

FCI Questions

Patryk Kozlowski

March 31, 2023

1. second quantization rules

$$a_{\kappa_1}^\dagger \equiv a_1^\dagger \dots a_{\kappa_n}^\dagger \equiv a_n^\dagger$$

$$a_{\kappa_1} \equiv a_1 \dots a_{\kappa_n} \equiv a_n$$

also, I frequently use these interchangeably

$$\kappa_1 \equiv 1 \dots \kappa_n \equiv n$$

so

$$\delta_{greekNumber,1} \equiv \delta_{GreekNumber,\kappa_1}$$

2. 2 determinants with no differences

$$\langle \Psi | V | \Psi \rangle = v^{\alpha\beta\gamma\delta} \langle 0 | \left(\prod_{\kappa} a_{\kappa} \right) a_{\alpha}^{\dagger} a_{\beta}^{\dagger} a_{\gamma} a_{\delta} \left(\prod_{\kappa'} a_{\kappa'}^{\dagger} \right) | 0 \rangle \quad (1)$$

$$= v^{\alpha\beta\gamma\delta} \langle 0 | \left(\prod_{\kappa} a_{\kappa} \right) \left(a_{\alpha}^{\dagger} a_{\beta}^{\dagger} a_{\gamma} a_{\delta} \left(a_1^{\dagger} a_1 - a_1 a_1^{\dagger} \right) \right) \left(\prod_{\kappa'} a_{\kappa'}^{\dagger} \right) | 0 \rangle \quad (2)$$

$$= v^{\alpha\beta\gamma\delta} \langle 0 | \left(\prod_{\kappa} a_{\kappa} \right) \left(a_{\alpha}^{\dagger} a_{\beta}^{\dagger} a_{\gamma} \delta_{\delta 1} a_1 - a_{\alpha}^{\dagger} a_{\beta}^{\dagger} a_{\gamma} a_1^{\dagger} a_{\delta} a_1 \right) \left(\prod_{\kappa'} a_{\kappa'}^{\dagger} \right) | 0 \rangle \quad (3)$$

$$\begin{aligned}
&= v^{\alpha\beta\gamma\delta} \langle 0 | \left(\prod_{\kappa} a_{\kappa} \right) \left(\delta_{\delta 1} a_{\alpha}^{\dagger} a_{\beta}^{\dagger} a_{\gamma} \left(a_2^{\dagger} a_2 - a_2 a_2^{\dagger} \right) a_1 \right. \\
&\quad \left. - a_{\alpha}^{\dagger} a_{\beta}^{\dagger} \delta_{\gamma 1} a_{\delta} a_1 + a_{\alpha}^{\dagger} a_{\beta}^{\dagger} a_1^{\dagger} a_{\gamma} a_{\delta} a_1 \right) \left(\prod_{\kappa'} a_{\kappa'}^{\dagger} \right) | 0 \rangle
\end{aligned} \tag{4}$$

$$\begin{aligned}
&= v^{\alpha\beta\gamma\delta} \langle 0 | \left(\prod_{\kappa} a_{\kappa} \right) \left(\delta_{\delta 1} a_{\alpha}^{\dagger} a_{\beta}^{\dagger} \delta_{\gamma 2} a_2 a_1 - \delta_{\delta 1} a_2^{\dagger} a_{\alpha}^{\dagger} a_{\beta}^{\dagger} a_{\gamma} a_2 a_1 \right. \\
&\quad \left. - \delta_{\gamma 1} a_{\alpha}^{\dagger} a_{\beta}^{\dagger} a_{\delta} \left(a_2^{\dagger} a_2 - a_2 a_2^{\dagger} \right) a_1 \right. \\
&\quad \left. + a_1^{\dagger} a_{\alpha}^{\dagger} a_{\beta}^{\dagger} a_{\gamma} a_{\delta} a_1 \right) \left(\prod_{\kappa'} a_{\kappa'}^{\dagger} \right) | 0 \rangle
\end{aligned} \tag{5}$$

$$\begin{aligned}
&= v^{\alpha\beta\gamma\delta} \langle 0 | \left(\prod_{\kappa} a_{\kappa} \right) \left(\delta_{\delta 1} \delta_{\gamma 2} a_{\alpha}^{\dagger} a_{\beta}^{\dagger} a_2 a_1 - \delta_{\gamma 1} a_{\alpha}^{\dagger} a_{\beta}^{\dagger} \delta_{\delta 2} a_2 a_1 \right. \\
&\quad \left. + \delta_{\gamma 1} a_{\alpha}^{\dagger} a_{\beta}^{\dagger} a_2^{\dagger} a_{\delta} a_2 a_1 + a_1^{\dagger} a_{\alpha}^{\dagger} a_{\beta}^{\dagger} a_{\gamma} a_{\delta} a_1 \right) \left(\prod_{\kappa'} a_{\kappa'}^{\dagger} \right) | 0 \rangle
\end{aligned} \tag{6}$$

$$\begin{aligned}
&= v^{\alpha\beta\gamma\delta} (\delta_{\delta 1} \delta_{\gamma 2} \delta_{\beta 2} \delta_{\alpha 1} - \delta_{\gamma 1} \delta_{\delta 2} \delta_{\beta 2} \delta_{\alpha 1}) \langle 0 | \left(\prod_{\kappa} a_{\kappa} \right) \left(\prod_{\kappa'} a_{\kappa'}^{\dagger} \right) | 0 \rangle \\
&\quad + v^{\alpha\beta\gamma\delta} \langle 0 | \left(\prod_{\kappa} a_{\kappa} \right) \left(-\delta_{\delta 1} a_2^{\dagger} a_{\alpha}^{\dagger} a_{\beta}^{\dagger} a_{\gamma} a_2 a_1 \right. \\
&\quad \left. + \delta_{\gamma 1} a_2^{\dagger} a_{\alpha}^{\dagger} a_{\beta}^{\dagger} a_{\delta} a_2 a_1 \right) \left(\prod_{\kappa'} a_{\kappa'}^{\dagger} \right) | 0 \rangle \\
&\quad + v^{\alpha\beta\gamma\delta} \langle 0 | \left(\prod_{\kappa=(n \dots 2)} a_{\kappa} \right) \left(a_{\alpha}^{\dagger} a_{\beta}^{\dagger} a_{\gamma} a_{\delta} \right) \left(\prod_{\kappa'=(2 \dots n)} a_{\kappa'}^{\dagger} \right) | 0 \rangle
\end{aligned} \tag{7}$$

$$= \sum_{\kappa_1, \kappa_2} (v^{\kappa_1 \kappa_2 \kappa_2 \kappa_1} - v^{\kappa_1 \kappa_2 \kappa_1 \kappa_2}) \tag{8}$$

+(these two terms same except for greek delta and gamma switch places, so can I cancel?)
 +(I notice the recursive pattern here, but I'm not sure what it means.)