FCI Questions

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1. 2 determinants with no differences

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

$$= v^{\alpha\beta\gamma\delta}\langle 0|\left(\sum_{\kappa} a_{\kappa}\right)\left(a_{\alpha}^{\dagger}a_{\beta}^{\dagger}a_{\gamma}\delta_{\delta\kappa_1}a_{\kappa_1} - a_{\alpha}^{\dagger}a_{\beta}^{\dagger}a_{\gamma}a_{\kappa_1}^{\dagger}a_{\delta}\right)\left(\sum_{\kappa'} a_{\kappa'}^{\dagger}\right)|0\rangle \tag{2}$$

$$= v^{\alpha\beta\gamma\delta}\langle 0|\left(\sum_{\kappa} a_{\kappa}\right) a_{\alpha}^{\dagger}a_{\beta}^{\dagger}\delta_{\delta\kappa_1}\delta_{\gamma\kappa_2} \tag{3}$$

$$\begin{aligned} &= v^{\alpha\beta\gamma\delta}\langle 0|\left(\prod_{\kappa} a_{\kappa}\right) a_{\alpha}^{\dagger}a_{\beta}^{\dagger}a_{\gamma}\delta_{\delta\kappa_1}\left(\prod_{\kappa'=(\kappa_2\ldots\kappa_n)} a_{\kappa'}^{\dagger}\right)|0\rangle \\ &\quad - v^{\alpha\beta\gamma\delta}\langle 0|\left(\prod_{\kappa} a_{\kappa}\right) a_{\alpha}^{\dagger}a_{\beta}^{\dagger}a_{\gamma}a_{\kappa_1}^{\dagger}a_{\delta}\left(\prod_{\kappa'=(\kappa_2\ldots\kappa_n)} a_{\kappa'}^{\dagger}\right)|0\rangle \end{aligned} \tag{4}$$

$$
\begin{aligned}
&= v^{\alpha\beta\gamma\delta}\delta_{\delta\kappa_1}\langle 0|\left(\prod_\kappa a_\kappa\right) a^\dagger_\alpha a^\dagger_\beta a_\gamma \left(\prod_{\kappa'=(\kappa_2\ldots\kappa_n)} a^\dagger_{\kappa'}\right)|0\rangle \\
&\quad - v^{\alpha\beta\gamma\delta}\langle 0|\left(\prod_\kappa a_\kappa\right)\Big(\delta_{\gamma\kappa_1} a^\dagger_\alpha a^\dagger_\beta a_\delta \\
&\qquad\qquad + a^\dagger_\alpha a^\dagger_\beta a^\dagger_{\kappa_1} a_\gamma a_\delta\Big)\left(\prod_{\kappa'=(\kappa_2\ldots\kappa_n)} a^\dagger_{\kappa'}\right)|0\rangle
\end{aligned}
\tag{5}
$$

$$
\begin{aligned}
&= v^{\alpha\beta\gamma\delta}\delta_{\delta\kappa_1}\delta_{\gamma\kappa_2}\langle 0|\left(\prod_\kappa a_\kappa\right) a^\dagger_\alpha a^\dagger_\beta \left(\prod_{\kappa'=(\kappa_3\ldots\kappa_n)} a^\dagger_{\kappa'}\right)|0\rangle \\
&\quad - v^{\alpha\beta\gamma\delta}\delta_{\delta\kappa_1}\langle 0|\left(\prod_\kappa a_\kappa\right) a^\dagger_\alpha a^\dagger_\beta a^\dagger_{\kappa_2} a_\gamma \left(\prod_{\kappa'=(\kappa_3\ldots\kappa_n)} a^\dagger_{\kappa'}\right)|0\rangle \\
&\quad - v^{\alpha\beta\gamma\delta}\langle 0|\left(\prod_\kappa a_\kappa\right) a^\dagger_\alpha a^\dagger_\beta a_\gamma a^\dagger_{\kappa'} a_\delta \left(\prod_{\kappa'=(\kappa_2\ldots\kappa_n)} a^\dagger_{\kappa'}\right)|0\rangle
\end{aligned}
\tag{6}
$$

$$
\begin{aligned}
&= \sum_{\kappa_1,\kappa_2} v^{\alpha\beta\gamma\delta}\delta_{\delta\kappa_1}\delta_{\gamma\kappa_2}\delta_{\beta\kappa_2}\delta_{\alpha\kappa_1} \\
&\quad - v^{\alpha\beta\gamma\delta}\delta_{\delta\kappa_1}\langle 0|\left(\prod_{\kappa=(\kappa_n\ldots\kappa_2)} a_\kappa\right) a_1 a^\dagger_\alpha a^\dagger_\beta a^\dagger_{\kappa_2} a_\gamma \left(\prod_{\kappa'=(\kappa_3\ldots\kappa_n)} a^\dagger_{\kappa'}\right)|0\rangle \\
&\quad - v^{\alpha\beta\gamma\delta}\langle 0|\left(\prod_\kappa a_\kappa\right) a^\dagger_\alpha a^\dagger_\beta a_\gamma a^\dagger_{\kappa'} a_\delta \left(\prod_{\kappa'=(\kappa_2\ldots\kappa_n)} a^\dagger_{\kappa'}\right)|0\rangle
\end{aligned}
\tag{7}
$$

$$
\begin{aligned}
&= \sum_{\kappa_1,\kappa_2} v^{\kappa_1\kappa_2\kappa_2\kappa_1} \\
&\quad -v^{\alpha\beta\gamma\delta}\delta_{\delta\kappa_1}\left\langle 0\right| \left(\prod_{\kappa=(\kappa_n\ldots\kappa_2)} a_\kappa\right) a_{\kappa_1}a^\dagger_{\kappa_2}a^\dagger_\alpha a^\dagger_\beta a_\gamma \left(\prod_{\kappa'=(\kappa_3\ldots\kappa_n)} a^\dagger_{\kappa'}\right)\left|0\right\rangle \\
&\quad - v^{\alpha\beta\gamma\delta}\left\langle 0\right| \left(\prod_{\kappa} a_\kappa\right) a^\dagger_\alpha a^\dagger_\beta a_\gamma a^\dagger_{\kappa'} a_\delta \left(\prod_{\kappa'=(\kappa_2\ldots\kappa_n)} a^\dagger_{\kappa'}\right)\left|0\right\rangle
\end{aligned}
\tag{8}
$$

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

$$
= v^{\alpha\beta\gamma\delta}\left\langle 0\right| \left(\sum_{\kappa} a_\kappa\right)\left(a^\dagger_\alpha a^\dagger_\beta a_\gamma \delta_{\delta\kappa_1} a_{\kappa_1} - a^\dagger_\alpha a^\dagger_\beta a_\gamma a^\dagger_{\kappa_1} a_\delta\right)\left(\sum_{\kappa'} a^\dagger_{\kappa'}\right)\left|0\right\rangle
\tag{10}
$$

$$
= v^{\alpha\beta\gamma\delta}\left\langle 0\right| \left(\sum_{\kappa} a_\kappa\right) a^\dagger_\alpha a^\dagger_\beta \delta_{\delta 1}\delta_{\gamma 2} a_1 a_2
\tag{11}
$$