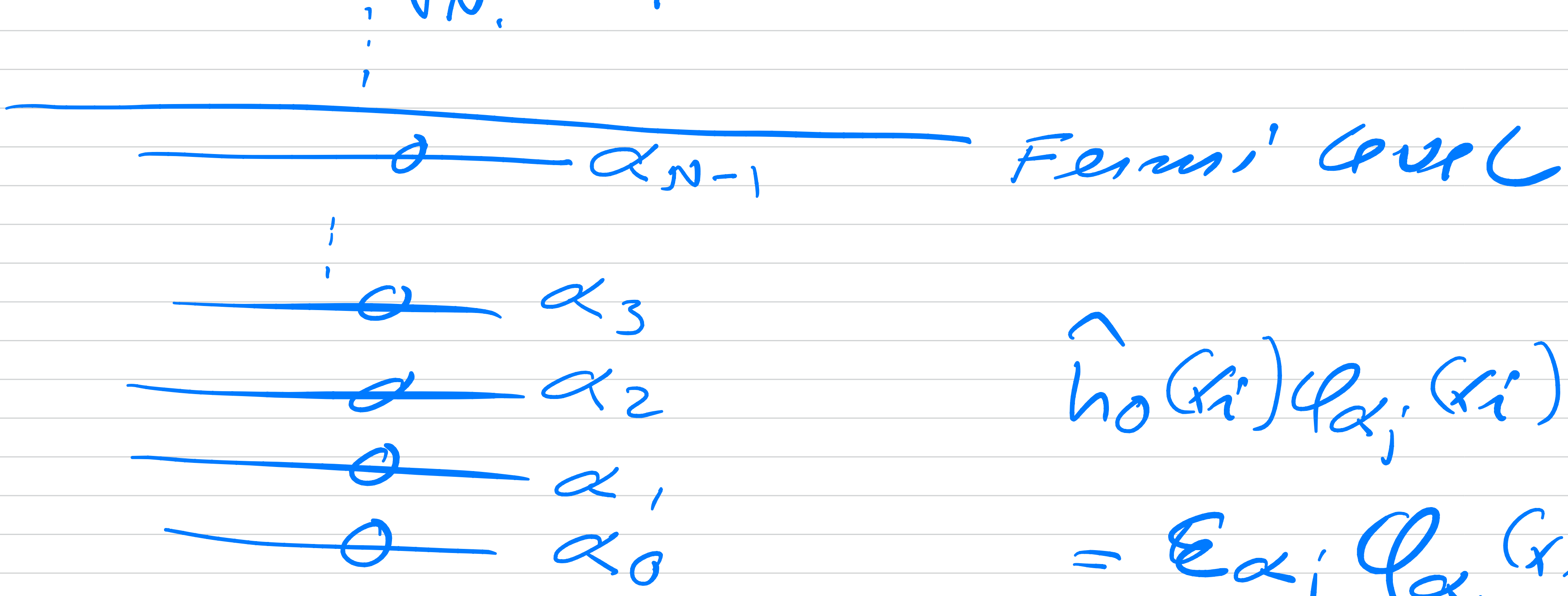
Lecture FYS4480/9480, August 30, 2024

FYS 4480/9480 AUG 30

$$\Phi_0 = \frac{1}{\sqrt{N!}} \sum_P (-)^P \hat{P}\, \varphi_{\alpha_0}(x_1)\, \varphi_{\alpha_1}(x_2) \cdots \varphi_{\alpha_{N-1}}(x_N)$$



$$\hat{h}_0(x_i)\varphi_{\alpha_j}(x_i) = \varepsilon_{\alpha_j}\varphi_{\alpha_j}(x_i)$$

$$\hat{H}_0 = \sum \hat{h}_0(x_i)$$

$$\hat{H}_0 \, \Phi_0(x_1, x_2 \ldots x_N ; \alpha_0 \ldots \alpha_{N-1})$$

$$= \varepsilon_0 \Phi_0$$

$N=2$

$$\langle \Phi_0 | \hat{H} | \Phi_0 \rangle = \underbrace{\varepsilon_{\alpha_0} + \varepsilon_{\alpha_1}}_{\langle \Phi_0 | \hat{H}_0 | \Phi_0 \rangle}$$

$$+ \underbrace{\langle \alpha_0 \alpha_1 | v | \alpha_0 \alpha_1 \rangle - \langle \alpha_0 \alpha_1 | v | \alpha_1 \alpha_0 \rangle}_{\langle \Phi_0 | H_1 | \Phi_0 \rangle}$$

N-general

$$\langle \Phi_0 | \hat{H}_0 | \Phi_0 \rangle = \sum_{\alpha_i = \alpha_0}^{\alpha_{N-1}} \varepsilon_{\alpha_i} = \mathcal{E}_0$$

$$\langle \Phi_0 | H_1 | \Phi_0 \rangle =$$

$$N! \int d\tau \, \Phi_H^* \hat{A} H_I \hat{A} \Phi_H$$

$$= \int d\tau \, \Phi_H^* H_I \sum_P (-)^P \hat{P} \Phi_H$$

$N=3$

$$\sum_{i<j} v(r_{ij}) = \sum_{i<j} v_{ij} = v_{12}+v_{13}$$
$$+\, v_{23}$$

$$\int dx_1\, dx_2\, dx_3\; \varphi^*_{\alpha_0}(x_1)\, \varphi^*_{\alpha_1}(x_2)\, \varphi^*_{\alpha_2}(x_3)$$
$$\times\, v_{12} \Big(\varphi_{\alpha_0}(x_1)\, \varphi_{\alpha_1}(x_2)\, \varphi_{\alpha_3}(x_3)$$
$$-\, \varphi_{\alpha_0}(x_1)\, \varphi_{\alpha_1}(x_3)\, \varphi_{\alpha_2}(x_2)$$
$$(2 \leftrightarrow 3) \quad P_{132}$$

$$-\, \varphi_{\alpha_0}(x_2)\, \varphi_{\alpha_1}(x_1)\, \varphi_{\alpha_2}(x_3) \; +$$
$$P_{213} \qquad\qquad 3 \text{ more} \Big)$$

$$\Rightarrow \quad \langle \Phi_0 | H_1 | \Phi_0 \rangle$$

$$= \frac{1}{2} \sum_{\alpha_i \alpha_j = \alpha_0}^{\alpha_2} \left(\langle \alpha_i \alpha_j | v | \alpha_i \alpha_j \rangle - \langle \alpha_i \alpha_j | v | \alpha_j \alpha_i \rangle \right)$$

$$\Rightarrow \quad \frac{1}{2} \sum_{\alpha_i \alpha_j}^{\alpha_{N-1}} \langle \alpha_i \alpha_j | v | \alpha_i \alpha_j \rangle_{AS}$$

$$|i\rangle = \sum_{\lambda} C_{i\lambda} |\lambda\rangle$$

$$|\underline{\Psi}_0^{(i)}\rangle = C |\Phi_0^{(\lambda)}\rangle$$

$$\Psi_0 = \frac{1}{\sqrt{N!}} \begin{vmatrix} \psi_1(x_1) & \cdots & \psi_1(x_N) \\ \psi_2(x_1) & & \psi_2(x_N) \\ \vdots & & \vdots \\ \psi_N(x_1) & & \psi_N(x_N) \end{vmatrix}$$

single-particle basis

$$\hat{h}_0 \psi_i(x_j) \neq \varepsilon_i \psi_i(x_j)$$

$$\langle \Psi_0 | \hat{H} | \Psi_0 \rangle = \sum_{i=1}^{N} \underbrace{\langle i | \hat{h}_0 | i \rangle}_{\varepsilon_i} + \frac{1}{2} \sum_{ij} \langle ij | v | ij \rangle_{AS}$$

$$\sum_{i=1}^{N} \sum_{\alpha\beta} C^*_{\alpha i} C_{\beta i} \langle \alpha | \hat{h}_c | \beta \rangle$$

$$\varepsilon_\alpha \delta_{\alpha\beta}$$

$$= \sum_{i=1}^{N} \sum_{\alpha} |C_{\alpha i}|^2 \varepsilon_\alpha$$

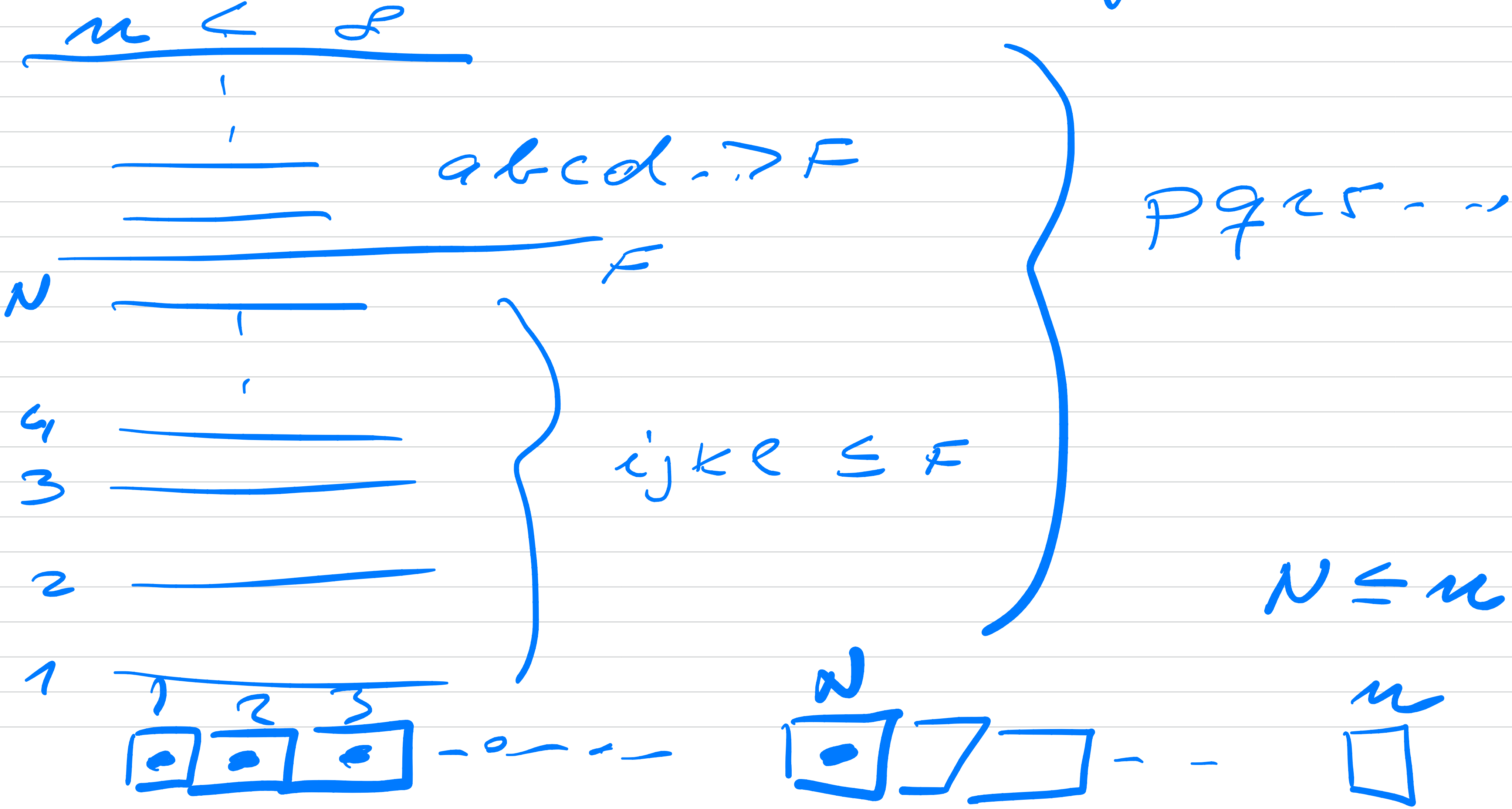
$$\frac{1}{2} \sum_{ij}^{N} \langle ij | v | ij \rangle_{AS}$$

$$= \frac{1}{2} \sum_{ij}^{N} \sum_{\alpha\beta\gamma\delta} C^*_{\alpha i} C^*_{\beta j} C_{\gamma i} C_{\delta j}$$

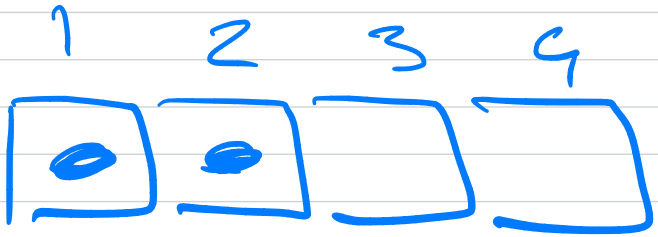
$$\times \langle \alpha\beta | v | \gamma\delta \rangle_{AS}$$

2nd quantization / Number representation

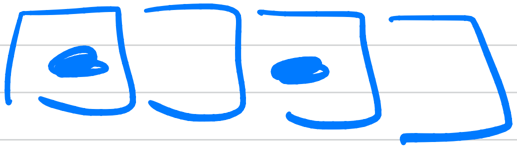
Fermionic systems first



$N=2$ $\qquad$ $n=4$



$|1100\rangle$



$|1010\rangle$

\# configurations

$$= \binom{n}{N} = \frac{n!}{(n-N)!\,N!}$$

$$= \frac{4}{2!\,2!} = \frac{\cancel{2}\cdot 3\,\cancel{4}^{\,2}}{\cancel{2}\cdot\cancel{2}}$$

$$= 6$$

Define a so-called creation operator

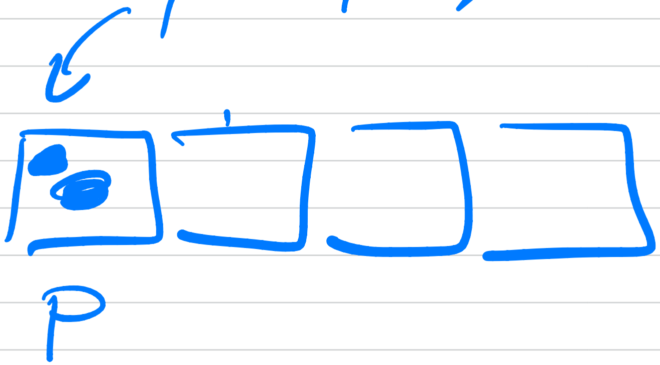
$$a_p^{\dagger}\,|0\rangle = |p\rangle$$

$|0\rangle$ ← True vacuum

Two particles

$$a_p^+ a_q^+ |0\rangle = |pq\rangle$$

$$a_p^+ |p\rangle = 0$$



want antisymmetric

$$|pq\rangle = - |qp\rangle$$

$$a_p^+ a_q^+ |0\rangle = - a_q^+ a_p^+ |0\rangle$$

$$\left(a_p^\dagger a_q^\dagger + a_q^\dagger a_p^\dagger\right)|0\rangle = 0$$

$\Rightarrow$ anticommutation rule

$$\{a_p^\dagger, a_q^\dagger\}|0\rangle = 0$$

$$[a_p^\dagger, a_q^\dagger]_+ |0\rangle = 0$$

$$\{a_p^\dagger, a_q^\dagger\} = 0$$

Define an annihilation operator

$$a_p|p\rangle = |0\rangle$$

$$a_p|0\rangle = 0 \qquad \Rightarrow$$

$$\{a_p, a_q\} = 0$$

$$\{a_p^\dagger, a_q\} = a_p^\dagger a_q + a_q a_p^\dagger$$
$$= \delta_{pq}$$

$N=3$

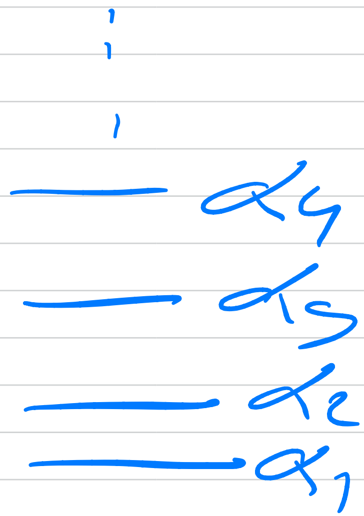
$$a_\alpha a_\alpha^\dagger |\alpha_1 \alpha_2 \alpha_3\rangle \qquad \alpha \notin \{\alpha_1 \alpha_2 \alpha_3\}$$

$$a_\alpha a_\alpha^\dagger a_{\alpha_1}^\dagger a_{\alpha_2}^\dagger a_{\alpha_3}^\dagger |0\rangle$$

$N=4$

$$a_\alpha |\alpha \alpha_1 \alpha_2 \alpha_3\rangle$$

$$|\alpha_1 \alpha_2 \alpha_3\rangle$$



$$\alpha = \alpha_4$$

$$a^{\dagger}_{\alpha_4} |\alpha_1 \alpha_2 \alpha_3\rangle = |\alpha_4 \alpha_1 \alpha_2 \alpha_3\rangle$$

$$a^{\dagger}_{\alpha_4} a^{\dagger}_{\alpha_1} = - a^{\dagger}_{\alpha_1} a^{\dagger}_{\alpha_4}$$

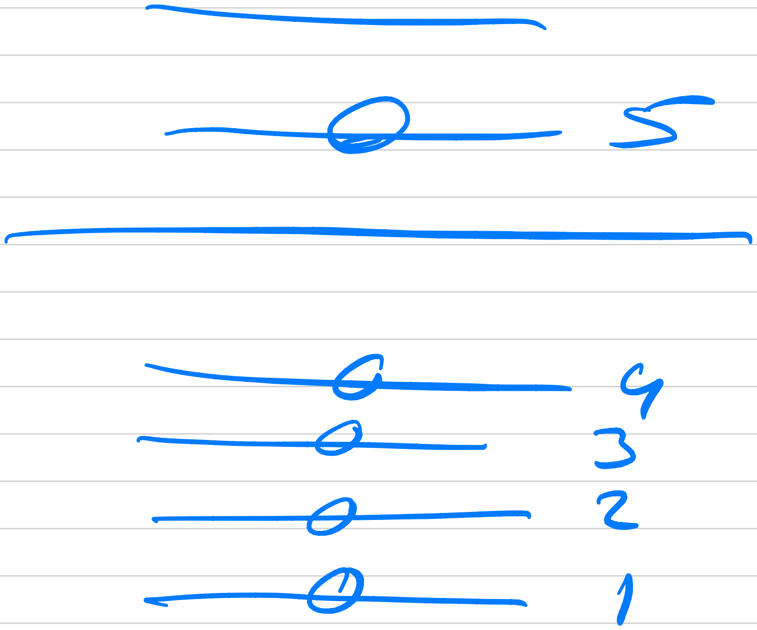
$$(-)^3 |\alpha_1 \alpha_2 \alpha_3 \alpha_4\rangle$$

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

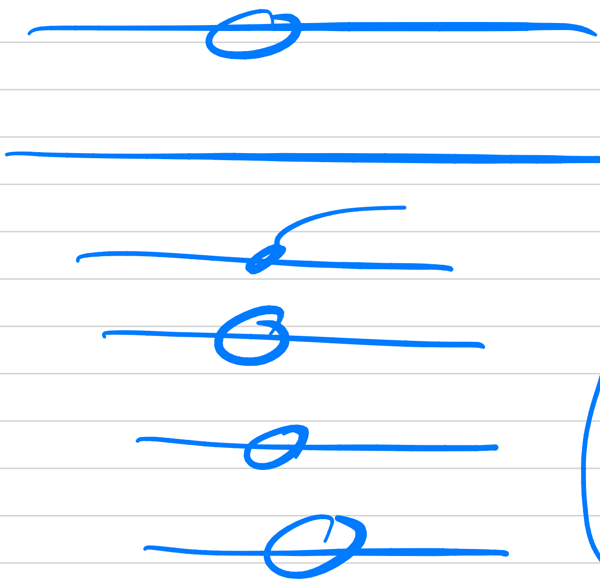
$$= -|\alpha_2 \alpha_1\rangle$$

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

$$\binom{40}{20}$$



$|12345\rangle$



$|1235\rangle$

$a^\dagger_\alpha |1235\rangle$

$= |\alpha 1235\rangle$

$\alpha = 4$

$$(-)^{(3)} \, |\alpha_1 \alpha_2 \alpha_3 \alpha_4\rangle$$

$$a_{\alpha_4} \, (-)^3 \, |\alpha_1 \alpha_2 \alpha_3 \alpha_4\rangle$$

$$a_{\alpha_4} \, |\alpha_4 \alpha_1 \alpha_2 \alpha_3\rangle = |\alpha_1 \alpha_2 \alpha_3\rangle$$

$$a^\dagger_\alpha a_\alpha \, |\alpha_1 \alpha_2 \alpha_3\rangle$$

if $\alpha \notin \{\alpha_1 \alpha_2 \alpha_3\}$

then zero $\quad a_\alpha |0\rangle = 0$

$$\alpha \in \{\alpha_1\, \alpha_2\, \alpha_3\}$$

$$\alpha = \alpha_1$$

$$a^\dagger_{\alpha_1} \underbrace{a_{\alpha_1} a^\dagger_{\alpha_1}}_{} a^\dagger_{\alpha_2} a^\dagger_{\alpha_3} |0\rangle$$

$$a^\dagger_{\alpha_1} a^\dagger_{\alpha_2} a^\dagger_{\alpha_3} |0\rangle = |\alpha_1\, \alpha_2\, \alpha_3\rangle$$

$$\left(a^\dagger_\alpha a_\alpha + a_\alpha a^\dagger_\alpha\right) |\alpha_1\, \alpha_2\, \alpha_3\rangle$$

$$= |\alpha_1\, \alpha_2\, \alpha_3\rangle$$

$$\{ a_\alpha^\dagger , a_\alpha \} = \underline{1}$$

$$\{ a_p^\dagger , a_q \} = \delta_{pq}$$

$$| \alpha_1 \alpha_2 \rangle$$

$$\hat{N} = \sum_p a_p^\dagger a_p$$

$$\langle \alpha_1 \alpha_2 | \hat{N} | \alpha_1 \alpha_2 \rangle$$

$$\sum_p \langle c| a_{\alpha_2} a_{\alpha_1} a_p^\dagger \underbrace{a_p a_{\alpha_1}^\dagger a_{\alpha_2}^\dagger}|0\rangle$$

$$\left(\delta_{p\alpha_1} - a_{\alpha_1}^\dagger a_p\right) a_{\alpha_2}^\dagger$$

$$\Big[\delta_{p\alpha_1} a_{\alpha_2}^\dagger - a_{\alpha_1}^\dagger \big(\delta_{p\alpha_2}$$

$$- a_{\alpha_1}^\dagger a_{\alpha_2}^\dagger a_p\big)\Big]|0\rangle$$