FYS4480 September 8

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

$$\hat{N}^2 = \hat{N} \qquad \langle i|j\rangle = \delta_{ij}$$

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

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

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

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

<u>Example</u>

$$[\hat{N}_i, \hat{N}_j] = \hat{N}_i \hat{N}_j - \hat{N}_j \hat{N}_i =$$

$(i \neq j)$

$$\underbrace{a_i^\dagger a_i a_j^\dagger a_j} - \underbrace{a_j^\dagger a_j a_i^\dagger a_i}$$

$$-\,"\,- \qquad - \left[a_j^\dagger (\delta_{ij} - a_i^\dagger a_j) \right] a_i$$

$$\{a_j^\dagger a_i^\dagger\} = 0$$

$$-\,"\,- \qquad + \underbrace{a_j^\dagger a_i^\dagger}\, \underbrace{a_j a_i} \qquad \{a_j a_i\} = 0$$

$+ \;\; '$

$$— \,'\, — \quad + a_i' \underbrace{a_j^+ a_i'} a_j'$$

$$— \,'\, — \quad + \Big(a_i^+ (\delta_{ij}' - a_i a_j^+) a_j'$$

$$— \,'\, — \quad - a_i^+ a_i \, a_j^+ a_j \equiv 0$$

$$[\hat{A}, \hat{B}]_- = \hat{A}\hat{B} - \hat{B}\hat{A}$$

$$[\hat{A}, \hat{B}]_+ = \hat{A}\hat{B} + \hat{B}\hat{A}$$

$$[\hat{A}, \hat{B}] = \hat{A}\hat{B} - \hat{B}\hat{A}$$

$$\{\hat{A}, \hat{B}\} = \hat{A}\hat{B} + \hat{B}\hat{A}$$

<u>Example</u>

$$[a_i^+, \hat{N}_j] =$$

$$a_i^+ a_j^+ a_j - a_j^+ a_j a_i^+$$

$$= a_i^+ a_j^+ a_j' - a_j^+ (\delta_{ij}' - a_i^+ a_j')$$

$$\langle 0 | a_i a_j^+ | 0 \rangle = \langle i j \rangle$$

$$= a_i^+ a_j^+ a_j + \underbrace{a_j^+ a_i^+}\, a_j - a_j^+ \delta_{ij}$$

$$a_i^+ a_j^+ a_j - a_i^+ a_j^+ a_j - a_i^+ \delta_{ij}$$

$$= - a_i^+ \delta_{ij}$$

$$[a_i, \hat{N}_j] = \delta_{ij}\, a_i$$

<u>Example</u>

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

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

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

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

$$= \int dx\, \varphi_\alpha^*(x)\, \varepsilon_\beta \varphi_\beta(x)$$

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

in 2nd quantization

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

$$= \sum_{\alpha} \varepsilon_\alpha a^+_\alpha a_\alpha$$

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

$$\sum_{\alpha} \varepsilon_\alpha \langle 0 | a_{\alpha_2} a_{\alpha_1} a^+_\alpha a_\alpha a^+_{\alpha_1} a^+_{\alpha_2} | 0 \rangle$$

$$= \sum_{\alpha_i} \varepsilon_{\alpha_i} = \varepsilon_{\alpha_1} + \varepsilon_{\alpha_2}$$

$$\langle 0 | a_{\alpha_2} a_{\alpha_1} a^+_\alpha \underline{a_\alpha a^+_{\alpha_1}} a^+_{\alpha_2} | 0 \rangle$$

$$a_{\alpha_2} a_{\alpha_1} a^+_\alpha \left[\delta_{\alpha\alpha_1} - a^+_{\alpha_1} a_\alpha \right] a^+_{\alpha_2}$$

$$a_{\alpha_2} \underline{a_{\alpha_1} a^+_{\alpha_1}} a^+_{\alpha_2} \underline{\delta_{\alpha\alpha_1}} \qquad \alpha_1 \neq \alpha_2$$

$$- a_{\alpha_2} a_{\alpha_1} a^+_\alpha a^+_{\alpha_1} a_\alpha a^+_{\alpha_2}$$

$$= a_{\alpha_2} \left(1 - a^+_{\alpha_1} a_{\alpha_1} \right) a^+_{\alpha_2}$$

$$- a_{\alpha_2} a_{\alpha_1} a^+_\alpha a^+_{\alpha_1} \left(\delta_{\alpha\alpha_2} - a^+_{\alpha_2} a_\alpha \right)$$

$$= a_{\alpha_2} a^+_{\alpha_2} - \underline{a_{\alpha_2}} a^+_{\alpha_1} a_{\alpha_1} a^+_{\alpha_2}$$

$$- \overline{a_{\alpha_1}^\dagger a_{\alpha_2} a_{\alpha_2}^\dagger a_{\alpha_1}}$$

$$- a_{\alpha_2} a_{\alpha_1} a_{\alpha_2}^+ a_{\alpha_1}^+$$

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

$$+ \delta_{\alpha_1\alpha_1} \quad \Rightarrow$$

$$\sum_\alpha \langle \alpha | h_0 | \alpha \rangle \langle \alpha_1 \alpha_2 | a_\alpha^+ a_\alpha | \alpha_1 \alpha_2 \rangle$$

$$= \varepsilon_{\alpha_1} + \varepsilon_{\alpha_2}$$

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

$$= \frac{1}{4} \sum_{\alpha\beta\gamma\delta} \left[\langle \alpha\beta | v | \gamma\delta \rangle + \langle \alpha\beta | v | \gamma\delta \rangle \right] \times a_\alpha^+ a_\beta^+ a_\delta a_\gamma$$

$$= \frac{1}{4} \sum_{\alpha\beta\gamma\delta} \langle \alpha\beta | v | \gamma\delta \rangle \underbrace{a_\alpha^+ a_\beta^+ a_\delta}\, a_\gamma$$

$$- \frac{1}{4} \sum_{\alpha\beta\gamma\delta} \langle \alpha\beta | v | \gamma\delta \rangle \underbrace{a_\alpha^+ a_\beta^+ a_\gamma a_\delta}$$

$$\gamma \leftrightarrow \delta$$

$$= \frac{1}{4} \sum_{\alpha\beta\gamma\delta} \left[\langle \alpha\beta | v | \gamma\delta \rangle - \langle \alpha\beta | v | \delta\gamma \rangle \right] \times a_\alpha^\dagger a_\beta^\dagger a_\delta a_\gamma$$

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

Wick's theorem

Definition

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

$$\langle c | a_\alpha a_\beta | 0 \rangle = \langle 0 | a_\alpha^\dagger a_\beta^\dagger | 0 \rangle$$

$$= \langle c | a_\alpha^\dagger a_\beta | 0 \rangle = 0$$

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

$$- \langle c | a_\beta^\dagger a_\alpha | 0 \rangle$$

$$= \overbracket{a_\alpha a_\beta^\dagger} + N[\underline{a_\alpha a_\beta^\dagger}]$$

contraction

$$\langle c| a_\alpha a_\beta^\dagger |c\rangle = -\langle c| \underline{a_\beta^\dagger a_\alpha} |c\rangle$$

$$\langle c| a_\alpha^\dagger = 0$$

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

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

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

Normal ordering of a chain of operators $XYZ \ldots W$

$$N[XYZ \cdots W] = (-)^P [\text{creation operators}][\text{annihilation operators}]$$

Example

$$a_1 a_2 a_3^\dagger = a_1 (\delta_{23} - a_3^\dagger a_2)$$

$$= a_1 \delta_{23} - (\delta_{13} - a_3^\dagger a_1) a_2$$

$$= a_1 \delta_{23} - \delta_{13} a_2 + a_3^\dagger a_1 a_2$$

$$\overbrace{a_2 a_3^\dagger}$$

$$N[a_1 \overbrace{a_2 a_3^\dagger}] + N[\overbrace{a_1 a_2 a_3^\dagger}]$$

$$N[a_1 a_2 a_3^\dagger]$$

Example

$$\langle 0 | a_1 a_2 a_3^\dagger a_4^\dagger | 0 \rangle$$

$$= a_1 (\delta_{23} - a_3^\dagger a_2) a_4^\dagger$$

$$a_1 a_4^\dagger \delta_{23} - a_1 a_3^\dagger a_2 a_4^\dagger$$

$$\text{— '' —} \quad -(\delta_{13} - a_3^\dagger a_1) a_2 a_4^\dagger$$

$$\underline{a_1 a_4^\dagger} \delta_{23} - \delta_{13} \underline{a_2 a_4^\dagger} + \underline{a_3^\dagger a_1} a_2 a_4^\dagger =$$

$$\delta_{23} \delta_{14} - \delta_{23} a_4^\dagger a_1$$

$$- \delta_{13} \delta_{24} + \delta_{13} a_4^\dagger a_2$$

$$+ \delta_{24} a_3^\dagger a_1 - a_3^\dagger a_2 \delta_{41}$$

$$+ a_3^\dagger a_4^\dagger a_1 a_2$$

$$\overbrace{a_j a_i^\dagger} \neq 0$$

$$\overbrace{a_i a_j} = 0$$

$$\overbrace{a_i^\dagger a_j} = 0$$

$$N[a_1 a_2 a_3^\dagger a_4^\dagger] + N[a_1 a_2 a_3^\dagger a_4^\dagger]$$

$$+ N[a_1 a_2 a_3^\dagger a_4^\dagger] + N[a_1 a_2 a_3^\dagger a_4^\dagger]$$

$$+ N[a_1 a_2 a_3^\dagger a_4^\dagger] + N[a_1 a_2 a_3^\dagger a_4^\dagger]$$

$$+ N[a_1 a_2 a_3^\dagger a_4^\dagger]$$

$$= N[a_1 a_2 a_3^\dagger a_4^\dagger]$$

$$+ \sum_{\text{(1) one contraction}} N[a_1 a_2 a_3^\dagger a_4^\dagger]$$

$$+ \sum_{\text{(2) two contraction}} N[a_1 a_2 a_3^\dagger a_4^\dagger]$$

$$XYZ \cdots W =$$

$$N[XYZ \cdots W] +$$

$$\sum_{(1)} N[XYZ \cdots W]$$

$$+ \sum_{(2)} N[XYZ \cdots W]$$

$$+ \quad \cdots$$

$$+ \sum_{\left(\frac{N}{2}\right)} N\left[x y z \cdots w \right]$$

Wick's theorem