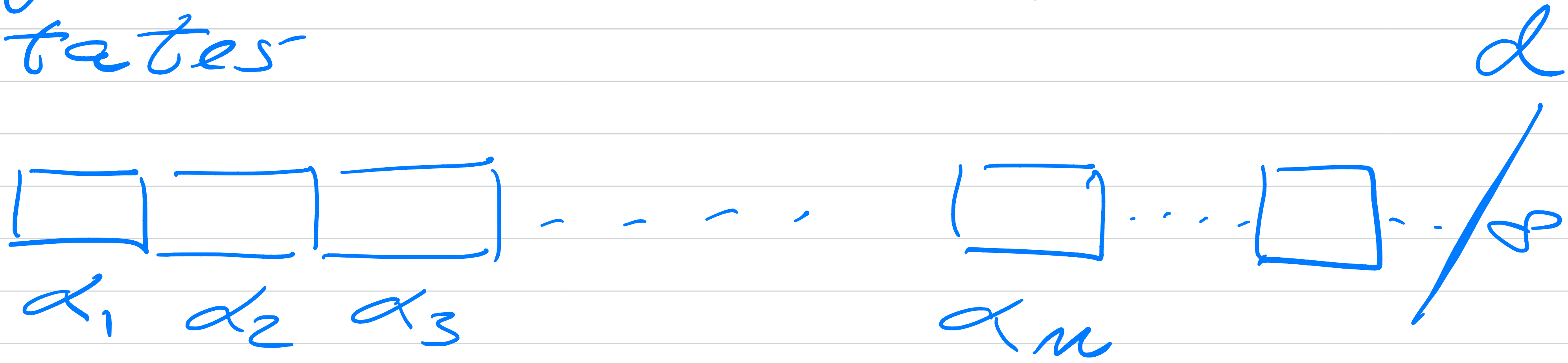
Lecture FYS4480, September 7

Define a vacuum state $|0\rangle$

Definition of single-particle states



Fermi level

$\alpha_n = F$

$$|\alpha\rangle = \varphi_{\alpha'}(x) \otimes \xi_{s m_s}$$

$$\alpha = \alpha' s m_s$$

Two particles

$$|\alpha_1\rangle \otimes |\alpha_2\rangle = |\alpha_1 \alpha_2\rangle$$

Example $|\alpha_1\rangle = \begin{bmatrix} 1 \\ 0 \end{bmatrix} = |0\rangle$

$|\alpha_2\rangle = \begin{bmatrix} 1 \\ 0 \end{bmatrix} \quad |0\rangle$

$$|\alpha_1\rangle \otimes |\alpha_2\rangle = \begin{bmatrix} 1 \\ 0 \\ 0 \\ 0 \end{bmatrix} = |\alpha_1 \alpha_2\rangle$$

$$= |00\rangle$$

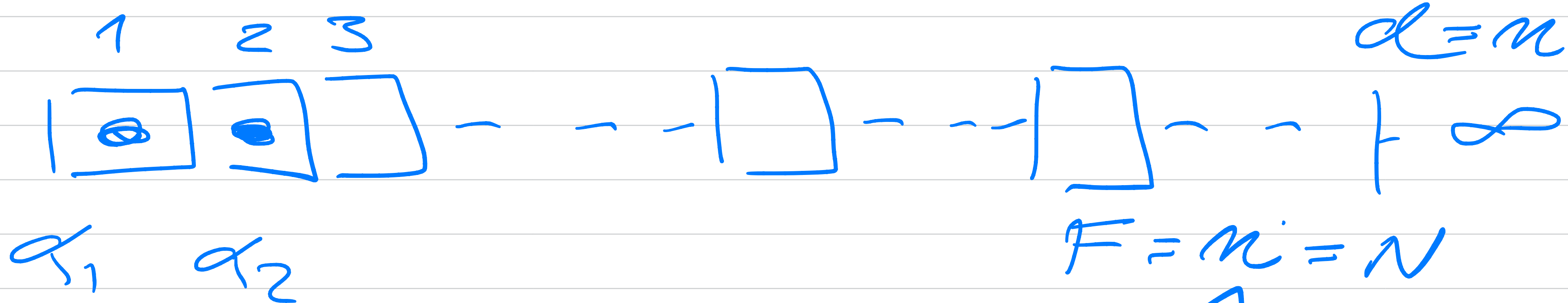
$$= |1\rangle$$

$$SD = |\alpha_1 \alpha_2 \dots \alpha_n\rangle_{AS}$$

$a_\alpha^\dagger |0\rangle = |\alpha\rangle \qquad a_\alpha^\dagger |\alpha\rangle = 0$

$a_\alpha |0\rangle = 0 \qquad a_\alpha |\alpha\rangle = |0\rangle$

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



$F = n_i = N$

sp states

$$\alpha_1 < \alpha_2 < \alpha_3 \quad \dots$$

$$\{a^\dagger_\alpha, a^\dagger_\beta\} = \{a_\alpha, a_\beta\} = 0$$

$$\{a^\dagger_\alpha\, a^\dagger_\beta\} = a^\dagger_\alpha a^\dagger_\beta + a^\dagger_\beta a^\dagger_\alpha$$

$$= [a^\dagger_\alpha\, a^\dagger_\beta]_+ \quad , \quad \{a_\alpha\, a^\dagger_\beta\} = \delta_{\alpha\beta}$$

$$a_\alpha^\dagger a_\alpha |\alpha_1 \alpha_2 \ldots \alpha_n\rangle$$

$$\alpha \notin \{\alpha_1 \alpha_2 \ldots \alpha_n\}$$

$$= 0$$

$$a_\alpha a_\alpha^\dagger |\alpha_1 \alpha_2 \ldots \alpha_n\rangle =$$

$$a_\alpha |\alpha\, \alpha_1 \alpha_2 \ldots \alpha_n\rangle = |\alpha_1 \alpha_2 \ldots \alpha_n\rangle$$

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

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

$$[x, p] = i\hbar$$

$$[J_x, J_y] \qquad (J_x J_y |\psi\rangle$$

$$- J_y J_x |\psi\rangle$$

$$|\alpha\rangle = a_\alpha^\dagger |0\rangle$$

$$a_\alpha^\dagger a_\alpha \, |\alpha_1, \alpha_2\rangle$$

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

$$\alpha = \alpha_2$$

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

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

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

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

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

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

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

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

Example ; norm of 2 body state $\langle \alpha_1 \alpha_2 | \alpha_1 \alpha_2 \rangle$

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

which strategy?

$$a_\alpha |0\rangle = 0 \qquad a^\dagger_\alpha |0\rangle = |\alpha\rangle \neq 0$$

$$\langle 0 | \{ a_{\alpha_2} (\delta_{\alpha_1 \alpha_1} - a^\dagger_{\alpha_1} a_{\alpha_1}) a^\dagger_{\alpha_2} \} | 0 \rangle$$

$$= \delta_{\alpha_1,\alpha_1} \underbrace{\langle 0 | a_{\alpha_2} a^\dagger_{\alpha_2} | 0 \rangle}_{\delta_{\alpha_2,\alpha_2}}$$

$$\left(\langle 0 | (\delta_{\alpha_2 \alpha_2} - a^\dagger_{\alpha_2} a_{\alpha_2}) | 0 \rangle \right)$$

$$- \langle 0 | a_{\alpha_2} a^\dagger_{\alpha_1} a_{\alpha_1} a^\dagger_{\alpha_2} | 0 \rangle$$

Last term

$$-\langle 0|a_{\alpha_2} a^\dagger_{\alpha_1} (\delta_{\alpha_1\alpha_2} - a^\dagger_{\alpha_2} a_{\alpha_1})|0\rangle$$

$= 0 \quad \Rightarrow$

$$\langle \alpha_1 \alpha_2 | \alpha_1 \alpha_2\rangle = \delta_{\alpha_1\alpha_1} \delta_{\alpha_2\alpha_2}$$

Example 2

$$\hat{N} = \sum_\alpha a^\dagger_\alpha a_\alpha$$

Number operator

$$\hat{N}^2 = \hat{N}$$

$$a_\alpha^\dagger a_\alpha \, |\alpha_1 \alpha_2 \cdots \alpha_n\rangle$$

$$= \begin{cases} 0 & \alpha \notin \{\alpha_1 \alpha_2 \ldots \alpha_n\} \\ |\alpha_1 \alpha_2 \cdots \alpha_n\rangle & \text{if } \alpha \in \{\alpha_1 \ldots \alpha_n\} \end{cases}$$

$$a_\alpha \, |\alpha_1 \alpha_2 \cdots \alpha_k \, \alpha \, \alpha_{k+1} \cdots \alpha_n\rangle$$

$$= a_\alpha^\dagger a_\alpha a_\alpha^\dagger (-)^k a_{\alpha_1}^\dagger a_{\alpha_2}^\dagger \cdots a_{\alpha_k}^\dagger a_{k+1}^\dagger \cdots a_{\alpha_n}^\dagger$$

$$= (-)^k a_\alpha^\dagger a_{\alpha_1}^\dagger a_{\alpha_2}^\dagger \cdots a_{\alpha_k}^\dagger a_{\alpha_{k+1}}^\dagger \cdots \times |0\rangle \quad |0\rangle$$

$$\hat{N}\,|\alpha_1, \alpha_2 \ldots \alpha_n\rangle$$

$$\hat{N} = \sum_{\alpha=\alpha_1}^{\alpha_n} a_\alpha^\dagger a_\alpha$$

$$\sum_{\alpha=\alpha_1}^{\alpha_n} a_\alpha^\dagger a_\alpha \,|\alpha_1, \alpha_2 \ldots \alpha_n\rangle$$

$$= n\,|\alpha_1, \alpha_2 \ldots \alpha_n\rangle$$

$$\langle \alpha_1, \alpha_2 \ldots \alpha_n | \hat{N} | \alpha_1, \alpha_2 \ldots \alpha_n\rangle$$

$$= n = \#\ \text{particles}$$

$$\hat{N}_i = a_i^\dagger a_i$$

$$\hat{N}_i^2 = (a_i^\dagger a_i)(a_i^\dagger a_i)$$

$$= a_i^\dagger (1 - a_i^\dagger a_i) a_i$$

$$= a_i^\dagger a_i - a_i^\dagger a_i^\dagger a_i a_i$$

$$(a_i^\dagger a_i - a_i^\dagger a_i^\dagger \underbrace{a_i a_i) |i\rangle}_{|0\rangle}$$

$$= a_i^\dagger a_i \Rightarrow \hat{N}_i^2 = \hat{N}_i$$

$$\Rightarrow \hat{N}^2 = \hat{N}$$

$$[N_i, N_j] = 0$$

$$[a_i, N_j] = \langle i | j \rangle a_i$$

$$[a_i^\dagger, N_j] = -\langle i | j \rangle a_i^\dagger$$

$$\searrow \delta_{ij}$$

Example 3

$$\hat{H}_0 = \sum_{i=1}^{N} \hat{h}_0(x_i) \qquad \hat{h}_0(x_i) = -\frac{\hbar^2}{2m} \partial_i^2 + v_{ext}(x_i)$$

in 2nd quantization

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

(show later)

$$\langle \alpha | \hat{h}_0 | \beta \rangle = \int_{x \in D} dx\, \varphi_\alpha^*(x) h_0 \varphi_\beta(x)$$

$$\hat{h}_0 | \varphi_\beta(x) \rangle = \varepsilon_\beta | \varphi_\beta \rangle$$

$$\hat{h}_0 | \beta \rangle = \varepsilon_\beta | \beta \rangle$$

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

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

2-particles $\quad |\alpha_1, \alpha_2\rangle$

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

$$\langle \alpha_1, \alpha_2 | H_0 | \alpha_1, \alpha_2 \rangle = \varepsilon_{\alpha_1} + \varepsilon_{\alpha_2}$$

$$\sum_{\alpha} \langle 0 | a_{\alpha_2} a_{\alpha_1} \; \varepsilon_\alpha a_\alpha^\dagger a_\alpha \; a_{\alpha_1}^\dagger a_{\alpha_2}^\dagger | 0 \rangle$$

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

skip $|0\rangle$

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

$$a_{\alpha_2} a_{\alpha_1} a_{\alpha_1}^\dagger a_{\alpha_2}^\dagger - \qquad - a_{\alpha_2} a_{\alpha_1} a_{\alpha_2}^\dagger a_{\alpha}^\dagger$$

$$a_{\alpha_2} a_{\alpha_1} a^\dagger_{\cdot} a_{\alpha_1}^\dagger a_\alpha a_{\alpha_2}^\dagger$$

$$a_{\alpha_2} \left(1 - a_{\alpha_1}^\dagger a_{\alpha_1} \right) a_{\alpha_2}^\dagger \qquad \alpha_1 \neq \alpha_2$$

$$- a_{\alpha_2} a_{\alpha_1} a_\alpha^\dagger a_{\alpha_1}^\dagger \left(\delta_{\alpha \alpha_2} - a_{\alpha_2}^\dagger a_\alpha \right) |$$

$$a_{\alpha_2}\left(1 - a^\dagger_{\alpha_1} a_{\alpha_1}\right) a^\dagger_{\alpha_2}$$

$$\underbrace{\delta_{\alpha_1\alpha_2} a_{\alpha_2} a^\dagger_{\alpha_2}} \quad - \quad a_{\alpha_2} a^\dagger_{\alpha_1} a_{\alpha_1} a^\dagger_{\alpha_2}$$

$$\delta_{\alpha_1\alpha_2}\left(\delta_{\alpha_2\alpha_2} - a^\dagger_{\alpha_2} a_{\alpha_2}\right)$$

$$\delta_{\alpha_1\alpha_2} \quad \delta_{\alpha_2\alpha_2} \qquad \delta_{\alpha\alpha_1}$$

$$\Rightarrow$$

$$\varepsilon_{\alpha_1}$$

Finally we get also a Term

$$\varepsilon_{\alpha_2}$$

Motivates the introduction of Wick's theorem, we need some definitions

$$\langle 0|a_\alpha a_\beta^\dagger|0\rangle = \delta_{\alpha\beta}\langle 0|0\rangle - \overbrace{\langle 0|a_\beta^\dagger a_\alpha|0\rangle}^{=0}$$

$$\langle 0|a_\alpha a_\beta^\dagger|0\rangle = \langle \alpha|\beta\rangle = \delta_{\alpha\beta}$$

$$= \underbrace{\overline{a_\alpha a_\beta^\dagger}}_{\text{contraction}} + N[a_\beta^\dagger a_\alpha]$$