

FCI Questions

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

$$= v^{\alpha\beta\gamma\delta} \langle 0 | \left(\prod_{\kappa} a_{\kappa} \right) \left(a_{\alpha}^{\dagger} a_{\beta}^{\dagger} a_{\gamma} \delta_{\delta 1} a_1 - a_{\alpha}^{\dagger} a_{\beta}^{\dagger} a_{\gamma} a_1^{\dagger} a_{\delta} a_1 \right) \left(\prod_{\kappa'} a_{\kappa'}^{\dagger} \right) | 0 \rangle \quad (2)$$

$$= v^{\alpha\beta\gamma\delta} \langle 0 | \left(\prod_{\kappa} a_{\kappa} \right) \left(\delta_{\delta 1} a_{\alpha}^{\dagger} a_{\beta}^{\dagger} a_{\gamma} \left(a_2^{\dagger} a_2 - a_2 a_2^{\dagger} \right) a_1 - a_{\alpha}^{\dagger} a_{\beta}^{\dagger} \delta_{\gamma 1} a_{\delta} a_1 \right. \\ \left. + a_{\alpha}^{\dagger} a_{\beta}^{\dagger} a_1^{\dagger} a_{\gamma} a_{\delta} a_1 \right) \left(\prod_{\kappa'} a_{\kappa'}^{\dagger} \right) | 0 \rangle \quad (3)$$

$$= v^{\alpha\beta\gamma\delta} \langle 0 | \left(\prod_{\kappa} a_{\kappa} \right) \left(\delta_{\delta 1} a_{\alpha}^{\dagger} a_{\beta}^{\dagger} \delta_{\gamma 2} a_2 a_1 - \delta_{\delta 1} a_2^{\dagger} a_{\alpha}^{\dagger} a_{\beta}^{\dagger} a_{\gamma} a_2 a_1 \right. \\ \left. - \delta_{\gamma 1} a_{\alpha}^{\dagger} a_{\beta}^{\dagger} a_{\delta} \left(a_2^{\dagger} a_2 - a_2 a_2^{\dagger} \right) a_1 + a_1^{\dagger} a_{\alpha}^{\dagger} a_{\beta}^{\dagger} a_{\gamma} a_{\delta} a_1 \right) \left(\prod_{\kappa'} a_{\kappa'}^{\dagger} \right) | 0 \rangle \quad (4)$$

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

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

$$\begin{aligned}
&= (v^{\kappa_1 \kappa_2 \kappa_2 \kappa_1} - v^{\kappa_1 \kappa_2 \kappa_1 \kappa_2}) \\
&+ v^{\alpha\beta\gamma\delta} \langle 0 | \left(\prod_{\kappa=(\kappa_n \dots \kappa_1)} a_{\kappa} \right) \left(\delta_{\gamma 1} a_2^{\dagger} a_{\alpha}^{\dagger} a_{\beta}^{\dagger} a_{\delta} a_2 a_1 \right. \\
&\quad \left. - \delta_{\delta 1} a_2 a_1 a_2^{\dagger} a_{\alpha}^{\dagger} a_{\beta}^{\dagger} a_{\gamma} a_2 a_1 \right) \left(\prod_{\kappa'=(\kappa_1 \dots \kappa_n)} a_{\kappa'}^{\dagger} \right) | 0 \rangle + \langle \Psi a_1^{\dagger} | V | a_1 \Psi \rangle
\end{aligned} \tag{7}$$

$$\begin{aligned}
&\langle 0 | \left(\prod_{\kappa=(\kappa_n \dots \kappa_3)} a_{\kappa} \right) \left(\delta_{\gamma 1} a_2 a_1 a_2^{\dagger} a_{\alpha}^{\dagger} a_{\beta}^{\dagger} a_{\delta} a_2 a_1 \right. \\
&\quad \left. - \delta_{\delta 1} a_2 a_1 a_2^{\dagger} a_{\alpha}^{\dagger} a_{\beta}^{\dagger} a_{\gamma} a_2 a_1 \right) \left(\prod_{\kappa'=(\kappa_3 \dots \kappa_n)} a_{\kappa'}^{\dagger} \right) | 0 \rangle \\
&= \langle 0 | \left(\prod_{\kappa=(\kappa_n \dots \kappa_3)} a_{\kappa} \right) \left(\delta_{\delta 1} a_1 a_{\alpha}^{\dagger} a_{\beta}^{\dagger} a_{\gamma} a_2 a_1 \right. \\
&\quad \left. - \delta_{\gamma 1} a_1 a_{\alpha}^{\dagger} a_{\beta}^{\dagger} a_{\delta} a_2 a_1 \right) \left(\prod_{\kappa'=(\kappa_3 \dots \kappa_n)} a_{\kappa'}^{\dagger} \right) | 0 \rangle
\end{aligned} \tag{8}$$

not sure where to go from here.

$$\begin{aligned}
&= \delta_{\delta\kappa_1} \delta_{\gamma\kappa_2} \delta_{\beta\kappa_2} \delta_{\alpha\kappa_1} \\
&\quad + \langle 0 | \left(\prod_{\kappa=(\kappa_n \dots \kappa_3)} a_\kappa \right) \delta_{\alpha\kappa_1} a_\beta^\dagger a_\gamma \left(\prod_{\kappa'=(\kappa_3 \dots \kappa_n)} a_{\kappa'}^\dagger \right) | 0 \rangle \\
&\quad - \langle 0 | \left(\prod_{\kappa=(\kappa_n \dots \kappa_3)} a_\kappa \right) a_\alpha^\dagger a_{\kappa_1} a_\beta^\dagger a_\gamma \left(\prod_{\kappa'=(\kappa_3 \dots \kappa_n)} a_{\kappa'}^\dagger \right) | 0 \rangle \\
&\quad \quad - \delta_{\gamma\kappa_1} \delta_{\delta\kappa_2} \delta_{\beta\kappa_2} \delta_{\alpha\kappa_1} \\
&\quad + \langle 0 | \left(\prod_{\kappa=(\kappa_n \dots \kappa_3)} a_\kappa \right) \delta_{\delta\kappa_2} \delta_{\alpha\kappa_2} a_\beta^\dagger a_\gamma \left(\prod_{\kappa'=(\kappa_3 \dots \kappa_n)} a_{\kappa'}^\dagger \right) | 0 \rangle \\
&\quad - \langle 0 | \left(\prod_{\kappa=(\kappa_n \dots \kappa_3)} a_\kappa \right) \delta_{\delta\kappa_2} a_\alpha^\dagger a_{\kappa_2} a_\beta^\dagger a_\gamma \left(\prod_{\kappa'=(\kappa_3 \dots \kappa_n)} a_{\kappa'}^\dagger \right) | 0 \rangle \\
&\quad \quad - \langle 0 | \left(\prod_{\kappa=(\kappa_n \dots \kappa_2)} a_\kappa \right) a_\alpha^\dagger a_\beta^\dagger \left(\prod_{\kappa'=(\kappa \dots \kappa_n)} a_{\kappa'}^\dagger \right) | 0 \rangle \quad (9)
\end{aligned}$$

$$\begin{aligned}
& - \langle 0 | \left(\prod_{\kappa=(\kappa_n \dots \kappa_3)} a_\kappa \right) \delta_{\gamma\kappa_1} \delta_{\alpha\kappa_1} a_\beta^\dagger a_\delta \left(\prod_{\kappa'=(\kappa_3 \dots \kappa_n)} a_{\kappa'}^\dagger \right) | 0 \rangle \\
& + \langle 0 | \left(\prod_{\kappa=(\kappa_n \dots \kappa_3)} a_\kappa \right) \delta_{\gamma\kappa_1} a_\alpha^\dagger a_{\kappa_1} a_\beta^\dagger a_\delta \left(\prod_{\kappa'=(\kappa_3 \dots \kappa_n)} a_{\kappa'}^\dagger \right) | 0 \rangle \\
& + \langle 0 | \left(\prod_{\kappa=(\kappa_n \dots \kappa_3)} a_\kappa \right) \delta_{\delta\kappa_2} \delta_{\alpha\kappa_2} a_\beta^\dagger a_\gamma \left(\prod_{\kappa'=(\kappa_3 \dots \kappa_n)} a_{\kappa'}^\dagger \right) | 0 \rangle \\
& - \langle 0 | \left(\prod_{\kappa=(\kappa_n \dots \kappa_3)} a_\kappa \right) \delta_{\delta\kappa_2} a_\alpha^\dagger a_{\kappa_2} a_\beta^\dagger a_\gamma \left(\prod_{\kappa'=(\kappa_3 \dots \kappa_n)} a_{\kappa'}^\dagger \right) | 0 \rangle \\
& + \langle 0 | \left(\prod_{\kappa=(\kappa_n \dots \kappa_3)} a_\kappa \right) \delta_{\gamma\kappa_2} \delta_{\alpha\kappa_2} a_\beta^\dagger a_\delta \left(\prod_{\kappa'=(\kappa_3 \dots \kappa_n)} a_{\kappa'}^\dagger \right) | 0 \rangle \text{ here} \\
& - \langle 0 | \left(\prod_{\kappa=(\kappa_n \dots \kappa_3)} a_\kappa \right) a_\alpha^\dagger a_{\kappa_2} a_\beta^\dagger a_\delta \left(\prod_{\kappa'=(\kappa_3 \dots \kappa_n)} a_{\kappa'}^\dagger \right) | 0 \rangle \\
& - \langle 0 | \left(\prod_{\kappa=(\kappa_n \dots \kappa_3)} a_\kappa \right) a_\alpha^\dagger a_\beta^\dagger a_\gamma a_\delta \left(\prod_{\kappa'=(\kappa_3 \dots \kappa_n)} a_{\kappa'}^\dagger \right) | 0 \rangle \text{ simp} \quad (10)
\end{aligned}$$

=

$$\begin{aligned}
& \delta_{\delta\kappa_1} \delta_{\gamma\kappa_2} \delta_{\beta\kappa_2} \delta_{\alpha\kappa_1} \\
& - \delta_{\gamma\kappa_1} \delta_{\delta\kappa_2} \delta_{\beta\kappa_2} \delta_{\alpha\kappa_1} \\
& - \langle 0 | \left(\prod_{\kappa=(\kappa_n \dots \kappa_3)} a_\kappa \right) \delta_{\gamma\kappa_1} \delta_{\alpha\kappa_1} a_\beta^\dagger a_\delta \left(\prod_{\kappa'=(\kappa_3 \dots \kappa_n)} a_{\kappa'}^\dagger \right) | 0 \rangle \\
& + \langle 0 | \left(\prod_{\kappa=(\kappa_n \dots \kappa_3)} a_\kappa \right) \delta_{\gamma\kappa_1} a_\alpha^\dagger \delta_{\beta\kappa_1} a_\delta \left(\prod_{\kappa'=(\kappa_3 \dots \kappa_n)} a_{\kappa'}^\dagger \right) | 0 \rangle \\
& - \langle 0 | \left(\prod_{\kappa=(\kappa_n \dots \kappa_3)} a_\kappa \right) \delta_{\gamma\kappa_1} a_\alpha^\dagger a_\beta^\dagger a_{\kappa_1} a_\delta \left(\prod_{\kappa'=(\kappa_3 \dots \kappa_n)} a_{\kappa'}^\dagger \right) | 0 \rangle \\
& + \langle 0 | \left(\prod_{\kappa=(\kappa_n \dots \kappa_3)} a_\kappa \right) \delta_{\delta\kappa_2} \delta_{\alpha\kappa_2} a_\beta^\dagger a_\gamma \left(\prod_{\kappa'=(\kappa_3 \dots \kappa_n)} a_{\kappa'}^\dagger \right) | 0 \rangle \\
& - \langle 0 | \left(\prod_{\kappa=(\kappa_n \dots \kappa_3)} a_\kappa \right) \delta_{\delta\kappa_2} a_\alpha^\dagger \delta_{\beta\kappa_2} a_\gamma \left(\prod_{\kappa'=(\kappa_3 \dots \kappa_n)} a_{\kappa'}^\dagger \right) | 0 \rangle \\
& + \langle 0 | \left(\prod_{\kappa=(\kappa_n \dots \kappa_3)} a_\kappa \right) \delta_{\delta\kappa_1} a_\alpha^\dagger a_\beta^\dagger a_{\kappa_2} a_\gamma \left(\prod_{\kappa'=(\kappa_3 \dots \kappa_n)} a_{\kappa'}^\dagger \right) | 0 \rangle \\
& + \langle 0 | \left(\prod_{\kappa=(\kappa_n \dots \kappa_3)} a_\kappa \right) \delta_{\gamma\kappa_2} \delta_{\alpha\kappa_2} a_\beta^\dagger a_\delta \left(\prod_{\kappa'=(\kappa_3 \dots \kappa_n)} a_{\kappa'}^\dagger \right) | 0 \rangle \\
& - \langle 0 | \left(\prod_{\kappa=(\kappa_n \dots \kappa_3)} a_\kappa \right) a_\alpha^\dagger \delta_{\beta\kappa_2} a_\delta \left(\prod_{\kappa'=(\kappa_3 \dots \kappa_n)} a_{\kappa'}^\dagger \right) | 0 \rangle \\
& + \langle 0 | \left(\prod_{\kappa=(\kappa_n \dots \kappa_3)} a_\kappa \right) a_\alpha^\dagger a_\beta^\dagger a_{\kappa_2} a_\delta \left(\prod_{\kappa'=(\kappa_3 \dots \kappa_n)} a_{\kappa'}^\dagger \right) | 0 \rangle \\
& \langle \Psi a_{\kappa_1}^\dagger | V | a_{\kappa_1} \Psi \rangle si \quad (11)
\end{aligned}$$

=

$$\begin{aligned}
& \delta_{\delta\kappa_1} \delta_{\gamma\kappa_2} \delta_{\beta\kappa_2} \delta_{\alpha\kappa_1} \\
& - \delta_{\gamma\kappa_1} \delta_{\delta\kappa_2} \delta_{\beta\kappa_2} \delta_{\alpha\kappa_1} \\
& + \delta_{\gamma\kappa_1} \delta_{\beta\kappa_1} \langle 0 | \left(\prod_{\kappa=(\kappa_n \dots \kappa_3)} a_\kappa \right) a_\alpha^\dagger a_\delta \left(\prod_{\kappa'=(\kappa_3 \dots \kappa_n)} a_{\kappa'}^\dagger \right) | 0 \rangle \\
& - \delta_{\gamma\kappa_1} \delta_{\alpha\kappa_1} \langle 0 | \left(\prod_{\kappa=(\kappa_n \dots \kappa_3)} a_\kappa \right) a_\beta^\dagger a_\delta \left(\prod_{\kappa'=(\kappa_3 \dots \kappa_n)} a_{\kappa'}^\dagger \right) | 0 \rangle \\
& - 0 \\
& + \delta_{\delta\kappa_1} \delta_{\alpha\kappa_2} \langle 0 | \left(\prod_{\kappa=(\kappa_n \dots \kappa_3)} a_\kappa \right) a_\beta^\dagger a_\gamma \left(\prod_{\kappa'=(\kappa_3 \dots \kappa_n)} a_{\kappa'}^\dagger \right) | 0 \rangle \\
& - \delta_{\delta\kappa_1} \delta_{\beta\kappa_2} \langle 0 | \left(\prod_{\kappa=(\kappa_n \dots \kappa_3)} a_\kappa \right) a_\alpha^\dagger a_\gamma \left(\prod_{\kappa'=(\kappa_3 \dots \kappa_n)} a_{\kappa'}^\dagger \right) | 0 \rangle \\
& + 0 \\
& + \langle \Psi a_{\kappa_1}^\dagger | V | a_{\kappa_1} \Psi \rangle
\end{aligned} \tag{12}$$

adding 2 electron int back in

$$= v^{\alpha\beta\gamma\delta}$$

$$\begin{aligned}
& (\delta_{\delta\kappa_1}\delta_{\gamma\kappa_2}\delta_{\beta\kappa_2}\delta_{\alpha\kappa_1} \\
& - \delta_{\gamma\kappa_1}\delta_{\delta\kappa_2}\delta_{\beta\kappa_2}\delta_{\alpha\kappa_1} \\
& + \delta_{\gamma\kappa_1}\delta_{\beta\kappa_1}\sum_{\kappa=3}\delta_{\alpha\kappa}\delta_{\delta\kappa} \\
& - \delta_{\gamma\kappa_1}\delta_{\alpha\kappa_1}\sum_{\kappa=3}\delta_{\beta\kappa}\delta_{\delta\kappa} \\
& + \delta_{\delta\kappa_1}\delta_{\alpha\kappa_2}\sum_{\kappa=3}\delta_{\beta\kappa}\delta_{\gamma\kappa} \\
& - \delta_{\delta\kappa_1}\delta_{\beta\kappa_2}\sum_{\kappa=3}\delta_{\alpha\kappa}\delta_{\gamma\kappa}) \\
& + \langle \Psi a_{\kappa_1}^\dagger | V | a_{\kappa_1} \Psi \rangle
\end{aligned} \tag{13}$$

$$\begin{aligned}
& = v^{\kappa_1\kappa_2\kappa_2\kappa_1} - v^{\kappa_1\kappa_2\kappa_1\kappa_2} \\
& + v^{\alpha\kappa_1\kappa_1\delta}\sum_{\tau=3}\delta_{\alpha\tau}\delta_{\delta\tau} - v^{\kappa_1\beta\kappa_1\delta}\sum_{\tau=3}\delta_{\beta\tau}\delta_{\delta\tau} + v^{\kappa_2\beta\gamma\kappa_1}\sum_{\tau=3}\delta_{\beta\tau}\delta_{\gamma\tau} - v^{\alpha\kappa_2\gamma\kappa_1}\sum_{\tau=3}\delta_{\alpha\tau}\delta_{\gamma\tau} \\
& + \langle \Psi a_{\kappa_1}^\dagger | V | a_{\kappa_1} \Psi \rangle
\end{aligned} \tag{14}$$

$$\kappa_* = \kappa + 1$$

$$\begin{aligned}
& = \sum_{\kappa=1}^{N-2} (v^{\kappa\kappa_*\kappa_*\kappa} - v^{\kappa\kappa_*\kappa\kappa_*} + \sum_{\tau=3} v^{\tau\kappa\kappa\tau} - \sum_{\tau=3} v^{\kappa\tau\kappa\tau} + \sum_{\tau=3} v^{\kappa_*\tau\tau\kappa} - \sum_{\tau=3} v^{\tau\kappa_*\tau\kappa}) \\
& + \left\langle \Psi \left(\prod_{\kappa'=(\kappa_1\ldots\kappa_{N-1})} a_{\kappa'}^\dagger \right) | 0 \right\rangle \left| V \right| \left\langle 0 \right| \left(\prod_{\kappa=(\kappa_{N-1}\ldots\kappa_1)} a_{\kappa} \right) \Psi \right\rangle
\end{aligned} \tag{15}$$

$$\begin{aligned}
& = \sum_{\kappa=1}^{N-2} (v^{\kappa\kappa_*\kappa_*\kappa} - v^{\kappa\kappa_*\kappa\kappa_*} + \sum_{\tau=3} v^{\tau\kappa\kappa\tau} - \sum_{\tau=3} v^{\kappa\tau\kappa\tau} + \sum_{\tau=3} v^{\kappa_*\tau\tau\kappa} - \sum_{\tau=3} v^{\tau\kappa_*\tau\kappa}) \\
& + 0
\end{aligned} \tag{16}$$

begone to do derivation, but I am only getting some double summations and I am kind of lost as to how I would implement this into my program. this derivation does suggest some ways to use the einstein summation convention, so that part is improved from what I had earlier in my program.