FCI Questions

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

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

$$\begin{aligned} = v^{\alpha\beta\gamma\delta} \langle 0| \left(\prod_{\kappa} a_{\kappa}\right) \Big(&\delta_{\delta 1} a_{\alpha}^{\dagger} a_{\beta}^{\dagger} a_{\gamma} \left(a_2^{\dagger} a_2 - a_2 a_2^{\dagger}\right) a_1 - a_{\alpha}^{\dagger} a_{\beta}^{\dagger} \delta_{\gamma 1} a_{\delta} a_1 \\ &+ a_{\alpha}^{\dagger} a_{\beta}^{\dagger} a_1^{\dagger} a_{\gamma} a_{\delta} a_1\Big) \left(\prod_{\kappa'} a_{\kappa'}^{\dagger}\right) |0\rangle \end{aligned} \tag{3}$$

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

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

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

$$
\begin{aligned}
&= \left(v^{\kappa_1\kappa_2\kappa_2\kappa_1} - v^{\kappa_1\kappa_2\kappa_1\kappa_2}\right) \\
&\quad + v^{\alpha\beta\gamma\delta}\langle 0|\left(\prod_{\kappa=(\kappa_n\ldots\kappa_1)} a_{\kappa}\right)\Big(\delta_{\gamma 1} a^{\dagger}_{2} a^{\dagger}_{\alpha} a^{\dagger}_{\beta} a_{\delta} a_{2} a_{1} \\
&\quad - \delta_{\delta 1} a_{2} a_{1} a^{\dagger}_{2} a^{\dagger}_{\alpha} a^{\dagger}_{\beta} a_{\gamma} a_{2} a_{1}\Big)\left(\prod_{\kappa'=(\kappa_1\ldots\kappa_n)} a^{\dagger}_{\kappa'}\right)|0\rangle + \left\langle \Psi a^{\dagger}_{1}\middle| V \middle| a_{1}\Psi\right\rangle
\end{aligned} \tag{7}
$$

$$
\begin{aligned}
&\langle 0|\left(\prod_{\kappa=(\kappa_n\ldots\kappa_3)} a_{\kappa}\right)\Big(\delta_{\gamma 1} a_{2} a_{1} a^{\dagger}_{2} a^{\dagger}_{\alpha} a^{\dagger}_{\beta} a_{\delta} a_{2} a_{1} \\
&\quad - \delta_{\delta 1} a_{2} a_{1} a^{\dagger}_{2} a^{\dagger}_{\alpha} a^{\dagger}_{\beta} a_{\gamma} a_{2} a_{1}\Big)\left(\prod_{\kappa'=(\kappa_3\ldots\kappa_n)} a^{\dagger}_{\kappa'}\right)|0\rangle \\
&\quad = \langle 0|\left(\prod_{\kappa=(\kappa_n\ldots\kappa_3)} a_{\kappa}\right)\Big(\delta_{\delta 1} a_{1} a^{\dagger}_{\alpha} a^{\dagger}_{\beta} a_{\gamma} a_{2} a_{1} \\
&\qquad - \delta_{\gamma 1} a_{1} a^{\dagger}_{\alpha} a^{\dagger}_{\beta} a_{\delta} a_{2} a_{1}\Big)\left(\prod_{\kappa'=(\kappa_3\ldots\kappa_n)} a^{\dagger}_{\kappa'}\right)|0\rangle
\end{aligned} \tag{8}
$$

not sure where to go from here.

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

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

$$=$$

$$\delta_{\delta\kappa_1}\delta_{\gamma\kappa_2}\delta_{\beta\kappa_2}\delta_{\alpha\kappa_1}$$

$$-\,\delta_{\gamma\kappa_1}\delta_{\delta\kappa_2}\delta_{\beta\kappa_2}\delta_{\alpha\kappa_1}$$

$$-\left\langle 0\right|\left(\prod_{\kappa=(\kappa_n\ldots\kappa_3)} a_\kappa\right)\delta_{\gamma\kappa_1}\delta_{\alpha\kappa_1}a^\dagger_\beta a_\delta\left(\prod_{\kappa'=(\kappa_3\ldots\kappa_n)} a^\dagger_{\kappa'}\right)\left|0\right\rangle$$

$$+\left\langle 0\right|\left(\prod_{\kappa=(\kappa_n\ldots\kappa_{30})} a_\kappa\right)\delta_{\gamma\kappa_1}a^\dagger_\alpha\delta_{\beta\kappa_1}a_\delta\left(\prod_{\kappa'=(\kappa_3\ldots\kappa_n)} a^\dagger_{\kappa'}\right)\left|0\right\rangle$$

$$-\left\langle 0\right|\left(\prod_{\kappa=(\kappa_n\ldots\kappa_3)} a_\kappa\right)\delta_{\gamma\kappa_1}a^\dagger_\alpha a^\dagger_\beta a_{\kappa_1}a_\delta\left(\prod_{\kappa'=(\kappa_3\ldots\kappa_n)} a^\dagger_{\kappa'}\right)\left|0\right\rangle$$

$$+\left\langle 0\right|\left(\prod_{\kappa=(\kappa_n\ldots\kappa_3)} a_\kappa\right)\delta_{\delta\kappa_2}\delta_{\alpha\kappa_2}a^\dagger_\beta a_\gamma\left(\prod_{\kappa'=(\kappa_3\ldots\kappa_n)} a^\dagger_{\kappa'}\right)\left|0\right\rangle$$

$$-\left\langle 0\right|\left(\prod_{\kappa=(\kappa_n\ldots\kappa_3)} a_\kappa\right)\delta_{\delta\kappa_2}a^\dagger_\alpha\delta_{\beta\kappa_2}a_\gamma\left(\prod_{\kappa'=(\kappa_3\ldots\kappa_n)} a^\dagger_{\kappa'}\right)\left|0\right\rangle$$

$$+\left\langle 0\right|\left(\prod_{\kappa=(\kappa_n\ldots\kappa_3)} a_\kappa\right)\delta_{\delta\kappa_1}a^\dagger_\alpha a^\dagger_\beta a_{\kappa_2}a_\gamma\left(\prod_{\kappa'=(\kappa_3\ldots\kappa_n)} a^\dagger_{\kappa'}\right)\left|0\right\rangle$$

$$+\left\langle 0\right|\left(\prod_{\kappa=(\kappa_n\ldots\kappa_3)} a_\kappa\right)\delta_{\gamma\kappa_2}\delta_{\alpha\kappa_2}a^\dagger_\beta a_\delta\left(\prod_{\kappa'=(\kappa_3\ldots\kappa_n)} a^\dagger_{\kappa'}\right)\left|0\right\rangle$$

$$-\left\langle 0\right|\left(\prod_{\kappa=(\kappa_n\ldots\kappa_3)} a_\kappa\right)a^\dagger_\alpha\delta_{\beta\kappa_2}a_\delta\left(\prod_{\kappa'=(\kappa_3\ldots\kappa_n)} a^\dagger_{\kappa'}\right)\left|0\right\rangle$$

$$+\left\langle 0\right|\left(\prod_{\kappa=(\kappa_n\ldots\kappa_3)} a_\kappa\right)a^\dagger_\alpha a^\dagger_\beta a_{\kappa_2}a_\delta\left(\prod_{\kappa'=(\kappa_3\ldots\kappa_n)} a^\dagger_{\kappa'}\right)\left|0\right\rangle$$

$$\left\langle \Psi a^\dagger_{\kappa_1}\middle| V \middle| a_{\kappa_1}\Psi\right\rangle si \quad (11)$$

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

adding 2 electron int back in

$$
\begin{aligned}
&= v^{\alpha\beta\gamma\delta} \\
&\qquad (\delta_{\delta\kappa_1}\delta_{\gamma\kappa_2}\delta_{\beta\kappa_2}\delta_{\alpha\kappa_1} \\
&\qquad - \delta_{\gamma\kappa_1}\delta_{\delta\kappa_2}\delta_{\beta\kappa_2}\delta_{\alpha\kappa_1} \\
&\qquad + \delta_{\gamma\kappa_1}\delta_{\beta\kappa_1}\sum_{\kappa=3}\delta_{\alpha\kappa}\delta_{\delta\kappa} \\
&\qquad - \delta_{\gamma\kappa_1}\delta_{\alpha\kappa_1}\sum_{\kappa=3}\delta_{\beta\kappa}\delta_{\delta\kappa} \\
&\qquad + \delta_{\delta\kappa_1}\delta_{\alpha\kappa_2}\sum_{\kappa=3}\delta_{\beta\kappa}\delta_{\gamma\kappa} \\
&\qquad - \delta_{\delta\kappa_1}\delta_{\beta\kappa 2}\sum_{\kappa=3}\delta_{\alpha\kappa}\delta_{\gamma\kappa}) \\
&\qquad + \left\langle \Psi a^{\dagger}_{\kappa_1} \middle| V \middle| a_{\kappa_1}\Psi \right\rangle
\end{aligned} \tag{13}
$$

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

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

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

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

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.