Lecture FYS4480, September 8, 2023

Example

$$H_0 = \sum_{\alpha\beta} \langle \alpha | h_0 | \beta \rangle a_\alpha^\dagger a_\beta$$

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

$$= \sum_{\alpha\beta} \langle \alpha | h_0 | \beta \rangle \times$$

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

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

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

First term

$$a_{\alpha_2} a_{\alpha_1} a^{+}_{\alpha} a^{+}_{\alpha_2} \delta_{\alpha_1 \beta} \qquad \Big| \sum_{\alpha\beta} \langle \alpha | h_0 | \beta \rangle$$

$$\sum_{\alpha} \langle \alpha | h_0 | \alpha_1 \rangle$$

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

$$\boxed{\langle \alpha_1 | h_0 | \alpha_1 \rangle} \quad \varepsilon_{\alpha_1}$$

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

$$= \langle 0 | \delta_{\alpha_2\alpha_2} - a^{+}_{\alpha_2} a_{\alpha_2} | 0 \rangle$$

2nd term

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

$$- a_{\alpha_2} a^{+}_{\alpha} \Big(\underbrace{\delta_{\alpha_1\alpha_2}}_{=0} - a^{+}_{\alpha_2} \underbrace{a_{\alpha_1}}_{0} \Big)$$

Second term:

$$-a_{\alpha_2} a_{\alpha_1} a_\alpha^+ a_{\alpha_1}^+ (\delta_{\beta\alpha_2} - \underbrace{a_{\alpha_2}^+ a_\beta}_{=0})$$

$$-a_{\alpha_2} a_{\alpha_1} a_\alpha^+ a_{\alpha_1}^+ \delta_{\beta\alpha_2} \rightarrow \langle \alpha | h_0 | \alpha_2 \rangle$$

$$-a_{\alpha_2} a_{\alpha_1} a_\alpha^+ a_{\alpha_1}^+ \quad \underbrace{\langle \alpha_2 | h_0 | \alpha_2 \rangle}_{= \varepsilon_{\alpha_2}}$$

$$= -a_{\alpha_2} (\delta_{\alpha\alpha_1} - a_\alpha^+ a_{\alpha_1}) a_{\alpha_1}^+$$

$$-a_{\alpha_2} a_{\alpha_1}^+ \langle \alpha_1 | h_0 | \alpha_2 \rangle$$

$$-(\underbrace{\delta_{\alpha_1\alpha_2}}_{=0} - \underbrace{a_{\alpha_1}^+ a_{\alpha_2}}_{=0})$$

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

Wick's theorem

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

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

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

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

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

Normal-ordered product

$$N[xyz\cdots w]$$

$$= (-1)^P [\text{creation operator}]$$

$$\times [\text{annihilation ops}]$$

P = # of interchanges

$$N[a^\dagger_{\alpha_1} a_{\alpha_2} a_{\alpha_3} a^\dagger_{\alpha_4} a_{\alpha_5} a^\dagger_{\alpha_8}]$$

$$= (-)^5 \; a^\dagger_{\alpha_1} a^\dagger_{\alpha_4} a^\dagger_{\alpha_8} a_{\alpha_2} a_{\alpha_3} a_{\alpha_5}$$

$$\langle 0 | N[xyz\cdots w] | 0 \rangle = 0$$

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

Example

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

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

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

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

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

no $a_1 a_2$ $\quad (a_\alpha^\dagger a_\beta^\dagger = 0)$

Example

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

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

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

$$= \text{———}\;|\;\text{———} - (\delta_{13} - a_3^\dagger a_1) a_2 a_4^\dagger$$

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

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

$$\delta_{23}\left(\delta_{14} - a_4^\dagger a_1\right)$$

$$- \delta_{13}\left(\delta_{24} - a_4^\dagger a_2\right)$$

$$+ a_3^\dagger a_1\left(\delta_{24} - a_4^\dagger a_2\right) =$$

$$\delta_{23}\delta_{14} - \delta_{23} a_4^\dagger a_1 - \delta_{13}\delta_{24}$$

$$+ \delta_{13} a_4^\dagger a_2 + \delta_{24} a_3^\dagger a_1 -$$

$$a_3^\dagger a_2 \delta_{41} + a_3^\dagger a_4^\dagger a_2 a_1$$

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

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

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

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

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

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

$$\overbrace{a_i a_j^\dagger} = \overbrace{a_i a_j^\dagger} = \langle 0| a_i a_j^\dagger |0\rangle$$

Wick's theorem states the following

$$\langle 0| x y z \cdots w |0\rangle =$$

$$x y z \cdots w = N[x y z, \cdots, w]$$

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

sum over all terms with one contraction

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

sum over all pair(s) with contraction

$$+ \cdots +$$

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

all pairs of contractions

N = # of creation & annihilation operators

$$= \langle 0 | \sum_{\left(\frac{N}{2}\right)} N[x\,y\,z\,\cdots\,w] \,|0\rangle$$

Example

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

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

$$= \frac{1}{2} \sum_{\alpha\beta\gamma\delta} \langle 0 | a_{\alpha_2} a_{\alpha_1} a^\dagger_\alpha a^\dagger_\beta a_\delta a_\gamma a^\dagger_{\alpha_1}$$

$$\times \, a^\dagger_{\alpha_2} | 0 \rangle \, \langle \alpha\beta | v | \gamma\delta \rangle$$

$$\langle 0 | a_{\alpha_2} a_{\alpha_1} a^\dagger_{\alpha} a^\dagger_{\beta} a_{\delta} a_{\gamma} a^\dagger_{\alpha_1} a^\dagger_{\alpha_2} | 0 \rangle$$

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

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

$$\delta_{\alpha_1 \alpha} \delta_{\alpha_2 \beta} \; \delta_{\gamma \alpha_1} \delta_{\delta \alpha_2}$$

$$\langle \alpha \beta | v | \gamma \delta \rangle$$

$$\{a_\delta a_\gamma\} = 0$$

(ii) $a_{\alpha_2} a_{\alpha_1} a_\alpha^\dagger a_\beta^\dagger a_\delta a_\gamma a_{\alpha_1}^\dagger a_{\alpha_2}^\dagger$

$$a_\delta a_\gamma = -a_\gamma a_\delta$$

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

(iii)

$$\delta_{\alpha_1 \beta}\, \delta_{\alpha_2 \alpha_1}\, \delta_{\alpha_1 \delta}\, \delta_{\alpha_2 \gamma}$$

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

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

(iv) $a_{\alpha_2} a_{\alpha_1} a^\dagger_{\alpha} a^\dagger_{\beta} a_\delta a_\gamma a^\dagger_{\alpha_1} a^\dagger_{\alpha_2}$

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

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

$\Rightarrow$

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

$$= \underbrace{\langle \alpha_1 \alpha_2 | v | \alpha_1 \alpha_2 \rangle}_{\text{Direct}} - \underbrace{\langle \alpha_2 \alpha_1 | v | \alpha_1 \alpha_2 \rangle}_{\text{exchange}}$$

Proof of Wick's theorem
We need a lemma.

a chain of operators
$[x y z \ldots w]$ and add
a new operator Ω

$$N[x y z \ldots w]\,\Omega =$$

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

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

(i) valid immediately if Ω is an annihilation operator since then

$N[xyz\ldots w]\Omega$ is already normal-ordered ($a^+a = 0 = a^-a$)

(ii) we have assumed that the sequence is normal-ordered ($xyz\ldots w$)

(iii) if Ω is a creation operator we need to move the comma if all $xyz\ldots w$ are annihilation operators since all

$$\overline{a^{\dagger}a}^{\dagger} = 0$$

(ii) in (iii) we anticommute Ω through all x y z -- w operators get the first term all anticommutations which are then produced give the second term of the lemma.