FYS 4480/9480

November

28, 2024

FYS 4480/9480 November 28

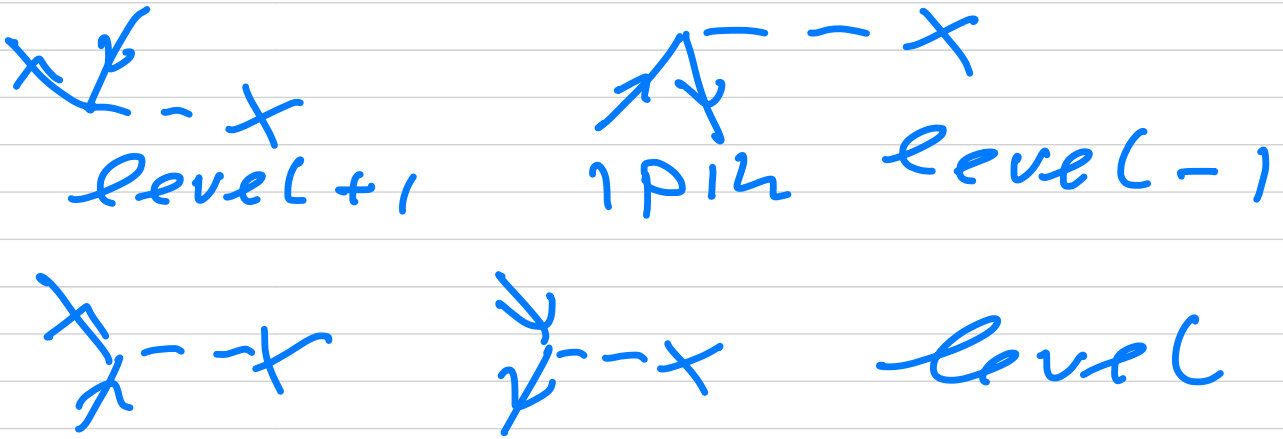
$$\langle \Phi_0 | \hat{H} e^{\hat{T}_2} | \Phi_0 \rangle = E_{CCD}$$

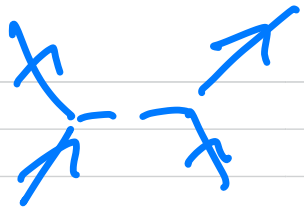
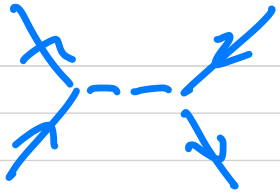
$$\langle \Phi_{ij}^{ab} | \hat{H} e^{\hat{T}_2} | \Phi_0 \rangle = E_{CCD} \cdot \langle \Phi_{ij}^{ab} | e^{\hat{T}_2} | \Phi_0 \rangle$$

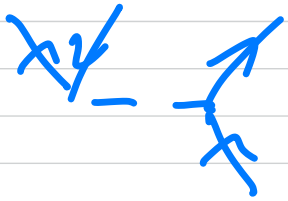
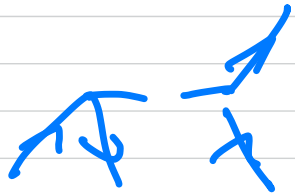
$$= E_{CCD}\, t_{ij}^{ab}$$

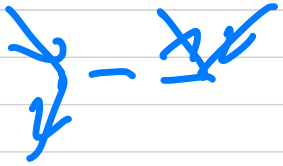
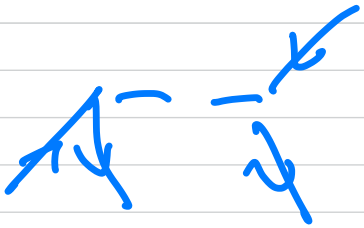
CCD equations →

F_N :



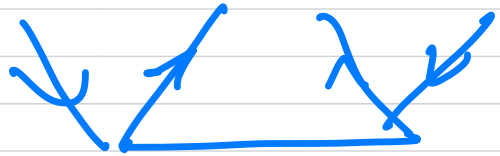
V_N :    level 0

 level 1  -1

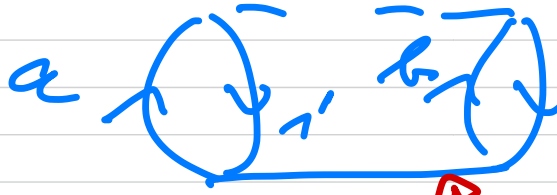
 level 1  -1

 level -2

 level $+2$

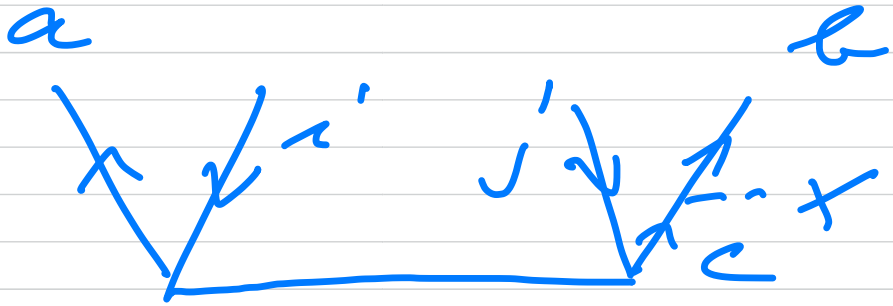
$\overline{I_2}$:  level 2

Energy ΔE_{CCD}

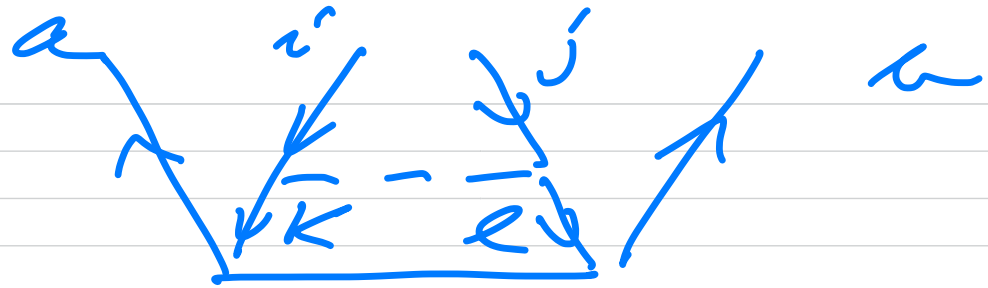


$$\frac{1}{4}\sum_{\substack{ab \\ i'j'}} t_{ij}^{ab} \langle ij||ab\rangle$$

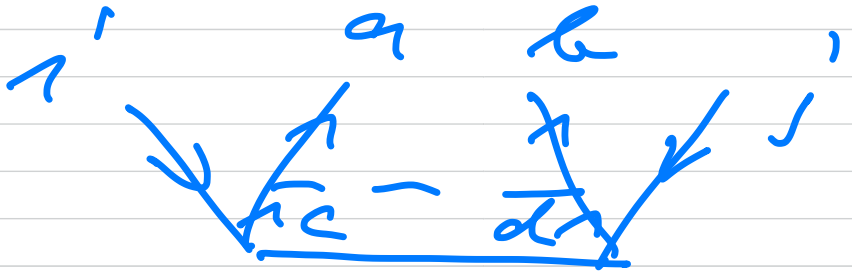
$\langle 1$



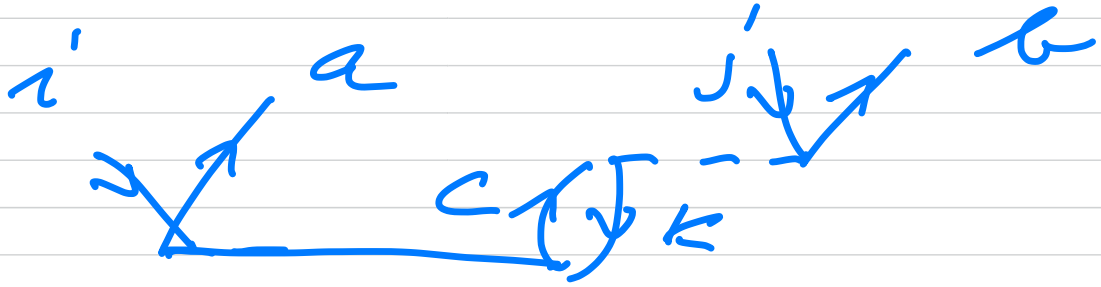
$\angle 2$



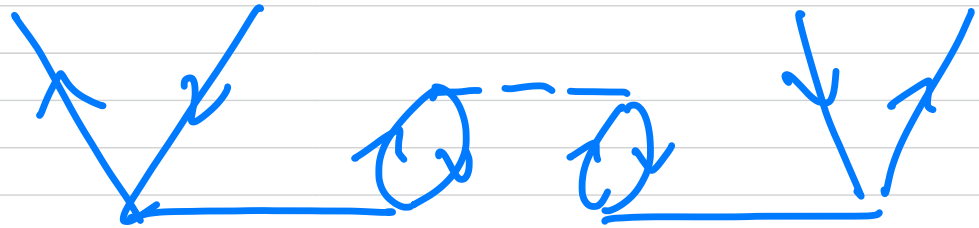
+



+ $\langle \Phi_0 | H_I R_{--}$

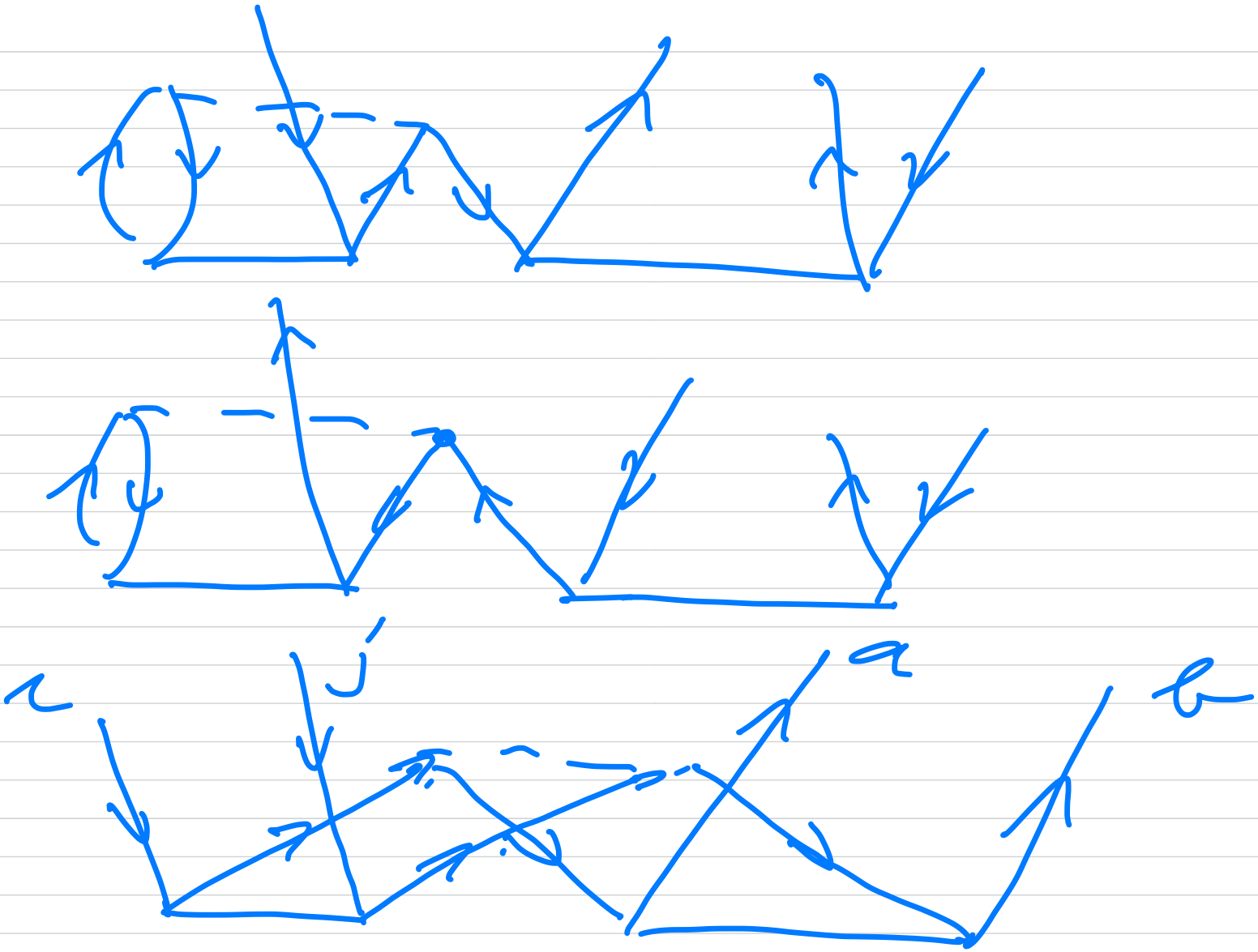


$\angle 3$

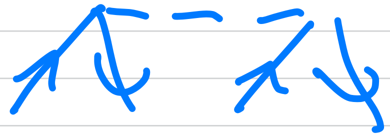


$H_N T_2^2$ $\quad e^{T_2}|\Phi_0\rangle =$

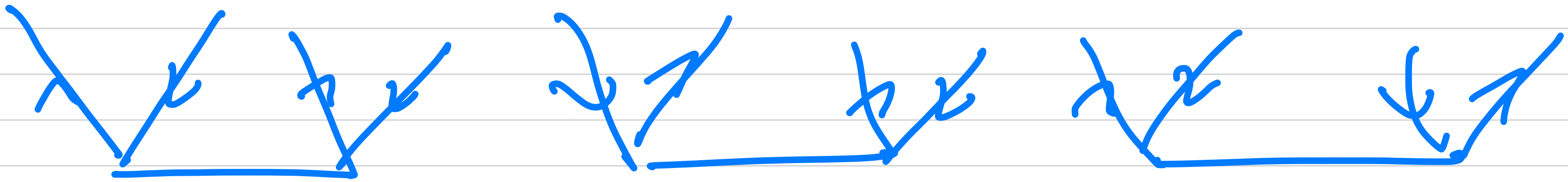
$(1 + T_2 + T_2^2/2 + T_2^3/3! + \cdots)$


a
b

$K_N T_2^3$



level -2



open level 6

$$\Delta E_{CCD} = \frac{1}{4} \sum_{\substack{ab \\ ij}} t_{ij}^{ab} \langle ij||ab \rangle$$

$(ij) \rightarrow I$ contains all 2h configs

$(ab) \rightarrow A$ contains all 2p configs

Example: pairing model

2p config

$|3\uparrow 5\downarrow\rangle$

$|4\uparrow 4\downarrow\rangle$

p=4

p=3

p=2

p=1

2h config : $|1\uparrow 1\downarrow\rangle$

$|2\uparrow 2\downarrow\rangle$

config I = 2

config A = 2

$t_{ij}^{ab} \rightarrow T_{IA}$

$\langle ab||ij\rangle \rightarrow V_{AI}$

$$\Delta E_{CCD} = \frac{1}{4} \sum_{\substack{ab \\ ij}} t_{ij}^{ab} v_{ij}^{ab}$$

$$= \frac{1}{4} \sum_{IA} \overline{I_A} V_{AI}$$

MBPT(2)

$$\Delta E_0^{(2)} = \langle \Phi_0 | H_I | \Phi_M \rangle \langle \Phi_M | H_I \frac{}{E_0} \times | \Phi_0 \rangle$$

$$= \langle \Phi_0 | H_I \; R^{(1)} | \Phi_0 \rangle$$

$$R^{(1)} = \frac{|\Phi_m\rangle\langle\Phi_m|\mathcal{H}_I|\Phi_k\rangle}{E_0 - E_m}$$

$$= \frac{\langle ab|r|ij\rangle}{\varepsilon_i + \varepsilon_j - \varepsilon_a - \varepsilon_b}$$

$$\Delta E_0^{(2)} = \frac{1}{4} \sum_{\substack{ab \\ ij}} \frac{\langle ij|r|ab\rangle\langle ab|r|ij\rangle}{\varepsilon_i + \varepsilon_j - \varepsilon_a - \varepsilon_b}$$

$$\Delta E_{FCI} = \sum c_{ij}^{ab} \langle ab|r|ij\rangle$$

$$\Delta E_{CCD} = \frac{1}{4} \sum_{\substack{ab \\ ij}} t_{ij}^{ab} \langle ab|r|ij\rangle$$

Final oral exam

- 25-30 min
- 10-15 min questions

- contain
  - Background (2nd quant, Wick's theorem)
  - methods
    - FCI, HF+DFT, MBPT
    - CC
  - link with calculations (2nd midterm)
  - conclusions