



FYS 4480/9480 November 14

$$\Delta E_0^{(2)} = \langle \Phi_0 | \hat{H} | \frac{\hat{e}_0}{\epsilon_0} \hat{A}_1 | \Phi_0 \rangle$$

$$\overline{\hat{R}} = \sum_{M>0} \frac{|\Phi_M\rangle \langle \Phi_M|}{\epsilon_0 - \epsilon_M}$$

$$\hat{R} |\Phi_N\rangle = \frac{|\Phi_N\rangle}{\epsilon_0 - \epsilon_N} \quad N \neq 0$$

wave operator :

$$\hat{R} H_1 |\Psi_0\rangle =$$

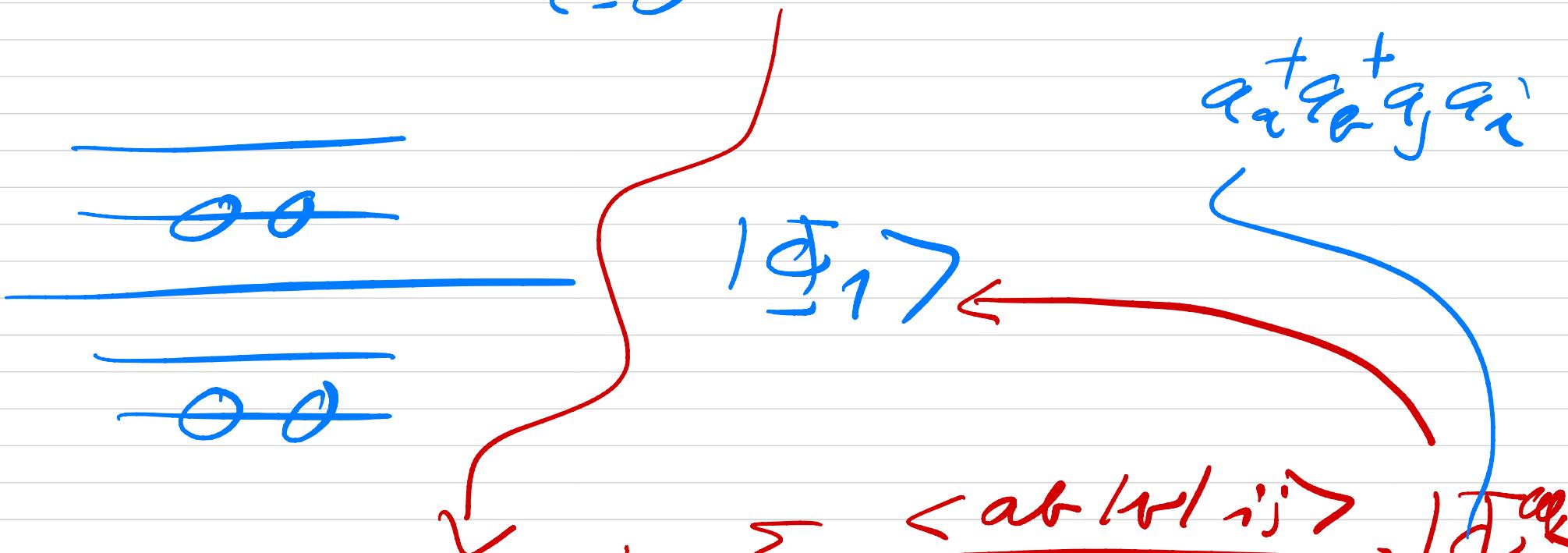
$$\frac{1}{4} \sum_{\substack{ab \\ ij}} \frac{\langle ab | v | ij \rangle}{\epsilon_i + \epsilon_j - \epsilon_a - \epsilon_b} |\Psi_{ij}^{ab}\rangle$$

$$\left( \sum_{ai} \frac{\langle alf | i \rangle}{\epsilon_i - \epsilon_a} |\Psi_a^i\rangle \right)$$

in 2nd mid term = 0

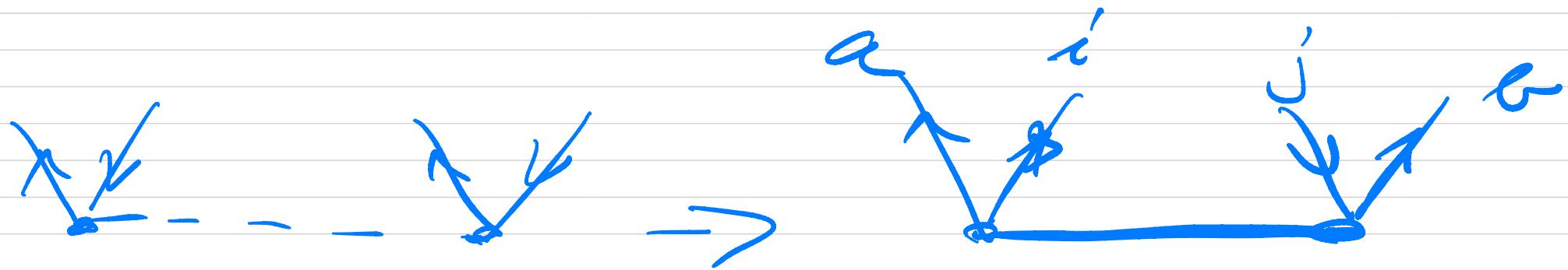
$\text{FCI}$ -case<sub>5</sub>

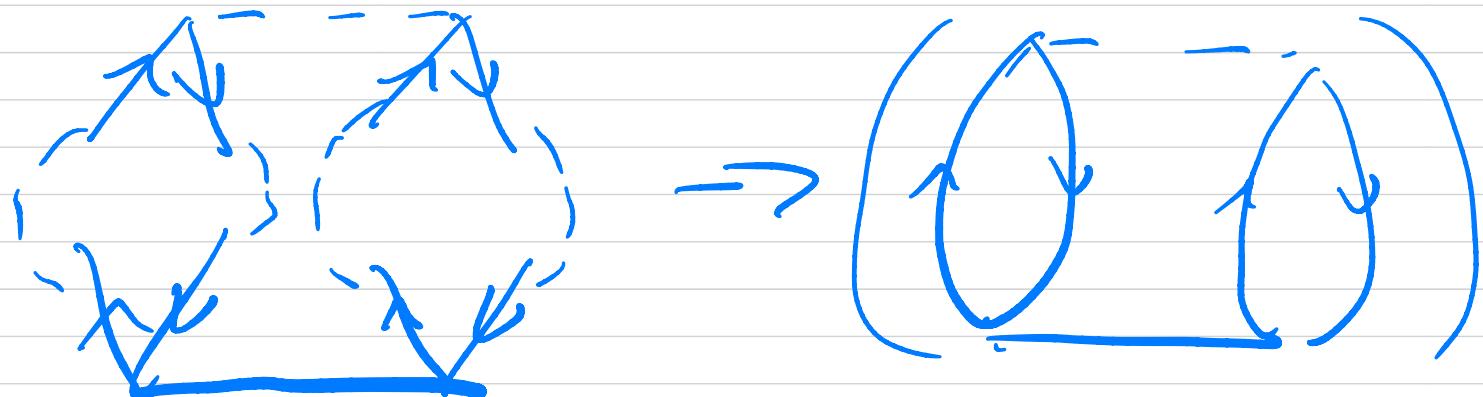
$$|\Psi_0\rangle = \sum_{i=0}^5 c_{0i} |\Phi_i\rangle$$



$$a_n^{+} a_i^{+} P_n P_j$$

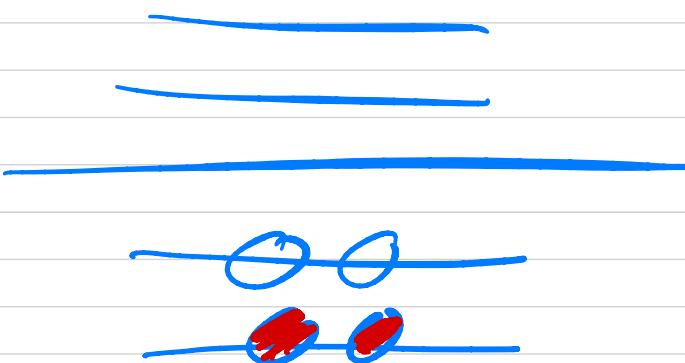
$$\Rightarrow \frac{1}{4} \sum_{ab} \sum_{i,j} \frac{\langle ab|v|i,j\rangle}{\epsilon_i + \epsilon_j - \epsilon_a - \epsilon_b} |\Phi_{ij}^{ab}\rangle$$
$$\frac{1}{4} \sum_{ab} \sum_{i,j} t_{ij}^{ab} |\Phi_{ij}^{ab}\rangle$$



$$\langle \vec{E}_0 | H, \hat{R} | H, | \vec{E}_0 \rangle$$




$$= \sum_{ai} \frac{\langle a | g | i \rangle}{\varepsilon_i - \varepsilon_a} | \Xi_i^a \rangle$$



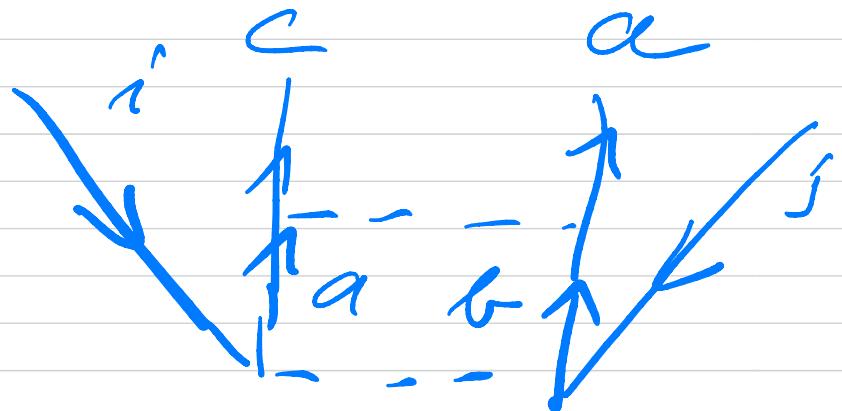
$$\langle i | g | i \rangle = \langle i | k_0 | i \rangle$$

$$+ \sum_j \langle i j | v | i j \rangle$$

$$\varepsilon_i' - g$$

wave operator to 2nd order

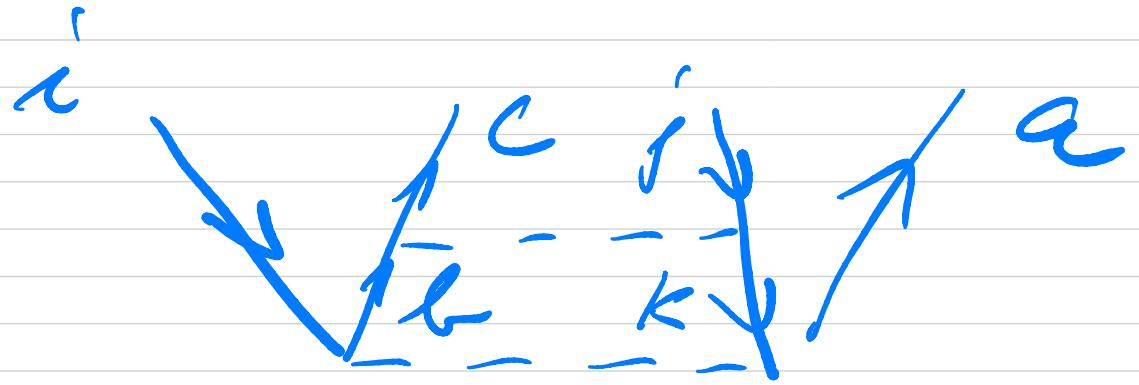
$$|\Psi^{(2)}\rangle = \hat{R}^\dagger H_1 \hat{R}^\dagger H_1 |\Phi_0\rangle$$



$$\frac{1}{8} \sum_{abcd} \frac{\langle cd|a|ab\rangle \langle ab|vij\rangle}{(\epsilon_i + \epsilon_j - \epsilon_a - \epsilon_b)}$$

$$ij \quad \times (\epsilon_i + \epsilon_j - \epsilon_c - \epsilon_d)$$

$$\times |\Phi_{ij}^{cd}\rangle$$



$$\sum_{\substack{abc \\ ijk}} \frac{\langle c k | v | b j \rangle \langle b a | v | i k \rangle}{(\varepsilon_i + \varepsilon_k - \varepsilon_b - \varepsilon_a)(\varepsilon_i + \varepsilon_j - \varepsilon_c - \varepsilon_a)} \\
 \times \left| \Phi_{i,j}^{ca} \right\rangle$$

$2P \approx h$

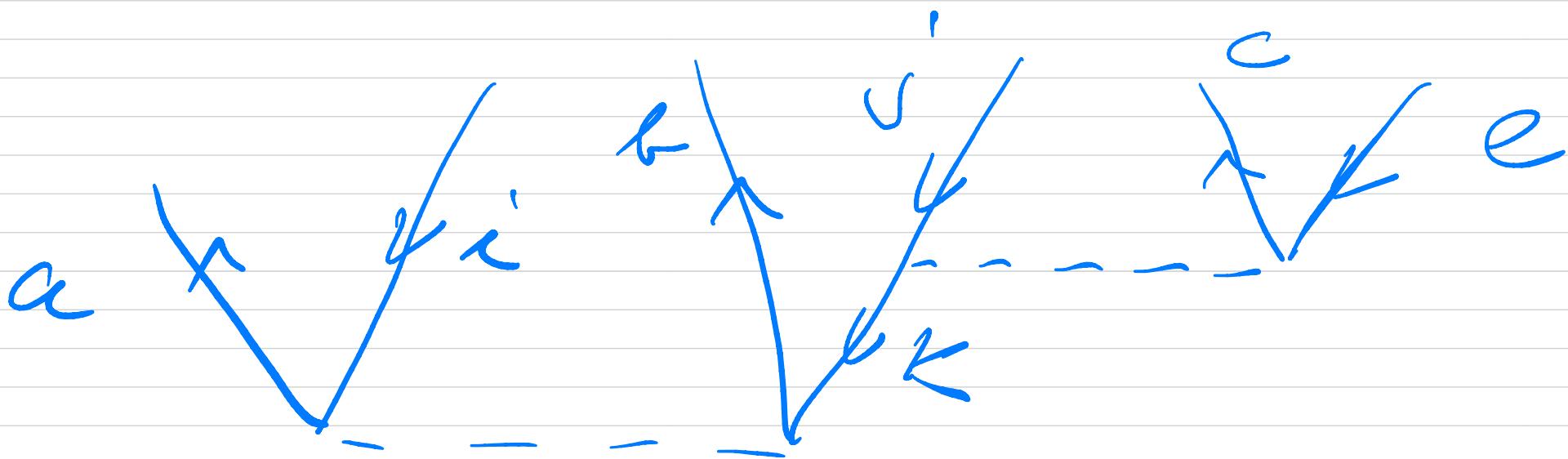
$\langle \psi | \psi \rangle$   
 $\psi = c_i|j\rangle + c_j|i\rangle + c_k|k\rangle$

$\langle \psi | \psi \rangle$

$\langle \psi | \psi \rangle$

$$-\frac{1}{2} \sum_{\substack{abc \\ i'j'}} \frac{\langle a_j | v | b_c \rangle \langle b_c | v | i_j' \rangle}{(\epsilon_{i'} + \epsilon_{j'} - \epsilon_b - \epsilon_c)(\epsilon_{i'} - \epsilon_a)} \\
 \times \left| \bigoplus_c \right|^a$$

$\langle \Phi_0 | H, \bar{\psi} \psi \rangle$



$$\sim \sum_{\substack{abc \\ ijk}} \dots | \bar{\Phi}_{ijk}^{abc} \rangle$$

3p3k