Lecture FYS4480/9480, November 1, 2024

FYS4480/9480 NOV 1

$$\Delta E_0 = E_0 - \mathcal{E}_0$$

$$\hat{H}_0 |\Phi_0\rangle = \mathcal{E}_0 |\Phi_0\rangle \qquad \langle \Phi_i | \Phi_j \rangle = \delta_{ij}$$

$$\mathcal{E}_0 = \sum_{i \leq F} \varepsilon_i$$

$$\hat{H}_0 = \sum_p \hat{h}_0(x_p) \qquad \hat{h}_0 |p\rangle = \varepsilon_p |p\rangle$$

$$\Delta E_0 = \sum_{n=0}^{\infty} \langle \Phi_0 | \hat{H}_1 \left\{ \frac{\hat{Q}}{\omega - H_0} \hat{H}_1 (\omega - E_0 + H_1) \right\}^n \times |\Phi_0\rangle$$

RS: $\omega = \mathcal{E}_0 \quad \wedge \quad$ BW: $\omega = E_0$

RS: $\quad \Delta E_0 = \sum_{n=1}^{\infty} \Delta E^{(n)}$

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

$$E_0^{\mathrm{Ref}} = \mathcal{E}_0 + \Delta E^{(1)}$$

$$\Delta E^{(2)} = \langle \Phi_0 | \hat{H}_1 \frac{\hat{Q}}{\mathcal{E}_0 - \hat{H}_0} \hat{H}_1 | \Phi_0 \rangle$$

$$\hat{H}_N = E_0^{ref} + \hat{F}_N + \hat{V}_N$$

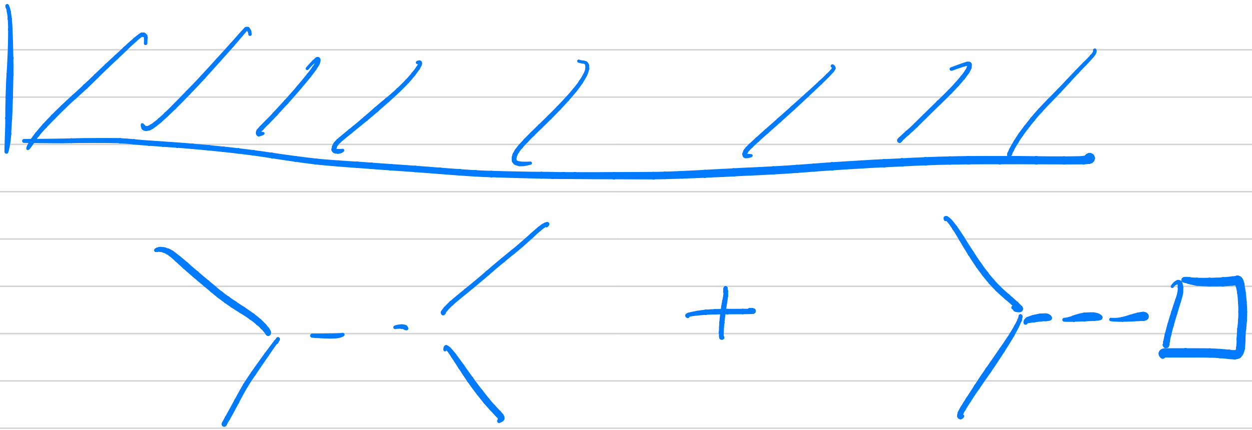
$$\hat{F}_N = \sum_{pq} \langle p | \hat{f} | q \rangle a_p^\dagger a_q$$

$$\langle p | \hat{f} | q \rangle = \langle p | \hat{h}_0 | q \rangle + \underbrace{\langle p | u^{HF} | q \rangle}_{\sum_{j \leq F} \langle pj | v | qj \rangle_{AS}}$$

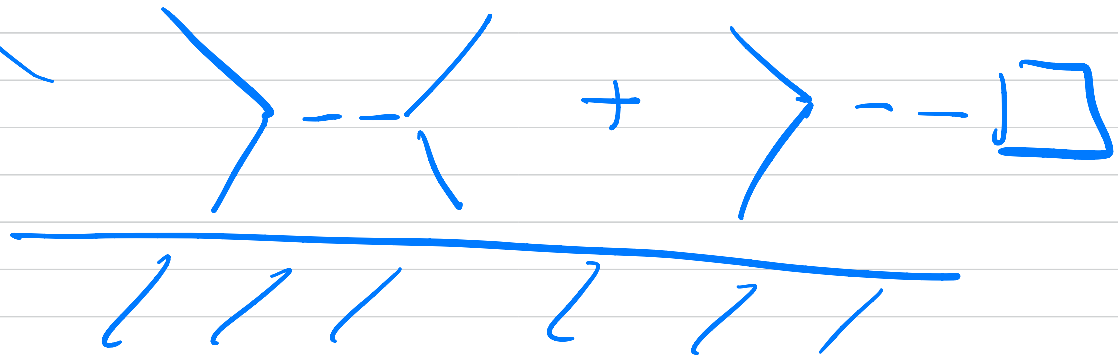
$$V_N = \frac{1}{4} \sum_{pqrs} \langle pq | v | rs \rangle_{AS} \, a_p^\dagger a_q^\dagger a_s a_r$$

$$\langle \Phi_0 | (\hat{F}_N + \hat{V}_N) \frac{\hat{Q}}{E_0 - \hat{H}_0} (\hat{F}_N + \hat{V}_N) | \Phi_0 \rangle$$

$\langle \Phi_0 |$



intermediate state



$| \Phi_0 \rangle$

$$\frac{1}{16}\sum_{\substack{pqrs\\ tuvw}} \langle \Phi_0 | a_t^\dagger a_u^\dagger a_w a_v a_p^\dagger a_q^\dagger a_s a_r | \Phi_0 \rangle \times \langle tu|v|vw\rangle_{AS} \langle pq|v|rs\rangle_{AS}$$

(Leave out $\frac{1}{\mathcal{E}_0 - \hat{H}_0}$)

$$a_t^\dagger a_u^\dagger a_w a_v a_p^\dagger a_q^\dagger a_s a_r$$

$\delta_{tr}\delta_{us}$ $\quad \underset{i\,j}{\leq F}$

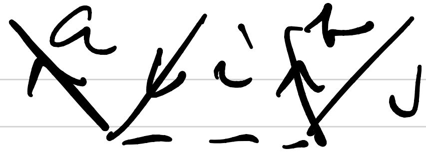
$\delta_{vp}\delta_{wq}$

$-\delta_{vq}\delta_{wp}$

$$\langle ab|v|ij\rangle_{AS} \quad \underset{a\;b}{>F}$$

$$-\langle ba|v|ij\rangle_{AS} = 2\langle ab|v|ij\rangle$$

$$\langle ab|v|ij\rangle_{AS} =$$



$+$

2p2h excitation

$$\langle ij|v|ab\rangle_{AS}$$

$$\frac{4}{16}\langle ij|v|ab\rangle\langle ab|v|ij\rangle$$

$\Rightarrow$

$$\frac{1}{4}\sum_{\substack{ab\\ij}} \langle ij|v|ab\rangle\langle ab|v|ij\rangle$$

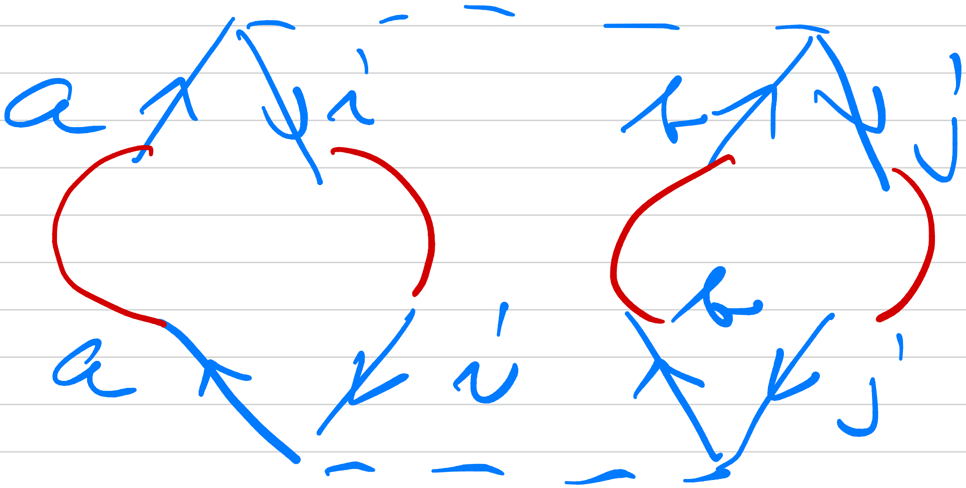
intermediate state

$$\mathcal{E}_M = \varepsilon_a + \varepsilon_b - \varepsilon_i - \varepsilon_j + \mathcal{E}_0$$

$$\mathcal{E}_0 - \mathcal{E}_M = \varepsilon_i + \varepsilon_j - \varepsilon_a - \varepsilon_b$$

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

Diagrammatic representation



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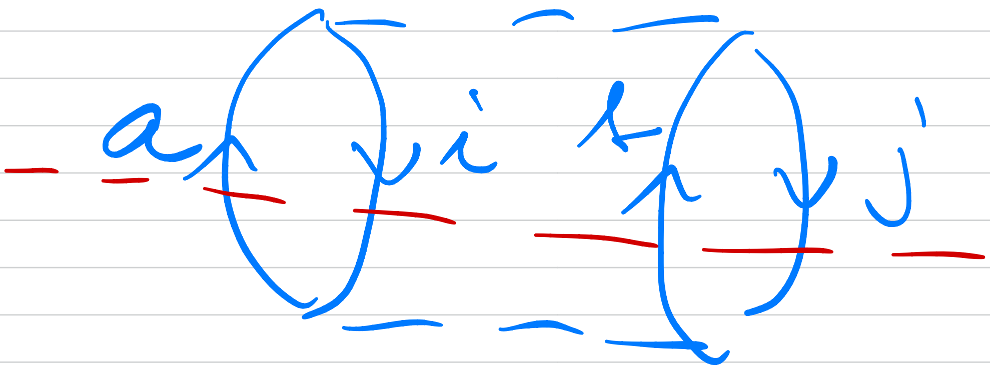
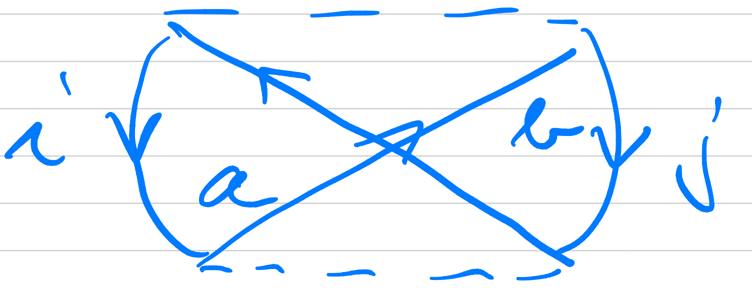
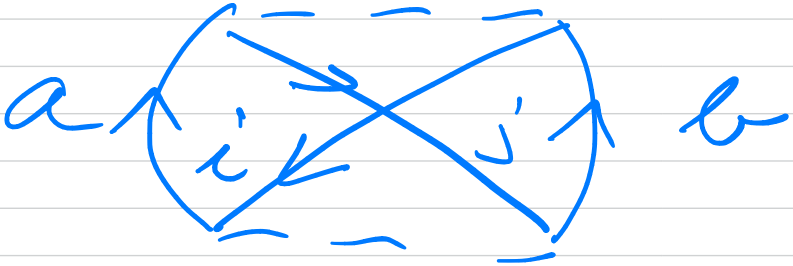
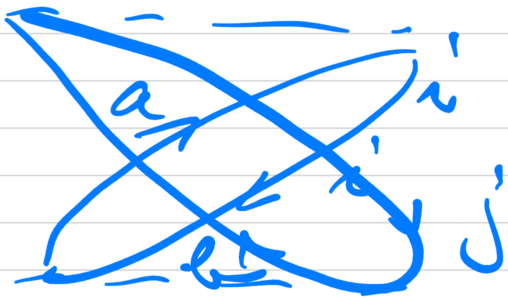
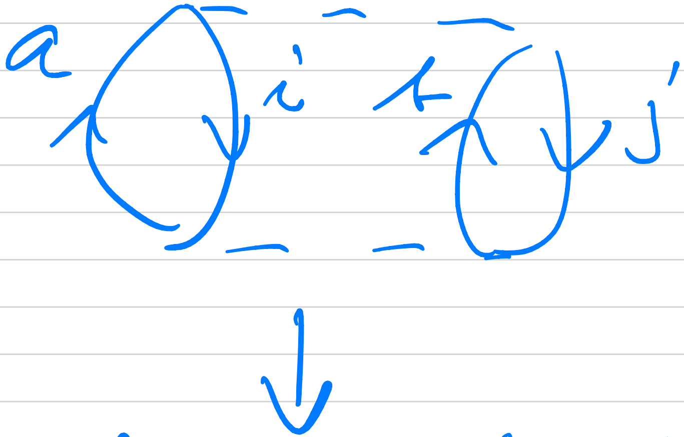


2p2h contribution

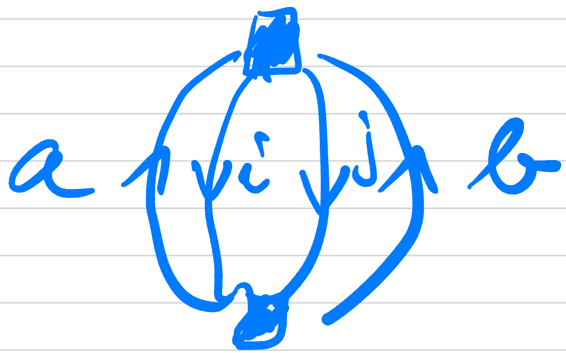








Hugenholtz



$$\sum_{\substack{pq\\tu}} \langle \Phi_0 | a_p^\dagger a_q \, a_t^\dagger a_u | \Phi_0 \rangle \times \langle p|g|q\rangle \langle t|g|u\rangle$$

$$a_p^\dagger a_q \, a_t^\dagger a_u$$

δ_{pu}

$i, j \leq F$

δ_{qt}

$a, b \ldots$

H_1

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

$$\langle p|\hat{f}|q\rangle = \langle p|h_0|q\rangle + \langle p|u^{HF}|q\rangle$$

Here only

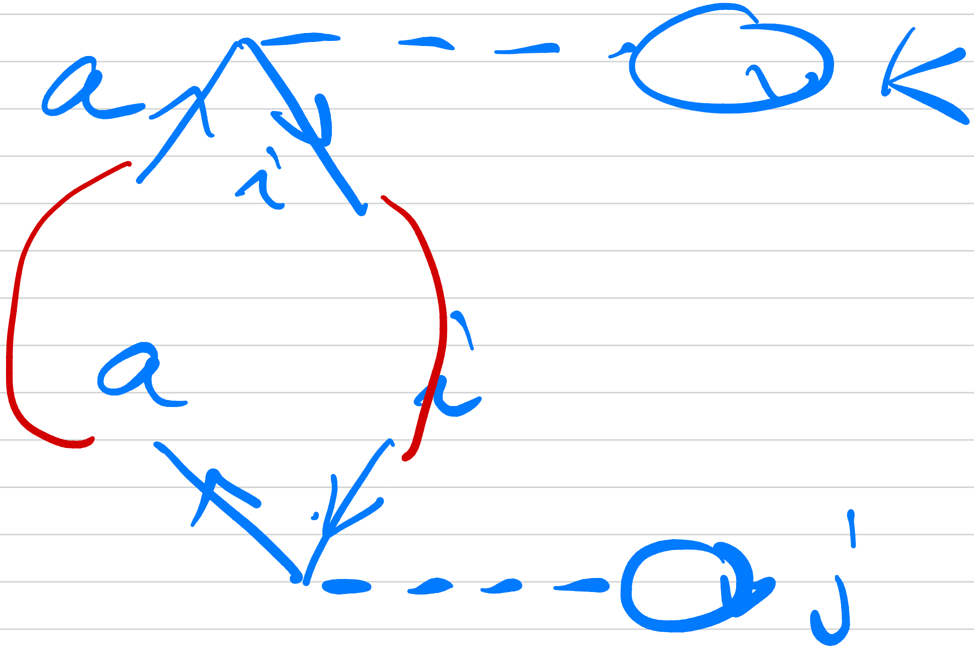
$$\langle p|u^{HF}|q\rangle = \sum_{j\le R} \langle pj|v|qj\rangle_{AS}$$

$$\sum_{ai} \frac{|\langle a|u^{HF}|i\rangle|^2}{\varepsilon_i - \varepsilon_a} =$$

$$\sum_{ai} \sum_{jK} \langle ij|v|aj\rangle \langle ik|v|ak\rangle$$

$$\times \frac{1}{\varepsilon_i - \varepsilon_a}$$

$$\langle a|h^{HF}|i\rangle = 0$$



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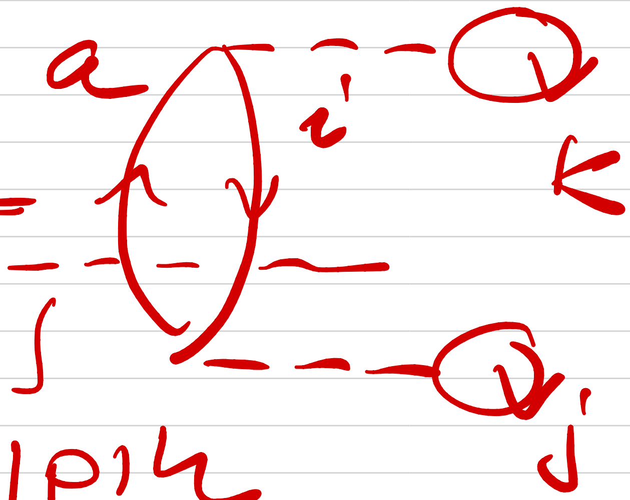
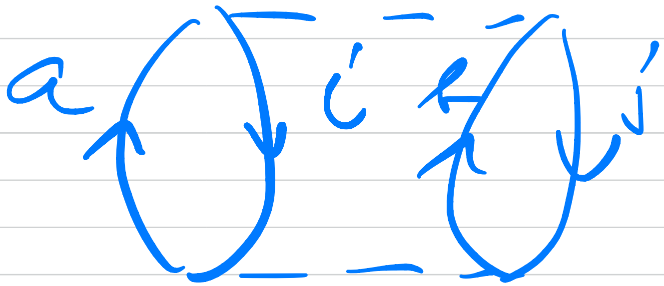
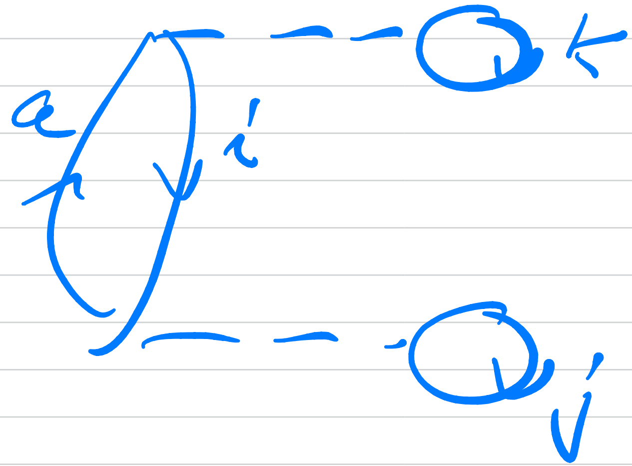


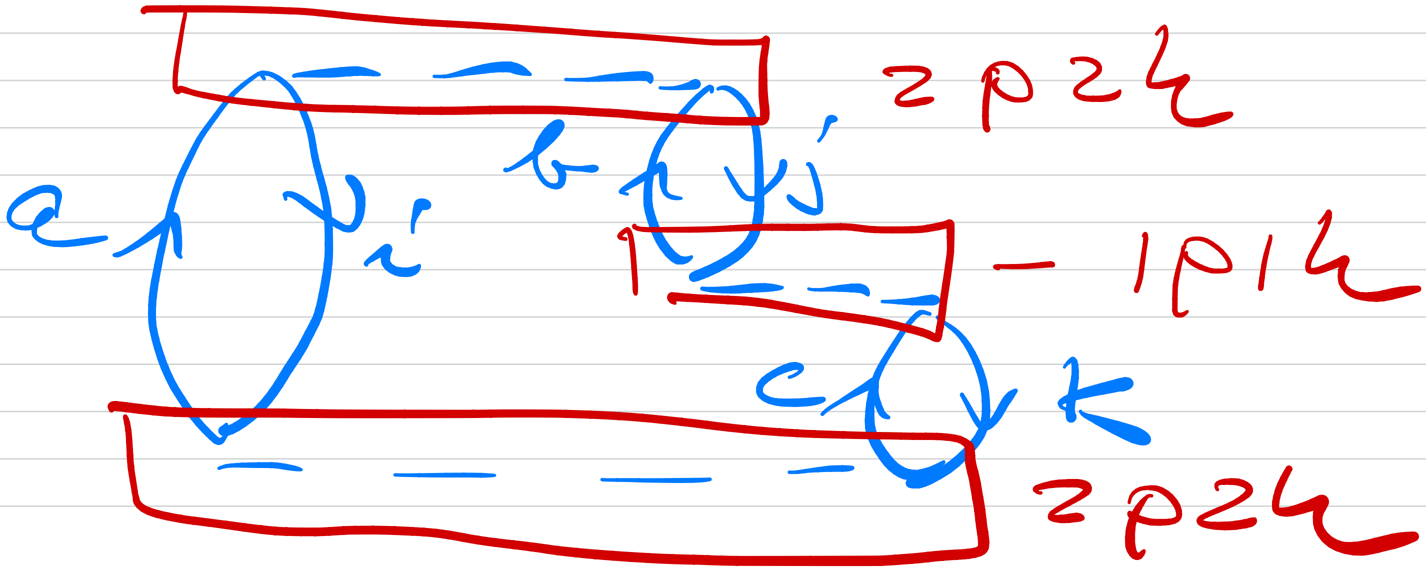
1p1h

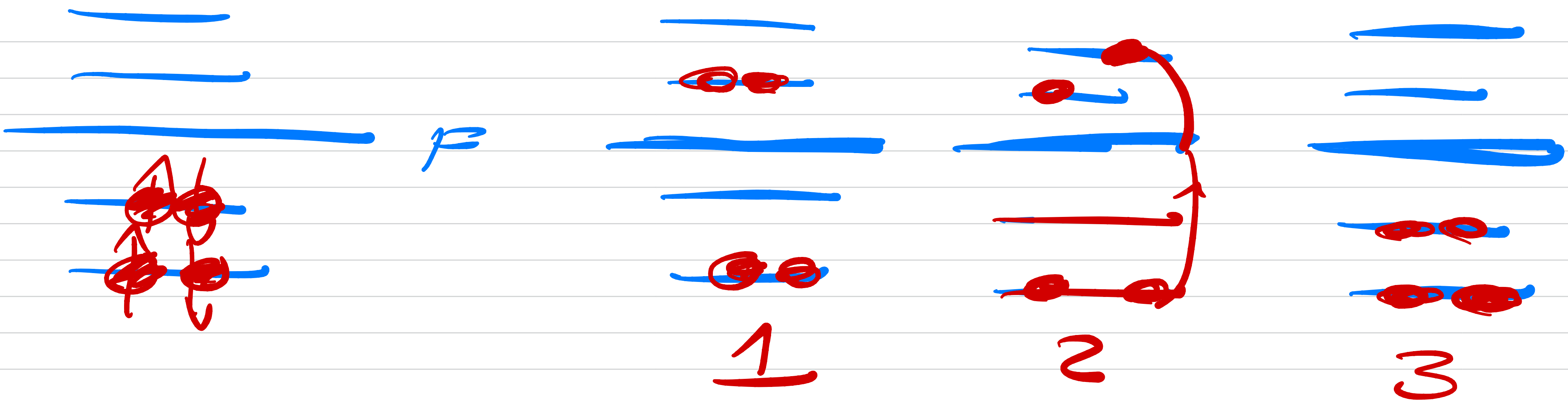
$$\Delta E^{(2)} =$$ 

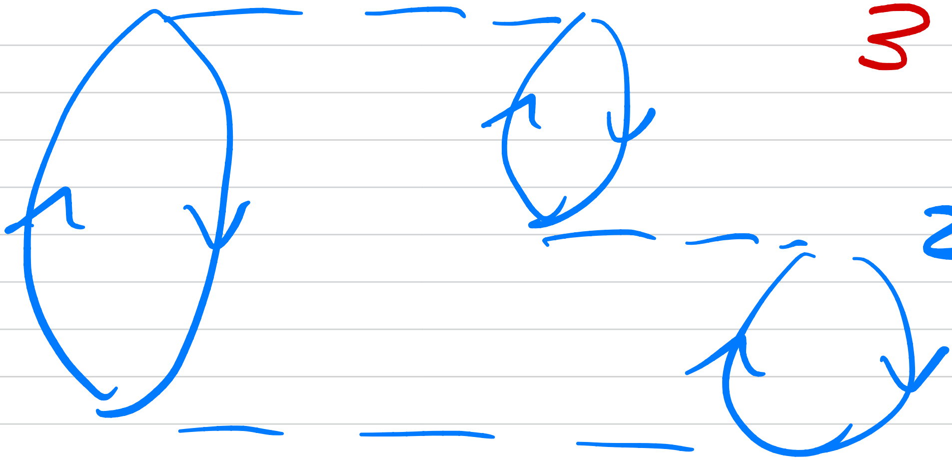
$+$ 

3rd-order

Example



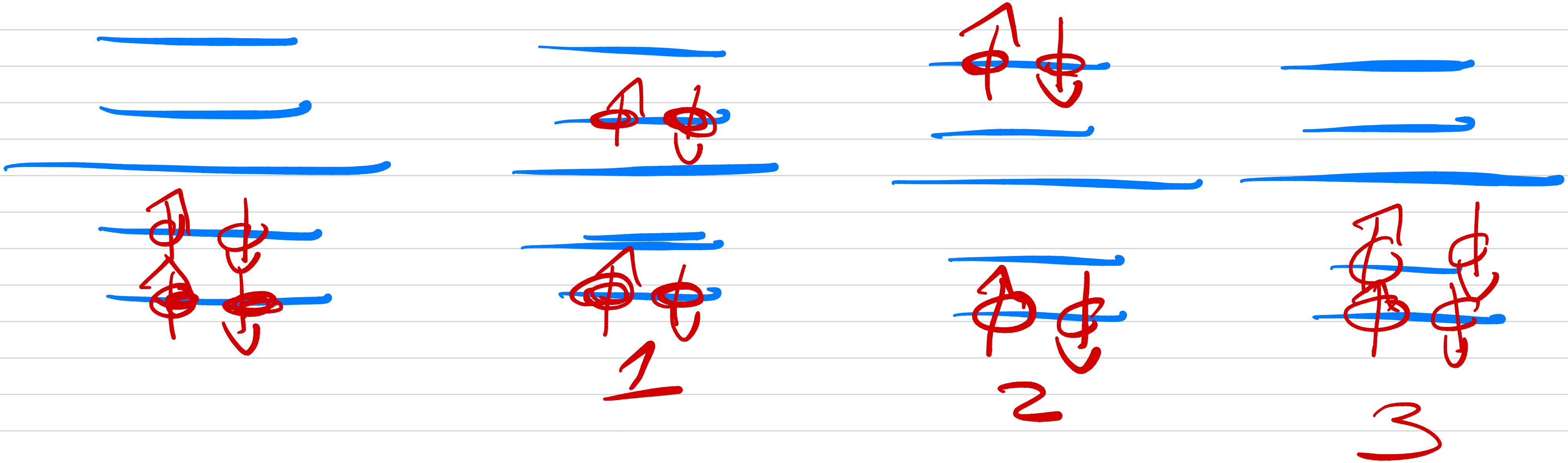


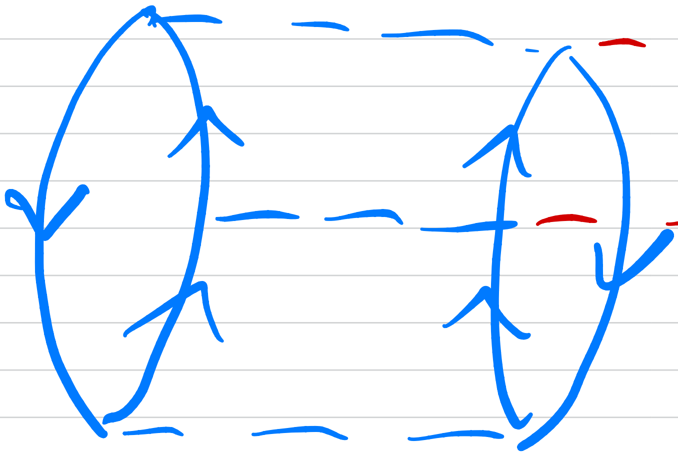


3 2p2h

2 1p1h

1 2p2h





2p2h 3

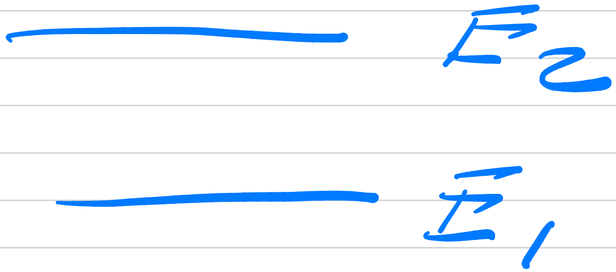
2p'2h 2

1 2p2h

2p-diagram

Example

$$\hat{H} = \sum_{i=1}^{2} a_i^{\dagger} a_i \varepsilon_i' + \lambda \sum_{i \neq j = 1,2} a_i^{\dagger} a_j$$



$$H|\psi_1\rangle = E_1 |\psi_1\rangle$$

$$H|\psi_2\rangle = E_2 |\psi_2\rangle$$

$$H_0 = \sum_{i=1}^{2} a_i^{\dagger} a_i \varepsilon_i'$$

$$|\phi_1\rangle = a_1^{\dagger}|0\rangle \wedge |\phi_2\rangle = a_2^{\dagger}|0\rangle$$

$$H_0|\phi_1\rangle = \varepsilon_1 |\phi_1\rangle \wedge H_0|\phi_2\rangle = \varepsilon_2 |\phi_2\rangle$$

$$\langle \Phi_1 | H_0 | \Phi_1 \rangle = \sum_{i=1}^{2} \langle 0 | a_1 a_i^\dagger a_i a_1^\dagger | 0 \rangle \times \varepsilon_i$$

$$= \varepsilon_1$$

$$\langle \Phi_1 | H_1 | \Phi_1 \rangle = \lambda \sum_{i \neq j} \langle 0 | a_1 a_i^\dagger a_j a_1^\dagger \times | 0 \rangle$$

$$= 0$$

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

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

$$|\psi_1\rangle = \alpha|\Phi_1\rangle + \beta|\Phi_2\rangle$$

$$H = \begin{bmatrix} \varepsilon_1 & \lambda \\ \lambda & \varepsilon_2 \end{bmatrix}$$

E_1 (lowest state)

$$(E_1 - \varepsilon_1)(E_1 - \varepsilon_2) - \lambda^2 = 0$$

$$E_1 = \frac{1}{2}\left(\varepsilon_1 + \varepsilon_2 - \sqrt{(\varepsilon_1 - \varepsilon_2) + 4\lambda^2}\right)$$

BW - PT $\quad \lambda \sum_{i \neq j} a_i^\dagger a_j$

$$\Delta E_1 = \underbrace{\langle \Phi_1 | H_1 | \Phi_1 \rangle}_{= 0}$$

$$+ \frac{\langle \Phi_1 | H_1 | \Phi_2 \rangle \langle \Phi_2 | H_1 | \Phi_1 \rangle}{E_1 - \varepsilon_2}$$

$$+ \frac{\langle \Phi_1 | H_1 | \Phi_2 \rangle \langle \Phi_2 | H_1 | \Phi_2 \rangle \times \langle \Phi_2 | H_1 | \Phi_1 \rangle}{(E_1 - \varepsilon_2)^2} + \ldots$$

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

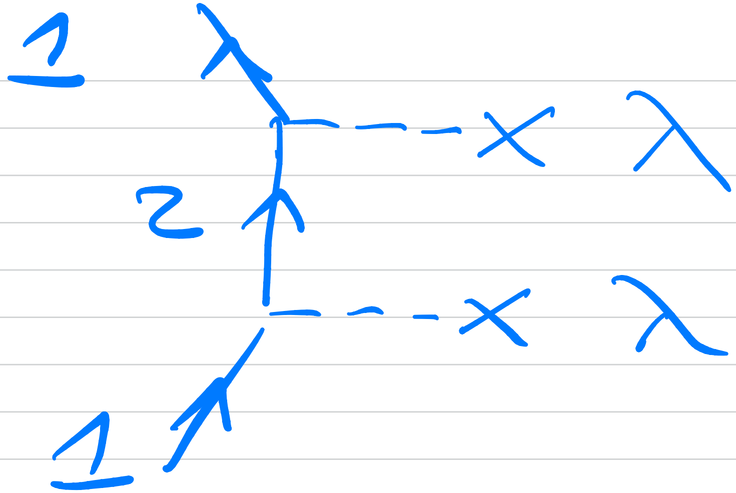
$$\Delta E_1 = E_1 - \varepsilon_1 = \frac{\lambda^2}{E_1 - \varepsilon_2} \Rightarrow$$

$$(E_1 - \varepsilon_1)(E_1 - \varepsilon_2) - \lambda^2 = 0$$

same as

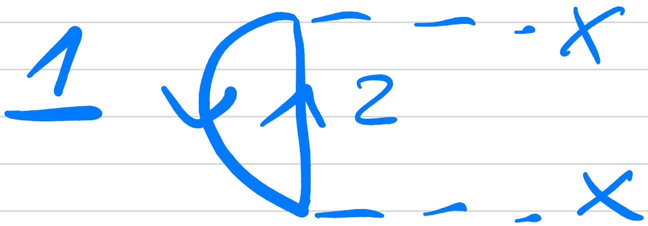
$$\det \begin{bmatrix} E_1 - \varepsilon_1 & \lambda \\ \lambda & E_1 - \varepsilon_2 \end{bmatrix} = 0$$

$$\frac{X^2}{E_1 - E_2} \quad :$$



particle formalism

particle-hole formalism



RS-theory (3rd-order)

$$E_1 \Rightarrow \varepsilon_1$$

$$\Delta E_1 = \underbrace{\langle \Phi_1 | H_1 | \Phi_1 \rangle}_{=0}$$

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

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

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

$$\Delta E_1^{(3rd)} = \frac{\lambda^2}{\varepsilon_1 - \varepsilon_2} \quad \Big| \; E_1 \simeq \varepsilon_1 + \frac{\lambda^2}{\varepsilon_1 - \varepsilon_2}$$

$$E_1 = \frac{1}{2}\left(\varepsilon_1 + \varepsilon_2 - \sqrt{(\varepsilon_1 - \varepsilon_2)^2 + 4\lambda^2}\right)$$

$$= \boxed{\varepsilon_1 + \frac{\lambda^2}{\varepsilon_1 - \varepsilon_2}} - \frac{\lambda^4}{(\varepsilon_1 - \varepsilon_3)^3} + \ldots$$