$$\sum_{pqrs} \langle pq|\hat{v}|rs\rangle_{AS} \times \langle \Phi_c | a_p^\dagger a_q^\dagger a_r a_s a_a^\dagger a_i | \Phi_c\rangle = 0$$