# FCI Questions

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## 1 0 differences between two determines

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

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

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

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

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

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

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

$$=\delta_{\alpha\kappa_1}\delta_{\beta\kappa_2}\delta_{\gamma\kappa_2}\delta_{\delta\kappa_1} \tag{3aa}$$

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

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

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

$$=\delta_{\alpha\kappa_1}\delta_{\beta\kappa_2}\delta_{\gamma\kappa_2}\delta_{\delta\kappa_1} \tag{3aa}$$

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

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

$$-\delta_{\alpha\kappa_1}\delta_{\beta\kappa_2}\delta_{\gamma\kappa_1}\delta_{\delta\kappa_2} \tag{3ca}$$

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

$$= \delta_{\alpha\kappa_1}\delta_{\beta\kappa_2}\delta_{\gamma\kappa_2}\delta_{\delta\kappa_1} \tag{4aa}$$

$$+\delta_{\delta\kappa_1}\delta_{\alpha\kappa_1}\langle 0|\left(\prod_{\kappa=(\kappa_n\ldots\kappa_3)} a_\kappa\right) a^\dagger_\beta a_\gamma \left(\prod_{\kappa'=(\kappa_3\ldots\kappa_n)} a^\dagger_{\kappa'}\right)|0\rangle \tag{4aba}$$

$$-\langle 0|\left(\prod_{\kappa=(\kappa_n\ldots\kappa_3)} a_\kappa\right) \delta_{\delta\kappa_1} a^\dagger_\alpha \delta_{\beta\kappa_1} a_\gamma \left(\prod_{\kappa'=(\kappa_3\ldots\kappa_n)} a^\dagger_{\kappa'}\right)|0\rangle \tag{4abba}$$

$$+\langle 0|\left(\prod_{\kappa=(\kappa_n\ldots\kappa_3)} a_\kappa\right) \delta_{\delta\kappa_1} a^\dagger_\alpha a_{\kappa_1} a^\dagger_\beta a_\gamma \left(\prod_{\kappa'=(\kappa_3\ldots\kappa_n)} a^\dagger_{\kappa'}\right)|0\rangle \tag{4abbb}$$

$$-\delta_{\alpha\kappa_1}\delta_{\beta\kappa_2}\delta_{\gamma\kappa_1}\delta_{\delta\kappa_2} \tag{4ca}$$

$$-\langle 0|\left(\prod_{\kappa=(\kappa_n\ldots\kappa_3)} a_\kappa\right) \delta_{\gamma\kappa_1}\delta_{\alpha\kappa_1} a^\dagger_\beta a_\gamma \left(\prod_{\kappa'=(\kappa_3\ldots\kappa_n)} a^\dagger_{\kappa'}\right)|0\rangle \tag{4cba}$$

$$+\langle 0|\left(\prod_{\kappa=(\kappa_n\ldots\kappa_3)} a_\kappa\right) \delta_{\gamma\kappa_1} a^\dagger_\alpha a_{\kappa_1} a^\dagger_\beta a_\gamma \left(\prod_{\kappa'=(\kappa_3\ldots\kappa_n)} a^\dagger_{\kappa'}\right)|0\rangle \tag{4cbb}$$

$$= \delta_{\alpha\kappa_1}\delta_{\beta\kappa_2}\delta_{\gamma\kappa_2}\delta_{\delta\kappa_1} \tag{3aa}$$

$$+\delta_{\alpha\kappa_1}\delta_{\delta\kappa_1}\langle\Psi|a^\dagger_{\kappa_1}a^\dagger_{\kappa_2}H_0 a_{\kappa_2}a_{\kappa_1}|\Psi\rangle \tag{3aba}$$

$$-\delta_{\beta\kappa_1}\delta_{\delta\kappa_1}\langle\Psi|a^\dagger_{\kappa_1}a^\dagger_2 H_0 a_2 a_1 a_{\kappa_2}|\Psi\rangle \tag{3abba}$$

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

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

$$-\delta_{\alpha\kappa_1}\delta_{\beta\kappa_2}\delta_{\gamma\kappa_1}\delta_{\delta\kappa_2} \tag{3c}$$

$$-\delta_{\gamma\kappa_1}\delta_{\alpha\kappa_1}\langle\Psi|a^\dagger_{\kappa_1}a^\dagger_{\kappa_2}H_0a_{\kappa_2}a_{\kappa_1}|\Psi\rangle \tag{3da}$$

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

$$-0 \tag{3dbb}$$

$$=\delta_{\alpha\kappa_1}\delta_{\beta\kappa_2}\delta_{\gamma\kappa_2}\delta_{\delta\kappa_1} \tag{3aa}$$

$$+\delta_{\alpha\kappa_1}\delta_{\delta\kappa_1}\langle\Psi|a^\dagger_{\kappa_1}a^\dagger_{\kappa_2}H_0a_{\kappa_2}a_{\kappa_1}|\Psi\rangle \tag{3aba}$$

$$-\delta_{\beta\kappa_1}\delta_{\delta\kappa_1}\langle\Psi|a^\dagger_{\kappa_1}a^\dagger_2H_0a_2a_1a_{\kappa_2}|\Psi\rangle \tag{3abba}$$

$$+\delta_{\beta\kappa_1}\delta_{\delta\kappa_1}\langle\Psi|a^\dagger_{\kappa_1}a^\dagger_{\kappa_2}H_0a_{\kappa_2}a_{\kappa_1}|\Psi\rangle \tag{3abbba}$$

$$-0 \tag{3abbbb}$$

$$-\delta_{\alpha\kappa_1}\delta_{\beta\kappa_2}\delta_{\gamma\kappa_1}\delta_{\delta\kappa_2} \tag{3c}$$

$$-\delta_{\gamma\kappa_1}\delta_{\alpha\kappa_1}\langle\Psi|a^\dagger_{\kappa_1}a^\dagger_{\kappa_2}H_0a_{\kappa_2}a_{\kappa_1}|\Psi\rangle \tag{3da}$$

$$+\delta_{\gamma\kappa_1}\delta_{\beta\kappa_1}\langle\Psi|a^\dagger_{\kappa_1a^\dagger_{\kappa_2}}H_0a_{\kappa_2}a_{\kappa_1}|\Psi\rangle \tag{3dba}$$

$$-0 \tag{3dbb}$$

$$= \delta_{\alpha\kappa_1}\delta_{\beta\kappa_2}\delta_{\gamma\kappa_2}\delta_{\delta\kappa_1} \tag{3aa}$$

$$-\delta_{\alpha\kappa_1}\delta_{\beta\kappa_2}\delta_{\gamma\kappa_1}\delta_{\delta\kappa_2} \tag{3ab}$$

$$+\delta_{\alpha\kappa_1}\delta_{\delta\kappa_1}\left\langle\Psi|a^\dagger_{\kappa_1}a^\dagger_{\kappa_2}H_0 a_{\kappa_2}a_{\kappa_1}|\Psi\right\rangle \tag{3ba}$$

$$+\delta_{\gamma\kappa_1}\delta_{\beta\kappa_1}\left\langle\Psi|a^\dagger_{\kappa_1 a^\dagger_{\kappa_2}}H_0 a_{\kappa_2}a_{\kappa_1}|\Psi\right\rangle \tag{3bb}$$

$$-\delta_{\gamma\kappa_1}\delta_{\alpha\kappa_1}\left\langle\Psi|a^\dagger_{\kappa_1}a^\dagger_{\kappa_2}H_0 a_{\kappa_2}a_{\kappa_1}|\Psi\right\rangle \tag{3bc}$$

adding the integrals back in.

$$= v^{\kappa_1\kappa_2\kappa_2\kappa_1} \tag{3aa}$$

$$-v^{\kappa_1\kappa_2\kappa_1\kappa_2} \tag{3ab}$$

$$+v^{\kappa_1\beta\gamma\kappa_1} \tag{3ba}$$

$$+v^{\alpha\kappa_1\kappa_1\delta} \tag{3bb}$$

$$-v^{\kappa_1\beta\kappa_1\delta} \tag{3bc}$$

# 2 conclusions

feeling like so close, but still no sigar.in einsum notation, it looks like (0.5)*(np.einsum('ijji', h2e)-np.einsum('ijij', h2e)+np.einsum('ijji', h2e)+np.einsum('ijji', h2e)-np.einsum('ijij', h2e)). what ami still messing?