FYS 4480, NOV 11, 2022

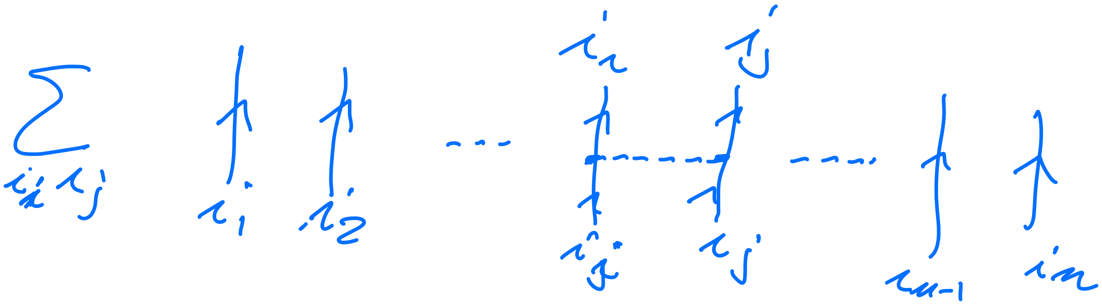
Many-body pert theory

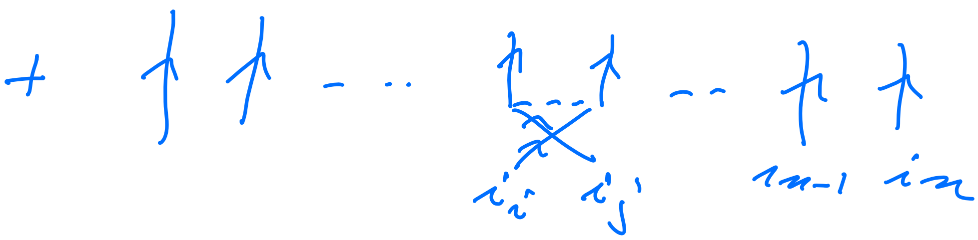
$$\Delta E^{(1)} = \langle \Phi_0 | H_1 | \Phi_0 \rangle$$

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

$$\Delta E^{(1)} = \frac{1}{2} \sum_{ij} \left\{ \langle ij | v | ij \rangle - \langle ij | v | ji \rangle \right\}$$

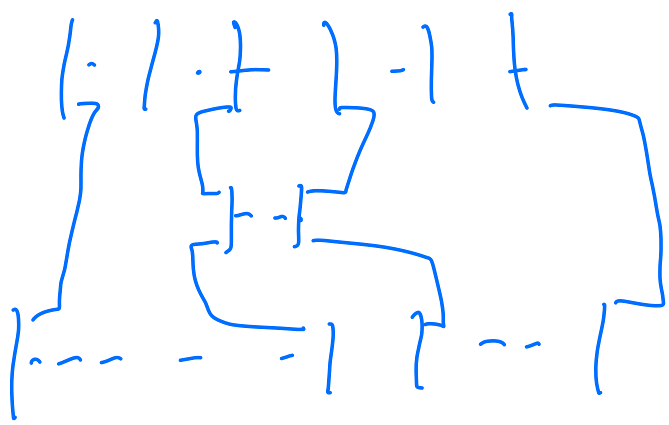
in particle formalism





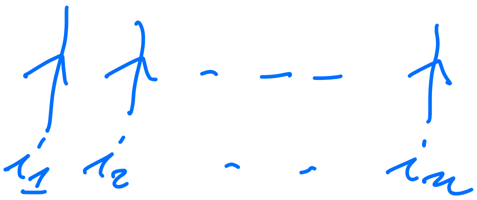
$$|\Phi_0\rangle = \prod_{i=1}^{n} a_i^{+} |0\rangle$$

$\langle \Phi_0 |$

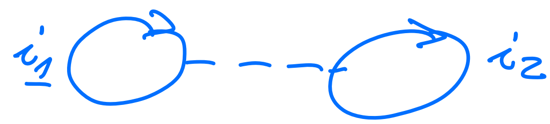


$|\Phi_0\rangle$

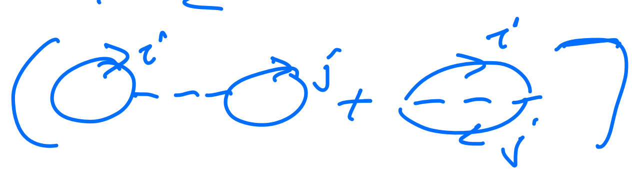
in particle-hole formalism

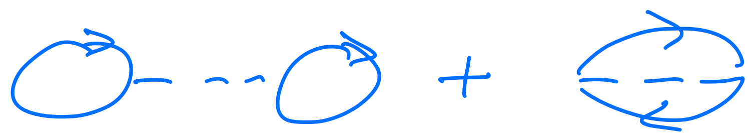
$\langle\Phi_0|\Phi_0\rangle =$ 

$\langle i_1 i_2 | v | i_1 i_2\rangle - \langle i_1 i_2 | v | i_2 i_1\rangle$

$=$ 

$+$ 

$\Delta E^{(1)} = \frac{1}{2}\sum_{ij}$ 

$=$ 

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

$$= \sum_{m\neq 0} \frac{\langle\Phi_0|V|\Phi_m\rangle\langle\Phi_m|V|\Phi_0\rangle}{w_0 - w_m}$$

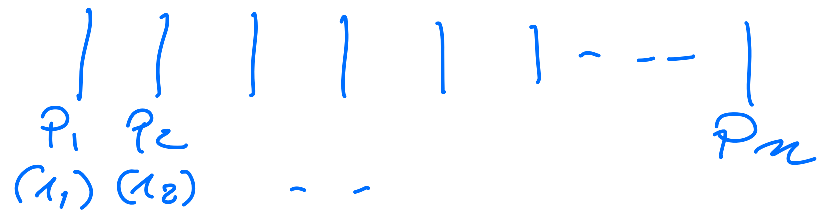
$$\hat{Q} = \sum_{m\neq 0} |\Phi_m\rangle\langle\Phi_m|$$

$$e = W_0 - H_0$$

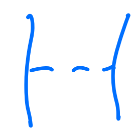
$$H_0 |\Phi_m\rangle = W_m |\Phi_m\rangle$$

Schematic plot in particle formalism

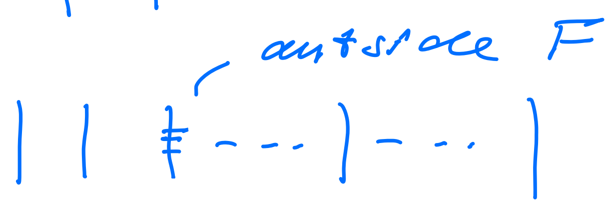
$\langle \Phi_0 |$:



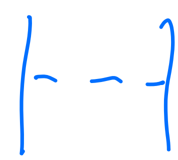
V

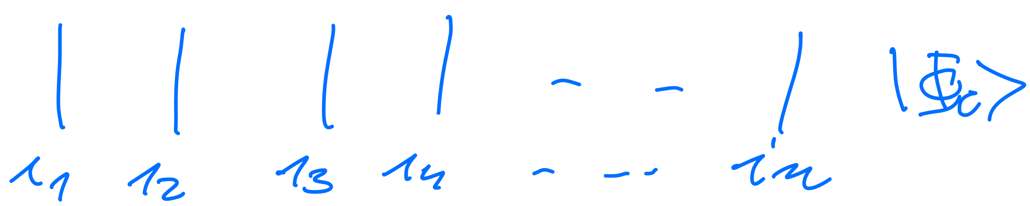


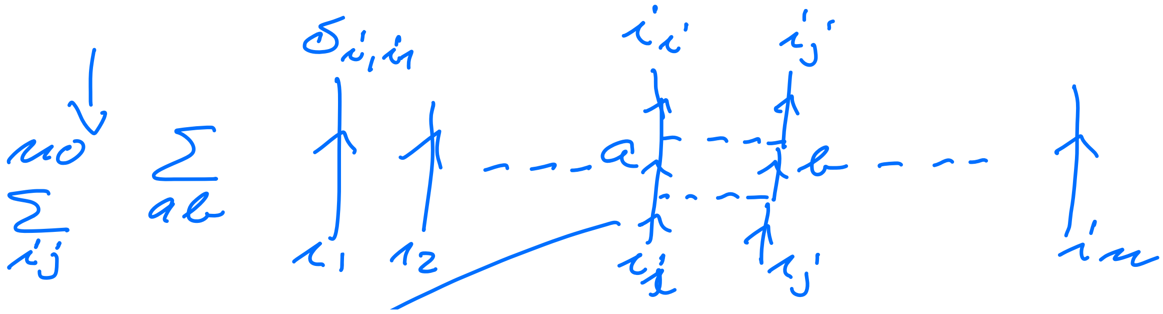
$$\frac{|\Phi_m\rangle\langle\Phi_m|}{W_0 - W_m}$$



V

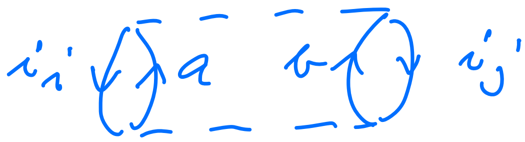






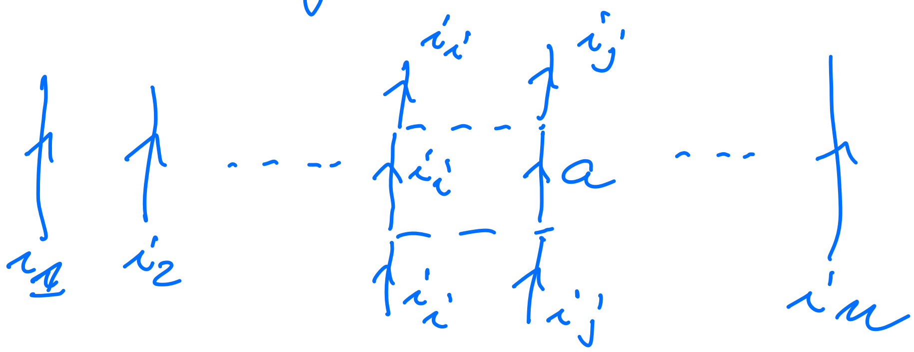
$$\sum_{ab} \frac{\langle i_i i_j | v | ab \rangle \langle ab | v | i_i i_j \rangle}{\varepsilon_{i_i} + \varepsilon_{i_j} - \varepsilon_a - \varepsilon_b}$$

in particle-hole formalism

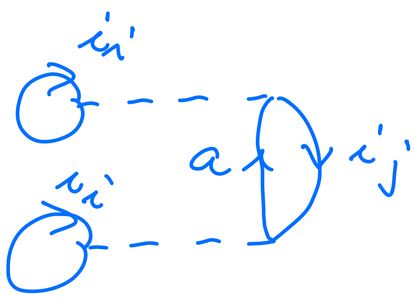


another contribution

particle formalism

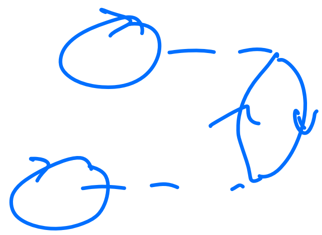


$\longrightarrow$ ph-formalism

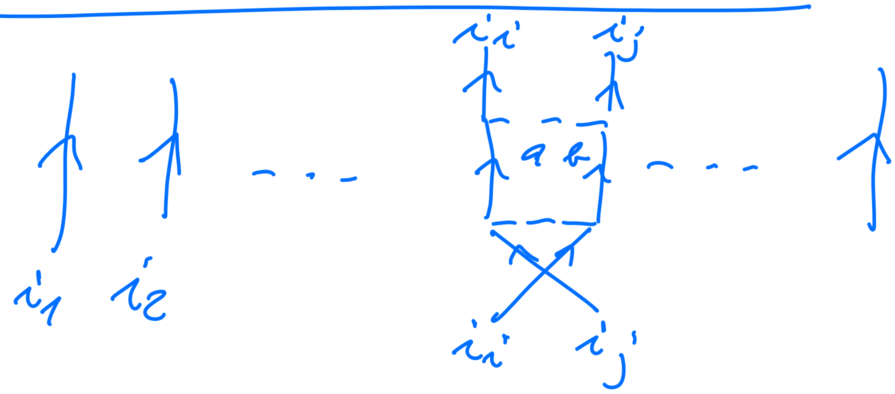


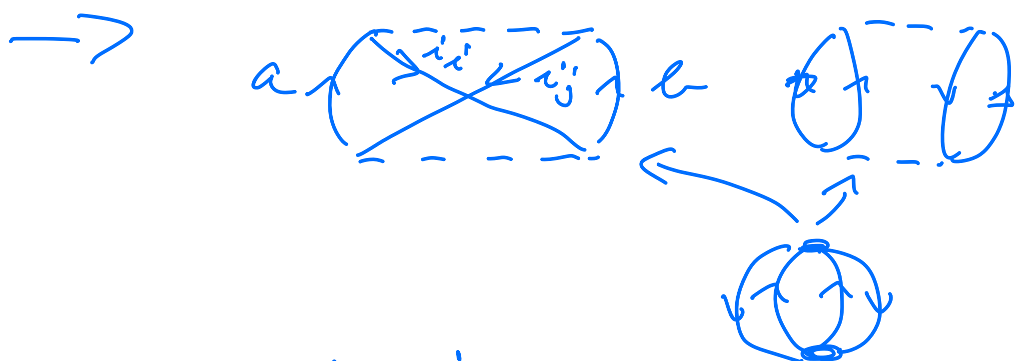
Final contribution

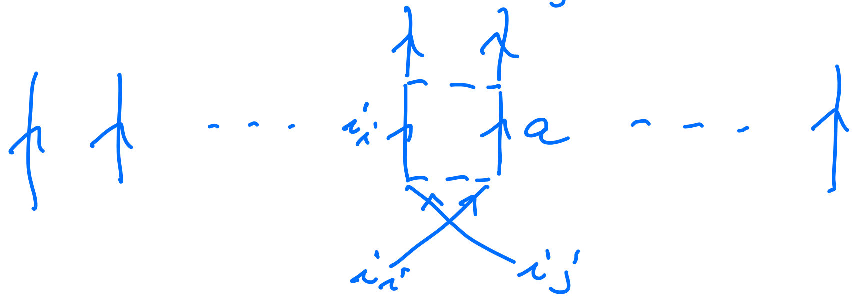
$$\sum_{ija}$$ 

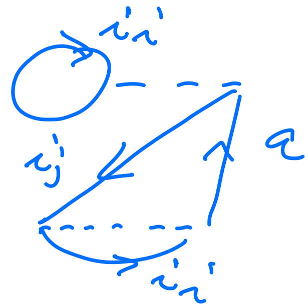
$=$ 

Further examples

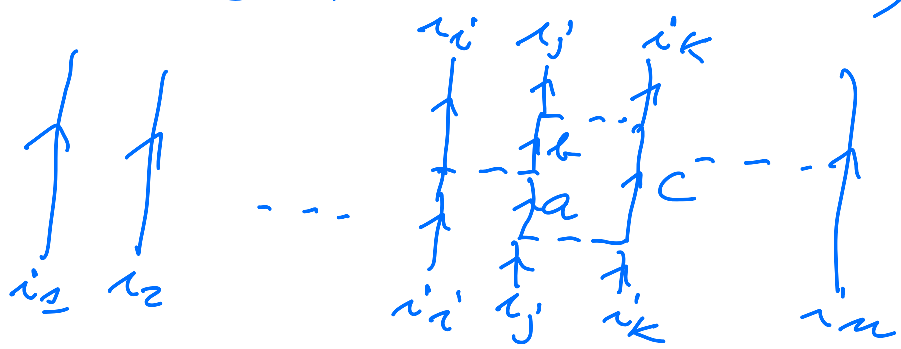


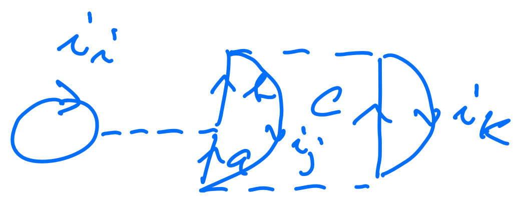


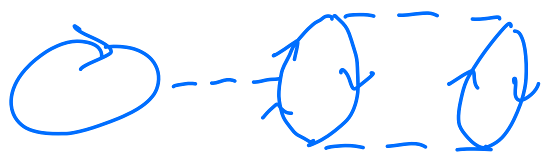


$\rightarrow$ 

Third-order contribution (RS)

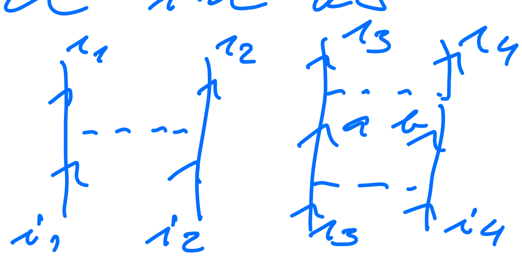
$\sum_{abc}$ 

$\rightarrow \sum_{abc}$ 

$\rightarrow$ 

Unlinked diagrams + Pauli violating diagrams

3rd in RS

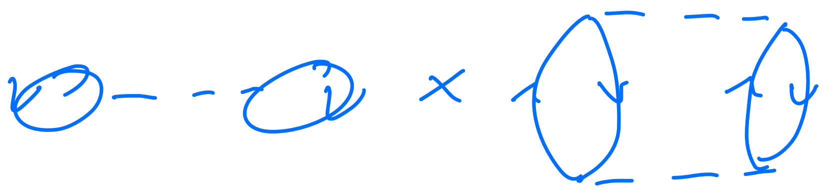


$$- \langle \Phi_0 | V | \Phi_0 \rangle \times \frac{\langle \Phi_0 | V | \Phi_m \rangle \langle \Phi_m | V | \Phi_0 \rangle}{(w_0 - w_m)^2}$$

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

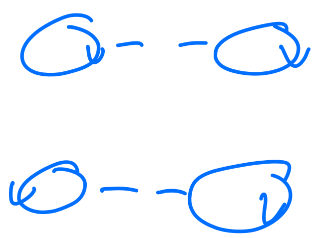
$$- \langle \Phi_0 | V | \Phi_0 \rangle \langle \Phi_0 | V \frac{Q}{(W_0 - H_0)^2} V | \Phi_0 \rangle$$

in ph-formalism



unlinked diagram

$\Delta E^{(2)}$:



$|\phi_m\rangle\langle\phi_m|$

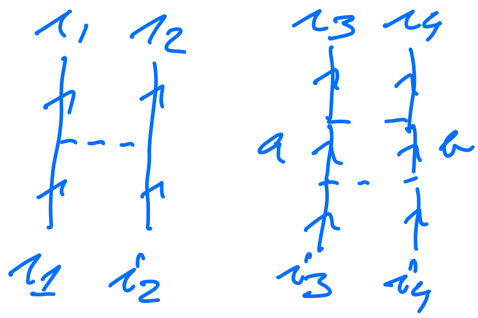
$|\Phi_m\rangle \in |\Phi_c\rangle$

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

$e = W_0 - H_0$

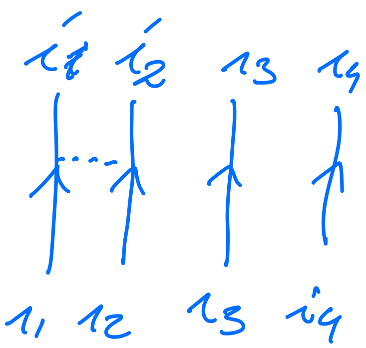
$$- \langle \Phi_0 | V \left(\frac{Q}{e}\right)^2 V | \Phi_0 \rangle \times \underbrace{\langle \Phi_0 | V | \Phi_0 \rangle}_{\Delta E^{(1)}}$$

First term

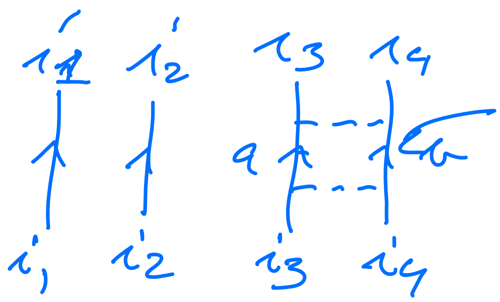


$$= \frac{\langle i_3 i_4 | v | ab \rangle \langle i_1 i_2 | v | i_1 i_2 \rangle \times \langle ab | v | i_3 i_4 \rangle}{(i_3 + i_4 - \varepsilon_a - \varepsilon_b)(i_3 + i_4 - \varepsilon_a - \varepsilon_b)}$$

this will be canceled by



$\times$



$$\frac{1}{e^2}$$

$\langle \Phi_0 | v | \Phi_0 \rangle$

Example : Exercise 1, week45

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

—— E_2 $\qquad H_0|\Phi_1\rangle = \varepsilon_1|\phi_1\rangle$

—— E_1 $\qquad H_0|\Phi_2\rangle = \varepsilon_2|\Phi_2\rangle$

For the ground state

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

$$H_1 = \lambda a_1^+ a_2 \qquad \langle\Phi_1|H_1|\Phi_2\rangle = \langle\Phi_2|H_1|\phi_1\rangle = \lambda$$

$$P = |\phi_1\rangle\langle\phi_1|$$

$$Q = |\phi_2\rangle\langle\Phi_2| \qquad \langle\Phi_2|H_1|\Phi_2\rangle = 0$$

$$\text{RS}: \ \Delta E_1^{(2)} = \frac{\langle\Phi_1|H_1|\phi_2\rangle\langle\Phi_2|H_1|\Phi_1\rangle}{\varepsilon_1-\varepsilon_2} = \frac{\lambda^2}{\varepsilon_1-\varepsilon_2}$$

$$\text{BW}: \ \Delta E_1^{(2)} = \frac{\lambda^2}{E_1-\varepsilon_2}$$

$$\text{BW}: \ \Delta E_1^{(3)} = \frac{\langle\Phi_1|H_1|\Phi_2\rangle\langle\Phi_2|H_1|\phi_2\rangle \times \langle\Phi_2|H_1|\phi_1\rangle}{(E_1-\varepsilon_2)(E_1-\varepsilon_2)}$$

$$= 0$$

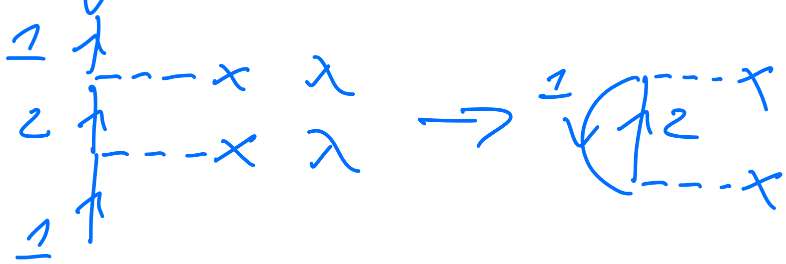
BW : $\Delta E_1 = E_1 - \varepsilon_1$

$$= \frac{\lambda^2}{E_1 - \varepsilon_2} \Rightarrow$$

$$E_1 = \varepsilon_1 + \frac{\lambda^2}{E_1 - \varepsilon_2} \qquad \left((E_1-\varepsilon_1)(E_1-\varepsilon_2) - \lambda^2 = 0 \right)$$

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

Diagrammatically in the particle formalism



in ph formalism

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

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

$$|\Phi_2\rangle = a_2^\dagger |0\rangle$$

<u>RS to 3rd order</u>

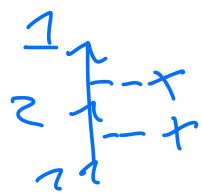
$E_1 \to \varepsilon_1$ in the expansion

$$\Delta E_1 = \overset{=0}{\langle \Phi_1 | H_1 | \Phi_1 \rangle} + \frac{\langle \Phi_1 | H_1 | \phi_2 \rangle \langle \Phi_2 | H_1 | \phi_1 \rangle}{\varepsilon_1 - \varepsilon_2}$$

$$+ \frac{\langle \Phi_1 | H_1 | \phi_2 \rangle \overset{=0}{\langle \phi_2 | H_1 | \phi_2 \rangle} \langle \Phi_2 | H_1 | \phi_1 \rangle}{(\varepsilon_1 - \varepsilon_2)^2}$$

$$- \overset{=0}{\langle \Phi_1 | H_1 | \phi_1 \rangle} \frac{\langle \Phi_1 | H_1 | \Phi_2 \rangle \langle \Phi_2 | H_1 | \phi_1 \rangle}{(\varepsilon_1 - \varepsilon_2)^2}$$

$$= \frac{\lambda^2}{\varepsilon_1 - \varepsilon_2}$$



FCI: Hamiltonian matrix

$$H = \begin{bmatrix} \varepsilon_1 & \lambda \\ \lambda & \varepsilon_2 \end{bmatrix} = \begin{bmatrix} \langle \Phi_1 | H | \Phi_1 \rangle & \langle \Phi_1 | H | \Phi_2 \rangle \\ \langle \Phi_2 | H | \Phi_1 \rangle & \langle \Phi_2 | H | \Phi_2 \rangle \end{bmatrix}$$

$$E = \frac{1}{2}\left[(\varepsilon_1+\varepsilon_2) \pm \sqrt{(\varepsilon_1-\varepsilon_2)^2+4\lambda^2}\right]$$

$$= \frac{1}{2}\left[\varepsilon_1+\varepsilon_2-(\varepsilon_2-\varepsilon_1)\sqrt{1+\frac{4\lambda^2}{(\varepsilon_2-\varepsilon_1)^2}}\right]$$

$$= \frac{1}{2}\left(\varepsilon_1+\varepsilon_2-(\varepsilon_2-\varepsilon_1)\left\{1+\frac{4\lambda^2}{2(\varepsilon_2-\varepsilon_1)^2} - \frac{2\lambda^4}{(\varepsilon_2-\varepsilon_1)^4}+\ldots\right\}\right)$$

$$\varepsilon_1 - \frac{\lambda^2}{\varepsilon_2-\varepsilon_1} + \frac{\lambda^4}{(\varepsilon_2-\varepsilon_1)^3} + \ldots$$

$$\Delta E_1(BW) = \frac{\lambda^2}{E_1-\varepsilon_2} = \frac{\lambda^2}{\varepsilon_1-\varepsilon_2+\Delta E_1}$$

$$= \frac{\lambda^2}{\varepsilon_1-\varepsilon_2}\,\frac{1}{1+\frac{\Delta E_1}{\varepsilon_1-\varepsilon_2}} =$$

$$\frac{\lambda^2}{\varepsilon_1-\varepsilon_2}\left(1-\frac{\Delta E_1}{\varepsilon_1-\varepsilon_2}+\frac{(\Delta E_1)^2}{(\varepsilon_1-\varepsilon_2)^2}+\ldots\right)$$

$$= \frac{\lambda^2}{\varepsilon_1-\varepsilon_2}\left(1-\frac{\lambda^2}{(\varepsilon_1-\varepsilon_2)^2}+\ldots\right)$$

$$\Delta E_1^{(4)}(RS) = \langle H_1 \overset{\leftarrow \Phi_1 \rangle}{\frac{Q}{e}} H_1 \frac{Q}{e} \overset{=0}{H_1} \frac{Q}{e} H_1 \rangle$$

$$e = \varepsilon_1 - \hat{H}_0$$

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

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

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

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

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

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

$$\frac{\langle \Phi_1 | H_1 | \Phi_2 \rangle \langle \Phi_2 | H_1 | \Phi_1 \rangle}{\varepsilon_1 - \varepsilon_2}$$

$$= \frac{\chi^2}{\varepsilon_1 - \varepsilon_2}$$

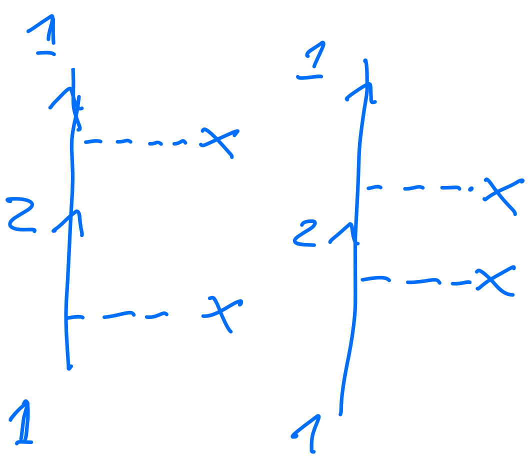
$$\frac{\lambda^2}{\varepsilon_1-\varepsilon_2} \langle \Phi_1 | H_1 \frac{Q}{e} \frac{Q}{e} H_1 | \Phi_1 \rangle$$

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

$$= \frac{\lambda^4}{(\varepsilon_1-\varepsilon_2)^3} = - \frac{\lambda^4}{(\varepsilon_2-\varepsilon_1)^3}$$

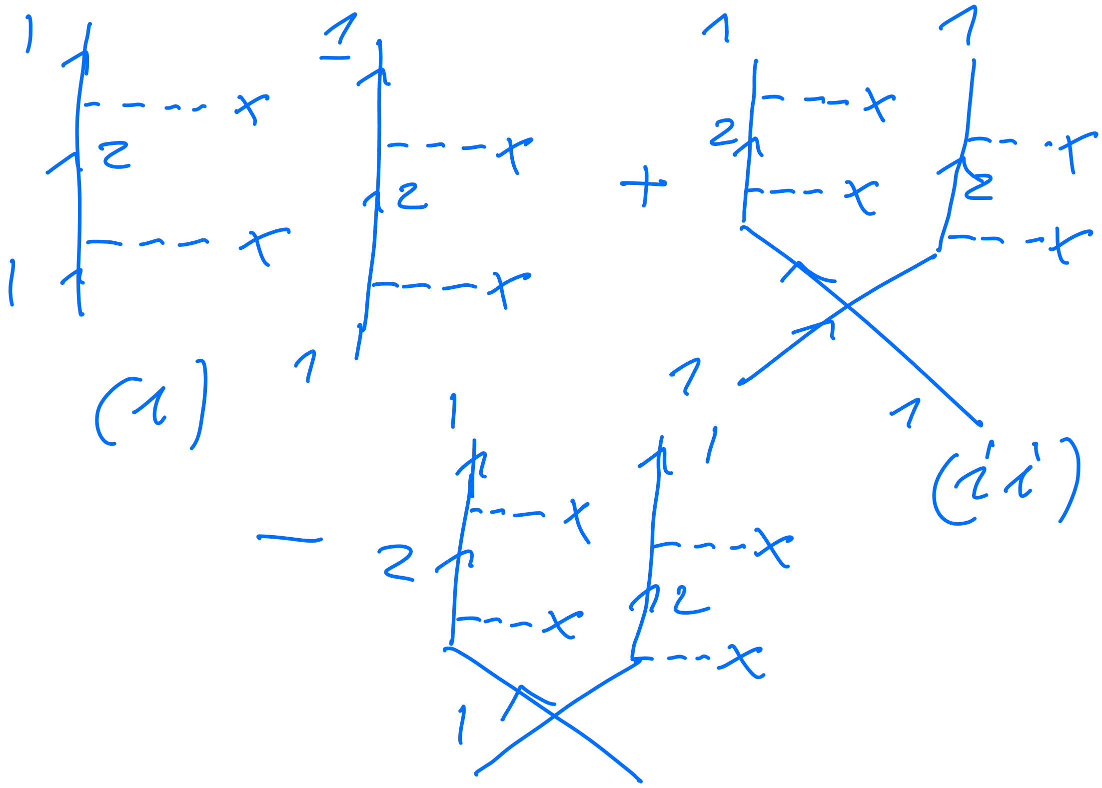
$$\Delta E_1^{(2)} + \Delta E_1^{(4)} = \frac{\lambda^2}{(\varepsilon_1-\varepsilon_2)^2} - \frac{\lambda^4}{(\varepsilon_2-\varepsilon_1)^4}$$

$$= \frac{\lambda^2}{(\varepsilon_2-\varepsilon_1)^2} - \frac{\lambda^4}{(\varepsilon_2-\varepsilon_1)^4}$$



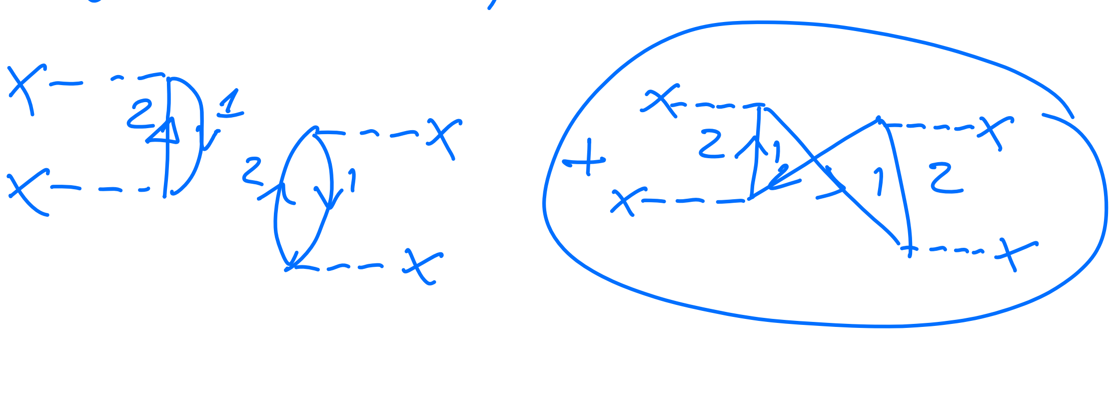
$$= \langle \Phi_1 | H_1 \frac{Q}{e} \langle \Phi_1 | H_1 \frac{Q}{e} H_1 | \Phi_1 \rangle \frac{Q}{e} H_1 | \Phi_1 \rangle$$

$$= \langle \Phi_1 | H_1 | \Phi_2 \rangle \left[\frac{\langle \Phi_1 | H_1 | \Phi_2 \rangle \langle \Phi_2 | H_1 | \phi_1 \rangle}{\varepsilon_1 - \varepsilon_2} \right] \times \frac{\langle \Phi_2 | H_1 | \phi_1 \rangle}{(\varepsilon_1 - \varepsilon_2)^2}$$

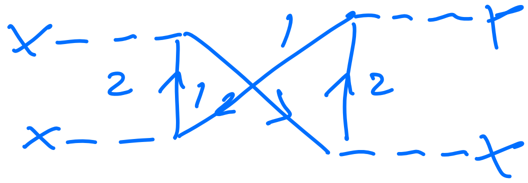


(i) (ii) (iii)

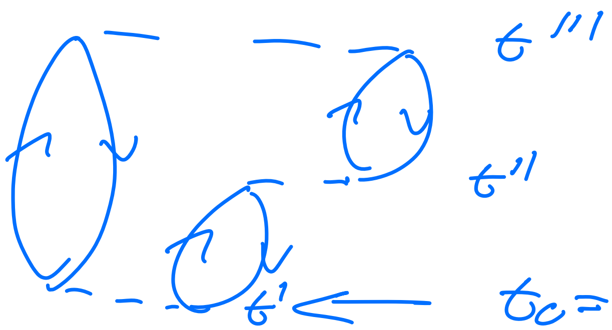
(i) + (ii)



we are left with the



$$\longrightarrow -\frac{\chi^4}{(\varepsilon_2-\varepsilon_1)^3}$$



$t_c = -\infty \quad |\Phi_c\rangle$

$u(t', t_c)\,|\Phi_c\rangle$