FCI Questions

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1. 2 determinants with no differences

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

The 2 electron ints have been omitted until needed to avoid repetition.

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

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

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

$$= \langle 0|\left(\prod_{\kappa=(\kappa_n\ldots\kappa_1)} a_\kappa\right) \delta_{\delta\kappa_1}\delta_{\gamma\kappa_2} a^\dagger_\alpha a^\dagger_\beta \left(\prod_{\kappa'=(\kappa_3\ldots\kappa_n)} a^\dagger_{\kappa'}\right)|0\rangle \tag{4aa}$$

$$- \langle 0| \left(\prod_{\kappa=(\kappa_n \ldots \kappa_3)} a_\kappa \right) \delta_{\delta\kappa_1} a_{\kappa_2} a_{\kappa_1} a^\dagger_{\kappa_2} a^\dagger_\alpha a^\dagger_\beta a_\gamma \left(\prod_{\kappa'=(\kappa_3 \ldots \kappa_n)} a^\dagger_{\kappa'} \right) |0\rangle \quad \text{(4ab)}$$

$$- \langle 0| \left(\prod_{\kappa=(\kappa_n \ldots \kappa_1)} a_\kappa \right) \delta_{\gamma\kappa_1} a^\dagger_\alpha a^\dagger_\beta \delta_{\delta\kappa_2} \left(\prod_{\kappa'=(\kappa_3 \ldots \kappa_n)} a^\dagger_{\kappa'} \right) |0\rangle \quad \text{(4baa)}$$

$$+ \langle 0| \left(\prod_{\kappa=(\kappa_n \ldots \kappa_1)} a_\kappa \right) \delta_{\gamma\kappa_1} a^\dagger_\alpha a^\dagger_\beta a^\dagger_{\kappa_2} a_\delta \left(\prod_{\kappa'=(\kappa_3 \ldots \kappa_n)} a^\dagger_{\kappa'} \right) |0\rangle \quad \text{(4bab)}$$

$$+ \langle 0| \left(\prod_{\kappa=(\kappa_n \ldots \kappa_2)} a_\kappa \right) a_{\kappa_1} a^\dagger_{\kappa_1} a^\dagger_\alpha a^\dagger_\beta a_\gamma \delta_{\delta\kappa_2} \left(\prod_{\kappa'=(\kappa_3 \ldots \kappa_n)} a^\dagger_{\kappa'} \right) |0\rangle \quad \text{(4bba)}$$

$$- \langle 0| \left(\prod_{\kappa=(\kappa_n \ldots \kappa_2)} a_\kappa \right) a_{\kappa_1} a^\dagger_{\kappa_1} a^\dagger_\alpha a^\dagger_\beta a_\gamma a^\dagger_{\kappa_2} a_\delta \left(\prod_{\kappa'=(\kappa_3 \ldots \kappa_n)} a^\dagger_{\kappa'} \right) |0\rangle \quad \text{(4bbb)}$$

$$= \delta_{\delta\kappa_1} \delta_{\gamma\kappa_2} \delta_{\beta\kappa_2} \delta_{\alpha\kappa_1} \quad \text{(3aa)}$$

$$+ \langle 0| \left(\prod_{\kappa=(\kappa_n \ldots \kappa_3)} a_\kappa \right) \delta_{\delta\kappa_1} \delta_{\alpha\kappa_1} a^\dagger_\beta a_\gamma \left(\prod_{\kappa'=(\kappa_3 \ldots \kappa_n)} a^\dagger_{\kappa'} \right) |0\rangle \quad \text{(2aa)}$$

$$- \langle 0| \left(\prod_{\kappa=(\kappa_n \ldots \kappa_3)} a_\kappa \right) \delta_{\delta\kappa_1} a^\dagger_\alpha a_{\kappa_1} a^\dagger_\beta a_\gamma \left(\prod_{\kappa'=(\kappa_3 \ldots \kappa_n)} a^\dagger_{\kappa'} \right) |0\rangle \quad \text{(2ab)}$$

$$- \delta_{\gamma\kappa_1} \delta_{\delta\kappa_2} \delta_{\beta\kappa_2} \delta_{\alpha\kappa_1} \quad \text{(2b)}$$

$$+ \langle 0| \left(\prod_{\kappa=(\kappa_n \ldots \kappa_3)} a_\kappa \right) \delta_{\gamma\kappa_1} a_{\kappa_2} a_{\kappa_1} a^\dagger_{\kappa_2} a^\dagger_\alpha a^\dagger_\beta a_\delta \left(\prod_{\kappa'=(\kappa_3 \ldots \kappa_n)} a^\dagger_{\kappa'} \right) |0\rangle \tag{2c}$$

$$+ \langle 0| \left(\prod_{\kappa=(\kappa_n \ldots \kappa_3)} a_\kappa \right) \delta_{\delta\kappa_2} a_{\kappa_2} a^\dagger_\alpha a^\dagger_\beta a_\gamma \left(\prod_{\kappa'=(\kappa_3 \ldots \kappa_n)} a^\dagger_{\kappa'} \right) |0\rangle \tag{2d}$$

$$- \langle 0| \left(\prod_{\kappa=(\kappa_n \ldots \kappa_2)} a_\kappa \right) a^\dagger_\alpha a^\dagger_\beta \delta_{\gamma\kappa_2} a_\delta \left(\prod_{\kappa'=(\kappa_3 \ldots \kappa_n)} a^\dagger_{\kappa'} \right) |0\rangle \tag{2ea}$$

$$+ \langle 0| \left(\prod_{\kappa=(\kappa_n \ldots \kappa_2)} a_\kappa \right) a^\dagger_\alpha a^\dagger_\beta a^\dagger_{\kappa_2} a_\gamma a_\delta \left(\prod_{\kappa'=(\kappa_3 \ldots \kappa_n)} a^\dagger_{\kappa'} \right) |0\rangle \tag{2eb}$$

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

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

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

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

$$-\delta_{\gamma\kappa_1} \delta_{\delta\kappa_2} \delta_{\beta\kappa_2} \delta_{\alpha\kappa_1} \tag{6c}$$

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

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

$$+ \langle 0| \left(\prod_{\kappa=(\kappa_n \ldots \kappa_3)} a_\kappa \right) \delta_{\delta\kappa_2} \delta_{\alpha\kappa_2} a^\dagger_\beta a_\gamma \left(\prod_{\kappa'=(\kappa_3 \ldots \kappa_n)} a^\dagger_{\kappa'} \right) |0\rangle \tag{6ea}$$

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

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

$$+ \langle 0| \left(\prod_{\kappa=(\kappa_n \ldots \kappa_3)} a_\kappa \right) \delta_{\gamma\kappa_2} a^\dagger_\alpha a_{\kappa_2} a^\dagger_\beta a_\delta \left(\prod_{\kappa'=(\kappa_3 \ldots \kappa_n)} a^\dagger_{\kappa'} \right) |0\rangle \tag{6fab}$$

$$+ \left\langle \Psi a^\dagger_{\kappa_2} a^\dagger_{\kappa_1} \middle| V \middle| a_{\kappa_1} a_{\kappa_2} \Psi \right\rangle \tag{6fba}$$

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