

FYS 4480, NOV 11, 2022

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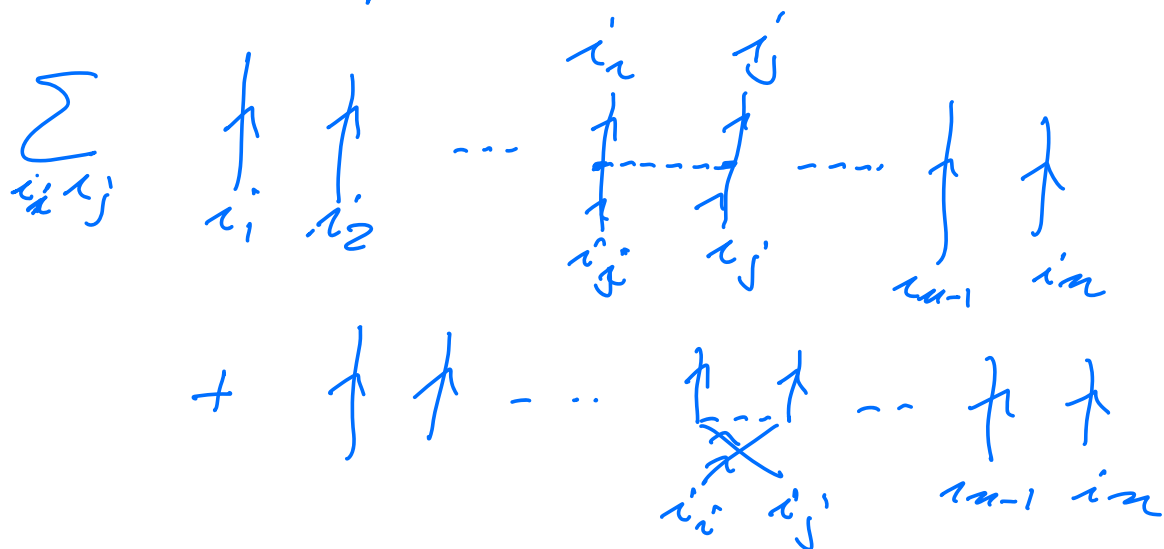
Many-body pert theory

$$\Delta E^{(1)} = \langle \Phi_0 | H_1 | \Phi_0 \rangle$$

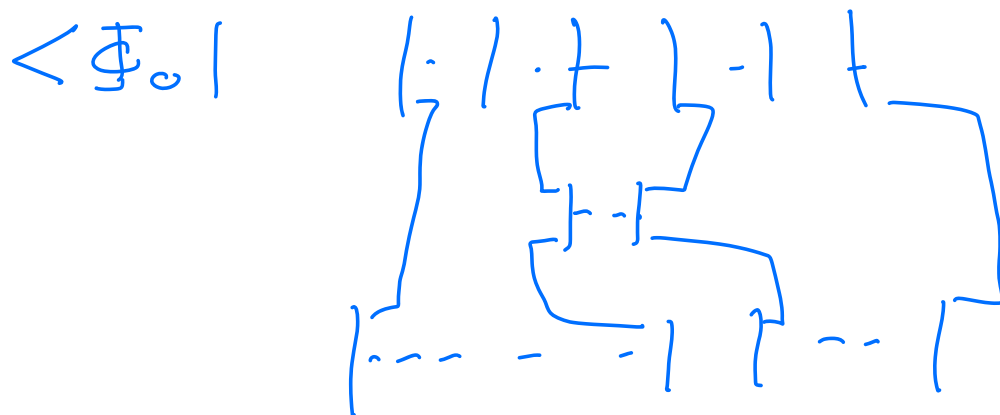
$$= \langle \Phi_0 | V | \Phi_0 \rangle$$

$$\Delta E^{(1)} = \frac{1}{2} \sum_{i,j} \{ \langle i j | v | i j \rangle - \langle i j | v | j i \rangle \}$$

in particle formalism



$$|\Phi_0\rangle = \prod_{i=1}^n a_i^\dagger |0\rangle$$



$$|\Phi_0\rangle$$

in particle-hole formalism

$$\langle \Phi_0 | \Phi_0 \rangle = \uparrow \uparrow \cdots \uparrow$$

$i_1 \quad i_2 \quad \cdots \quad i_n$

$$\langle i_1 i_2 | v | i_1' i_2' \rangle = \langle i_1' i_2' | v | i_2 i_1 \rangle$$

$$= i_1 \circlearrowright \cdots \circlearrowright i_2$$

$$+ \begin{array}{c} i_1' \\ \circlearrowleft \\ \cdots \\ \circlearrowright \\ i_2' \end{array}$$

$$\Delta E^{(1)} = \frac{1}{2} \sum_{i,j} \left( \circlearrowright^i \cdots \circlearrowright^j + \begin{array}{c} i \\ \circlearrowleft \\ \cdots \\ \circlearrowright \\ j \end{array} \right)$$

$$= \circlearrowright \cdots \circlearrowright + \begin{array}{c} \circlearrowright \\ \cdots \\ \circlearrowleft \end{array}$$

$$\Delta E^{(2)} = \langle \Phi_0 | v \frac{Q}{\epsilon} v | \Phi_0 \rangle$$

$$= \sum_{m \neq 0} \frac{\langle \Phi_0 | v | \Phi_m \rangle \langle \Phi_m | v | \Phi_0 \rangle}{\omega_0 - \omega_m}$$

$$Q = \sum_{m \neq 0} |\Phi_m\rangle \langle \Phi_m|$$

$$e = W_0 - H_0$$

$$H_0 |\Phi_m\rangle = W_m |\Phi_m\rangle$$

Schematic plot in  
particle formalism

$$\langle \Phi_0 | : \quad \begin{array}{ccccccc} | & | & | & | & | & | & \cdots | \\ p_1 & p_2 & & & & & p_n \\ (x_1) & (x_2) & & & & & \end{array}$$

V

$\{ - \}$

$$\frac{|\Phi_m\rangle \langle \Phi_m|}{W_0 - W_m}$$

$$\begin{array}{ccccccc} | & | & \{ - \} & \cdots & | & \cdots & | \\ & & \text{outside } F & & & & \end{array}$$

V

$\{ - \}$

$$\begin{array}{ccccccc} | & | & | & | & \cdots & | & |\Phi_0\rangle \\ x_1 & x_2 & x_3 & x_4 & \cdots & x_n & \end{array}$$

$$\sum_{i,j} \downarrow$$

$$\sum_{a,b}$$

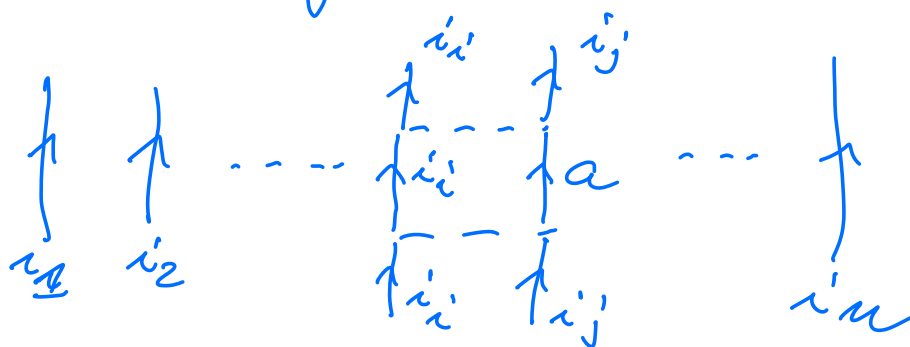
$$\begin{array}{ccccccc} \delta_{x_i, x_j} & & x_i & & x_j & & \\ \uparrow & \uparrow & \uparrow & \uparrow & \uparrow & \uparrow & \uparrow \\ x_1 & x_2 & x_i & x_j & x_i & x_j & x_n \end{array}$$

$$\sum_{ab} \frac{\langle i_i' i_j' | v | ab \rangle \langle ab | v | i_i i_j \rangle}{\epsilon_{i_i'} + \epsilon_{i_j'} - \epsilon_a - \epsilon_b}$$

in particle-hole formalism

$$i_i' \left( \overline{a} \overline{b} \right) i_j'$$

another contribution  
particle formalism



→ ph-formalism

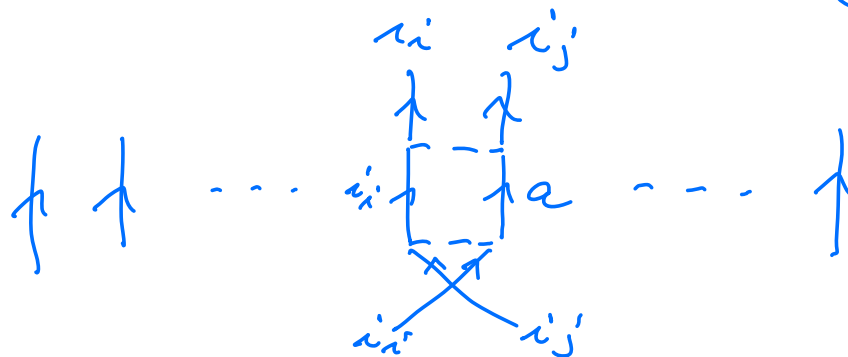
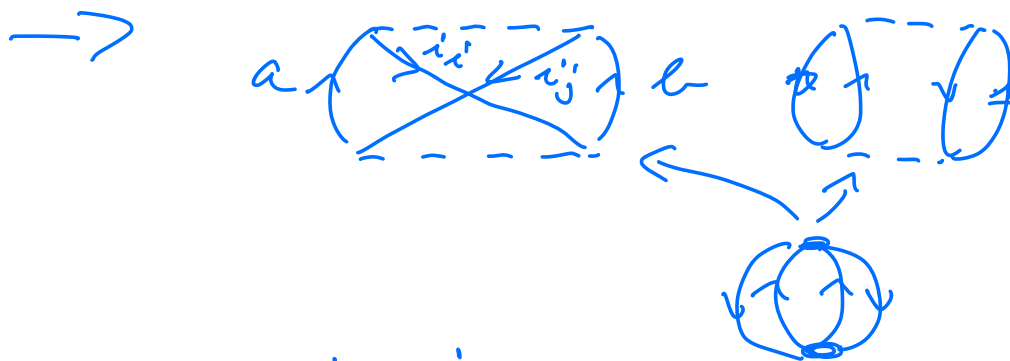
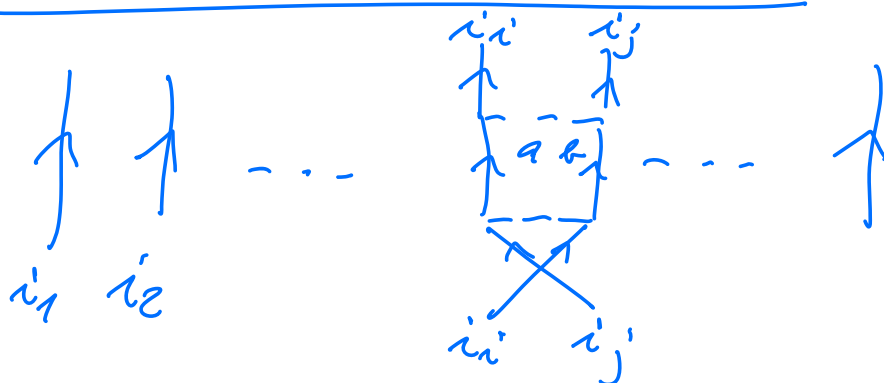


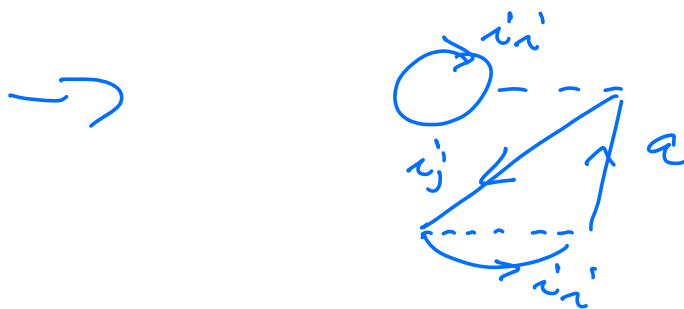
Final contribution

$$\sum_{i,j,a} \begin{array}{c} i \\ \bigcirc \text{---} \bigcirc \\ i \end{array} a \begin{array}{c} \bigcirc \text{---} \bigcirc \\ j \end{array}$$

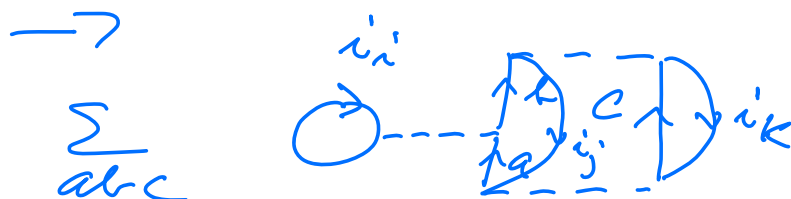
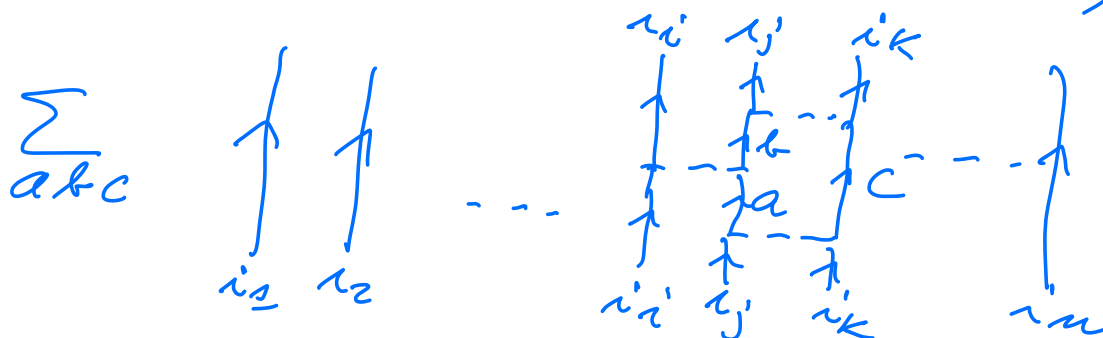
$$= \begin{array}{c} \bigcirc \text{---} \bigcirc \\ \bigcirc \text{---} \bigcirc \end{array}$$

Further examples



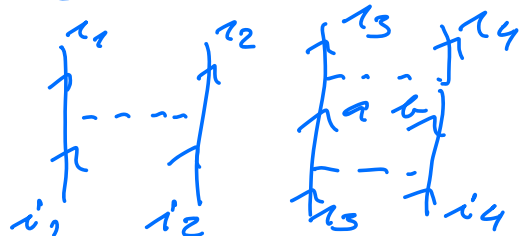


Third-order contribution (RS)



Unlinked diagrams +  
Pauli violating diagrams

3rd in RS

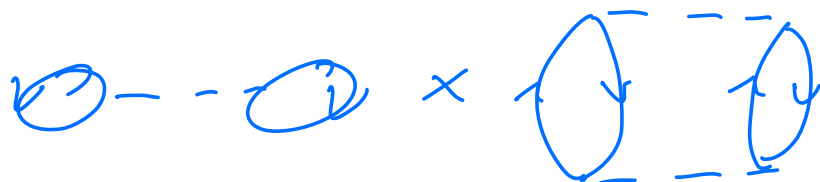


$$- \langle \Phi_0 | v | \Phi_0 \rangle \times$$

$$\frac{\langle \Phi_0 | v | \Phi_m \rangle \langle \Phi_m | v | \Phi_0 \rangle}{(\omega_0 - \omega_m)^2}$$

$$\Delta E^{(3)} = \langle \Phi_0 | V \frac{Q}{W_0 - H_0} V \frac{Q}{W_0 - H_0} V | \Phi_0 \rangle \\ - \langle \Phi_c | V | \Phi_c \rangle \langle \Phi_0 | V \frac{Q}{(W_0 - H_0)^2} V | \Phi_c \rangle$$

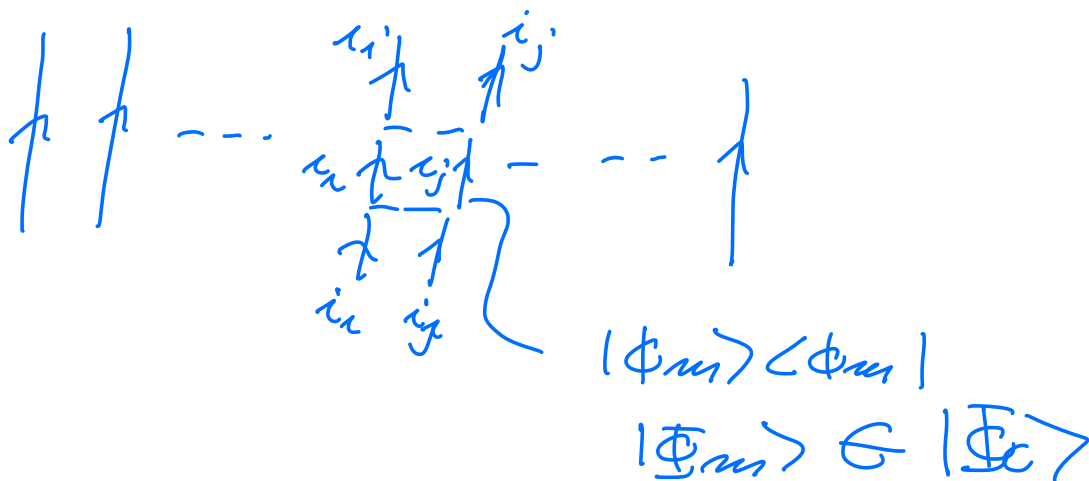
in ph-formalism



unlinked diagram

$$\Delta E^{(2)} : \quad \text{Diagram 1}$$

$$\text{Diagram 2}$$



$$\Delta E_c^{(3)} = \langle \Phi_0 | v \frac{Q}{e} v \frac{Q}{e} v | \Phi_0 \rangle$$

$$E = W_0 - H_0 - \langle \Phi_0 | V \left( \frac{Q}{e} \right)^2 V | \Phi_0 \rangle + \langle \Phi_c | V | \Phi_c \rangle$$

## First term

$$\begin{array}{cc} \begin{array}{c} \tau_1 \quad \tau_2 \\ | \quad | \\ | \quad | \\ | \quad | \\ | \quad | \\ \tau_1 \quad \tau_2 \end{array} & \begin{array}{c} \tau_3 \quad \tau_4 \\ | \quad | \\ | \quad | \\ | \quad | \\ | \quad | \\ \tau_3 \quad \tau_4 \end{array} \end{array} = \frac{\langle i_3 i_4 | v | a b \rangle \langle i_3 i_2 | v | i_1 i_4 \rangle \times \langle a b | v | i_3 i_4 \rangle}{(i_3 + i_4 - \epsilon_a - \epsilon_b)(i_3 + i_4 - \epsilon_a - \epsilon_c)}$$

this will be canceled by

$$\underbrace{\begin{array}{cccc} i_1 & i_2 & i_3 & i_4 \\ \uparrow & \uparrow & \uparrow & \uparrow \\ 1 & 2 & 3 & 4 \end{array}} \times \begin{array}{cccc} i_1 & i_2 & i_3 & i_4 \\ \uparrow & \uparrow & \uparrow & \uparrow \\ 1 & 2 & 3 & 4 \end{array} \frac{1}{e^2}$$

Example: Exercise 1, weeks

$$H = \underbrace{\sum_{i=1}^2 \epsilon_i a_i^\dagger a_i}_{H_0} + \lambda \underbrace{\sum_{i \neq j} a_i^\dagger a_j}_{H_1}$$



$$\begin{aligned} & \text{--- } E_2 & H_0 |\Phi_1\rangle &= E_1 |\Phi_1\rangle \\ & \text{--- } E_1 & H_0 |\Phi_2\rangle &= E_2 |\Phi_2\rangle \end{aligned}$$

For the ground state

$$\Delta E_1^{(1)} - \langle \Phi_1 | H_1 | \Phi_1 \rangle = 0$$

$$\begin{aligned} H_1 &= \lambda a_1^\dagger a_2 & \langle \Phi_1 | H_1 | \Phi_2 \rangle \\ & & = \langle \Phi_2 | H_1 | \Phi_1 \rangle \end{aligned}$$

$$\hat{P} = |\Phi_1\rangle \langle \Phi_1|$$

$$= \lambda$$

$$\hat{Q} = |\Phi_2\rangle \langle \Phi_2|$$

$$\langle \Phi_2 | H_1 | \Phi_2 \rangle = 0$$

$$\text{RS: } \Delta E_1^{(2)} = \frac{\langle \Phi_1 | H_1 | \Phi_2 \rangle \langle \Phi_2 | H_1 | \Phi_1 \rangle}{E_1 - E_2} = \frac{\lambda^2}{E_1 - E_2}$$

$$\text{BW: } \Delta E_1^{(2)} = \frac{\lambda^2}{E_1 - E_2}$$

$$\begin{aligned} \text{BW: } \Delta E_1^{(3)} &= \langle \Phi_1 | H_1 | \Phi_2 \rangle \langle \Phi_2 | H_1 | \Phi_2 \rangle \\ &\quad \times \langle \Phi_2 | H_1 | \Phi_1 \rangle \\ &= \frac{\langle \Phi_2 | H_1 | \Phi_1 \rangle}{(E_1 - E_2)(E_1 - E_2)} \end{aligned}$$

$$= 0$$

$$BW : \Delta E_1 = E_1 - \epsilon_1$$

$$= \frac{\lambda^2}{E_1 - \epsilon_2} \Rightarrow$$

$$E_1 = \epsilon_1 + \frac{\lambda^2}{E_1 - \epsilon_2} \left( \frac{(E_1 - \epsilon_1)(E_1 - \epsilon_2)}{-\lambda^2} = 0 \right)$$

$$\Delta E_1(BW) = \langle \Phi_0 | H_1 + \frac{1}{E_1 - H} H_1 | \Phi_0 \rangle$$

Diagrammatically in the  
particle formalism

$$\begin{array}{c} 1 \\ 2 \\ 1 \end{array} \begin{array}{c} \uparrow \\ \uparrow \\ \uparrow \end{array} \begin{array}{c} \text{---} x \\ \text{---} x \\ \text{---} x \end{array} \begin{array}{c} \lambda \\ \lambda \\ \lambda \end{array} \rightarrow \begin{array}{c} 1 \\ 2 \end{array} \begin{array}{c} \uparrow \\ \uparrow \end{array} \begin{array}{c} \text{---} x \\ \text{---} x \end{array}$$

in ph formalism

$$|\Phi_2\rangle = a_2^\dagger a_1 |\Phi_1\rangle$$

$$|\Phi_1\rangle = a_1^\dagger |0\rangle$$

$$|\Phi_0\rangle = a_2^\dagger |0\rangle$$

RS to 3rd order

$E_1 \rightarrow E_1$  in the expansion

$$\begin{aligned} \Delta E_1 &= \langle \Phi_1 | H_1 | \Phi_1 \rangle + \\ &\quad \frac{\langle \Phi_1 | H_1 | \Phi_2 \rangle \langle \Phi_2 | H_1 | \Phi_1 \rangle}{E_1 - E_2} \\ &\quad + \frac{\langle \Phi_1 | H_1 | \Phi_2 \rangle \langle \Phi_2 | H_1 | \Phi_2 \rangle \langle \Phi_2 | H_1 | \Phi_1 \rangle}{(E_1 - E_2)^2} \\ &\quad - \frac{\langle \Phi_1 | H_1 | \Phi_1 \rangle \langle \Phi_1 | H_1 | \Phi_2 \rangle \langle \Phi_2 | H_1 | \Phi_1 \rangle}{(E_1 - E_2)^2} \\ &= \frac{\lambda^2}{E_1 - E_2} \end{aligned}$$

$$\begin{array}{c} 1 \\ \uparrow \\ 2 \\ \uparrow \\ 1 \end{array} \begin{array}{c} -x \\ -x \\ -x \end{array}$$

FCI: Hamiltonian matrix

$$H = \begin{bmatrix} E_1 & \lambda \\ \lambda & E_2 \end{bmatrix}$$

$$\begin{bmatrix} \langle \Phi_1 | H | \Phi_1 \rangle & \langle \Phi_1 | H | \Phi_2 \rangle \\ \langle \Phi_2 | H | \Phi_1 \rangle & \langle \Phi_2 | H | \Phi_2 \rangle \end{bmatrix}$$

$$E = \frac{1}{2} \left[ (\epsilon_1 + \epsilon_2) \pm \sqrt{(\epsilon_1 - \epsilon_2)^2 + 4\lambda^2} \right]$$

$$= \frac{1}{2} \left[ \epsilon_1 + \epsilon_2 - (\epsilon_2 - \epsilon_1) \sqrt{1 + \frac{4\lambda^2}{(\epsilon_2 - \epsilon_1)^2}} \right]$$

$$= \frac{1}{2} \left( \epsilon_1 + \epsilon_2 - (\epsilon_2 - \epsilon_1) \left\{ 1 + \frac{4\lambda^2}{2(\epsilon_2 - \epsilon_1)^2} - \frac{2\lambda^4}{(\epsilon_2 - \epsilon_1)^4} + \dots \right\} \right)$$

$$\epsilon_1 - \frac{\lambda^2}{\epsilon_2 - \epsilon_1} + \frac{\lambda^4}{(\epsilon_2 - \epsilon_1)^3} + \dots$$

$$\Delta E_1(BW) = \frac{\lambda^2}{\epsilon_1 - \epsilon_2} = \frac{\lambda^2}{\epsilon_1 - \epsilon_2 + \Delta E_1}$$

$$= \frac{\lambda^2}{\epsilon_1 - \epsilon_2} \frac{1}{1 + \frac{\Delta E_1}{\epsilon_1 - \epsilon_2}} =$$

$$\frac{\lambda^2}{\epsilon_1 - \epsilon_2} \left( 1 - \frac{\Delta E_1}{\epsilon_1 - \epsilon_2} + \frac{(\Delta E_1)^2}{(\epsilon_1 - \epsilon_2)^2} + \dots \right)$$

$$= \frac{\lambda^2}{\epsilon_1 - \epsilon_2} \left( 1 - \frac{\lambda^2}{(\epsilon_1 - \epsilon_2)^2} + \dots \right)$$

$$\Delta E_1^{(4)}(RS) = \langle \overset{\leftarrow \Phi_1}{H_1} \frac{Q}{e} H_1 \frac{Q}{e} \overset{\leftarrow \Phi_1}{H_1} \frac{Q}{e} H_1 \rangle$$

$$e = E_1 - \overset{\leftarrow}{H_0}$$

$$- \langle H_1 \frac{Q}{e} \langle H_1 \rangle \frac{Q}{e} H_1 \frac{Q}{e} \overset{=0}{H_1} \rangle$$

$$- \langle H_1 \frac{Q}{e} H_1 \frac{Q}{e} \langle H_1 \rangle \frac{Q}{e} \overset{=0}{H_1} \rangle$$

$$+ \langle H_1 \frac{Q}{e} \langle H_1 \rangle \frac{Q}{e} \langle H_1 \rangle \frac{Q}{e} \overset{=0}{H_1} \rangle$$

$$- \langle H_1 \frac{Q}{e} \langle H_1 \frac{Q}{e} H_1 \rangle \frac{Q}{e} H_1 \rangle$$

$$\langle \Phi_1 | H_1 | \Phi_1 \rangle = \langle \Phi_2 | H_1 | \Phi_2 \rangle = 0$$

$$\Delta E_1^{(4)} = - \langle H_1 \frac{Q}{e} \langle H_1 \frac{Q}{e} H_1 \rangle \frac{Q}{e} H_1 \rangle$$

$$\frac{\langle \Phi_1 | H_1 | \Phi_2 \rangle \langle \Phi_2 | H_1 | \Phi_1 \rangle}{E_1 - E_2}$$

$$= \frac{\lambda^2}{E_1 - E_2}$$

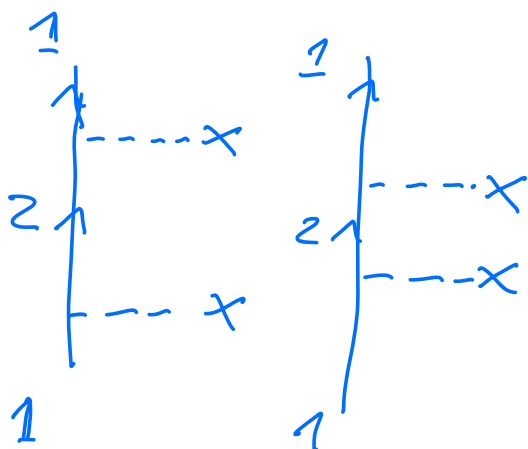
$$\frac{\lambda^2}{\epsilon_1 - \epsilon_2} \langle \Phi_1 | H_1 \frac{Q}{\epsilon} \frac{Q}{\epsilon} H_1 | \Phi_1 \rangle$$

$$= \frac{\lambda^2}{\epsilon_1 - \epsilon_2} \frac{\langle \Phi_1 | H_1 | \Phi_2 \rangle \langle \Phi_2 | H_1 | \Phi_1 \rangle}{(\epsilon_1 - \epsilon_2)^2}$$

$$= \frac{\lambda^4}{(\epsilon_1 - \epsilon_2)^3} = - \frac{\lambda^4}{(\epsilon_2 - \epsilon_1)^3}$$

$$\Delta E_1^{(2)} + \Delta E_1^{(4)} = \frac{\lambda^2}{(\epsilon_1 - \epsilon_2)^2} - \frac{\lambda^4}{(\epsilon_2 - \epsilon_1)^4}$$

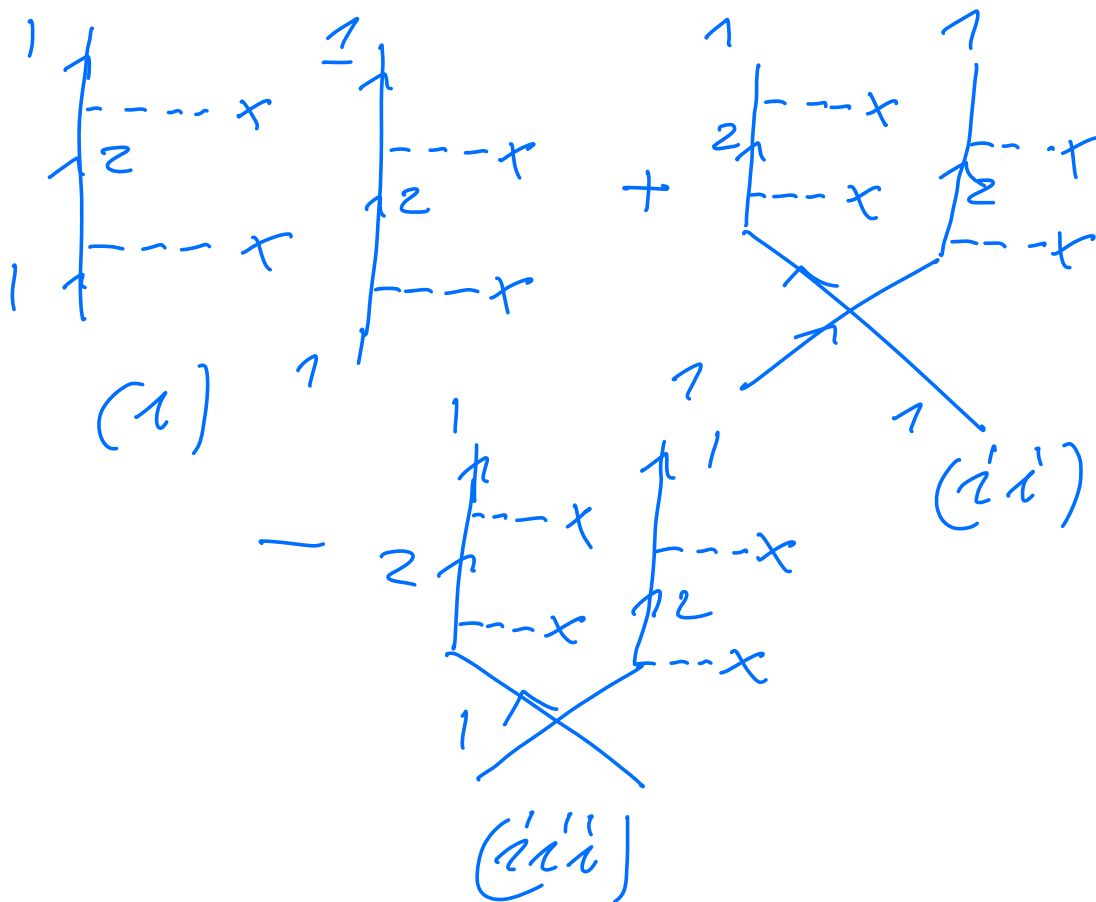
$$= \frac{\lambda^2}{(\epsilon_2 - \epsilon_1)^2} - \frac{\lambda^4}{(\epsilon_2 - \epsilon_1)^4}$$



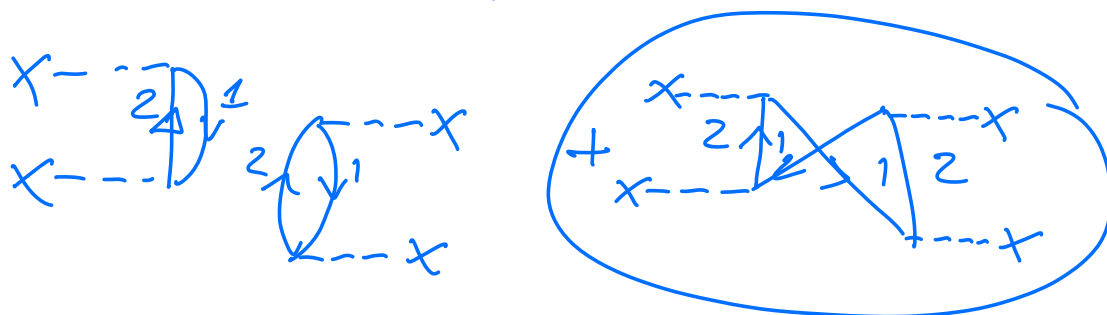
$$= \langle \Phi_1 | H_1 \frac{Q}{\epsilon} \langle \Phi_1 | H_1 \frac{Q}{\epsilon} H_1 | \Phi_1 \rangle \frac{Q}{\epsilon} H_1 | \Phi_1 \rangle$$

$$= \langle \Phi_1 | H_1 | \Phi_2 \rangle \left[ \frac{\langle \Phi_1 | H_1 | \Phi_2 \rangle \langle \Phi_2 | H_1 | \Phi_1 \rangle}{\varepsilon_1 - \varepsilon_2} \right]$$

$$\times \frac{\langle \Phi_2 | H_1 | \Phi_1 \rangle}{(\varepsilon_1 - \varepsilon_2)^2}$$



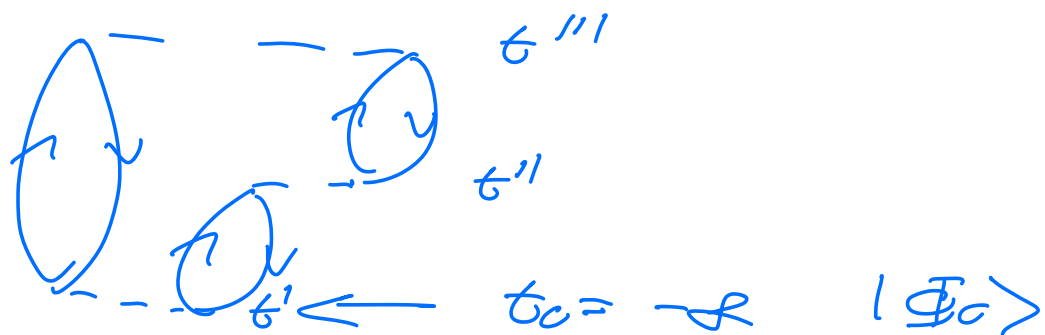
$$(i') + (ii')$$



we are left with the

$$\rightarrow - \frac{\chi^9}{(\epsilon_2 - \epsilon_1)^3}$$

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$$u(t_1, t_0) |\Phi_0\rangle$$

