FYS4480/9480 lecture, September 4, 2025

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Operators in 2nd quantization and Wick's time independent theorem.

Normal ordering

$$N[XYZ\ldots W]$$

$$:XYZ\ldots W:$$

$$\{XYZ\ldots W\}$$

$$\hat{H}_0 = \sum_{\alpha\beta} \underbrace{\langle \alpha | h_0 | \beta \rangle}_{\text{integral}} a_\alpha^\dagger a_\beta$$

$$\int dx\, \varphi_\alpha^*(x)\, \hat{h}_0(x)\, \varphi_\beta(x)$$

$$\left(\text{if } h_0 |\beta\rangle = \varepsilon_\beta |\beta\rangle \quad \sum_\alpha \varepsilon_\alpha a_\alpha^\dagger a_\alpha \right)$$

$$\hat{H}_{\text{II}} = \frac{1}{2} \sum_{\alpha\beta\gamma\delta} \langle \alpha\beta | v | \gamma\delta \rangle \times a_\alpha^\dagger a_\beta^\dagger a_\delta a_\gamma$$

$$\int dx_1 \int dx_2\, \varphi_\alpha^*(x_1)\, \varphi_\beta^*(x_2)\, v(x_1 x_2)\, \varphi_\gamma(x_1)\, \varphi_\delta(x_2)$$

$$\hat{H}_0 = \sum_{i=1}^{N} \hat{h}_0(x_i)$$

$$\left(-\frac{\hbar^2}{2m} \nabla_i^2 + V_{ext}(x_i) \right)$$

spectral decomposition

ONB $\{ |0\rangle, |1\rangle \, - - \, |n-1\rangle \}$

$i = 0, 1, - \; n-1$

$|i\rangle$

operator A has $|i\rangle$ as eigenbasis

$$|\psi\rangle = \sum_{i=0}^{n-1} \alpha_i |i\rangle$$

$$\left(\sum_{i=0}^{n-1} |\alpha_i|^2 = 1 \right) \qquad \langle\psi|\psi\rangle = 1$$

$$\hat{A}|\psi\rangle = \sum_{i=0}^{n-1} \alpha_i \underbrace{\hat{A}|i\rangle}_{\lambda_i |i\rangle}$$

Define a projection

$$\hat{P}_j = |j\rangle\langle j| \qquad \langle j|i\rangle = \delta_{ij}$$

$$\hat{P}_j|\psi\rangle = |j\rangle\langle j| \left(\sum_i \alpha_i |i\rangle \right)$$

$$= \alpha_j |j\rangle$$

$$\hat{A}|\psi\rangle = \sum_{i=0}^{n-1} \alpha_i \lambda_i |i\rangle$$

$$= \left(\sum_{i=0}^{n-1} \lambda_i \hat{P}_i\right)|\psi\rangle$$

$$\hat{A} = \sum_{i=0}^{n-1} \lambda_i \hat{P}_i$$

spectral decomposition.

$$\Phi(x_1\, x_2 \ldots x_N;\, \alpha_1\, \alpha_2 \ldots \alpha_N)$$

$$= \frac{1}{\sqrt{N}} \begin{vmatrix} \varphi_{\alpha_1}(x_1) & \varphi_{\alpha_1}(x_2) & \ldots & \varphi_{\alpha_1}(x_N) \\ \varphi_{\alpha_2}(x_1) & - & - & - \\ \vdots & - & - & \vdots \\ \varphi_{\alpha_N}(x_1) & - & - & \varphi_{\alpha_N}(x_N) \end{vmatrix}$$

Same SD in 2nd quant

$$|\alpha_1\, \alpha_2 \ldots \alpha_N\rangle = a^\dagger_{\alpha_1}\, a^\dagger_{\alpha_2} \ldots a^\dagger_{\alpha_N} |0\rangle$$

Define

$$\hat{h}_0(x_i)\,\varphi_{\alpha_i'}(x_i) = \sum_{\alpha_k'} \langle \alpha_k' | \hat{h}_0 | \alpha_k \rangle \, \varphi_{\alpha_k'}(x_i)$$

no permutations

$$\left(\sum_i \hat{h}_0(x_i) \right) \varphi_{\alpha_1}(x_1)\,\varphi_{\alpha_2}(x_2) \cdots \varphi_{\alpha_N}(x_N)$$

$$= \sum_{\alpha_1'} \langle \alpha_1' | \hat{h}_0 | \alpha_1 \rangle \, \varphi_{\alpha_1'}(x_1)\,\varphi_{\alpha_2}(x_2) \cdots \varphi_{\alpha_N}(x_N)$$

$$+$$

$$+ \sum_{\alpha_2'} \langle \alpha_2' | \hat{h}_0 | \alpha_2 \rangle \, \varphi_{\alpha_1}(x_1) \, \varphi_{\alpha_2'}(x_2) \cdots \varphi_{\alpha_N}(x_N)$$

$$+$$

$$\vdots$$

$$+ \sum_{\alpha_N'} \langle \alpha_N' | \hat{h}_0 | \alpha_N \rangle \, \varphi_{\alpha_1}(x_1) \, \varphi_{\alpha_2}(x_2) \cdots \varphi_{\alpha_N'}(x_N)$$

interchange $x_1 \leftrightarrow x_2$

$$\mathcal{H}_0 \, \varphi_{\alpha_1}(x_2)\, \varphi_{\alpha_2}(x_1) \cdots \varphi_{\alpha_N}(x_N)$$

$$= \sum_{\alpha_2'} \langle \alpha_2' | h_0 | \alpha_2 \rangle \, \varphi_{\alpha_1}(x_2)\, \varphi_{\alpha_2'}(x_1) \cdots \varphi_{\alpha_N}(x_N)$$

$$+ \sum_{\alpha_1'} \langle \alpha_1' | h_0 | \alpha_1 \rangle \, \varphi_{\alpha_1'}(x_2)\, \varphi_{\alpha_2}(x_1) \cdots \varphi_{\alpha_N}(x_N)$$

$$+ \cdots \sum_{\alpha_N'} \cdots\cdots \varphi_{\alpha_N'}(x_N)$$

By computing all permutations we can rewrite the equation (taking care of all permutations phases)

$$\hat{H}_0 |\alpha_1 \alpha_2 \cdots \alpha_N\rangle$$

$$= \sum_{\alpha_1'} \langle \alpha_1' | h_0 | \alpha_1 \rangle |\alpha_1' \alpha_2 \cdots \alpha_N\rangle$$

$$+ \sum_{\alpha_2'} \langle \alpha_2' | h_0 | \alpha_2 \rangle |\alpha_1 \alpha_2' \cdots \alpha_N\rangle$$

$$+ \cdots + \sum_{\alpha_N'} \langle \alpha_N' | \hat{h}_0 | \alpha_N \rangle |\alpha_1 \alpha_2 \cdots \alpha_N'\rangle$$

$$|\alpha_1 \alpha_2 \cdots \alpha_k' \cdots \alpha_N\rangle$$

$$= a^\dagger_{\alpha_k'} a_{\alpha_k} |\alpha_1 \alpha_2 \cdots \alpha_k \cdots \alpha_N\rangle$$

$$\hat{H}_0 |\alpha_1 \alpha_2 \cdots \alpha_N\rangle$$

$$= \sum_{\alpha_1'} \langle \alpha_1' | \hat{h}_0 | \alpha_1 \rangle a^\dagger_{\alpha_1'} a_{\alpha_1} |\alpha_1 \alpha_2 \cdots \alpha_N\rangle$$

$$+ \sum_{\alpha_2'} \langle \alpha_2' | \hat{h}_0 | \alpha_2 \rangle a^\dagger_{\alpha_2'} a_{\alpha_2} | \cdots \rangle$$

$$+ \cdots + \sum_{\alpha_N'} \langle \alpha_N' | \hat{h}_0 | \alpha_N \rangle a^\dagger_{\alpha_N'} a_{\alpha_N} | \cdots \rangle$$

$$= \sum_{\alpha\beta} \langle \alpha | \hat{h}_0 | \beta \rangle a_\alpha^\dagger a_\beta$$

$$\times \, | \alpha_1 \alpha_2 \dots \alpha_N \rangle$$

$$= \hat{H}_0 | \alpha_1 \alpha_2 \dots \alpha_N \rangle$$

$$\Rightarrow$$

$$\hat{H}_0 = \sum_{\alpha\beta} \langle \alpha | \hat{h}_0 | \beta \rangle a_\alpha^\dagger a_\beta$$

$$\langle \alpha | \beta \rangle = \delta_{\alpha\beta} \quad \langle \alpha | \hat{h}_0 | \beta \rangle = \varepsilon_\alpha \delta_{\alpha\beta}$$

$$[\quad \hat{H}_0 = \sum_{\alpha} \varepsilon_\alpha a_\alpha^\dagger a_\alpha$$

$$\hat{H}_I = \frac{1}{2} \sum_{\alpha\beta\gamma\delta} \langle \alpha\beta | v | \gamma\delta \rangle \, a^\dagger_\alpha a^\dagger_\beta a_\delta a_\gamma$$

$$= \frac{1}{4} \sum_{\alpha\beta\gamma\delta} \langle \alpha\beta | v | \gamma\delta \rangle_{AS} \, a^\dagger_\alpha a^\dagger_\beta a_\delta a_\gamma$$

$$\langle \alpha\beta | v | \gamma\delta \rangle_{AS} =$$

$$\langle \alpha\beta | v | \gamma\delta \rangle - \langle \alpha\beta | v | \delta\gamma \rangle$$

$$\overbracket{a_i a_j^\dagger} = \langle 0 | a_i a_j^\dagger | 0 \rangle = \delta_{ij}$$

$$\overbracket{a_i a_j} = \langle 0 | a_i a_j | 0 \rangle = 0$$

$$\overbracket{a_i^\dagger a_j} = \langle 0 | a_i^\dagger a_j | 0 \rangle = 0$$

$$\overbracket{a_i^\dagger a_j^\dagger} = \langle 0 | a_i^\dagger a_j^\dagger | 0 \rangle = 0$$

$$N[\hat{A}\hat{B}\hat{C}\hat{D} \ldots \hat{Z}\hat{X}\hat{Y}]$$

$$= (-)^P \begin{bmatrix}\text{creation} \\ \text{operator}\end{bmatrix} \begin{bmatrix}\text{annihilation} \\ \text{operator}\end{bmatrix}$$

$$N[a_1 a_2 a_3^\dagger] = (-)^2 \, a_3^\dagger a_4 a_2$$

$$= (-1)^2 \langle 0 | a_3^\dagger a_1 a_2 | 0 \rangle = 0$$

Wick's theorem

$$\langle 0 | \hat{A}\hat{B}\hat{C}\hat{D} \cdots \hat{X}\hat{Y}\hat{Z}\hat{W} | 0 \rangle$$

$$= N[\hat{A}\hat{B}\hat{C}\hat{D} \cdots \hat{X}\hat{Y}\hat{Z}\hat{W}]$$

$$+ \sum_{(1)} N[\hat{A}\hat{B}\hat{C}\hat{D} \cdots \hat{X}\hat{Y}\hat{Z}\hat{W}]$$

$$+ \sum_{(2)} N[\hat{A}\hat{B}\hat{C}\hat{D} \cdots \hat{X}\hat{Y}\hat{Z}\hat{W}]$$

$$+ \cdots + \sum_{\left(\frac{N}{2}\right)} N[\hat{A}\hat{B}\hat{C}\hat{D} \cdots \hat{X}\hat{Y}\hat{Z}\hat{W}]$$

$$= \sum_{\left(\frac{N}{2}\right)} N[\hat{A}\hat{B}\hat{C}\hat{D} \cdots \hat{X}\hat{Y}\hat{Z}\hat{W}]$$

$$|12\rangle = a_1^{\dagger} a_2^{\dagger} |0\rangle$$

$$\langle a_1 a_2 | H_0 | a_1^{\dagger} a_2^{\dagger} \rangle = \varepsilon_1 + \varepsilon_2$$

$$\langle a_i | h_0 | a_j \rangle = \delta_{ij}\, \varepsilon_i$$

$$\hat{N} = \sum_{i=1}^{N} a_i^{\dagger} a_i$$

$$\langle 12 | \mathcal{H}_1 | 12 \rangle$$

$$= \frac{1}{2} \sum_{\alpha\beta\gamma\delta} \langle \alpha\beta | v | \gamma\delta \rangle$$

$$\times \langle 0 | a_2 a_1 \, a_\alpha^\dagger a_\beta^\dagger a_\delta a_\gamma \, a_1^\dagger a_2^\dagger | 0 \rangle$$

$$a_2 a_1 a_\alpha^\dagger a_\beta^\dagger a_\delta a_\gamma a_1^\dagger a_2^\dagger$$

$\delta_{\beta 2}\,\delta_{\alpha 1}$ $\qquad$ $\delta_{\gamma 1}$ $\delta_{\delta 2}$

$\delta_{\beta 1}\,\delta_{\alpha 2}$ $\qquad$ $\delta_{\gamma 1}\,\delta_{\delta 2}$

$$\langle 12 | v | 12 \rangle \qquad - \langle 21 | v | 12 \rangle$$

$$\langle \alpha\beta | v | \gamma\delta \rangle \qquad - \langle 21 | v | 12 \rangle$$

$\delta_{\beta 2}\,\delta_{\alpha 1}$ $\qquad$ $\delta_{\gamma 2}\,\delta_{\delta 1}$

$\delta_{\beta 1}\,\delta_{\alpha 2}$ $\qquad$ $- \langle 12 | v | 21 \rangle$

$\delta_{\gamma 2}\,\delta_{\delta 1}$

$$\langle 21 | v | 21 \rangle = \langle 12 | v | 12 \rangle$$

$$\langle 12 | f(I | 12 \rangle = \langle 12 | v | 12 \rangle$$

$$- \langle 12 | v | 21 \rangle$$

$$= \langle 12 | v | 12 \rangle_{AS}$$

$$= \langle 21 | v | 21 \rangle_{AS}$$

$$= - \langle 12 | v | 21 \rangle_{AS}$$

$$= - \langle 21 | v | 12 \rangle_{AS}$$

$$|1234\rangle = a_1^\dagger a_2^\dagger a_3^\dagger a_4^\dagger |0\rangle$$

$$\langle 1234| \mathcal{H}_I | 1234\rangle =$$

$$\frac{1}{2}\sum_{\alpha\beta\gamma\delta} \langle\alpha\beta|v|\gamma\delta\rangle \times$$

$$\langle 0| a_4 a_3 a_2 a_1\, a_\alpha^\dagger a_\beta^\dagger a_\delta a_\gamma\, a_1^\dagger a_2^\dagger a_3^\dagger a_4^\dagger$$

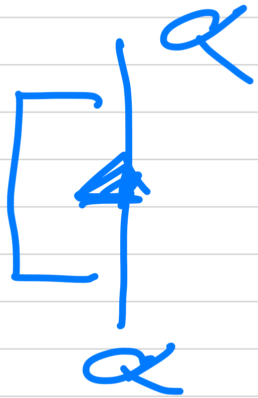
$$\times |0\rangle$$

$\hookrightarrow$ redefine vacuum $|0\rangle$

$\longrightarrow |c\rangle$

Diagrammatic notation

(i) $\overbrace{a_\alpha \, a_\alpha^{+}}$



arrow pointing up represents a particle on top of $|\Phi\rangle$, with a true $|0\rangle$ all states are particle states

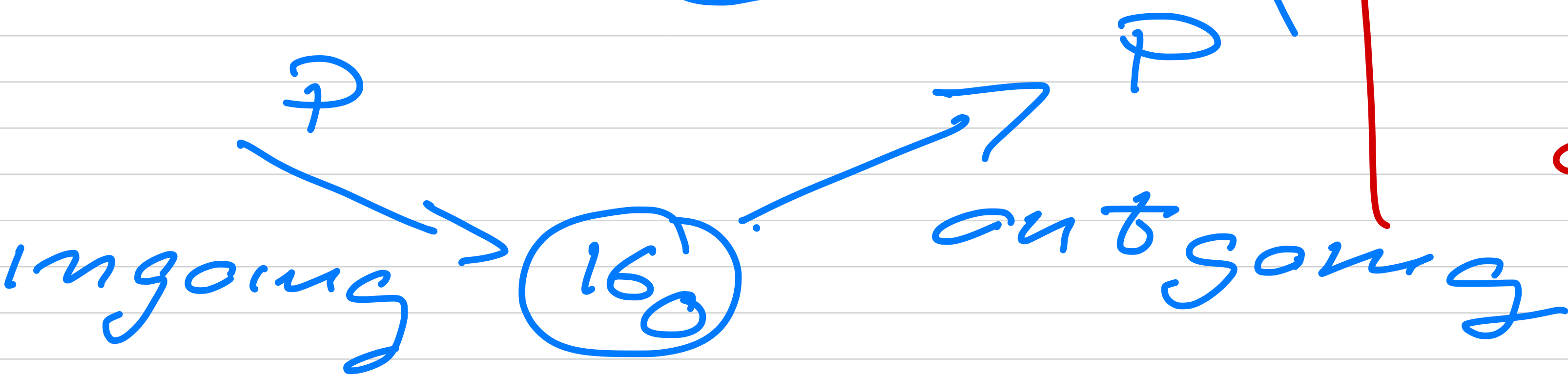
(ii) one body operator

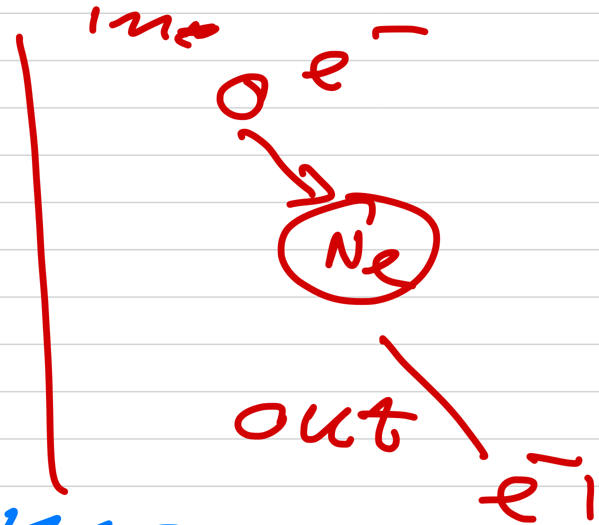
Example $H_0 = \sum_{\alpha\beta} \langle \alpha | h_0 | \beta \rangle \, a^\dagger_\alpha a_\beta$

$\langle \alpha | h_0 | \beta \rangle$

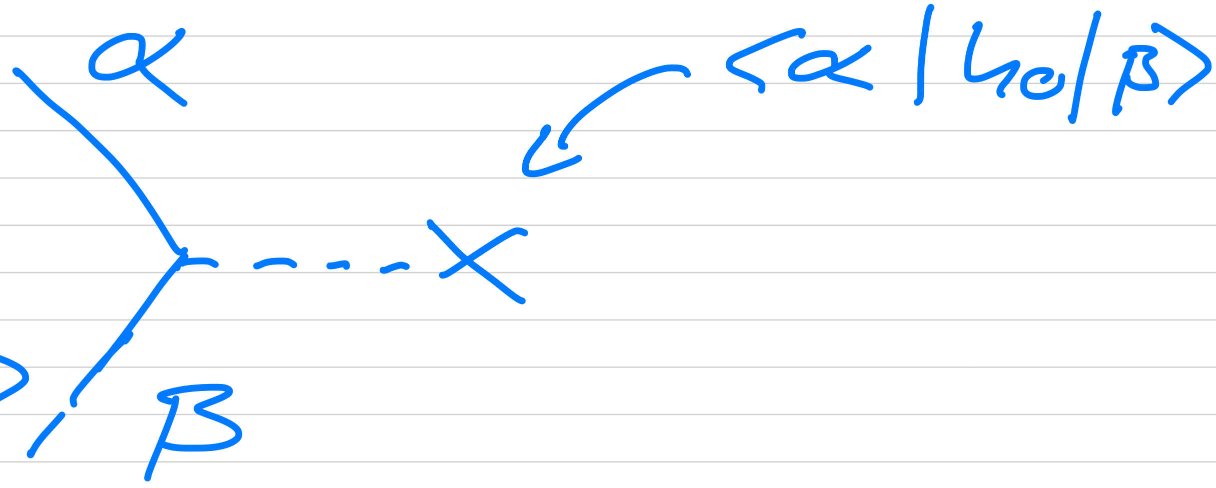
ingoing states

outgoing state



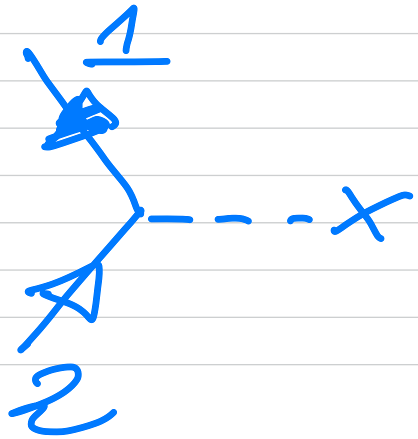


$$\sum_{\alpha\beta} \langle \alpha | \hat{h}_0 | \beta \rangle \, a^\dagger_\alpha a_\beta$$



$$\langle c | a_1 a^\dagger_\alpha a_\beta a^\dagger_2 | c \rangle$$

$$\langle 1 | \mathcal{H}_0 | 2 \rangle = \langle 1 | h_0 | 2 \rangle$$

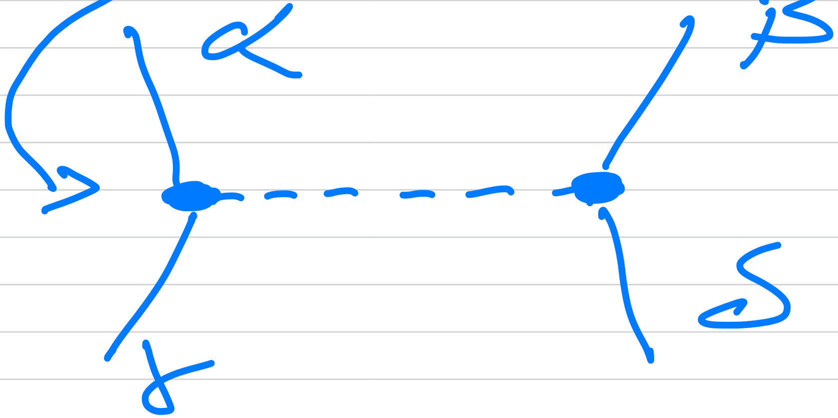


outgoing label $\langle \alpha |$

incoming label $| \beta \rangle$

(iii) Two-body operator

$$\frac{1}{2} \sum_{\alpha\beta\gamma\delta} \langle \alpha\beta | v | \gamma\delta \rangle \, a^\dagger_\alpha a^\dagger_\beta a_\delta a_\gamma$$



left

$\langle \alpha\beta |$ right

outgoing

incoming

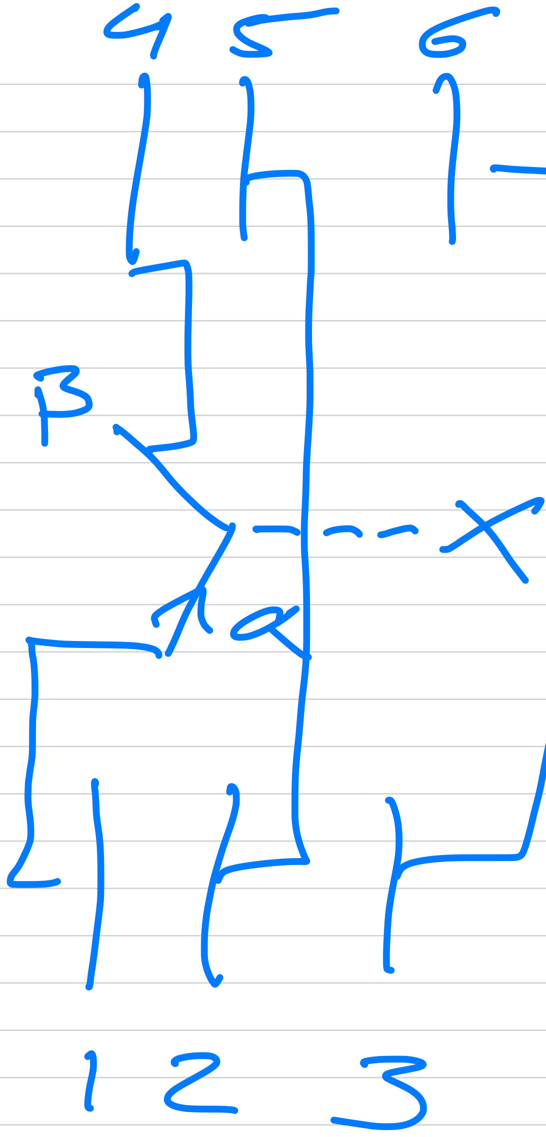
left $| \gamma\delta \rangle$ right

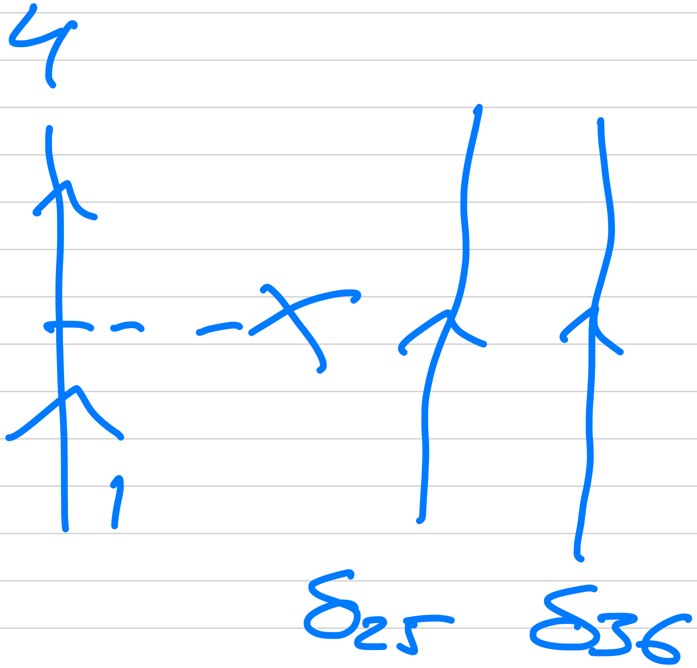
(iv) a given (with $|0\rangle$)

$$a_1^\dagger a_2^\dagger a_3^\dagger |0\rangle = |123\rangle$$

1 2 3

(v) action of H_0 on this state





$$\langle 4|V_0|1\rangle$$

$$\times\, \delta_{25}\,\delta_{36}$$