FCI Questions

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April 17, 2023

1 one difference between two determinants

$$\langle\Psi|V|\Psi(k\to k')\rangle = v^{\alpha\beta\gamma\delta}\,(-1)^{\varepsilon\left(\kappa_1,\ldots,\kappa'_i,\ldots,\kappa_n\right)} \tag{1a}$$

$$\langle 0|\left(\prod_{\kappa=(\kappa_n\ldots\kappa_2)} a_\kappa\right) a_{\kappa_1} a^\dagger_\alpha a^\dagger_\beta a_\gamma a_\delta a^\dagger_{\kappa'_1}\left(\prod_{\kappa'=(\kappa_2\ldots\kappa_n)} a^\dagger_{\kappa'}\right)|0\rangle \tag{1b}$$

omitting into QUAL and face factor for now

$$\langle 0|\left(\prod_{\kappa=(\kappa_n\ldots\kappa_2)} a_\kappa\right) a_{\kappa_1} a^\dagger_\alpha a^\dagger_\beta a_\gamma \delta_{\delta\kappa'_1}\left(\prod_{\kappa'=(\kappa_2\ldots\kappa_n)} a^\dagger_{\kappa'}\right)|0\rangle \tag{2a}$$

$$-\langle 0|\left(\prod_{\kappa=(\kappa_n\ldots\kappa_2)} a_\kappa\right) a_{\kappa_1} a^\dagger_\alpha a^\dagger_\beta a_\gamma a^\dagger_{\kappa'_1} a_\delta\left(\prod_{\kappa'=(\kappa\ldots\kappa_n)} a^\dagger_{\kappa'}\right)|0\rangle \tag{2b}$$

$$=\langle 0|\left(\prod_{\kappa=(\kappa_n\ldots\kappa_2)} a_\kappa\right) \delta_{\delta\kappa'_1} a_{\kappa_1} a^\dagger_\alpha a^\dagger_\beta \delta_{\gamma\kappa_2}\left(\prod_{\kappa'=(\kappa_3\ldots\kappa_n)} a^\dagger_{\kappa'}\right)|0\rangle \tag{3aa}$$

$$-\langle 0|\left(\prod_{\kappa=(\kappa_n\ldots\kappa_2)} a_\kappa\right) \delta_{\delta\kappa'_1} a_{\kappa_1} a^\dagger_\alpha a^\dagger_\beta a^\dagger_{\kappa_2} a_\gamma\left(\prod_{\kappa'=(\kappa_3\ldots\kappa_n)} a^\dagger_{\kappa'}\right)|0\rangle \tag{3ab}$$

$$-\langle 0| \left(\prod_{\kappa=(\kappa_n \ldots \kappa_2)} a_\kappa \right) a_{\kappa_1} a^\dagger_\alpha a^\dagger_\beta \delta_{\gamma\kappa'_1} a_\delta \left(\prod_{\kappa'=(\kappa_2 \ldots \kappa_n)} a^\dagger_{\kappa'} \right) |0\rangle \tag{3ba}$$

$$+\langle 0| \left(\prod_{\kappa=(\kappa_n \ldots \kappa_2)} a_\kappa \right) a_{\kappa_1} a^\dagger_\alpha a^\dagger_\beta a^\dagger_{\kappa'_1} a_\gamma a_\delta \left(\prod_{\kappa'=(\kappa_2 \ldots \kappa_n)} a^\dagger_{\kappa'} \right) |0\rangle \tag{3bb}$$

$$=\langle 0| \left(\prod_{\kappa=(\kappa_n \ldots \kappa_2)} a_\kappa \right) \delta_{\delta\kappa'_1} \delta_{\gamma\kappa_2} \delta_{\alpha\kappa_1} a^\dagger_\beta \left(\prod_{\kappa'=(\kappa_3 \ldots \kappa_n)} a^\dagger_{\kappa'} \right) |0\rangle \tag{3aaa}$$

$$-\langle 0| \left(\prod_{\kappa=(\kappa_n \ldots \kappa_2)} a_\kappa \right) \delta_{\delta\kappa'_1} \delta_{\gamma\kappa_2} a^\dagger_\alpha a_{\kappa_1} a^\dagger_\beta \left(\prod_{\kappa'=(\kappa_3 \ldots \kappa_n)} a^\dagger_{\kappa'} \right) |0\rangle \tag{3aab}$$

$$+\langle 0| \left(\prod_{\kappa=(\kappa_n \ldots \kappa_3)} a_\kappa \right) \delta_{\delta\kappa'_1} a_{\kappa_1} a^\dagger_\alpha a^\dagger_\beta a_\gamma \left(\prod_{\kappa'=(\kappa_3 \ldots \kappa_n)} a^\dagger_{\kappa'} \right) |0\rangle \tag{3aba}$$

$$-\langle 0| \left(\prod_{\kappa=(\kappa_n \ldots \kappa_2)} a_\kappa \right) \delta_{\gamma\kappa'_1} \delta_{\alpha\kappa_1} a^\dagger_\beta a_\delta \left(\prod_{\kappa'=(\kappa_2 \ldots \kappa_n)} a^\dagger_{\kappa'} \right) |0\rangle \tag{3ca}$$

$$+\langle 0| \left(\prod_{\kappa=(\kappa_n \ldots \kappa_2)} a_\kappa \right) \delta_{\gamma\kappa'_1} a^\dagger_\alpha a_{\kappa_1} a^\dagger_\beta a_\delta \left(\prod_{\kappa'=(\kappa_2 \ldots \kappa_n)} a^\dagger_{\kappa'} \right) |0\rangle \tag{3cb}$$

$$+0 \tag{3da}$$

$$= \delta_{\delta\kappa'_1} \delta_{\gamma\kappa_2} \delta_{\alpha\kappa_1} \delta_{\beta\kappa_2} \tag{5aaa}$$

$$- \langle 0| \left(\prod_{\kappa=(\kappa_n \ldots \kappa_2)} a_\kappa \right) \delta_{\delta\kappa'_1} \delta_{\gamma\kappa_2} a^\dagger_\alpha \delta_{\beta\kappa_1} \left(\prod_{\kappa'=(\kappa_3 \ldots \kappa_n)} a^\dagger_{\kappa'} \right) |0\rangle \tag{5aab}$$

$$+ \langle 0| \left(\prod_{\kappa=(\kappa_n \ldots \kappa_3)} a_\kappa \right) \delta_{\delta\kappa'_1} \delta_{\rho\kappa_1} a^\dagger_\beta a_\gamma \left(\prod_{\kappa'=(\kappa \ldots \kappa_n)} a^\dagger_{\kappa'} \right) |0\rangle \tag{5aaca}$$

$$- \langle 0| \left(\prod_{\kappa=(\kappa_n \ldots \kappa_{30})} a_\kappa \right) \delta_{\delta\kappa'_1} a^\dagger_\alpha a_{\kappa_1} a^\dagger_\beta a_\gamma \left(\prod_{\kappa'=(\kappa_3 \ldots \kappa_n)} a^\dagger_{\kappa'} \right) |0\rangle \tag{5aacb}$$

$$-\delta_{\gamma\kappa'_1} \delta_{\alpha\kappa_1} \langle \Psi | a^\dagger_\beta a_\delta | \Psi \rangle \tag{5d}$$

$$+ \langle 0| \left(\prod_{\kappa=(\kappa_n \ldots \kappa_2)} a_\kappa \right) \delta_{\gamma\kappa'_1} a^\dagger_\alpha \delta_{\beta\kappa_1} a_\delta \left(\prod_{\kappa'=(\kappa \ldots \kappa_n)} a^\dagger_{\kappa'} \right) |0\rangle \tag{5ea}$$

$$-0 \tag{5eb}$$

$$= \delta_{\delta\kappa'_1} \delta_{\gamma\kappa_2} \delta_{\alpha\kappa_1} \delta_{\beta\kappa_2} \tag{6a}$$

$$-\delta_{\delta\kappa'_1} \delta_{\gamma\kappa_2} \delta_{\alpha\kappa_2} \delta_{\beta\kappa_1} \tag{6b}$$

$$+\delta_{\theta\kappa'_1} \delta_{\alpha\kappa_1} \langle \Psi | a^\dagger_\beta a_\gamma | \Psi \rangle \tag{6c}$$

$$- \langle 0| \left(\prod_{\kappa=(\kappa_n \ldots \kappa_3)} a_\kappa \right) \delta_{\delta\kappa'_1} a^\dagger_\alpha \delta_{\beta\kappa_1} a_\gamma \left(\prod_{\kappa'=(\kappa_3 \ldots \kappa_n)} a^\dagger_{\kappa'} \right) |0\rangle \tag{6da}$$

$$+0 \tag{6db}$$

$$-\delta_{\gamma\kappa_1'}\delta_{\alpha\kappa_1}\left\langle\Psi|a_\beta^\dagger a_\delta^\dagger|\Psi\right\rangle \tag{6e}$$

$$+\delta_{\gamma\kappa_1'}\delta_{\beta\kappa_1}\left\langle\Psi|a_\alpha^\dagger a_\delta|\Psi\right\rangle \tag{6f}$$

$$=\delta_{\delta\kappa_1'}\delta_{\gamma\kappa_2}\delta_{\alpha\kappa_1}\delta_{\beta\kappa_2} \tag{5a}$$

$$-\delta_{\delta\kappa_1'}\delta_{\gamma\kappa_2}\delta_{\alpha\kappa_2}\delta_{\beta\kappa_1} \tag{5b}$$

$$+\delta_{\theta\kappa_1'}\delta_{\alpha\kappa_1}\left\langle\Psi|a_\beta^\dagger a_\gamma|\Psi\right\rangle \tag{5c}$$

$$-\delta_{\delta\kappa_1'}\delta_{\beta\kappa_1}\left\langle\Psi|a_\alpha^\dagger a_\gamma|\Psi\right\rangle \tag{5da}$$

$$-\delta_{\gamma\kappa_1'}\delta_{\alpha\kappa_1}\left\langle\Psi|a_\beta^\dagger a_\delta^\dagger|\Psi\right\rangle \tag{5e}$$

$$+\delta_{\gamma\kappa_1'}\delta_{\beta\kappa_1}\left\langle\Psi|a_\alpha^\dagger a_\delta|\Psi\right\rangle \tag{5f}$$

introducing the ints, but not pf

$$=v^{1221'}-v^{2121'} \tag{5a}$$

$$+v^{1221'}-v^{2121'}-v^{121'2}+v^{211'2} \tag{5b}$$

$$=2(v^{1221'}-v^{2121'})-v^{121'2}+v^{211'2} \tag{6}$$

$$=(-1)^{\varepsilon\left(\kappa_1,\ldots,\kappa_i',\ldots,\kappa_n\right)}\left(2(v^{1221'}-v^{2121'})-v^{121'2}+v^{211'2}\right) \tag{7}$$