FYS4480/9480, lecture September 26

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$$(\mathcal{H} - E_0)\sum_{PH} c_H^P |\Phi_H^P\rangle$$

$$|\Phi_0^G\rangle = |\Phi_0\rangle$$

opou

$$\langle\Phi_0|(\mathcal{H} - E_0)|\Big(1 + \overbrace{\sum_{ai} c_i^a |\Phi_i^a\rangle}^{1p1h} + \sum_{abij} c_{ij}^{ab} |\Phi_{ij}^{ab}\rangle + \cdots\Big)|\Phi_0\rangle$$

$$\Delta E_0 = E_0 - E_0^{REF} = \sum_{ai} \langle i|f|a\rangle \boxed{c_i^a} + \sum_{abij} \langle ij|v|ab\rangle \boxed{c_{ij}^{ab}}$$

Hamiltonian matrix

$$
\begin{array}{c|cccccc}
 & 0p0h & 1p1h & 2p2h & 3p3h & \cdots & NpNh \\
\hline
0p0h & E_0^{Ref} & \langle \Phi_0 | H | \Phi_i^a \rangle & \langle \Phi_0 | H | \Phi_{ij}^{ab} \rangle & 0 & 0 \cdots & 0 \\
1p1h & & & \times & \times & 0 & \cdots \\
2p2h & & \times & \times & & & \\
3p3h & 0 & \times & \times & \times & & \\
\vdots & 0 & 0 & \times & \times & \times & \\
\vdots & \vdots & 0 & 0 & \times & & \\
\vdots & & & \vdots & 0 & & \\
 & \vdots & \vdots & \vdots & \vdots & & \\
NpNh & 0 & 0 & 0 & \vdots & 0 &
\end{array}
$$

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

$$\langle i | \hat{h}_0 | a \rangle + \sum_{j \in F} \langle ij | \hat{v} | aj \rangle_{AS}$$

Hartree-Fock algorithm

$$\langle i | \hat{f} | a \rangle = 0$$

$\hat{h}_0 |q\rangle$

$= \varepsilon_q |q\rangle$

$$\langle p | \hat{f} | q \rangle = \delta_{pq} \, \varepsilon_p^{HF}$$

$$\hat{f} |q\rangle \Rightarrow \hat{f} |q\rangle_{HF} = \varepsilon_q^{HF} |q\rangle_{HF}$$

$$\langle i | f | i \rangle = \varepsilon_i^{HF}$$

$$\langle a | f | a \rangle = \varepsilon_a^{HF}$$

$$\mathcal{H} c = \lambda c$$

$$U U^{+} = U^{+} U = \mathbb{1} \qquad U^{+} = U^{-1}$$

$$U \mathcal{H} \underset{\uparrow}{} c = \lambda U c$$

$$\mathbb{1}$$

$$\underbrace{U \mathcal{H} U^{+}}_{D} \underbrace{U c}_{y} = \lambda \underbrace{U c}_{y}$$

$$D = \begin{bmatrix} \lambda_1 & & & \\ & \lambda_2 & & \\ & & \ddots & \\ & & & \lambda_N \end{bmatrix}$$

$$\mathcal{U} = \mathcal{U}_p \, \mathcal{U}_{p-1} \cdots \mathcal{U}_1$$

$$\mathcal{U}_p \, \mathcal{U}_{p-1} \cdots \mathcal{U}_1 \, \mathcal{H} \, \mathcal{U}_1^{\dagger} \cdots \mathcal{U}_p^{\dagger}$$

$$\mathcal{U}_1 \, \mathcal{H} \, \mathcal{U}_1^{\dagger}$$

$$\begin{array}{c} \quad |p|2 \\ \begin{bmatrix} \times & \times & \times & 0 & 0 \; 0 & 0 \\ \times & \times & \times & - & - & - \\ \times & \times & \times & & & \\ 0 & \times & \times & - & - & \\ \vdots & 0 & \times & & & \\ \vdots & \vdots & \vdots & & & \\ 0 & & \vdots & & & \end{bmatrix} \end{array} \longrightarrow$$

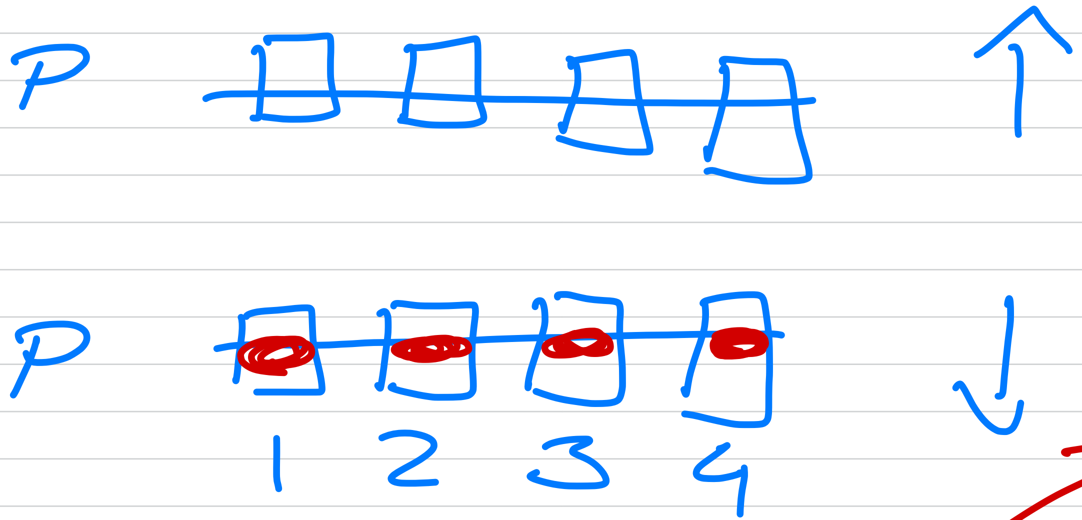
$$\begin{bmatrix} x & 0 & x & 0 & 0 & \cdots & 0 \\ 0 & x & x & x & 0 & - & - \\ x & x & \vdots & \vdots & & & \\ 0 & x & \vdots & & & & \\ 0 & x & \ddots & \vdots & & & \end{bmatrix}$$

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

$$= 0$$

Lipkin-model

$J_z = 2$



$\binom{8}{4} = 70$

$J_z = -2$

$$\mathcal{H}_0|\Phi_0\rangle = \varepsilon_0|\Phi_0\rangle$$

$J = 2$

$J_z = -2, -1, 0, +1, +2$

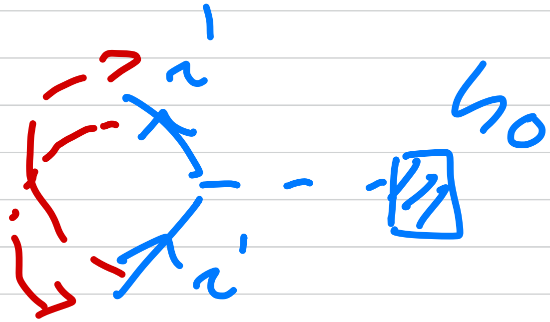
Diagrammatic representation

$$\Delta E_0 = E_0 - E_0^{Ref}$$

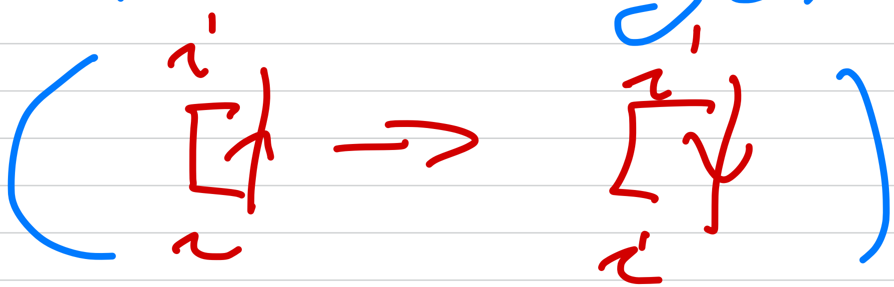
$$= \sum_{ai} \langle i|\hat{f}|a\rangle c_i^a + \sum_{\substack{ab\\ij}} \langle ij|v|ab\rangle_{AS} \times c_{ij}^{ab}$$

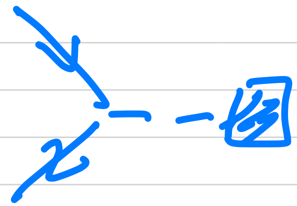
$$E_0^{Ref} = \sum_{i \le F} \langle i | \hat{h}_0 | i \rangle$$

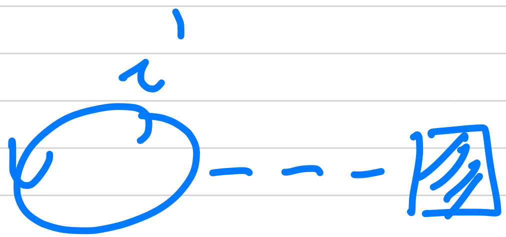
$$+ \frac{1}{2} \sum_{ij \le F} \left\{ \langle ij | v | ij \rangle - \langle ij | v | ji \rangle \right\}$$

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

Now: hole states are written as downgoing arrows



$$\sum_{i \le F} \langle i | h_0^2 | i \rangle \rightarrow \sum_{i \le F}$$ 

$=$ 

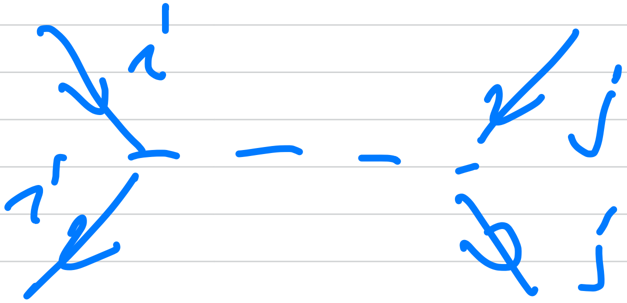
$(-)^{n_h + n_e}$

n_e = number of closed loops

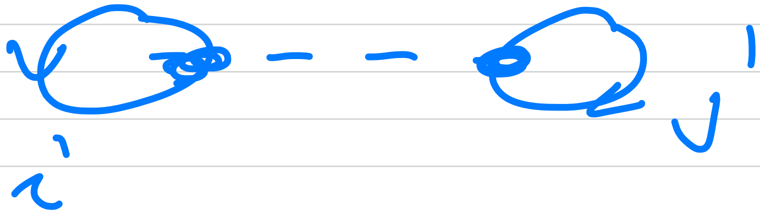
n_h = number of holes

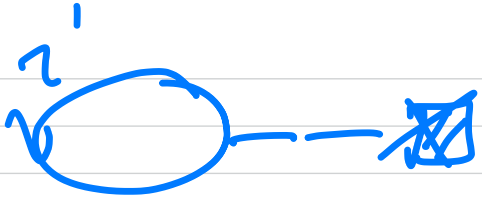
$$\sum_{i'j' \le F} \langle i'j' | v | i'j' \rangle \longrightarrow$$

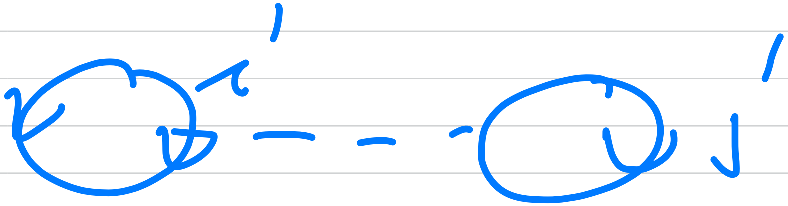
$$\sum_{i'j' \le F}$$  $\longrightarrow$ Ph-Formulierung

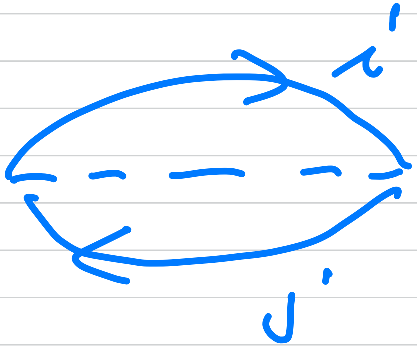
$$\sum_{i'j' \le F}$$ 

$n_h = 2$

$=$  $n_e = 2$

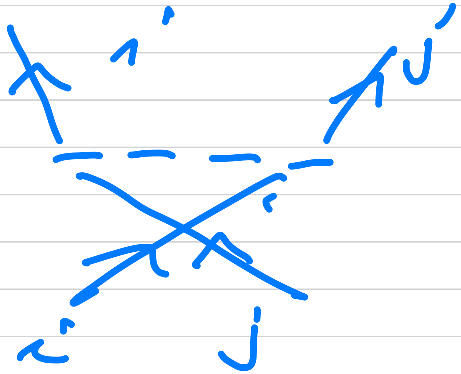
$$E_0^{Ref} =$$ 

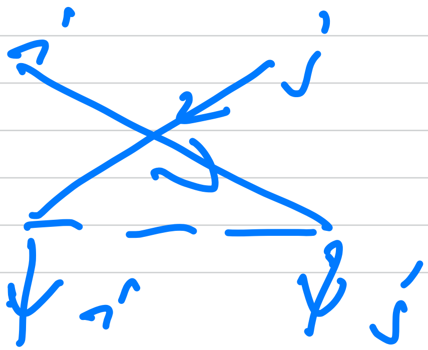
$$+$$ 

$$+$$ 

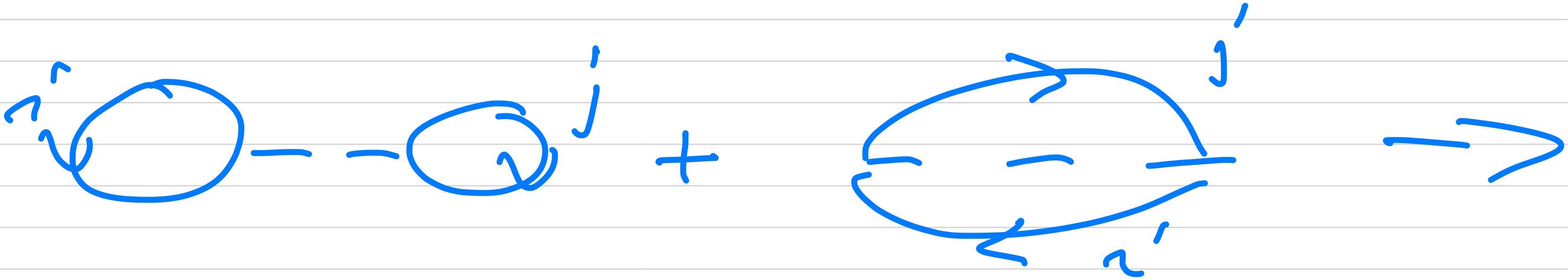
$n_h = 2$

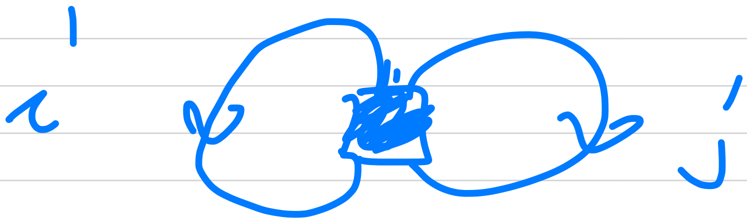
$n_\ell = 1$

$$- \sum_{i'j' \leq F} \langle i'j' | v | j'i' \rangle \Rightarrow \sum_{i'j' \leq F}$$ 

$$\xrightarrow{PH} \sum_{i'j' \leq F}$$ 

Hugenholtz (antisymm)



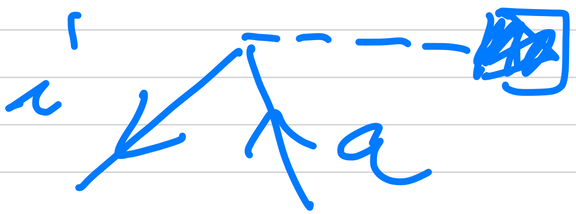


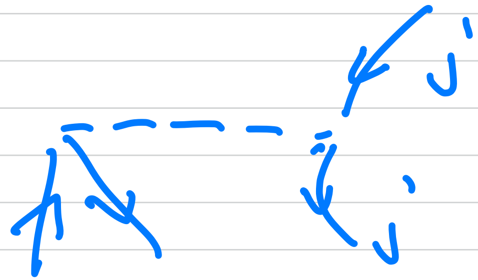
$$\langle i|\hat{f}|a\rangle = \langle \Phi_0|\hat{f}|\Phi_i^a\rangle$$

$$= \langle i|\hat{h}_0|a\rangle + \sum_{j\le F} \langle ij|v|aj\rangle_{AS}$$

$$\langle ij|v|aj\rangle - \langle ij|v|ja\rangle$$

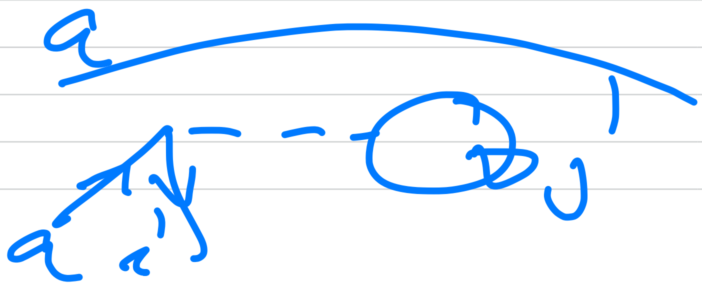
DH





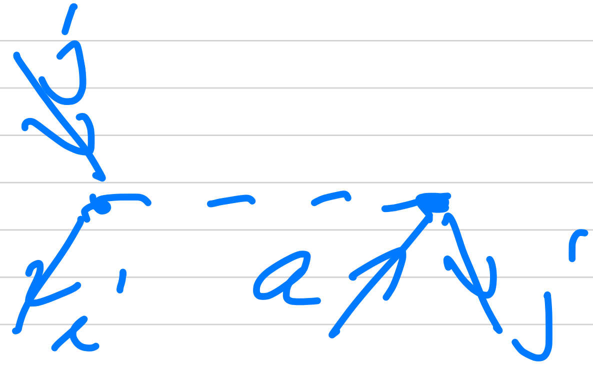
$$\sum_{j\le F}$$

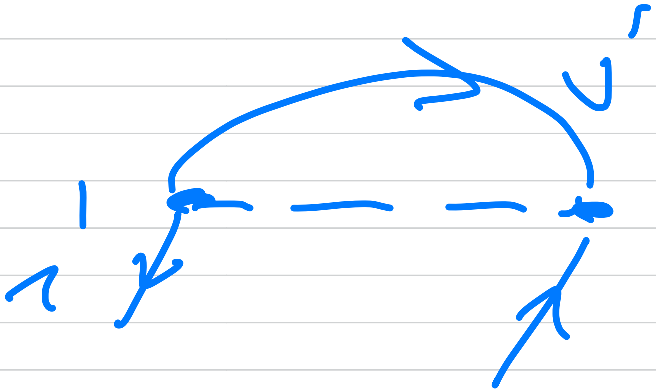
$$=$$



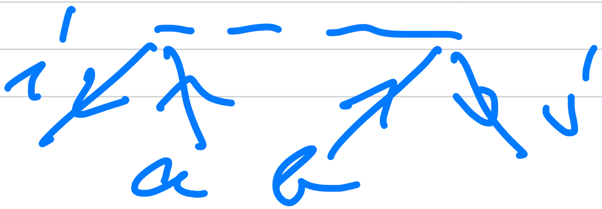
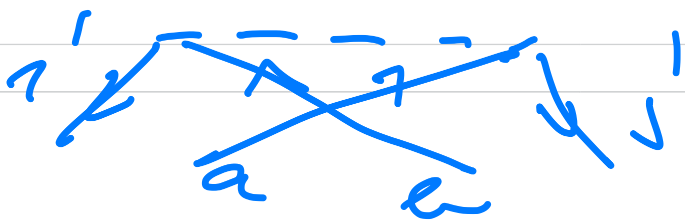
$$-\sum_{j\le F} \langle ij|v|ja\rangle$$

$$\rightarrow \sum_{j\le F}$$





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

2p2h  + 

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