Lecture FYS4480, September 14, 2023

Lemma

$$N[xyz \cdots w]\Omega =$$

$$N[xyz \cdots w\Omega] +$$

$$\sum_{(1)\Omega} N[xyz \cdots w\Omega]$$

Examples of (iii) and (iv)

$$N[a_1 a_2 \cdots a_N a_k]\, a_e^+ =$$

$$N[a_1 a_2 \cdots a_N a_e^+] +$$

$$\sum_{(1)} N[a_1 a_2 \cdots a_N a_e^+]$$

$N = 1$

$$N[a_1]\,a_e^\dagger = N[a_1 a_e^\dagger] +$$

$$N[\overbrace{a_1 a_e^\dagger}]$$

$$= -\langle 0| a_e^\dagger a_1 |0\rangle + \overbrace{a_1 a_e^\dagger}$$

$$\langle 0| a_1 a_e^\dagger |0\rangle = \delta_{1e} - \langle 0| a_e^\dagger a_1 |0\rangle$$

If it holds for N it should hold for $N+1$. Multiply ~~from~~ left with a_0

$$a_0\, N[a_1 a_2 \dots a_N]\, a_e^\dagger =$$

$$= a_0 N[a_1 a_2 \ldots a_N a_e^+]$$

$$+ \sum_{(1)} a_0 N[a_1 \ldots a_N a_e^+]$$

we have that

$$a_0 N[a_1 \ldots a_N] a_e^+ =$$

$$N[a_0 a_1 \ldots a_N] a_e^+$$

$$\sum_{(1)} a_0 N[a_1 \ldots a_N a_e^+]$$

$$= \sum_{(1)} N[a_0 a_1 a_2 \ldots a_N a_e^+]$$

Last term

$$(-)^N q_0 q_e^+ N[q_1 \cdots q_N]$$

$$= (-)^N \left[N[q_0 q_e^+] + \overbrace{q_0 q_e}^{}{}^{+} \right]$$

$$\times N[q_1 \cdots q_N]$$

$$N[q_0 q_e^+] = -N[q_e^+ q_0]$$

$$= (-)^N [q_e^+ q_0 \cdots q_N]$$

we can rewrite

$$\overline{a_0 a_e}^{\dagger} N[a_1 \cdots a_N] =$$

$$N[a_0 a_e^{\dagger} a_1 \cdots a_N]$$

$$= (-)^N N[a_0 a_1 \cdots a_N a_e^{\dagger}]$$

$$\Rightarrow$$

$$N[a_0 a_1 \cdots a_N] a_e^{\dagger} =$$

$$N[a_0 a_1 \cdots a_N a_e^{\dagger}] +$$

$$\sum_{(1)} N[a_0 a_1 \overline{\cdots a_N a_e^{\dagger}}]$$

Wick's theorem

$$x y z \ldots w \times \Omega =$$

$$N[x y z \ldots w \Omega] +$$

$$\sum_{(1)\neq\Omega} N[x y, z \ldots w \Omega]$$

$$+ \sum_{(1)\Omega} N[x y z \ldots w \Omega]$$

$$+ \sum_{(2)\neq\Omega} N[x y z \ldots w \Omega]$$

$$+ \sum_{(2)\Omega} N[x y z \ldots w \Omega]$$

$$+ \sum_{[\frac{N}{2}] \neq \Omega} N[\cdots] + \sum_{[\frac{N}{2}]\Omega} N[xy\cdots yx]$$

$$+ \sum_{[\frac{N+1}{2}] \neq \Omega} N[\cdots] + \sum_{[\frac{N+1}{2}]\Omega} N[\cdots]$$

if $N+1$ gives an odd number, then we end up with one operator which is uncontracted $\Rightarrow 0$

$$\sum_{[m] \neq \Omega} + \sum_{[m] = \Omega} = \sum_{[m]}$$

$\Rightarrow$

$$xyz \cdots w \cdot \Omega =$$

$$\langle c | \sum_{[\frac{N}{2}]} N[xyz \cdots w\Omega]$$

all contracted

Example that motivates Wick's generalized theorem

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

$$= N[a^\dagger_{\alpha_1} a^\dagger_{\alpha_2}] |0\rangle$$

$$\langle \alpha_1 \alpha_2 | = \langle 0 | a_{\alpha_2} a_{\alpha_1}$$

$$= \langle 0 | N[a_{\alpha_2} a_{\alpha_1}]$$

$$H_0 = \sum_{\alpha\beta} \langle \alpha | h_0 | \beta \rangle \underbrace{a_\alpha^\dagger a_\beta}_{\text{Normal ordered}}$$

$$\langle \alpha_1 \alpha_2 | H_0 | \alpha_1 \alpha_2 \rangle =$$

$$\sum_{\alpha\beta} \langle \alpha | h_0 | \beta \rangle \langle 0 | a_{\alpha_2} a_{\alpha_1} a_\alpha^\dagger a_\beta a_{\alpha_1} a_{\alpha_2} | 0 \rangle$$

$$a_{\alpha_2} a_{\alpha_1} a_{\alpha}^{\dagger} a_{\beta} a_{\alpha_1}^{\dagger} a_{\alpha_c}^{\dagger}$$

$$a_{\alpha} a_{\beta}^{\dagger} = \delta_{\alpha\beta}$$

$$a_{\alpha} a_{\beta} = a_{\alpha}^{\dagger} a_{\beta}^{\dagger} = a_{\alpha}^{\dagger} a_{\beta} = 0$$

$$a_{\alpha_2} a_{\alpha_1} a_{\alpha}^{\dagger} a_{\beta} a_{\alpha_1}^{\dagger} a_{\alpha_2}^{\dagger} \qquad \delta_{\alpha\alpha_1} \delta_{\beta\alpha_1} \times \delta_{\alpha_2\alpha_2}$$

$$a_{\alpha_2} a_{\alpha_1} a_{\alpha}^{\dagger} a_{\beta} a_{\alpha_1}^{\dagger} a_{\alpha_2}^{\dagger}$$

$$\delta_{\alpha\alpha_2} \delta_{\beta\alpha_2} \delta_{\alpha_1\alpha_1}$$

$$N[a_{\alpha_1} a_{\alpha_2}]\, N[a_{\alpha}^{\dagger} a_{\beta}]\, N[a_{\gamma_1}^{\dagger} a_{\gamma_2}^{\dagger}]$$

Wick's generalized theorem: an arbitrary product of creation and annihilation operators in which some operators are already in a normal-ordered form is given by

$$N[A_1 A_2 \ldots]\, N[B_1 B_2 \ldots]\, N[C_1 C_2 \ldots]$$

$$= N[A_1 A_2 \ldots B_1 B_2 \ldots C_1 C_2 \ldots]$$

$$+ \sum_{\text{All}} N[A_1 A_2 \ldots B_1 B_2 \ldots C_1 C_2 \ldots]$$

where the contractions run over contractions between operators from different normal-ordered products

$$H_I = \frac{1}{2}\sum_{\alpha\beta\gamma\delta} \langle \alpha\beta | v | \gamma\delta \rangle \boxed{a_\alpha^\dagger a_\beta^\dagger a_\delta a_\gamma}$$

Normal-ordered

$$|\alpha_1 \alpha_2\rangle = a_{\alpha_1}^\dagger a_{\alpha_2}^\dagger |0\rangle$$

$$\langle \alpha_1 \alpha_2 | H_I | \alpha_1 \alpha_2 \rangle \propto$$

$$N[\underbrace{a_{\alpha_2} a_{\alpha_1}}] \, N[\underbrace{a_\alpha^\dagger a_\beta^\dagger} \underbrace{a_\delta a_\gamma}] \, N[\underbrace{a_{\alpha_1}^\dagger a_{\alpha_2}^\dagger}]$$

Diagrammatic notations

(i) $\overline{a_\alpha a_\alpha^\dagger}$ $\qquad\qquad$ $\uparrow \alpha$

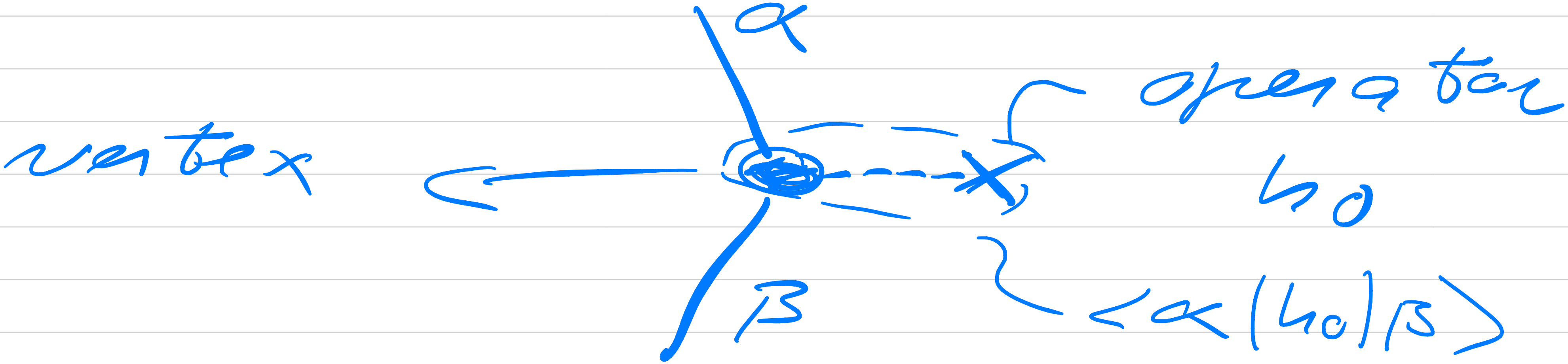
arrow: up, particle states
with $|0\rangle$ all states are
particle states

arrow: down $\downarrow$, hole
state. States below Fermi
level. applies to a
redefinition of $|0\rangle$

(ii) one body operator

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

no arrows

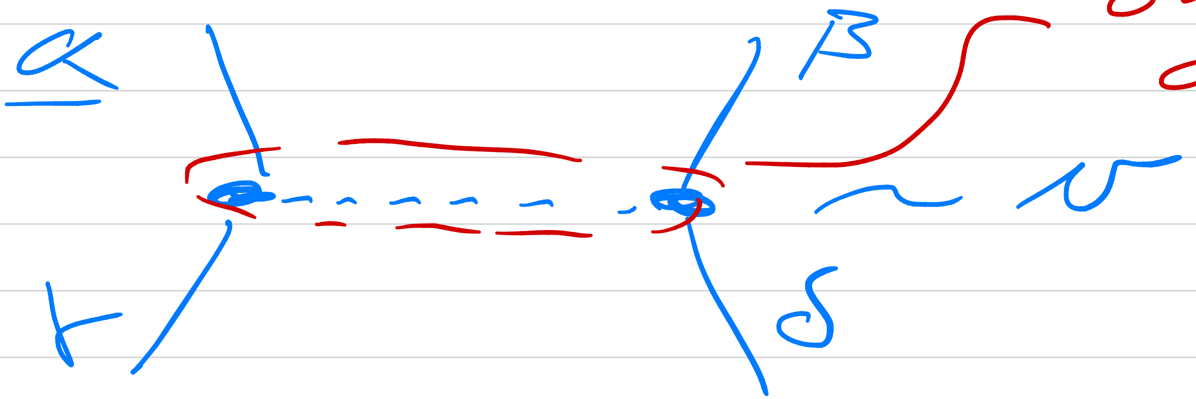


outgoing α represents $\langle \alpha |$

incoming β — " — $| \beta \rangle$

(iii) Two body

$$\langle \alpha \beta | v | \gamma \delta \rangle \, a^\dagger_\alpha a^\dagger_\beta a_\delta a_\gamma$$

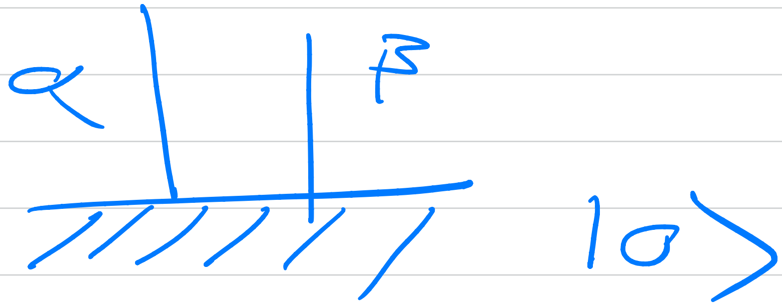


$$\langle \alpha \beta | = \langle \underset{\alpha}{\text{left}} \; \underset{\beta}{\text{right}} |$$

$$| \gamma \delta \rangle = | \underset{\gamma}{\text{left}} \; \underset{\delta}{\text{right}} \rangle$$

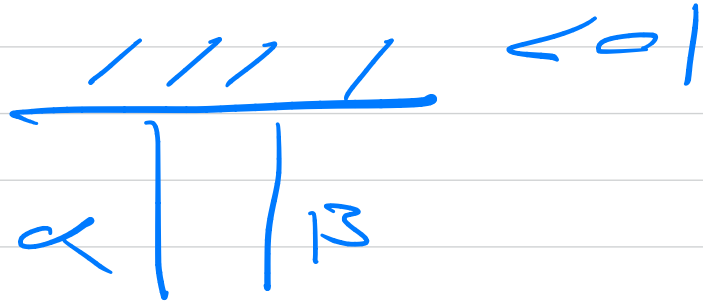
(v) specific state

$|\alpha\beta\rangle =$



$a^\dagger_\alpha a^\dagger_\beta |0\rangle$

$\langle \alpha\beta| =$

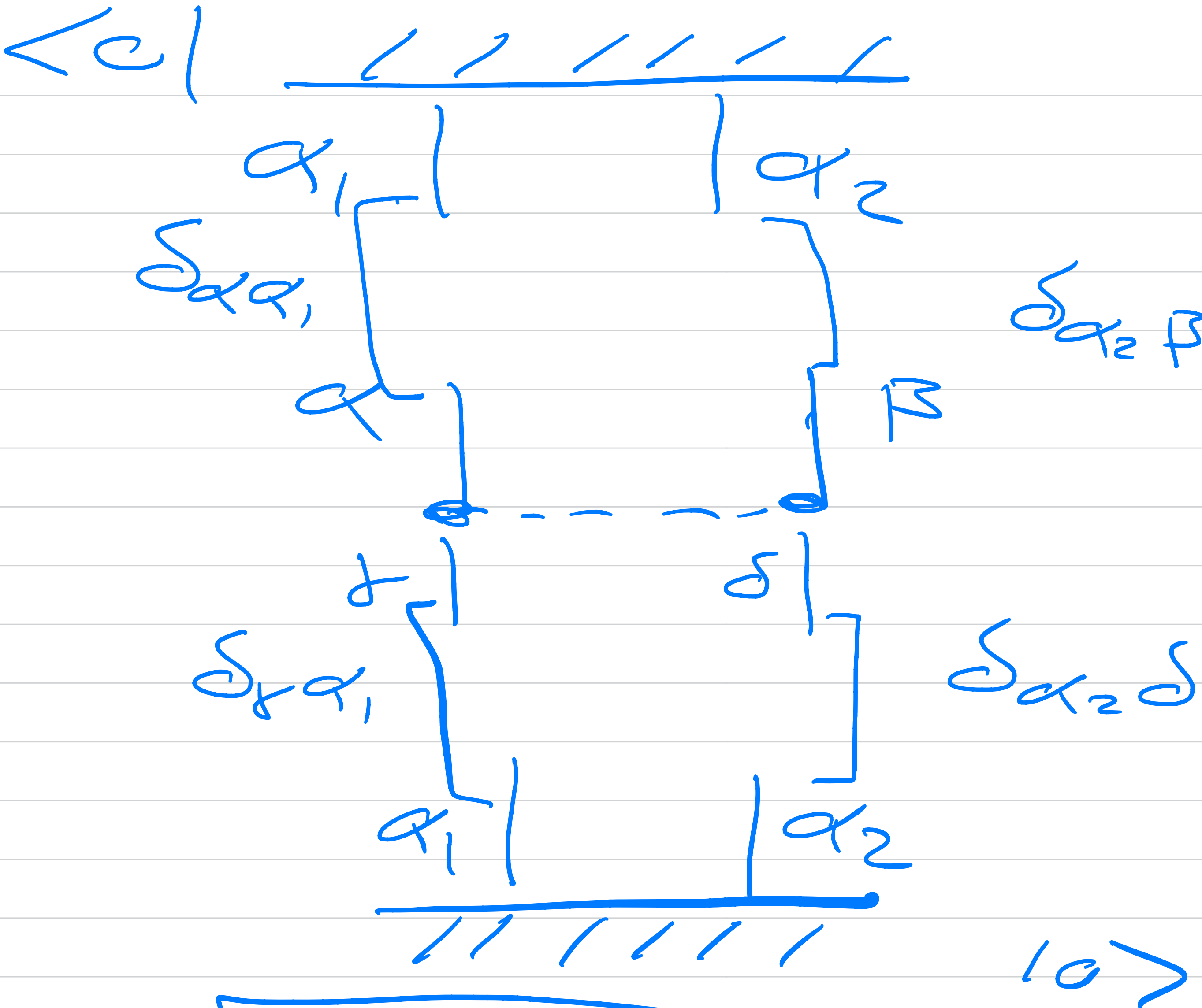


$= \langle 0| a_\beta a_\alpha$

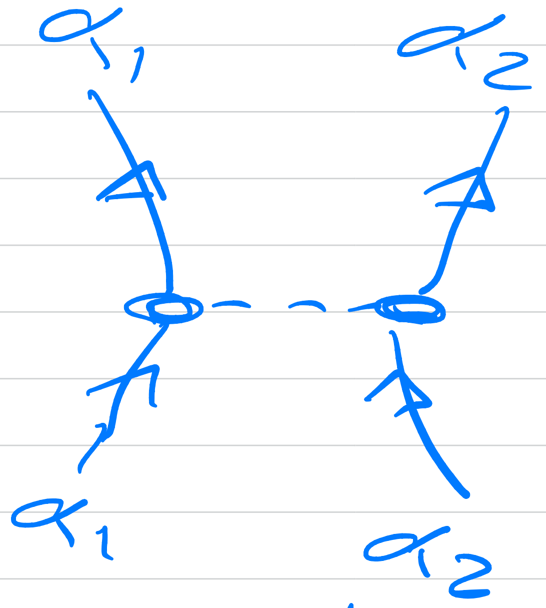
Example

$\langle \alpha_1 \alpha_2 | H_1 | \alpha_1 \alpha_2 \rangle$

Direct term



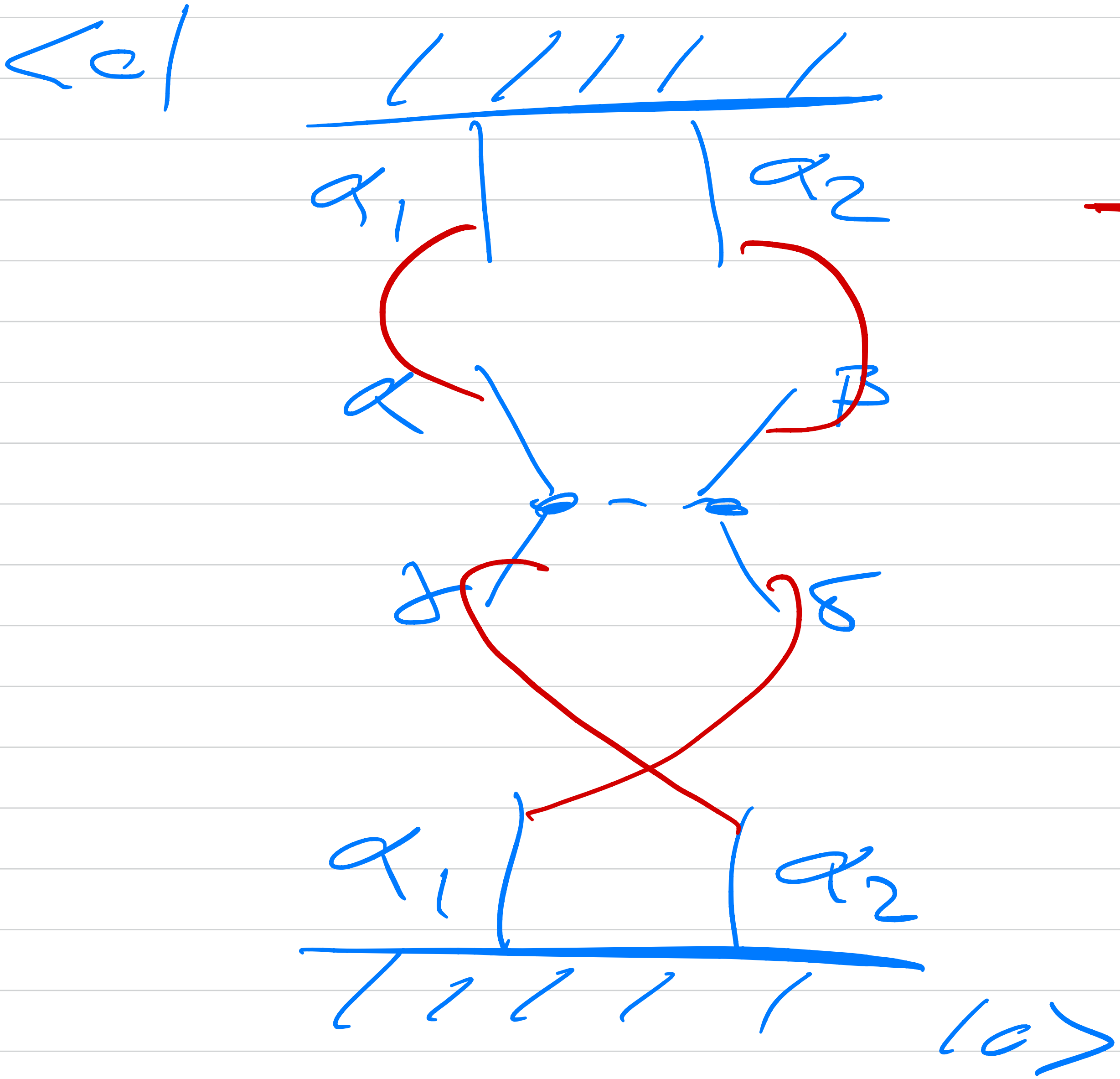
$=$



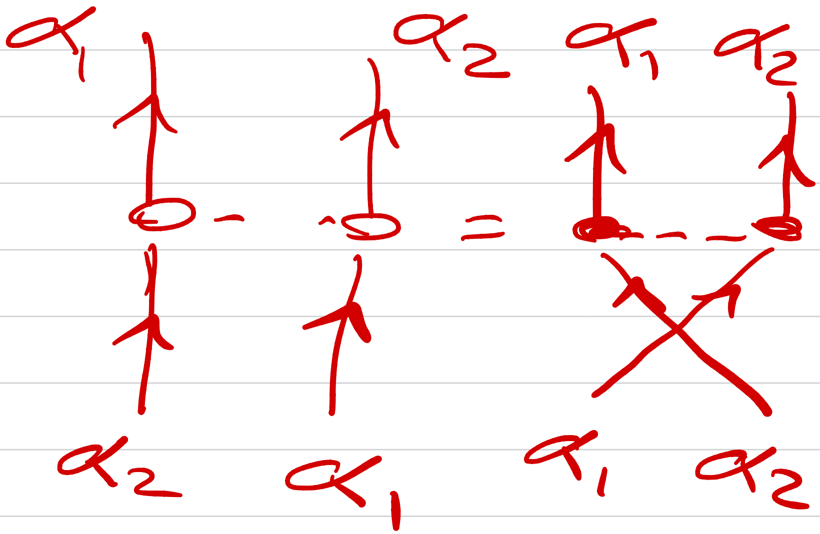
$\langle \alpha_1, \alpha_2 | v | \alpha_1, \alpha_2 \rangle$

$$a_{\alpha_2} a_{\alpha_1} a^{+}_{\alpha} a^{+}_{\beta} a_{\delta} a_{\gamma} a^{+}_{\alpha_1} a^{+}_{\alpha_2}$$

Exchange term



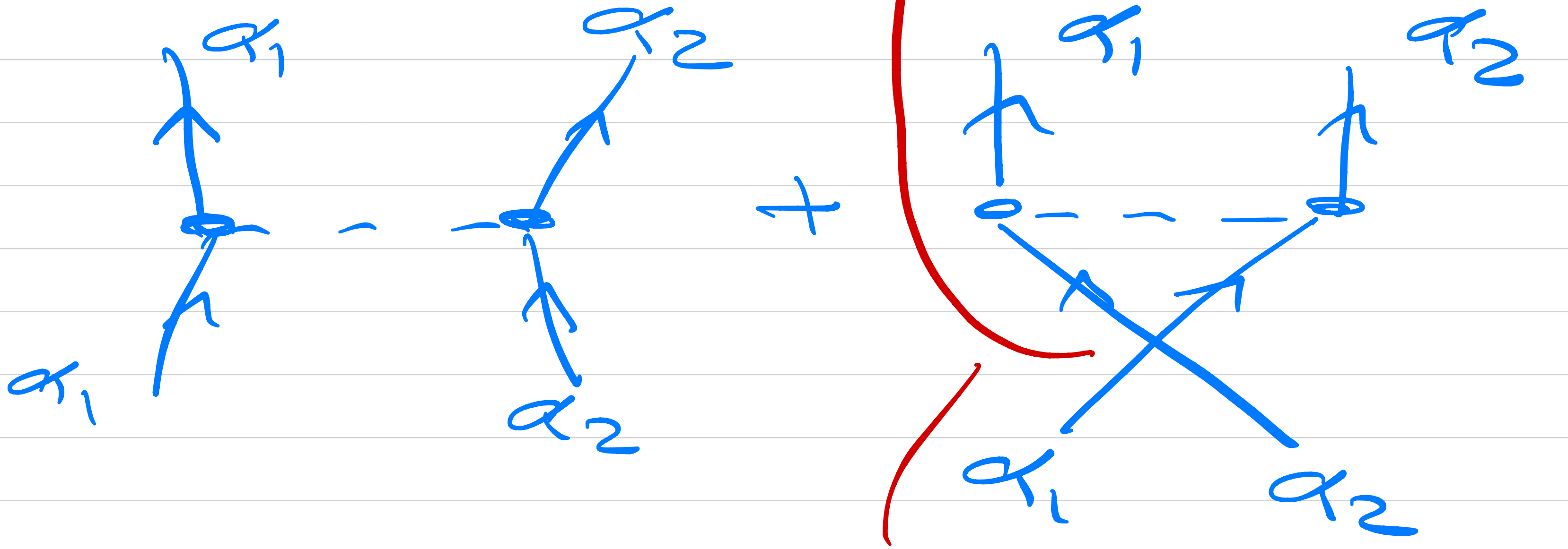
$- \langle \alpha_1 \alpha_2 | v | \alpha_2 \alpha_1 \rangle$



$|\alpha_1 \alpha_2\rangle$

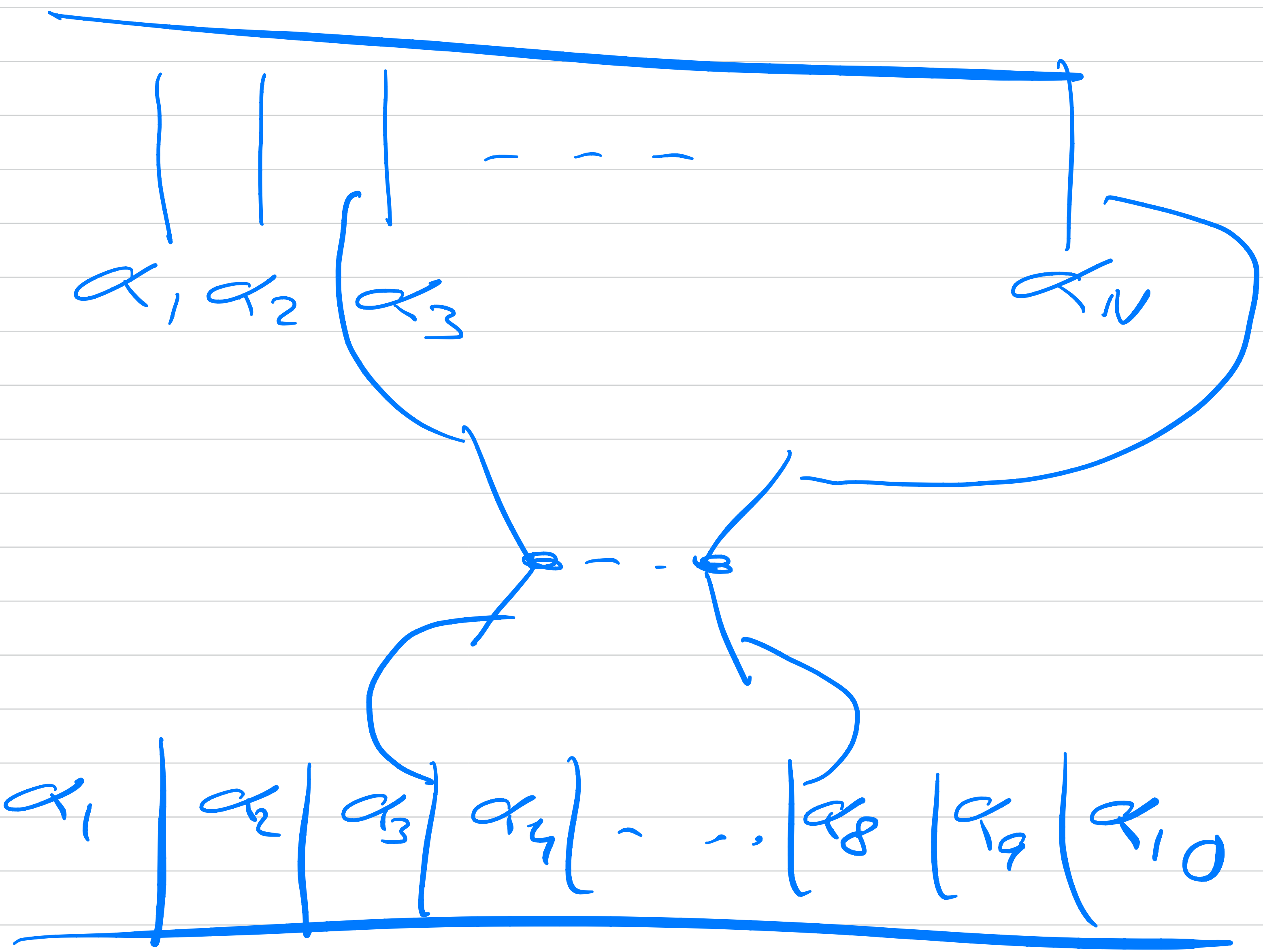
$$\langle \alpha_1 \alpha_2 | H_1 | \alpha_1 \alpha_2 \rangle$$

$$= \langle \alpha_1 \alpha_2 | v | \alpha_1 \alpha_2 \rangle - \langle \alpha_1 \alpha_2 | v | \alpha_2 \alpha_1 \rangle$$



crossing fermion lines

with many particles



particle-hole formalism;

redefine $|0\rangle \rightarrow |c\rangle$