

FCI Questions

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1 0 differences between two determines

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

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

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

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

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

$$- \langle 0 | \left(\prod_{\kappa=(\kappa_n \dots \kappa_1)} a_{\kappa} \right) a_{\gamma}^{\dagger} a_{\beta}^{\dagger} \delta_{\gamma\kappa_1} a_{\delta} \left(\prod_{\kappa'=(\kappa_2 \dots \kappa_n)} a_{\kappa'}^{\dagger} \right) | 0 \rangle \quad (3ba)$$

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

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

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

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

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

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

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

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

$$- \delta_{\alpha\kappa_1} \delta_{\beta\kappa_2} \delta_{\gamma\kappa_1} \delta_{\delta\kappa_2} \quad (3ca)$$

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

$$= \delta_{\alpha\kappa_1} \delta_{\beta\kappa_2} \delta_{\gamma\kappa_2} \delta_{\delta\kappa_1} \quad (4aa)$$

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

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

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

$$- \delta_{\alpha\kappa_1} \delta_{\beta\kappa_2} \delta_{\gamma\kappa_1} \delta_{\delta\kappa_2} \quad (4ca)$$

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

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

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

$$+ \delta_{\alpha\kappa_1} \delta_{\delta\kappa_1} \langle \Psi | a_{\kappa_1}^\dagger a_{\kappa_2}^\dagger H_0 a_{\kappa_2} a_{\kappa_1} | \Psi \rangle \quad (3aba)$$

$$- \delta_{\beta\kappa_1} \delta_{\delta\kappa_1} \langle \Psi | a_{\kappa_1}^\dagger a_2^\dagger H_0 a_2 a_1 a_{\kappa_2} | \Psi \rangle \quad (3abba)$$

$$+ \langle 0 | \left(\prod_{\kappa=(\kappa_n \dots \kappa_3)} a_\kappa \right) \delta_{\delta\kappa_1} a_\alpha^\dagger \delta_{\beta\kappa_1} a_\gamma \left(\prod_{\kappa'=(\kappa_3 \dots \kappa_n)} a_{\kappa'}^\dagger \right) | 0 \rangle \quad (3abbbba)$$

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

$$- \delta_{\alpha\kappa_1} \delta_{\beta\kappa_2} \delta_{\gamma\kappa_1} \delta_{\delta\kappa_2} \quad (3c)$$

$$- \delta_{\gamma\kappa_1} \delta_{\alpha\kappa_1} \langle \Psi | a_{\kappa_1}^{\dagger} a_{\kappa_2}^{\dagger} H_0 a_{\kappa_2} a_{\kappa_1} | \Psi \rangle \quad (3da)$$

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

$$- 0 \quad (3dbb)$$

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

$$+ \delta_{\alpha\kappa_1} \delta_{\delta\kappa_1} \langle \Psi | a_{\kappa_1}^{\dagger} a_{\kappa_2}^{\dagger} H_0 a_{\kappa_2} a_{\kappa_1} | \Psi \rangle \quad (3aba)$$

$$- \delta_{\beta\kappa_1} \delta_{\delta\kappa_1} \langle \Psi | a_{\kappa_1}^{\dagger} a_2^{\dagger} H_0 a_2 a_1 a_{\kappa_2} | \Psi \rangle \quad (3abba)$$

$$+ \delta_{\beta\kappa_1} \delta_{\delta\kappa_1} \langle \Psi | a_{\kappa_1}^{\dagger} a_{\kappa_2}^{\dagger} H_0 a_{\kappa_2} a_{\kappa_1} | \Psi \rangle \quad (3abbba)$$

$$- 0 \quad (3abbbb)$$

$$- \delta_{\alpha\kappa_1} \delta_{\beta\kappa_2} \delta_{\gamma\kappa_1} \delta_{\delta\kappa_2} \quad (3c)$$

$$- \delta_{\gamma\kappa_1} \delta_{\alpha\kappa_1} \langle \Psi | a_{\kappa_1}^{\dagger} a_{\kappa_2}^{\dagger} H_0 a_{\kappa_2} a_{\kappa_1} | \Psi \rangle \quad (3da)$$

$$+ \delta_{\gamma\kappa_1} \delta_{\beta\kappa_1} \langle \Psi | a_{\kappa_1 a_{\kappa_2}}^{\dagger} H_0 a_{\kappa_2} a_{\kappa_1} | \Psi \rangle \quad (3dba)$$

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

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

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

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

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

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

adding the integrals back in.

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

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

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

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

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

equation 3 part b similar to the Condon roles. not sure were to go with this, or with part a

2 math\`drafts.pdf

I'm confused about the steps you took to get from

$$\sum_{\kappa} h^{\kappa\kappa} \tag{3}$$

$$\sum_{\kappa} h^{(\kappa)(\kappa)} \delta_{[\kappa],[\kappa]} \tag{4}$$