# FYS4480/9480, lecture
November 23, 2025

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$$|\Psi_0\rangle = e^{T}|\Phi_c\rangle$$

$$T = T_1 + T_2 + \cdots + T_{NPNH}$$

FCI

$$|\Psi_c\rangle = (1 + \hat{C})|\Phi_c\rangle$$

$$\hat{C} = \sum_{PH>0} C_H^P |\Phi_H^P\rangle$$

$$|\Phi_H^P\rangle = \underbrace{a_{a_1}^{\dagger} a_{a_2}^{\dagger} \cdots a_{i_N} a_{i_{N-1}} \cdots a_{i_1}}_{NPNH} \times |\Phi_c\rangle$$

$$T \simeq T_2 = \frac{1}{4}\sum_{abij} t_{ij}^{ab} a_a^{\dagger} a_b^{\dagger} a_j a_i$$

$$\mathcal{H} e^{T_2} |\Phi_0\rangle = \mathcal{H}\left(1 + T_2 + \frac{1}{2!} T_2^2 + \cdots\right)$$

$$\times |\Phi_0\rangle$$

$$\left( \mathcal{H} |\Psi_0\rangle = E_0 |\Psi_0\rangle \right)$$

$$\langle \Phi_0 | \mathcal{H}\left(1 + T_2 + \frac{1}{2!} T_2^2 + \cdots\right) |\Phi_0\rangle$$

$$= \underbrace{\langle \Phi_0 | \mathcal{H} | \Phi_0 \rangle}_{E_0^{Ref}} + \langle \Phi_0 | \mathcal{H} T_2 | \Phi_0 \rangle$$

$$= \langle \Psi_0 | E_0 e^{T_2} | \Phi_0 \rangle$$

$$= \langle \Psi_0 | E_{CCD} e^{T_2} | \Phi_0 \rangle$$

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

$$= \langle \Phi_0 | \mathcal{H} T_2 | \Phi_0 \rangle$$

$$= \sum_{\substack{ab \\ ij}} t_{ij}^{ab} \langle ab | v | ij \rangle$$

$$\Big( \underbrace{\sum_{ai} t_i^a}_{T_1} \langle a | f | i \rangle \Big)$$

$$\langle \Phi_i^a | \mathcal{H} e^{T_2} | \Phi_0 \rangle = 0$$

$$\langle \Phi_{ij}^{ab} | \mathcal{H} e^{T_2} | \Phi_0 \rangle = E_{CCD} \langle \Phi_{ij}^{ab} | e^{T_2} | \Phi_0 \rangle$$

$$\langle \Phi_{ij}^{ab} | H \left(1 + T_2 + \frac{1}{2} T_2^2 + \cdots\right) | \Phi_0 \rangle$$

$$= E_{CCD} \langle \Phi_{ij}^{ab} | \left(1 + T_2 + \cdots\right) | \Phi_0 \rangle$$

$$= E_{CCD} \langle \Phi_{ij}^{ab} | \frac{1}{4} \sum_{\substack{cd\\kl}} t_{kl}^{cd}$$

$$\times\, a_c^\dagger a_d^\dagger a_l a_k | \Phi_0 \rangle$$

$$\langle \Phi_0 | a_i^\dagger a_j^\dagger a_b a_a$$

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

$$\langle \Phi_{ij}^{ab} | \left( E_0^{Ref} + F_N + V_N \right) \left( 1 + T_2 + \frac{1}{2} T_2^2 \right)$$

$$\times | \Phi_0 \rangle$$

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

$$E_0^{Ref}\, t_{ij}^{ab} + \langle \Phi_{ij}^{ab} | F_N T_2 | \Phi_0 \rangle$$

$$( = \langle ab | v | ij \rangle$$

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

$$+ \langle \Phi_{ij}^{ab} | V_N T_2 | \Phi_0 \rangle$$

$$+ \langle \Phi_{ij}^{ab} | V_N \frac{1}{2} T_2^2 | \Phi_0 \rangle$$

$$\langle ab||ij\rangle + \langle \Phi_{ij}^{ab} | F_N T_2 | \Phi_0 \rangle$$

$$+ \langle \Phi_{ij}^{ab} | V_N T_2 | \Phi_0 \rangle$$

$$+ \langle \Phi_{ij}^{ab} | V_N \frac{1}{2} T_2^2 | \Phi_0 \rangle$$

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

$$\sum_{\substack{cd \\ kl}} t_{kl}^{cd} \langle cd||kl\rangle$$

$$t_{ij}^{ab}(0) = \frac{\langle ab||ij\rangle}{\varepsilon_i + \varepsilon_j - \varepsilon_a - \varepsilon_b}$$

$$\langle \Phi_{ij}^{ab} | F_N T_2 | \Phi_0 \rangle$$

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

$$a_i^{\dagger} a_j^{\dagger} a_k a_a \; a_p^{\dagger} a_q \; a_c^{\dagger} a_d^{\dagger} a_l a_k$$

$$L1 = \Big( \sum_c \langle a | f | c \rangle t_{ij}^{cb} + \sum_d \langle b | f | d \rangle t_{ij}^{ad} \Big)$$

$$- \Big( \sum_l \langle l | f | j \rangle t_{il}^{ab} + \sum_k \langle k | f | i \rangle t_{kj}^{ab} \Big)$$

$$\langle \Phi_{ij}^{ab} | V_N T_2 | \Phi_0 \rangle$$

$$\frac{1}{16} \left\{ a_i^\dagger a_j^\dagger \{ a_b a_a \; a_p^\dagger a_q^\dagger a_s a_r \; a_c^\dagger a_d^\dagger \} a_l a_k \right\}$$

$$a_i^\dagger a_j^\dagger a_b a_a \; a_p^\dagger a_q^\dagger a_s a_r \; a_c^\dagger a_d^\dagger a_l a_k$$

$$L2a = \frac{1}{2} \sum_{cd} \langle ab \| cd \rangle t_{ij}^{cd}$$

$$L2b = \frac{1}{2} \sum_{kl} \langle kl \| ij \rangle t_{kl}^{ab}$$

$$L2C = -\sum_{kc} \Big( \langle lk|v|cj\rangle t_{ik}^{ac} - \langle lk|v|ci\rangle t_{jk}^{ac} - \langle ak|v|cj\rangle t_{ik}^{lc} + \langle ak|v|ci\rangle t_{jk}^{lc} \Big)$$

$$\langle \Phi_{ij}^{ab} | V_N \tfrac{1}{2} T_2^2 | \Phi_0 \rangle$$

$G_1$ :

$$a_i^\dagger a_j^\dagger a_b a_a \; a_p^\dagger a_q^\dagger a_s a_r \; a_c^\dagger a_d^\dagger a_e a_k \; a_e^\dagger a_f^\dagger a_n a_m$$

$$\langle pq||rs\rangle \qquad t_{ke}^{cd} \qquad t_{mn}^{ef}$$

$$G_1 = \frac{1}{4} \sum_{\substack{ke \\ cd}} \underbrace{\langle ke||cd\rangle}_{} \, t_{ij}^{cd} \, t_{ke}^{ab}$$

$$V_{IA} \cdot \overline{T_{AI}}$$

$$\times$$

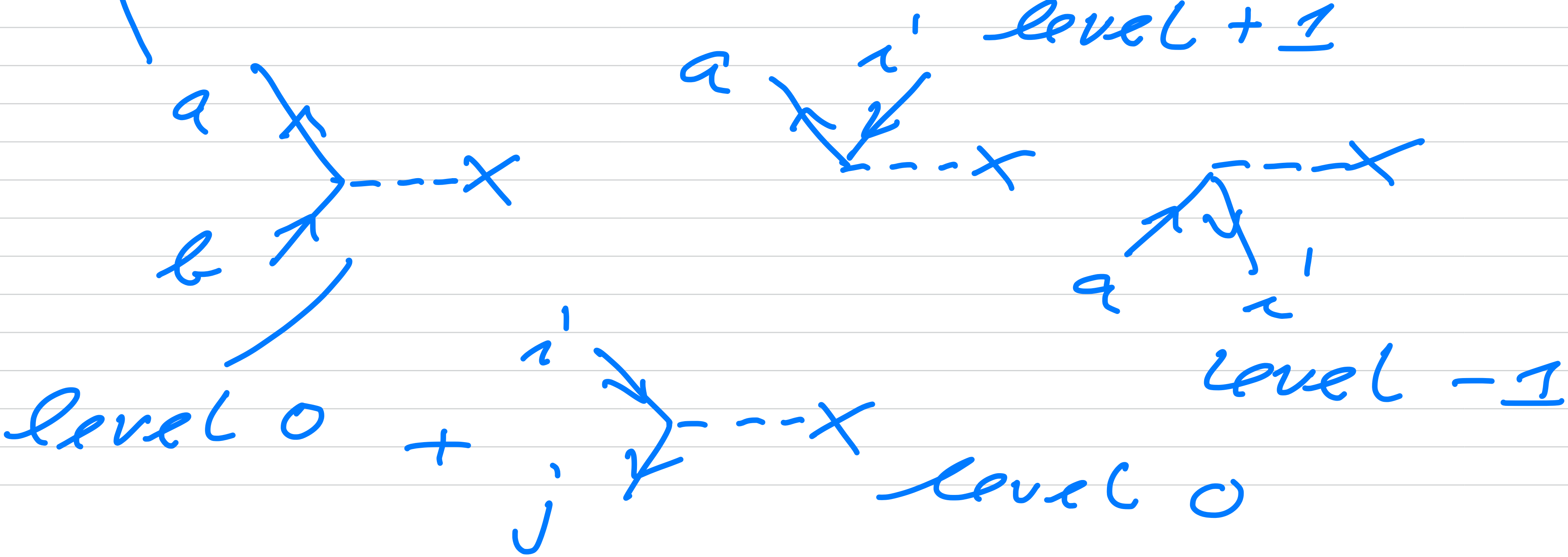
# Diagrammatic approach

$$T_2 = \frac{1}{4} \sum_{\substack{ab \\ ij}} t_{ij}^{ab} a_a^\dagger a_b^\dagger a_j a_i$$


excitation level 2
(2p2h states)

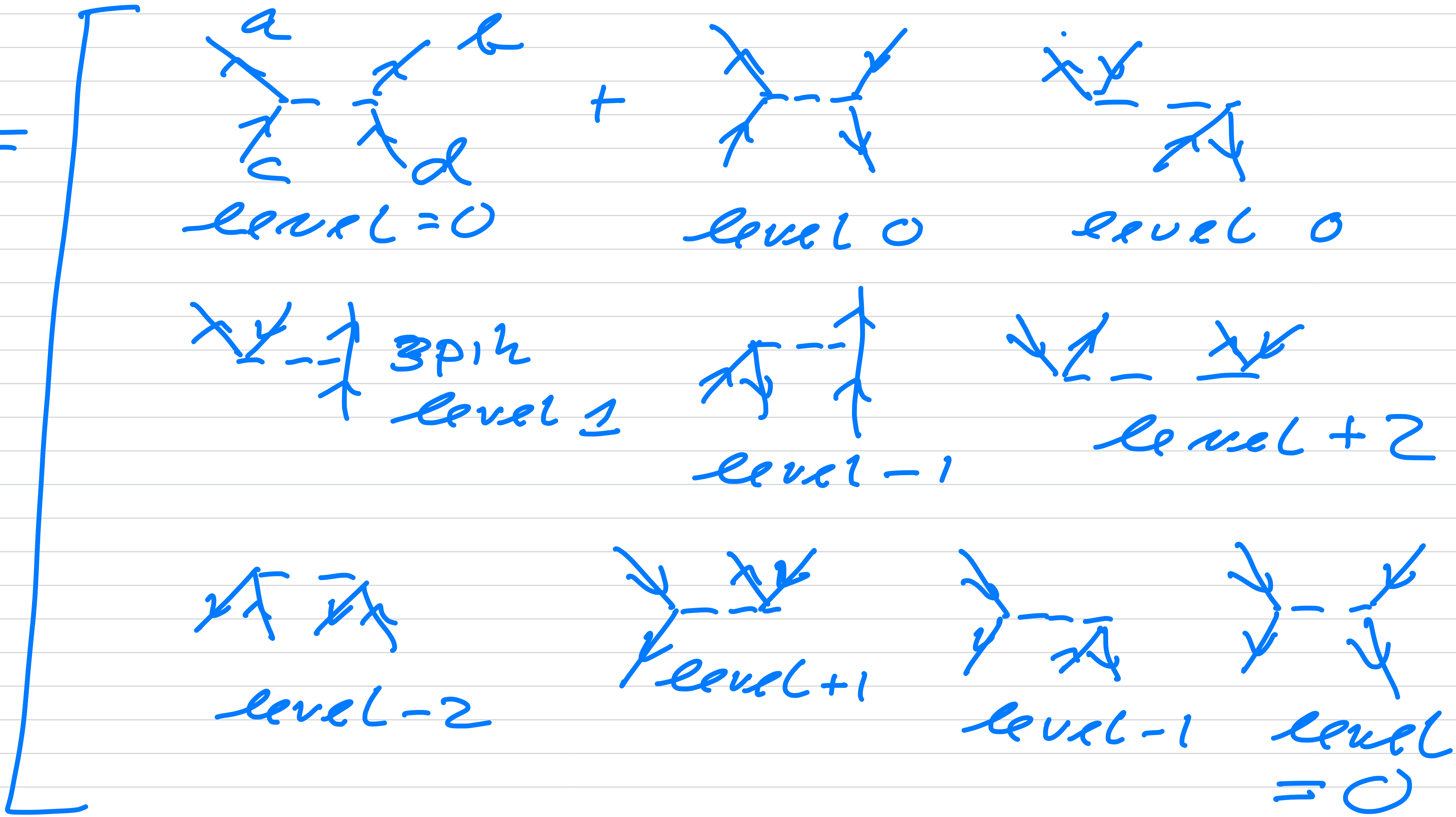
$$F_N = \sum_{pq} a_p^\dagger a_q \langle p|f|q\rangle$$

$$= \sum_{ab} a_a^\dagger a_b \langle a|f|b\rangle + \sum_{ai} a_a^\dagger a_i \langle a|f|i\rangle + \cdots$$



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

$=$

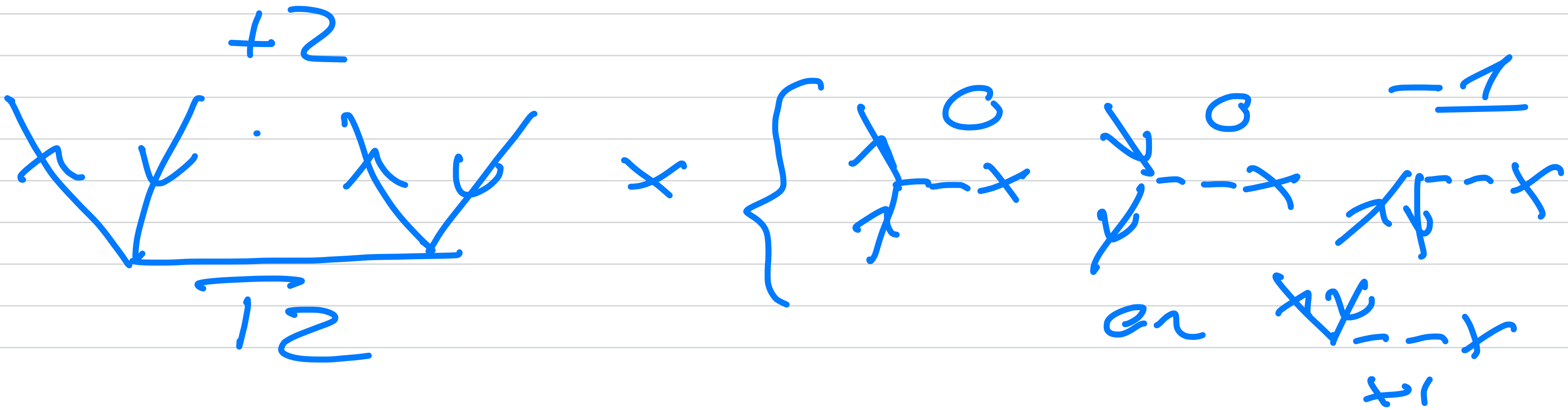


$$\langle \Phi_{ij}^{ab} | F_N T_2 | \Phi_0 \rangle$$

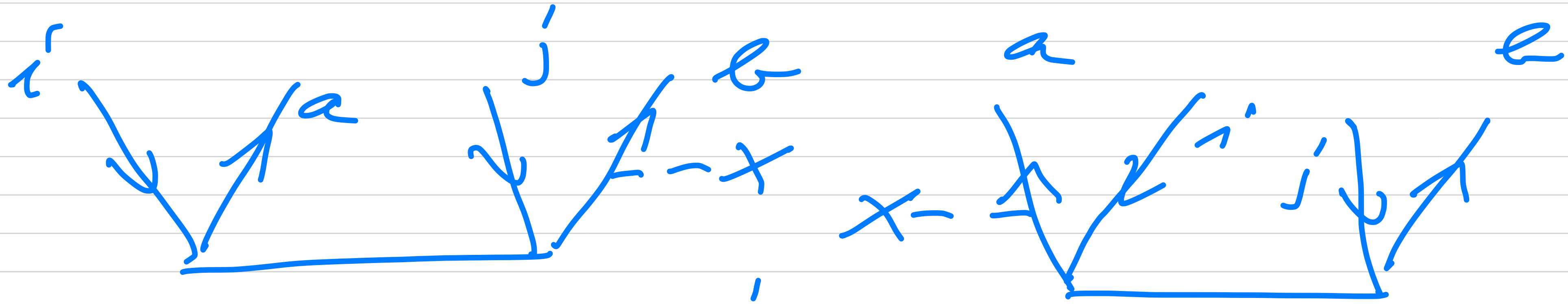
want to end in a 2p2h state

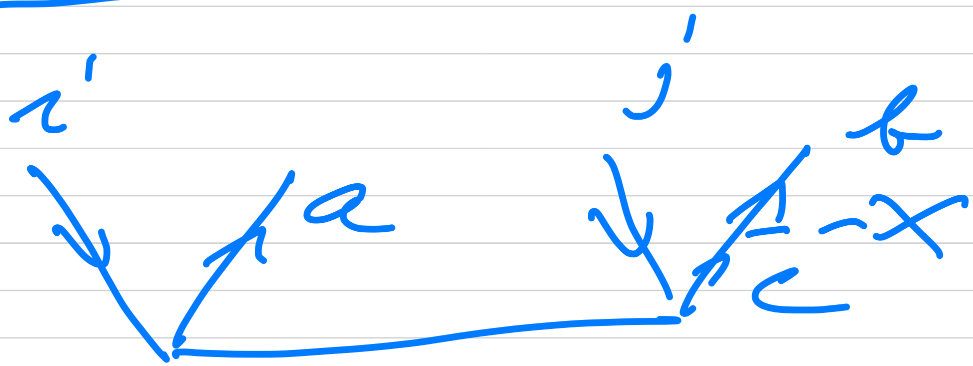
level +2 excitation

$|\Phi_0\rangle$ is level 0

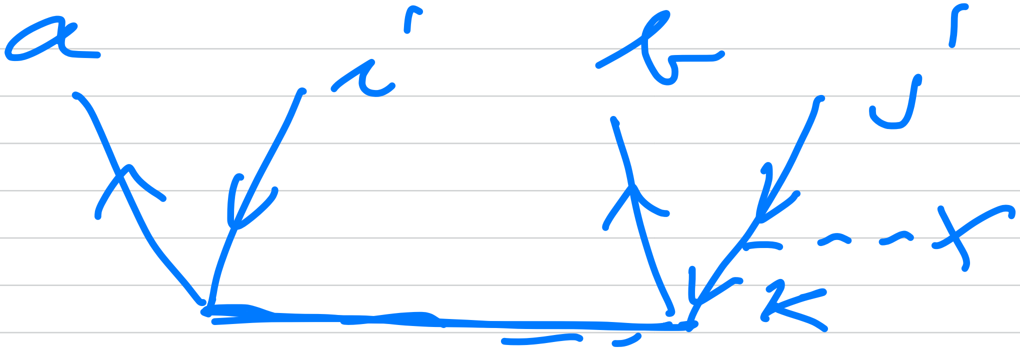



$+ \underline{1}$



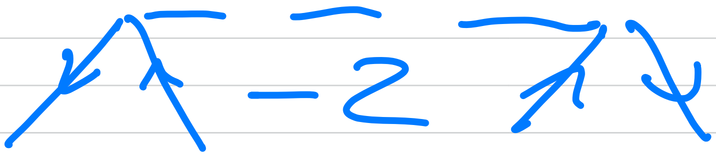

$=$ 


$$\sum_c \langle b|f|e\rangle \, t_{ij}^{ac}$$

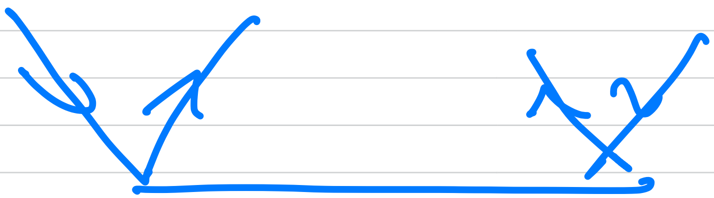



$$\Delta E_{CCD} = \frac{1}{4}\sum_{\substack{ab\\ij}} t_{ij}^{ab}\langle ij||ab\rangle$$

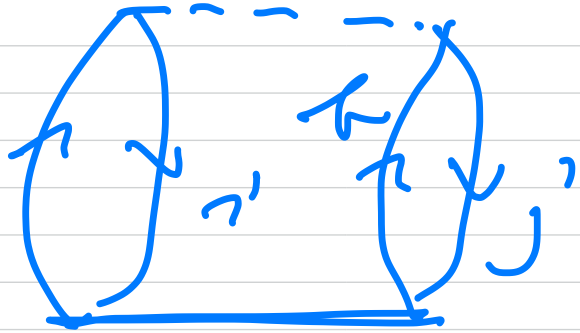
$V_N$




$T_2$



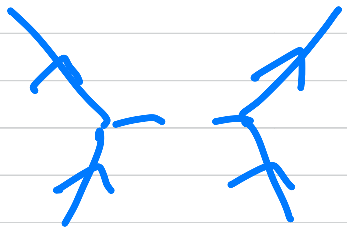
+2

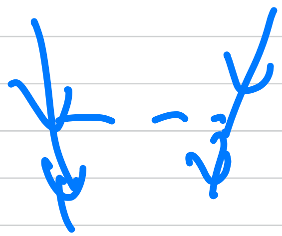


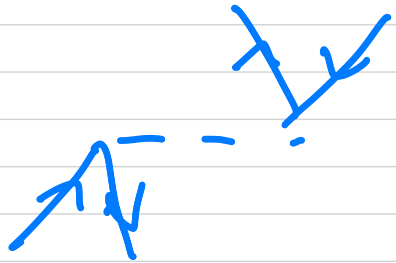

$$t_{ij}^{ab} = \langle \Phi_0 | V_N T_2 | \Phi_0 \rangle$$

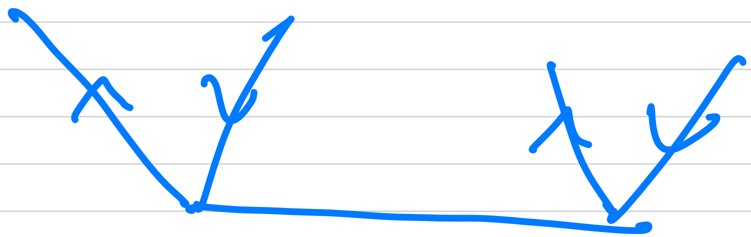
$$\langle \Phi_{ij}^{ab} | V_N T_2 | \Phi_0 \rangle$$

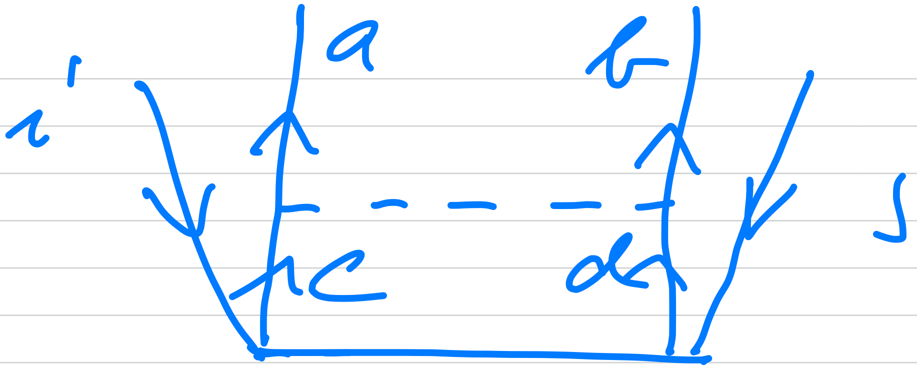
+2      +2      +0





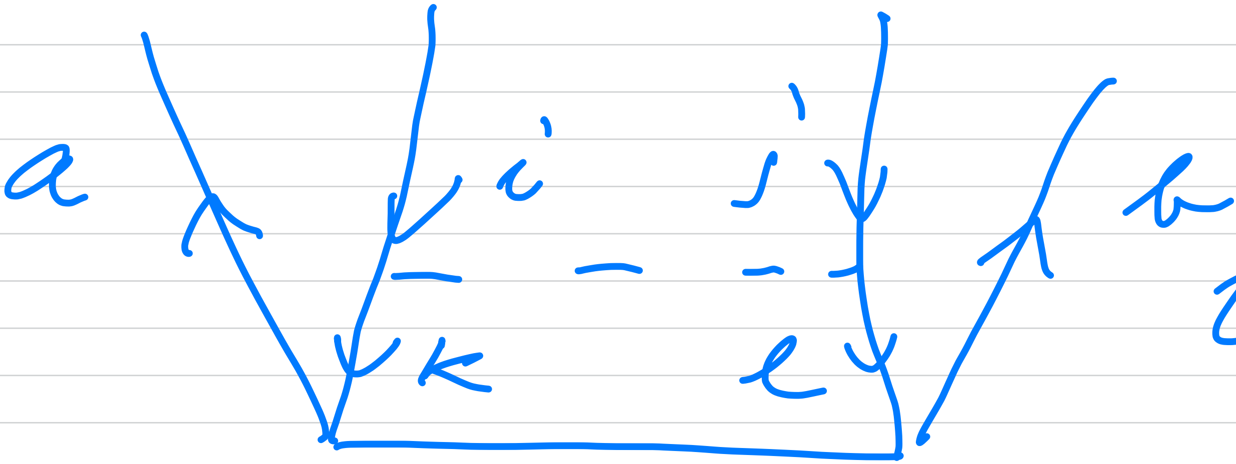






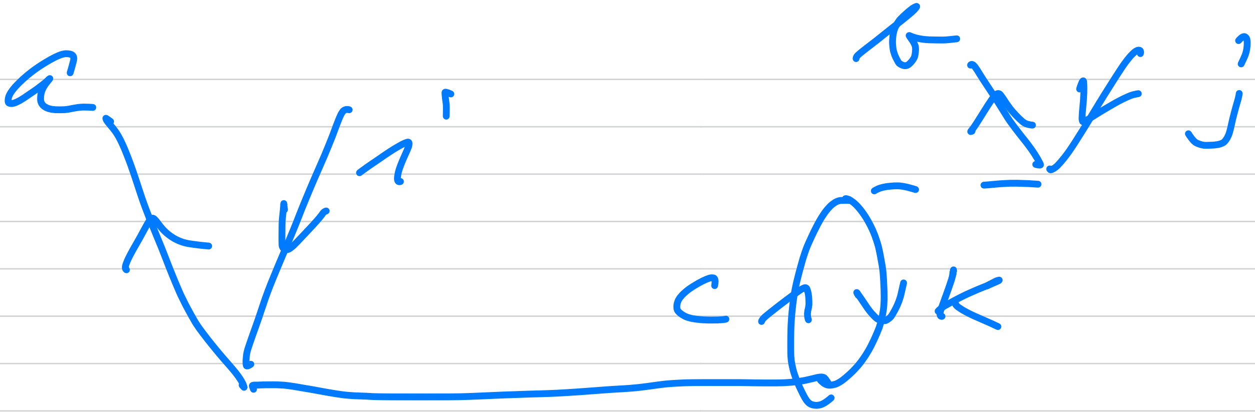

L2a 2p2h

$$\frac{1}{2}\sum_{cd}\langle ab||cd\rangle \times t_{ij}^{cd}$$




L2b

$$\frac{1}{2}\sum_{ke}\langle ke||ij\rangle\, t_{ke}^{ab}$$




$$\langle \Phi^{ak}_{ij} | V_N \frac{1}{2} T_2^2 | \Phi_0 \rangle$$

+2

+2 +2

level 0