FYS4480/9480, lecture
October 31, 2025

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$$\Delta E_0(FCI) = E_0 - E_0^{Ref}$$

$$= \sum_{ai} C_i^a \langle a|f|i\rangle + \sum_{\substack{ab\\ij}} C_{ij}^{ab} \langle ab|v|ij\rangle$$

$$\Delta E_0(MBPT) = E_0 - \varepsilon_0 =$$

$$\langle \Phi_0 | H_1 | \Phi_0 \rangle + \Delta E_0^{(2)} + \cdots +$$

$$\Delta E_c^{(2)} = \sum_{\lambda=1} \langle \Phi_0 | \mathcal{U}_I | \Phi_\lambda \rangle \times \frac{\langle \Phi_\lambda | \mathcal{U}_I | \Phi_0 \rangle}{\varepsilon_0 - \varepsilon_\lambda}$$

$$|\Phi_\lambda\rangle = \begin{cases} 1p1h \\ 2p2h \end{cases}$$

<u>1p1h</u>

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

FCI: $\sum_{ai} c_i^a \langle a | f | i \rangle =$

1p1h

$$\hat{f} = \hat{h}_0 + u^{HF}$$

$$\hat{h}_0 |a\rangle = \varepsilon_a |a\rangle$$

$$\hat{h}_0 |i\rangle = \varepsilon_i |i\rangle$$

FCI: $$\sum_{ai} C_i^a \langle a | u^{HF} | i \rangle$$

MBPT(2): $$\sum_{ai} \frac{\langle i | u^{HF} | a \rangle \langle a | u^{HF} | i \rangle}{\varepsilon_i - \varepsilon_a}$$

$$C_i^a(\text{MBPT}(2)) = \frac{\langle i | u^{HF} | a \rangle}{\varepsilon_i - \varepsilon_a} \simeq C_i^a(\text{FCI})$$

$$\langle i | u^{HF} | a \rangle = \sum_{j \le F} \langle ij | v | aj \rangle_{AS}$$

MBPT(2): [1P1h] $$\sum_{\substack{ai \\ jk}} \frac{\langle ij | v | aj \rangle_{AS} \langle ik | v | ak \rangle}{\varepsilon_i - \varepsilon_a}$$

MBPT(2) 2p2h : $\displaystyle \frac{1}{16}\sum_{\substack{\lambda \\ pqrs \\ tuvw}} \langle \Phi_0 | a_p^\dagger a_q^\dagger a_s a_r | \Phi_\lambda \rangle$

$$\times \frac{\langle \Phi_\lambda | a_t^\dagger a_u^\dagger a_w a_v | \Phi_0 \rangle}{\varepsilon_0 - \varepsilon_\lambda}$$

$$\times \langle pq | v | rs \rangle_{AS} \langle tu | v | vw \rangle_{AS}$$

$$|\Phi_\lambda\rangle \to |\Phi_{ij}^{ab}\rangle = a_a^\dagger a_b^\dagger a_j a_i \times |\Phi_0\rangle$$

$$\langle\Phi_0| a_p^\dagger a_q^\dagger a_s a_r a_a^\dagger a_b^\dagger a_j a_i |\Phi_0\rangle$$

$$\delta_{pi}\,\delta_{qj}\,\delta_{sb}\,\delta_{ra}$$

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

$$\delta_{pi}\,\delta_{qj}\,\delta_{sa}\,\delta_{rb}$$

$$-\langle ij|v|ba\rangle_{AS}$$

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

$$\Delta E_0^{(2)}(2p2h) =$$

$$\frac{1}{4}\sum_{\substack{ab\\ij}} \frac{\langle ij|v|ab\rangle_{AS}\langle ab|v|ij\rangle_{AS}}{\mathcal{E}_0 - \mathcal{E}_{ij}^{ab}}$$

$$\left\{ \mathcal{E}_{ij}^{ab} = \varepsilon_a + \varepsilon_b - \varepsilon_j - \varepsilon_i + \mathcal{E}_0 \right\}$$

$$= \frac{1}{4}\sum_{\substack{ab\\ij}} \frac{\langle ij|v|ab\rangle_{AS}\langle ab|v|ij\rangle_{AS}}{\varepsilon_i + \varepsilon_j - \varepsilon_a - \varepsilon_b}$$

$|\Phi_x\rangle\langle\Phi_x|$ needs a factor $\frac{1}{4}$

FCI (2p2h) : $\displaystyle\sum_{\substack{ab\\ij}} C_{ij}^{ab} \langle ab\|v\|ij\rangle_{AS}$

approx

MBPT$_2$ (2p2h) :

$$\frac{1}{4}\sum_{\substack{ab\\ij}} \frac{\langle ij\|v\|ab\rangle_{AS}\langle ab\|v\|ij\rangle_{AS}}{\varepsilon_i+\varepsilon_j-\varepsilon_a-\varepsilon_b}$$

$$\Delta E_0^{(2)} = \sum_{\substack{ai\\kj}} \frac{\langle ij\|v\|aj\rangle_{AS}\langle ak\|v\|ik\rangle_{AS}}{\varepsilon_i-\varepsilon_a} + \frac{1}{4}\sum_{\substack{ab\\ij}} \frac{\langle ij\|v\|ab\rangle_{AS}\langle ab\|v\|ij\rangle_{AS}}{\varepsilon_i+\varepsilon_j-\varepsilon_a-\varepsilon_b}$$

Slight iteration of our simple example:

$$\mathcal{H} = \underbrace{\sum_{i=1}^{2} \varepsilon_p a_p^\dagger a_p}_{\mathcal{H}_0} + \lambda \sum_{p \neq q} a_p^\dagger a_q$$

$$\underline{\qquad\qquad} \; E_2 \qquad\qquad \mathcal{H} |\psi_1\rangle = E_1 |\psi_1\rangle$$

$$\underline{\qquad\qquad} \; E_1 \qquad\qquad \mathcal{H} |\psi_2\rangle = E_2 |\psi_2\rangle$$

$$\mathcal{H}_0 |\phi_1\rangle = \varepsilon_1 |\phi_1\rangle = a_1^\dagger |0\rangle$$

$$\mathcal{H}_0 |\phi_2\rangle = \varepsilon_2 |\phi_2\rangle \qquad a_2^\dagger |0\rangle$$

$$\langle \phi_i | \phi_j \rangle = \delta_{ij}$$

$$|\Psi_1\rangle = \alpha|\Phi_1\rangle + \beta|\Phi_2\rangle$$

$$\langle\Phi_1|\mathcal{H}|\Phi_1\rangle = \varepsilon_1$$

$$\langle\Phi_2|\mathcal{H}|\Phi_2\rangle = \varepsilon_2$$

$$\langle\Phi_1|\mathcal{H}|\Phi_2\rangle = \lambda$$

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

$$\det(\mathbb{H} - E_i) = 0$$

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

(i) BWPT

$$\Delta E_1 = \overset{=0}{\langle \Phi_1 | \mathcal{H}_I | \Phi_1 \rangle}$$

$$+ \frac{\langle \Phi_1 | \mathcal{H}_I | \Phi_2 \rangle \langle \Phi_2 | \mathcal{H}_1 | \Phi_1 \rangle}{E_1 - \varepsilon_2} \quad \lambda^2$$

$$+ \overset{\sim\lambda}{\langle \phi_1 | \mathcal{H}_1 | \Phi_2 \rangle} \overset{=0}{\langle \Phi_2 | \mathcal{H}_1 | \Phi_2 \rangle}$$

$$\times \frac{\langle \Phi_2 | \mathcal{H}_1 | \phi_1 \rangle \sim \lambda}{(E_1 - \varepsilon_2)^2}$$

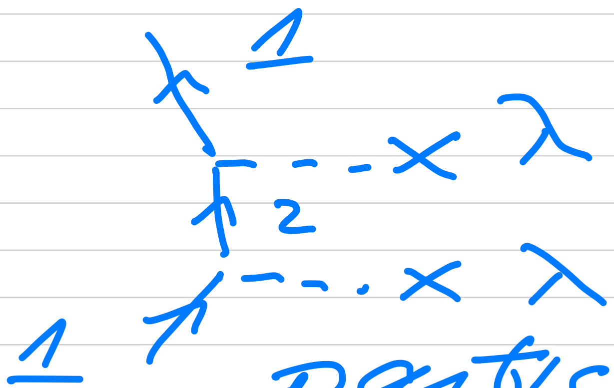
$$+ \ldots \; 0$$

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

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

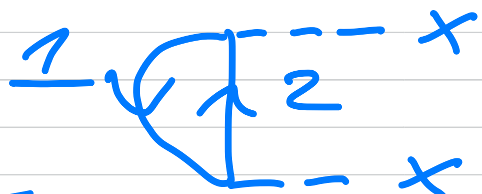
$$= \det(H - E_1)$$

$$\frac{\lambda^2}{E_1 - \varepsilon_2} = \frac{\langle \Phi_1 | H_1 | \Phi_2 \rangle \langle \Phi_2 | H_1 | \Phi_1 \rangle}{E_1 - \varepsilon_2}$$



ph

formalism



particle formalism

(iii) RSPT

$$\mathcal{E}_1 \to \varepsilon_1 \qquad (\mathcal{E}_2 - \varepsilon_2)$$

$$\Delta E_1 = \underbrace{\langle \Phi_1 | \mathcal{H}_1 | \Phi_1 \rangle}_{=0}$$

$$+ \frac{\langle \phi_1 | \mathcal{H}_1 | \phi_2 \rangle \langle \phi_2 | \mathcal{H}_1 | \phi_1 \rangle}{\varepsilon_1 - \varepsilon_2}$$

$$+ \frac{\langle \phi_1 | \mathcal{H}_1 | \phi_2 \rangle \overbrace{\langle \Phi_2 | \mathcal{H}_1 | \Phi_2 \rangle}^{=0} \langle \phi_2 | \mathcal{H}_1 | \phi_1 \rangle}{(\varepsilon_1 - \varepsilon_2)^2}$$

$$- \frac{\underbrace{\langle \phi_1 | \mathcal{H}_1 | \phi_1 \rangle}_{=0} \langle \phi_1 | \mathcal{H}_1 | \phi_2 \rangle \langle \phi_2 | \mathcal{H}_1 | \phi_1 \rangle}{(\varepsilon_1 - \varepsilon_2)^2}$$

$$\Delta E_1(\text{3rd-order}) = \frac{\lambda^2}{\varepsilon_1 - \varepsilon_2} + \Delta E_1(\text{BW})$$

$$E_1 \simeq \varepsilon_1 + \frac{\lambda^2}{\varepsilon_1 - \varepsilon_2}$$

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

$$x = \frac{4\lambda^2}{(\varepsilon_1 - \varepsilon_2)^2} \qquad \left|\frac{2\lambda}{\varepsilon_1 - \varepsilon_2}\right| < 1$$

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

$$E_1 = \varepsilon_1 + \frac{x^2}{\varepsilon_1-\varepsilon_2}\left[1 - \frac{x^2}{(\varepsilon_1-\varepsilon_2)^2} + \cdots\right]$$

$$\Delta E_1^{(4)}(\mathrm{RSPT}) = ?$$

Def $\langle \mathcal{H}_1 \rangle = \langle \phi_1 | \mathcal{H}_1 | \phi_1 \rangle$

$\langle \mathcal{H}_1 \frac{Q}{e_0} \mathcal{H}_I \rangle = \langle \phi_1 | \mathcal{H}_1 \frac{Q}{e_0} \mathcal{H}_1 | \phi_1 \rangle$

$e_0 = \varepsilon_1 - \mathcal{H}_0 \qquad Q = |\phi_2\rangle\langle\phi_2|$ $=0$

$$\langle \mathcal{H}_1 \frac{Q}{e_0} \mathcal{H}_1 \frac{Q}{e_0} \mathcal{H}_1 \frac{Q}{e_0} \mathcal{H}_1 \rangle$$

$$\langle \Phi_2 | \mathcal{H}_1 | \Phi_2 \rangle = 0$$

$$- \langle \mathcal{H}_1 \frac{Q}{e_0} \underbrace{\langle \mathcal{H}_1 \rangle}_{=0} \frac{Q}{e_0} \mathcal{H}_1 \frac{Q}{e_0} \mathcal{H}_1 \rangle$$

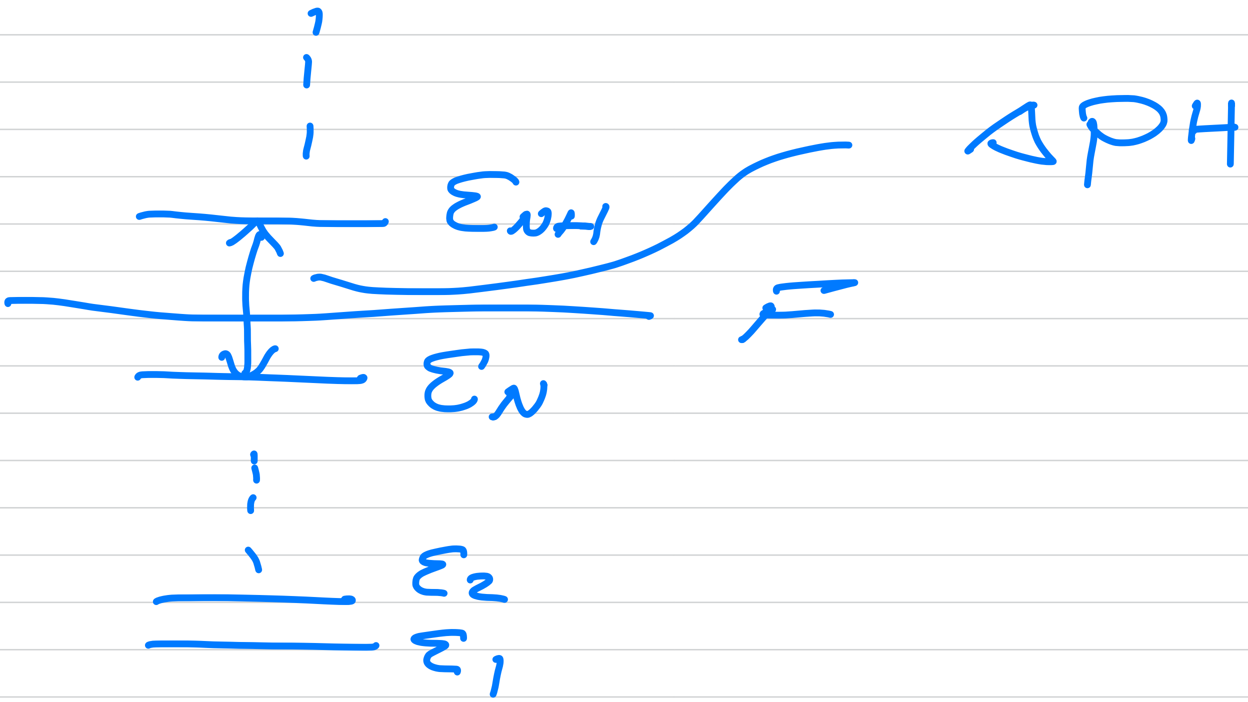
$$- \langle \mathcal{H}_1 \frac{Q}{e_0} \mathcal{H}_1 \frac{Q}{e_0} \underbrace{\langle \mathcal{H}_1 \rangle}_{=0} \frac{Q}{e_0} \mathcal{H}_1 \rangle$$

$$+ \langle \mathcal{H}_1 \frac{Q}{e_0} \overbrace{\langle \mathcal{H}_1 \rangle}^{=0} \frac{Q}{e_0} \overbrace{\langle \mathcal{H}_1 \rangle}^{=0} \frac{Q}{e_0} \mathcal{H}_1 \rangle$$

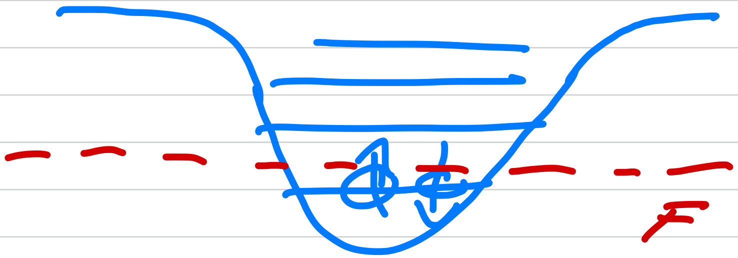
$$- \langle \mathcal{H}_1 \frac{Q}{e_0} \underbrace{\langle \mathcal{H}_1 \frac{Q}{e_0} \mathcal{H}_1 \rangle}_{\lambda^2/(\varepsilon_1 - \varepsilon_2)} \frac{Q}{e_0} \mathcal{H}_1 \rangle$$

$$\lambda^2/(\varepsilon_1 - \varepsilon_2)^2$$

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



Quantum dots



$$\varepsilon_{n_x n_y} = \hbar\omega(n_x + n_y + 1)$$

$$n_x, n_y = 0, 1, 2, \ldots$$

$\langle r \rangle$ larger

$\hbar\omega \gg 1$ (strong well potential)

spacing $\sim \hbar\omega$

$\langle r \rangle$ is small

$\hbar\omega$ smaller

ΔpH becomes smaller

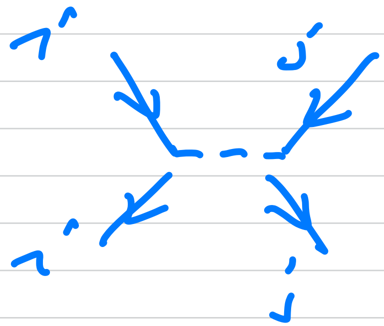
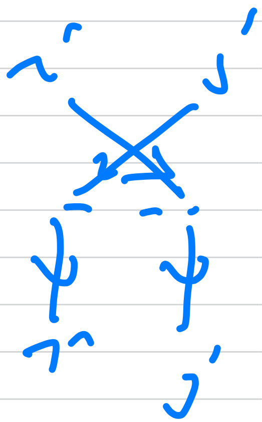
$$\frac{\lambda}{\Delta pH} \gg 1$$

Diagrams & Diagram rules

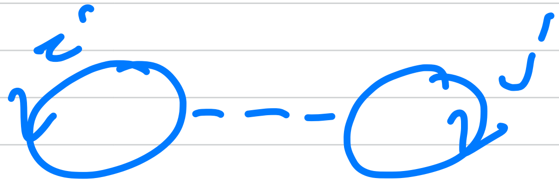
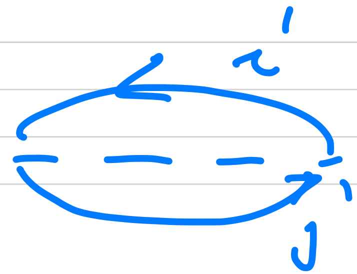
RSPT

$$\Delta E_0^{(1)} = \langle \Phi_0 | H_1 | \Phi_0 \rangle$$

$$= \frac{1}{2} \sum_{ij \leq F} \langle ij | v | ij \rangle_{AS}$$

$$= \frac{1}{2} \sum_{ij \leq F} \Big[$$  $$+$$  $$\Big]$$

$$= \frac{1}{2} \sum_{ij < F} \Big[\langle ij | v | ij \rangle - \langle ij | v | ji \rangle \Big]$$

$$=$$  $$+$$ 

$$\Delta E_0^{(2)}$$

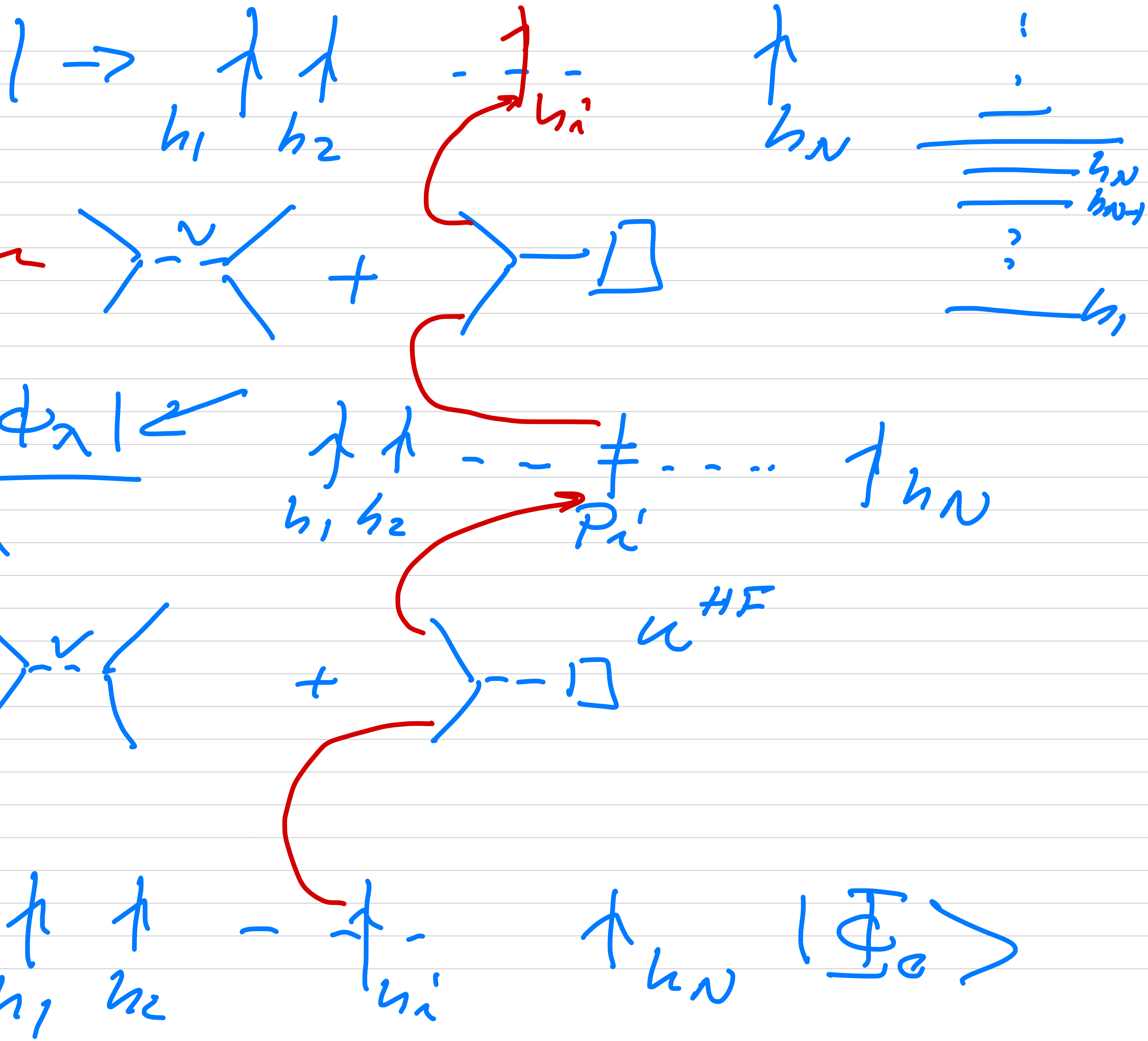
$$\text{IPIK}$$

$$\sum_{aijk} \frac{\langle kj \| v \| ka \rangle_{AS} \langle ia \| v \| ij \rangle_{AS}}{\varepsilon_i - \varepsilon_a}$$

$$= \sum_{\lambda \, (\text{IPIK})} \frac{\langle \Phi_0 | \mathcal{H}_1 | \Phi_\lambda \rangle \langle \Phi_\lambda | \mathcal{H}_1 | \Phi_0 \rangle}{\varepsilon_0 - \varepsilon_\lambda}$$

particle formalism

$$\langle \Phi_0 | \to$$



$$\frac{|\Phi_\lambda\rangle\langle\Phi_\lambda|}{\varepsilon_0 - \varepsilon_\lambda}$$