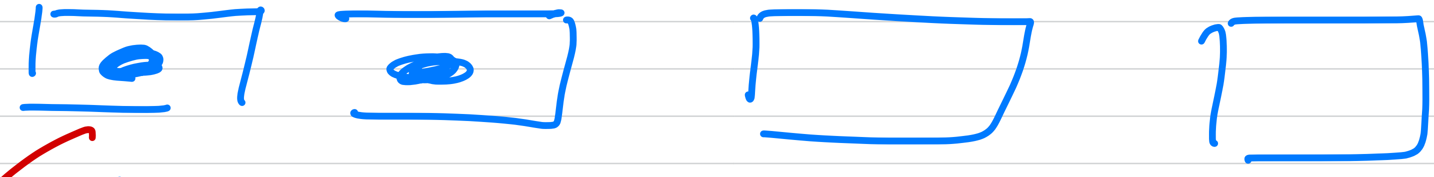
FYS4480/9480 August 29

$N = 2 \qquad n = 4$

$\alpha_1 \quad \alpha_2 \quad \alpha_3 \quad \alpha_4$



$1 \quad 2 \quad 3 \quad 4$

$$\frac{4!}{2!\,2!} = 6 \text{ possible configs}$$

$$|1100\rangle \rightarrow |1100\rangle$$

$$a_i^{\dagger}\,|0\rangle = |i\rangle$$

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

$$|i\rangle \qquad a_i |i\rangle = |0\rangle$$

$$a_i |0\rangle = 0$$

$$[a_p^\dagger, a_q^\dagger]_+ = \{a_p^\dagger, a_q^\dagger\}$$

$$= a_p^\dagger a_q^\dagger + a_q^\dagger a_p^\dagger = 0$$

$$\left([A, B] = AB - BA \right)$$

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

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

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

$$a_p^\dagger a_p \quad a_1^\dagger a_2^\dagger |0\rangle$$

$$p \in \{1, 2\}$$

$p=1$

$$a_{p=1}^\dagger \, a_1 \, a_1^\dagger a_2^\dagger |0\rangle$$

$$= a_1^\dagger \, a_2^\dagger |0\rangle = |12\rangle$$

$P = 2$

$$a_2^\dagger a_2 \quad a_1^\dagger a_2^\dagger |0\rangle$$

$$- \; a_2^\dagger \underbrace{a_2 a_2^\dagger}\, a_1^\dagger |0\rangle$$

$$\{a_1^\dagger, a_2^\dagger\} = a_1^\dagger a_2^\dagger + a_2^\dagger a_1^\dagger = 0$$

$$\Rightarrow a_1^\dagger a_2^\dagger = - a_2^\dagger a_1^\dagger$$

$$= - a_2^\dagger a_1^\dagger |0\rangle = - |21\rangle$$

$$= |12\rangle$$

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

$$a_\alpha^\dagger a_\alpha \quad a_{\alpha_1}^\dagger a_{\alpha_2}^\dagger \cdots a_{\alpha_k}^\dagger a_\alpha^\dagger \cdots$$

$$= \underline{a_\alpha^\dagger} \underbrace{a_\alpha \quad a_\alpha^\dagger \quad a_{\alpha_1}^\dagger a_{\alpha_2}^\dagger \cdots a_{\alpha_k}^\dagger}_{k} a_{\alpha_{k+1}}^\dagger \cdots$$

$$\times (-)^k$$

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

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

$$\phi_1(x_1 x_2) = \frac{1}{\sqrt{2}}\Big(\varphi_p(x_1)\varphi_q(x_2) - \varphi_p(x_2)\varphi_q(x_1)\Big)$$

$$\phi_2(x_1, x_2) = \frac{1}{\sqrt{2}}\Big(\varphi_r(x_1)\varphi_s(x_2) - \varphi_r(x_2)\varphi_s(x_1)\Big)$$

$$\langle \phi_2(x_1 x_2) | \phi_1(x_1, x_2) \rangle$$

$$= \frac{1}{2}\int dx_1 \int dx_2$$

ONB

$$\Big(\varphi_r^*(x_1)\varphi_s^*(x_2) - \varphi_r^*(x_2)\varphi_s^*(x_1)\Big) \times \Big(\varphi_p(x_1)\varphi_q(x_2) - \varphi_p(x_2)\varphi_q(x_1)\Big)$$

$$= \frac{1}{2} \int dx_1 \int dx_2 \Big[\varphi_r^*(x_1)\, \varphi_s^*(x_2)\, \varphi_p(x_1)\, \varphi_q(x_2$$

δ_{sp}

δ_{rp}

$$+ \varphi_r^*(x_2)\, \varphi_s^*(x_1)\, \varphi_p(x_2)\, \varphi_s(x_1)$$

$x_1 \longleftrightarrow x_2$

$\delta_{rp}\, \delta_{sq}$

$\delta_{sp}\, \delta_{rq}$

$$- \varphi_r^*(x_1)\, \varphi_s^*(x_2)\, \varphi_p(x_2)\, \varphi_q(x_1)$$

$x_1 \Leftrightarrow x_2$

$$- \varphi_r^*(x_2)\, \varphi_s^*(x_1)\, \varphi_p(x_1)\, \varphi_q(x_2) \Big]$$

$$= \delta_{rp}\delta_{sq} - \delta_{rq}\delta_{sp}$$

2nd-quantization

$$\langle p|q\rangle = \langle 0|a_p a_q^\dagger|0\rangle$$

$$= \langle 0|\delta_{pq} - a_q^\dagger a_p|0\rangle$$

$$= \delta_{pq}$$

Normal-ordering of operators

$$N[xyz\ldots w] = (-)^k \langle 0|\underbrace{x'y'z'\ldots w'}_{\substack{\text{all creation operators}\\ \text{to the left}\\ \text{all annihilation}\\ \text{operators to the}\\ \text{right}}}|0\rangle$$

k = number of times we need to swap operators

contractions

$$\overline{a_p a_q^\dagger} = \langle 0 | a_p a_q^\dagger | 0 \rangle$$
$$= \delta_{pq}$$

$$\overline{a_p a_q} = \langle 0 | a_p a_q | 0 \rangle = 0$$

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

$$= \overline{a_p^\dagger a_p^\dagger}$$

$$\langle p|q\rangle = \langle 0|a_p a_q^\dagger|0\rangle$$

$$= \overline{a_p a_q^\dagger} + \underbrace{N[a_p a_q^\dagger]}_{= -\langle 0|a_q^\dagger a_p|0\rangle}$$

$$\langle rs | pq \rangle$$

$$|rs\rangle = a_r^\dagger a_s^\dagger |0\rangle$$

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

$$\langle 0 | a_s a_r \, a_p^\dagger a_q^\dagger |0\rangle$$

$$= a_s \left(\delta_{rp} - a_p^\dagger a_r \right) a_q^\dagger$$

$$\delta_{rp} \left(\delta_{sq} - a_q^\dagger a_s \right)$$

$$- \; a_s a_p^\dagger a_r a_q^\dagger$$

$$\underbrace{\delta_{rp}\delta_{sq}}_{N[a_s a_r a_p^\dagger a_q^\dagger]} - \underbrace{\delta_{rp} a_q^\dagger a_s}_{N[a_s a_r a_p^\dagger a_q^\dagger]} \leftarrow 0$$

$$- a_s a_p^\dagger a_r a_q^\dagger$$

$$- a_s a_p^\dagger (\delta_{rq} - a_q^\dagger a_r)$$

$$a_s a_p^\dagger a_q^\dagger a_r - \delta_{rq} a_s a_p^\dagger$$

$$-\delta_{rq}(\delta_{sp} - a_p^\dagger a_s)$$

$$N[a_s a_r a_p^\dagger a_q^\dagger] + N[a_s a_r a_p^\dagger a_q^\dagger]$$

$$= 0$$

$$\underline{a_s a_p^\dagger a_q^\dagger a_r}$$

$$(\delta_{sp} - a_p^\dagger a_s) a_q^\dagger a_r$$

$$N[a_s a_r a_p^\dagger a_q^\dagger]$$

$$- \boxed{a_p^\dagger a_s a_q^\dagger a_r}$$

$$- a_p^\dagger \left(\delta_{sq} - a_q^\dagger a_s \right) a_r$$

$$= \underbrace{a_p^\dagger a_q^\dagger a_s a_r} - \underbrace{a_p^\dagger a_r \delta_{sq}}$$

$$N\left[a_s a_r a_p^\dagger a_q^\dagger \right] + N\left[a_s a_r a_p^\dagger a_q^\dagger \right]$$

$$= 0 \qquad\qquad\qquad = 0$$

$$\delta_{rp} \delta_{sq} - \delta_{sp} \delta_{rq}$$

$$\langle 0 | X Y Z \cdots W | 0 \rangle =$$

Wick's theorem

$$N[X Y Z \cdots W]$$

$$+ \sum_{\substack{\text{all} \\ \text{1 pair} \\ \text{contractions}}} N[X Y Z \cdots W]$$

$$+ \sum_{\substack{\text{all} \\ \text{2 pairs}}} N[X Y Z \cdots W]$$

$$+ \cdots + \underbrace{\sum_{\substack{\text{all}\\ \text{pairs}\\ \text{of operators}}} N\left[x y z \cdots w \right]}_{\text{only non-zero}}$$

Example :

number operator

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

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

$$\sum_{i=1}^{n} \varepsilon_{i} \langle 0 | a_2 a_1 \, a_i^\dagger a_{i} \, a_1^\dagger a_2^\dagger |0\rangle$$

$$a_2 a_1 a_i^\dagger a_{i} a_1^\dagger a_2^\dagger \qquad \delta_{22}\,\delta_{i1}$$

$$\delta_{i2}\,\delta_{11}$$

$$= 2 = N$$

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

$$\hat{h}_0(x_1) \longrightarrow \sum_{pq=1}^{n} \langle p | h_0 | q \rangle a_p^\dagger a_q$$

$$\delta_{pq} \varepsilon_p$$

$$\sum_{p=1}^{n} \varepsilon_p a_p^\dagger a_p$$

$$\langle 12 | H_0 | 12 \rangle$$

$$= \sum_p \varepsilon_p \langle 0 | a_2 a_1 a_p^\dagger a_p a_1^\dagger a_2^\dagger | 0 \rangle$$

$$= \varepsilon_1 + \varepsilon_2$$

$$\hat{H}_I = \frac{1}{2} \sum_{pqrs} \langle pq|v|rs\rangle \, a_p^\dagger a_q^\dagger a_s a_r$$

$$\langle 12|\hat{H}_I|12\rangle =$$

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