Lecture Fys4480/9480, November 9, 2023

Rayleigh-schrödinger theory

$$\Delta E = \sum_{i=1}^{\infty} \Delta E^{(i)}$$

$$\hat{P} = |\Phi_0\rangle\langle\Phi_0| \qquad \hat{Q} = \sum_{i=1}^{\infty} |\Phi_M\rangle\langle\Phi_M|$$

$$\langle\Phi_0|\Phi_M\rangle = 0 \quad M = 0$$

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

$$\Delta E^{(2)} = \sum_M \frac{\langle\Phi_0|H_1|\Phi_M\rangle\langle\Phi_M|H_1|\Phi_0\rangle}{W_0 - W_M}$$

$$H_0|\Phi_0\rangle = W_0|\Phi_0\rangle$$

$$|\Phi_0\rangle = \frac{1}{\sqrt{N!}} \sum_P (-1)^P \hat{P} \left(\varphi_{\alpha_1}(x_1) \cdots \varphi_{\alpha_N}(x_N) \right)$$

$$h_0 \varphi_{\alpha_i}(x_i) = \varepsilon_{\alpha_i} \varphi_{\alpha_i}(x_i)$$

$$h_0 |\alpha_i\rangle = \varepsilon_{\alpha_i} |\alpha_i\rangle \Rightarrow \langle a|h_0|i\rangle = 0$$

$$H = H_0 + H_1 = E_0^{Ref} + \underbrace{F_N + V_N}_{H_N}$$

$$E_0^{Ref}(MBPT) = W_0 \quad \text{unperturbed energy}$$

$$\Delta E(MBPT) = E_0 - W_0$$

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

$$E_0^{Ref}(FCI) = \underbrace{W_0}_{\sum_{i\leq F} \varepsilon_i} + \underbrace{\frac{1}{2}\sum_{ij} \langle ij|v|ij\rangle_{AS}}_{\Delta E^{(1)}}$$

$$= E_0 - (W_0 + \Delta E^{(1)})$$

Define wave operator

$$\Omega = \sum_{i=1}^{\infty} \Omega^{(i)}$$

$$\Omega^{(1)} = \sum_{M} \frac{|\Phi_M\rangle\langle\Phi_M|H_1|\Phi_0\rangle}{W_0 - W_M}$$

$$\Delta E^{(2)} = \langle\Phi_0|H_1\Omega^{(1)}|\Phi_0\rangle$$

$$\Omega^{(2)} = \sum_{MN} \frac{|\Phi_M\rangle\langle\Phi_M|H_1|\Phi_N\rangle \times \langle\Phi_N|H_1|\Phi_0\rangle}{(W_0 - W_M)(W_0 - W_N)} -$$

$$-\left\{\sum_{M} \frac{|\Phi_M\rangle\langle\Phi_M|H_1|\Phi_0\rangle}{(\omega_0-\omega_M)^2}\right\}.$$

$$\times \underbrace{\langle\Phi_0|H_1|\Phi_0\rangle}_{\Delta E^{(1)}}$$

Examples

$$\Delta E^{(2)} = \sum_{\underbrace{ai}_{M}} \frac{\langle\Phi_0|H_1|\Phi_i^a\rangle\langle\Phi_i^a|H_1|\Phi_0\rangle}{\varepsilon_i-\varepsilon_a}$$

$1p1h$

$$\langle\Phi_0|H_1|\Phi_i^a\rangle$$

$$= \langle i|f|a\rangle =$$

$$= \underbrace{\langle i|h_0|a\rangle}_{=0} + \sum_{j\leq F} \langle ij|v|aj\rangle_{AS}$$

But we have also $2p2h$

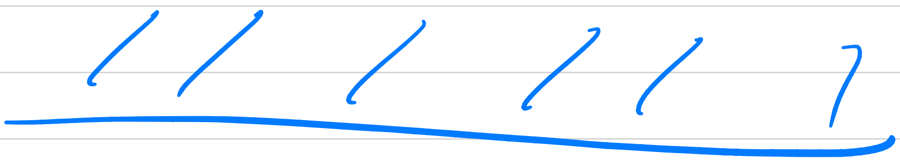
$$\langle \Phi_0|H_1|\Phi_{ij}^{ab}\rangle = \langle ij|v|ab\rangle_{AS}$$

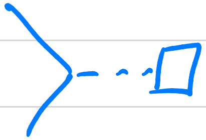
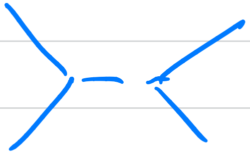
collecting

$$\Delta E^{(2)} = \sum_{ai} \frac{|\langle i|f|a\rangle|^2}{\varepsilon_i - \varepsilon_a}$$

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

Diagrammatic representation

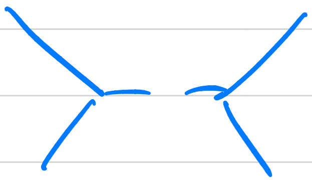
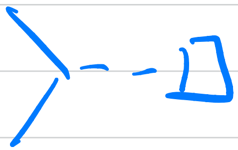
$\langle \Phi_0 |$ 

 or 

$$\frac{|\Phi_M\rangle\langle\Phi_M|}{\omega_0-\omega_M}$$

$|\Phi_M\rangle = a_a^\dagger a_i |\Phi_0\rangle$

or $a_a^\dagger a_b^\dagger a_j a_i |\Phi_0\rangle$

 or 

 $|\Phi_0\rangle$

Let us study the V_N case (without the $1/\omega_\sigma - \omega_{a}$ denom)

$$\frac{1}{16}\sum_{\substack{pqrs\\tuwv}} \langle \Phi_0 | a_p^\dagger a_q^\dagger a_s a_r\, a_t^\dagger a_u^\dagger a_w a_v |\Phi_0\rangle$$

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

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

2p

2h

$$\langle \Phi_0 | a_p^\dagger a_q^\dagger a_s a_r\, a_a^\dagger a_i |\Phi_0\rangle \qquad a_e^\dagger a_q$$

$$\underbrace{\delta_{rt}\,\delta_{su}}_{\text{particle states}} \qquad \underbrace{\delta_{pv}\,\delta_{qw}}_{\text{hole states}}$$

$$\sum_{\substack{pqrs\\tuvw}} \longrightarrow \sum_{pqrs} \longrightarrow \sum_{\substack{ab\\ij}}$$

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

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

$$-\,\delta_{pv}\,\delta_{qw}\,\delta_{ru}\,\delta_{s\cdot}$$

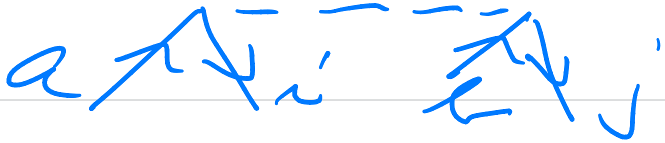
$$-\,\langle ij|v|ba\rangle_{AS}\,\langle ab|v|ij\rangle_{AS}$$

$$\Rightarrow \frac{1}{16} \cdot 4 \sum_{\substack{ij \\ ab}} \langle ij|v|ab\rangle_{AS} \langle ab|v|ij\rangle_{AS}$$

$$= \frac{1}{4} \sum_{\substack{ij \\ ab}} \langle ij|v|ab\rangle_{AS} \langle ab|v|ij\rangle_{AS}$$

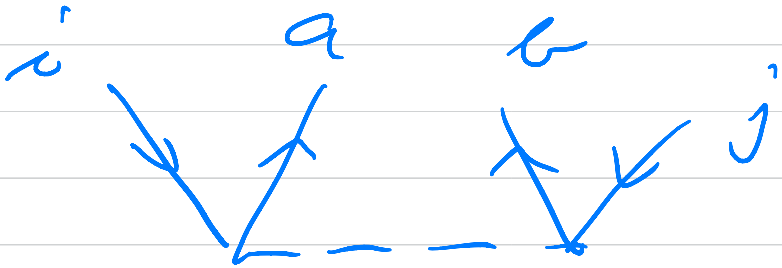
with the denominators

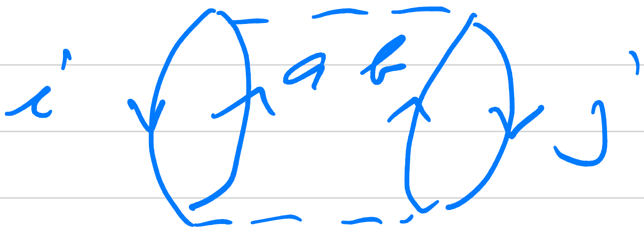
$$= \frac{1}{4} \sum_{\substack{ij \\ ab}} \frac{\langle ij|v|ab\rangle_{AS} \langle ab|v|ij\rangle_{AS}}{\varepsilon_i + \varepsilon_j - \varepsilon_a - \varepsilon_b}$$

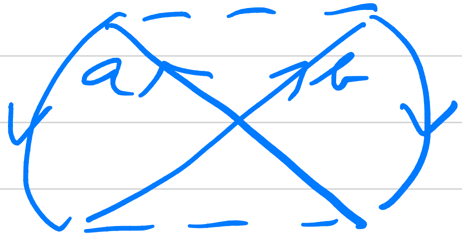


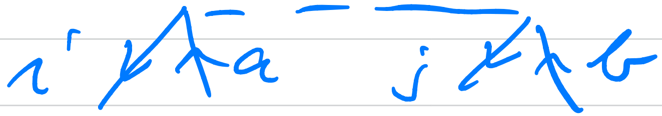
$\langle \Phi_0 | H_1 | \Phi_M \rangle$

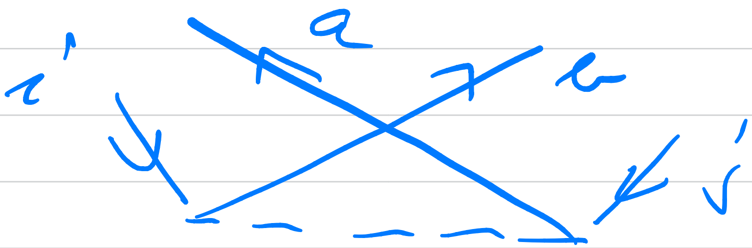
$\langle \Phi_M | H_1 | \Phi_c \rangle$



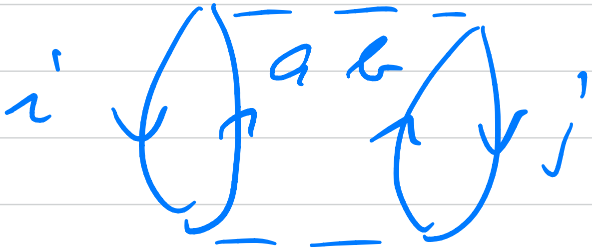








Feynman Goldstone diagrams



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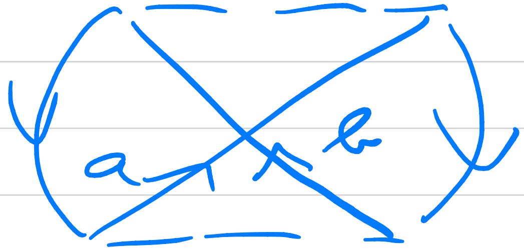

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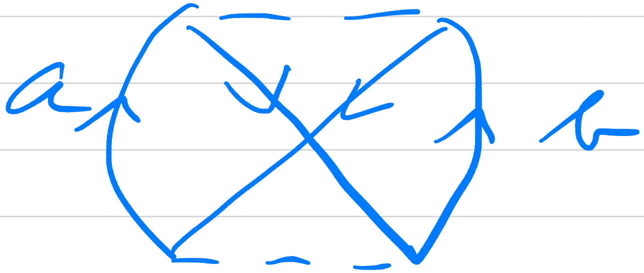

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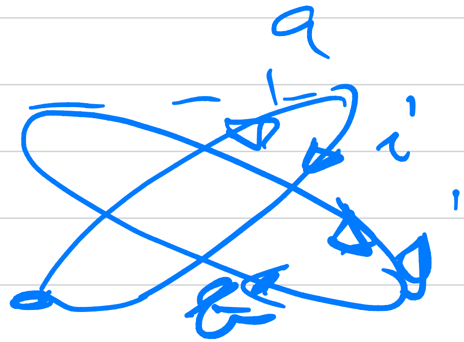
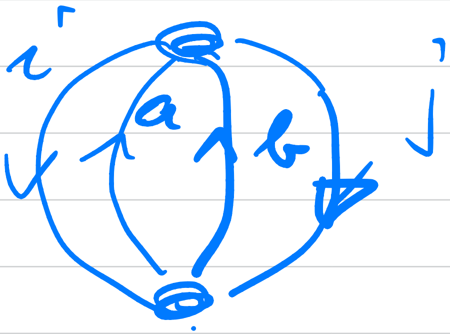


$\langle ji|v|ba\rangle\langle ab|v|ij\rangle$

$=$



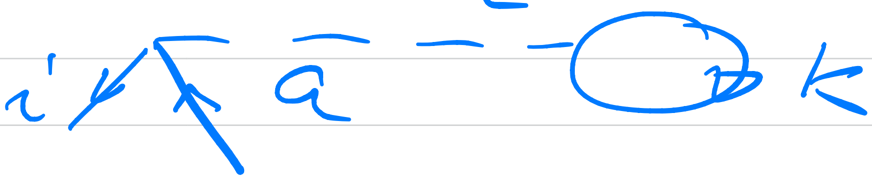
$$= \frac{1}{4}\sum_{\substack{ij\\ab}} \frac{\langle ij|v|ab\rangle_A\langle ab|v|ij\rangle_A}{\varepsilon_i+\varepsilon_j-\varepsilon_a-\varepsilon_b}$$

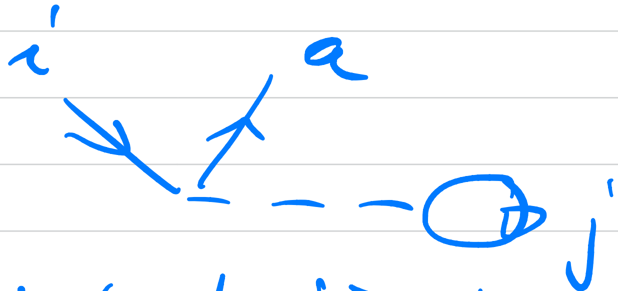
one-body operator

$$\langle \Phi_0 | a_p^\dagger a_q | \Phi_M \rangle \langle \Phi_M | \underbrace{a_p^\dagger a_q | \Phi_0 \rangle}$$

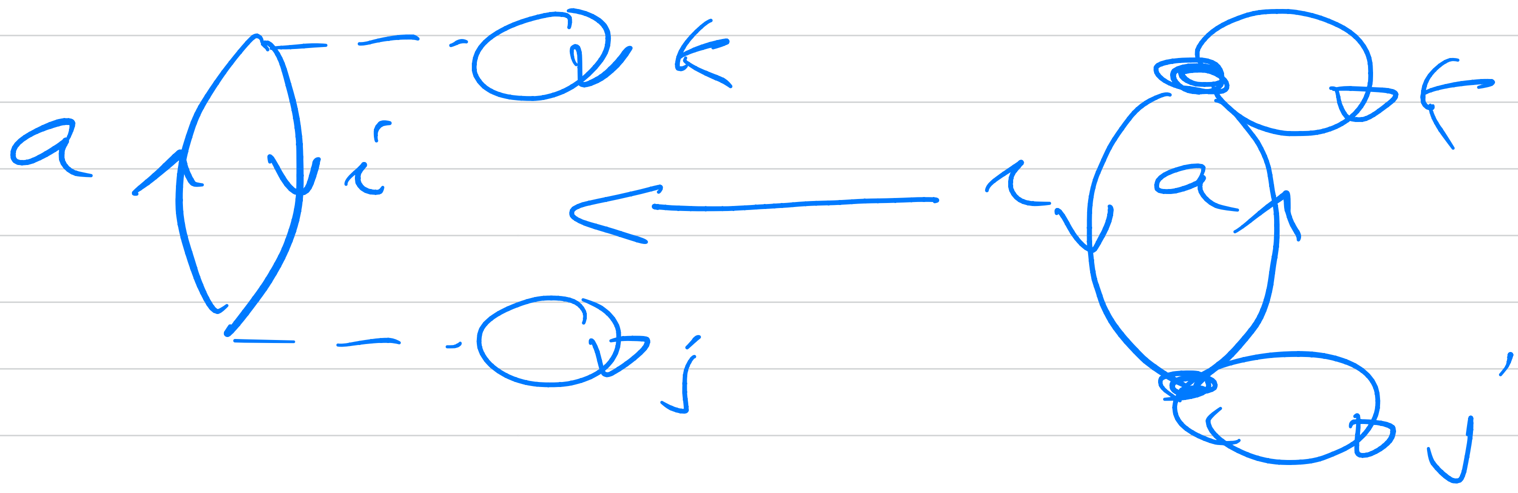
$$\langle i | f | a \rangle = \sum_j \langle ij | v | aj \rangle_{AS}$$

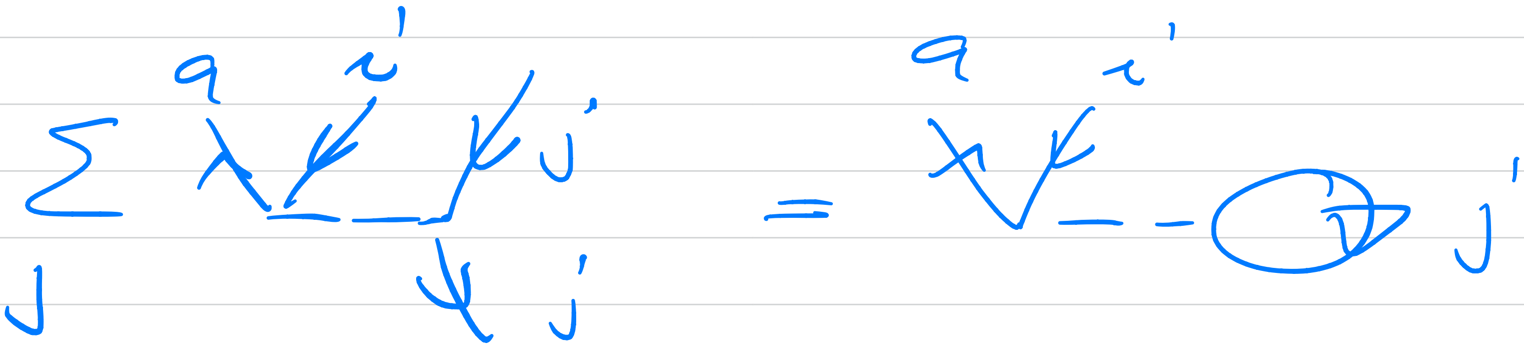
$$\sum_{ai} \frac{\langle i | f | a \rangle \langle a | f | i \rangle}{\varepsilon_i - \varepsilon_a}$$





$$= \sum_{\substack{ai \\ jk}} \frac{\langle ij | v | aj \rangle_{AS} \langle ak | v | ik \rangle_{AS}}{\varepsilon_i - \varepsilon_a}$$



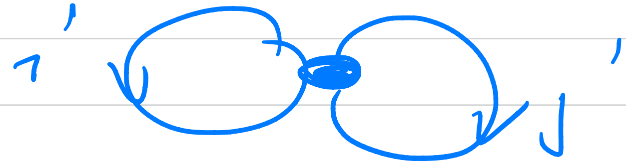


$$E_0^{(2)} = W_0 + \underbrace{\frac{1}{2}\sum_{i'j'} \langle i'j' | v | i'j' \rangle_{AS}}_{\Delta E^{(1)}}$$

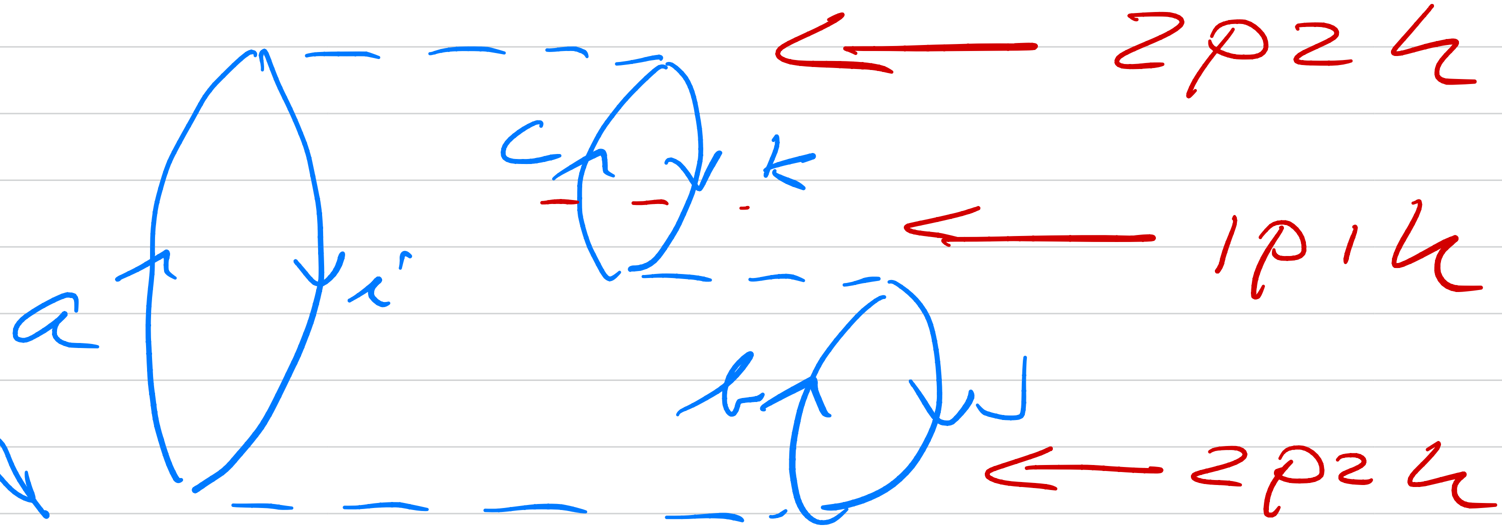
$$+ \; \Delta E^{(2)}$$

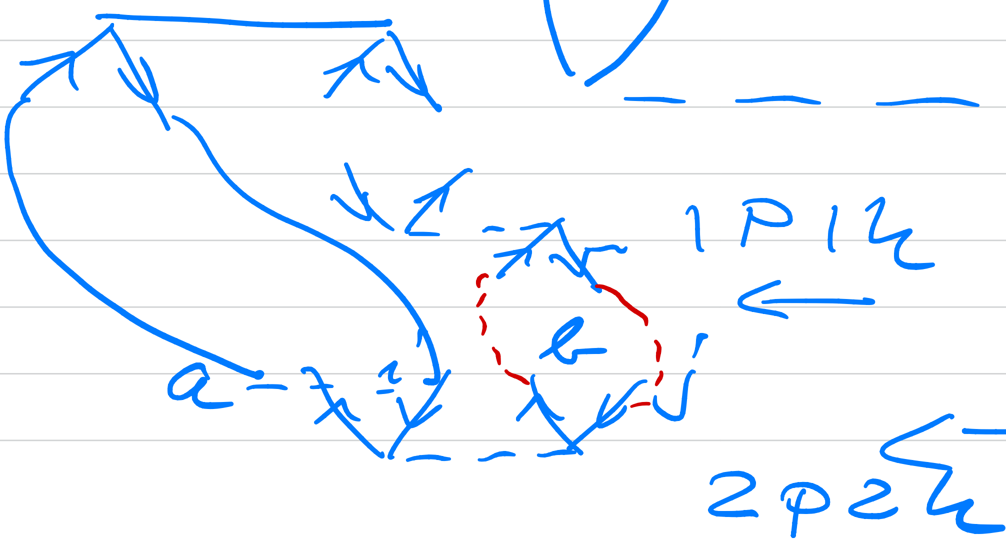
$\Delta E^{(1)} =$

$=$

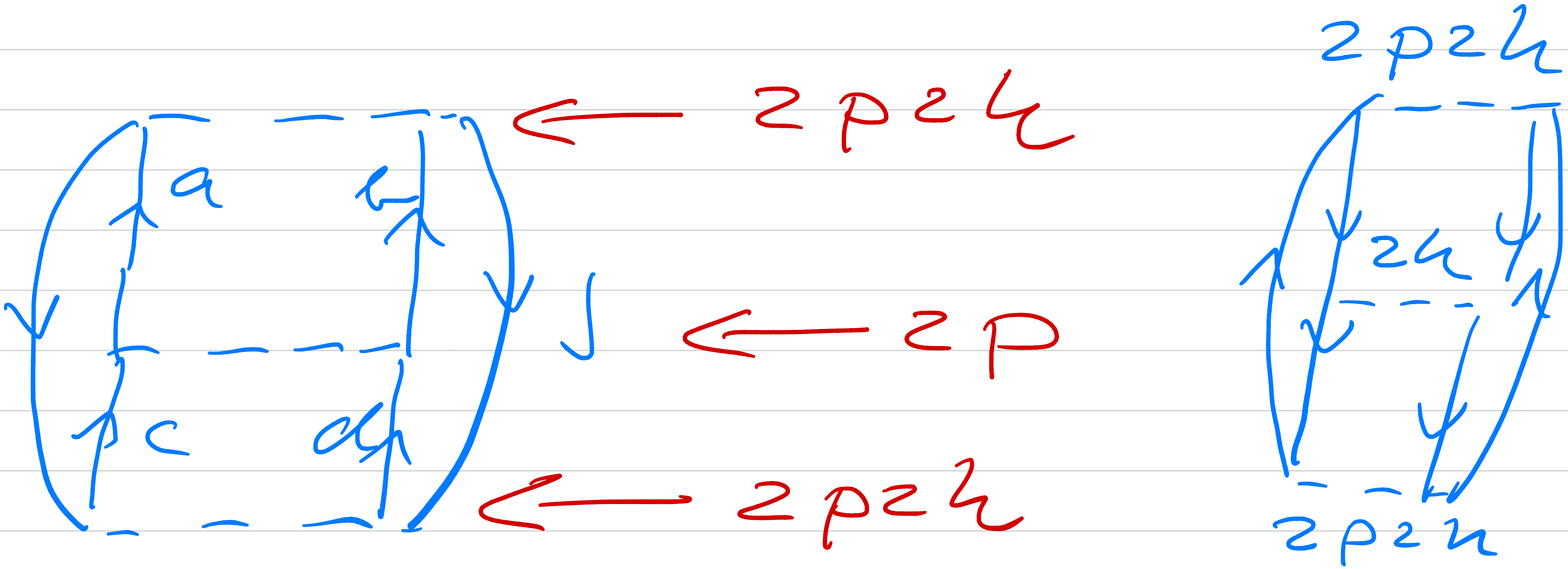


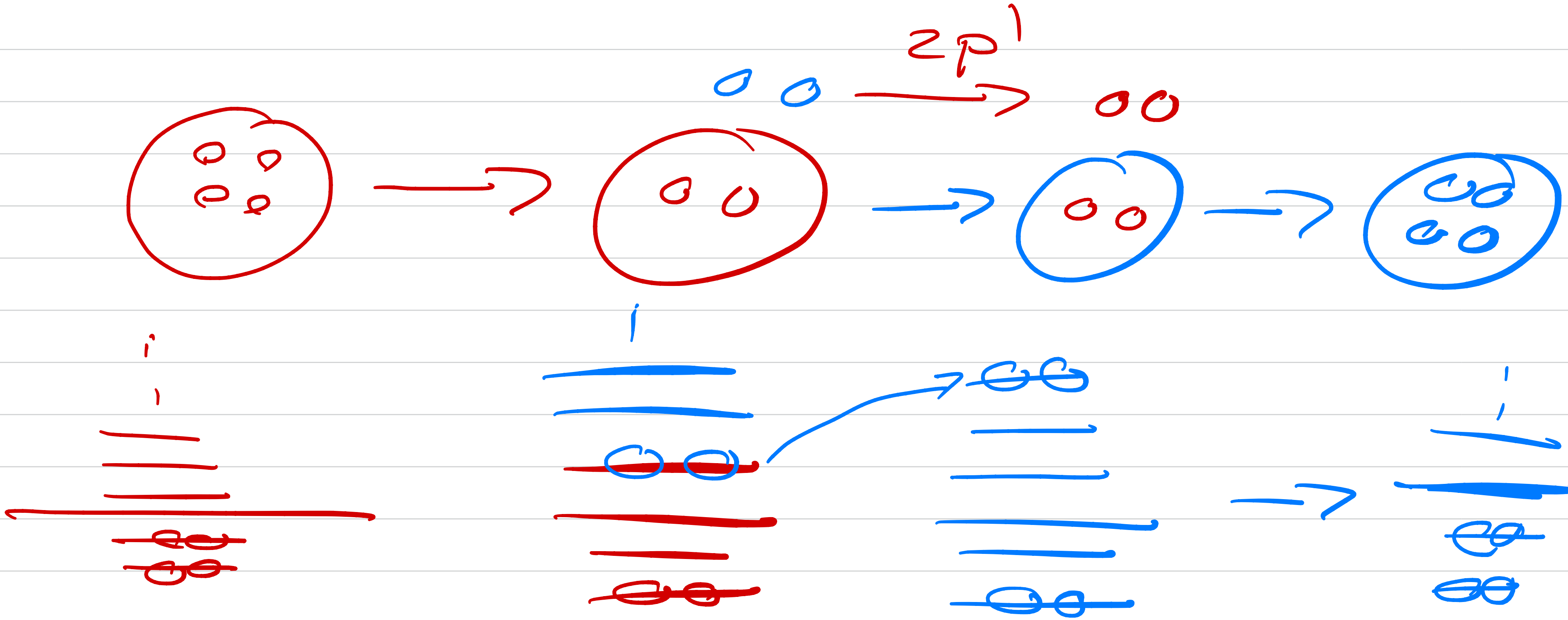
$\Delta E^{(3)}$





$H_1|\Phi_0\rangle$


a
b
c
d
2p2h
2p
2p2h
2p2h
2h
2p2h


2p'