

FCI Questions

Patryk Kozłowski

April 25, 2023

1 one difference between two determinants

$$\langle \Psi | V | \Psi(k \rightarrow k') \rangle = v^{\alpha\beta\gamma\delta} (-1)^{\varepsilon(\kappa_1, \dots, \kappa'_i, \dots, \kappa_n)} \quad (1a)$$

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

omitting into QUAL and face factor for now

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

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

$$= \langle 0 | \left(\prod_{\kappa=(\kappa_n \dots \kappa_2)} a_\kappa \right) \delta_{\delta\kappa'_1} \delta_{\alpha\kappa_1} a_\beta^\dagger a_\gamma \left(\prod_{\kappa'=(\kappa_2 \dots \kappa_n)} a_{\kappa'}^\dagger \right) | 0 \rangle \quad (3)$$

$$- \langle 0 | \left(\prod_{\kappa=(\kappa_n \dots \kappa_2)} a_\kappa \right) \delta_{\delta\kappa'_1} a_\alpha^\dagger a_1 a_\beta^\dagger a_\gamma \left(\prod_{\kappa'=(\kappa_2 \dots \kappa_n)} a_{\kappa'}^\dagger \right) | 0 \rangle \quad (4)$$

$$- \langle 0 | \left(\prod_{\kappa=(\kappa_n \dots \kappa_2)} a_\kappa \right) a_1 a_\alpha^\dagger a_\beta^\dagger \delta_{\gamma\kappa'_1} a_\delta \left(\prod_{\kappa'=(\kappa_2 \dots \kappa_n)} a_{\kappa'}^\dagger \right) | 0 \rangle \quad (5)$$

$$+0 \quad (6)$$

$$= \delta_{\delta\kappa_1'} \delta_{\alpha\kappa_1} \delta_{\beta\kappa_2} \delta_{\gamma\kappa_2} \quad (7)$$

$$- \langle 0 | \left(\prod_{\kappa=(\kappa_n \dots \kappa_2)} a_{\kappa} \right) \delta_{\delta\kappa_1'} a_{\alpha}^{\dagger} \delta_{\beta\kappa_1} a_{\gamma} \left(\prod_{\kappa'=(\kappa_2 \dots \kappa_n)} a_{\kappa'}^{\dagger} \right) | 0 \rangle \quad (8)$$

$$+0 \quad (9)$$

$$- \langle 0 | \left(\prod_{\kappa=(\kappa_n \dots \kappa_2)} a_{\kappa} \right) \delta_{\alpha\kappa_1} a_{\beta}^{\dagger} \delta_{\gamma\kappa_1'} a_{\delta} \left(\prod_{\kappa'=(\kappa_2 \dots \kappa_n)} a_{\kappa'}^{\dagger} \right) | 0 \rangle \quad (10)$$

$$+ \langle 0 | \left(\prod_{\kappa=(\kappa_n \dots \kappa_2)} a_{\kappa} \right) a_{\alpha}^{\dagger} a_1 a_{\beta}^{\dagger} \delta_{\gamma\kappa_1'} a_{\delta} \left(\prod_{\kappa'=(\kappa_2 \dots \kappa_n)} a_{\kappa'}^{\dagger} \right) | 0 \rangle \quad (11)$$

$$= \delta_{\delta\kappa_1'} \delta_{\alpha\kappa_1} \delta_{\beta\kappa_2} \delta_{\gamma\kappa_2} \quad (12)$$

$$- \delta_{\alpha\kappa_2} \delta_{\beta\kappa_1} \delta_{\gamma\kappa_2} \delta_{\delta\kappa_1'} \quad (13)$$

$$- \delta_{\alpha\kappa_1} \delta_{\beta\kappa_2} \delta_{\gamma\kappa_1'} \delta_{\delta\kappa_2} \quad (14)$$

$$+ \langle 0 | \left(\prod_{\kappa=(\kappa_n \dots \kappa_2)} a_{\kappa} \right) a_{\alpha}^{\dagger} \delta_{\beta\kappa_1} \delta_{\gamma\kappa_1'} a_{\delta} \left(\prod_{\kappa'=(\kappa_2 \dots \kappa_n)} a_{\kappa'}^{\dagger} \right) | 0 \rangle \quad (15)$$

$$-0 \quad (16)$$

$$= \delta_{\delta\kappa_1'} \delta_{\alpha\kappa_1} \delta_{\beta\kappa_2} \delta_{\gamma\kappa_2} \quad (17)$$

$$- \delta_{\alpha\kappa_2} \delta_{\beta\kappa_1} \delta_{\gamma\kappa_2} \delta_{\delta\kappa_1'} \quad (18)$$

$$- \delta_{\alpha\kappa_1} \delta_{\beta\kappa_2} \delta_{\gamma\kappa_1'} \delta_{\delta\kappa_2} \quad (19)$$

$$+ \delta_{\alpha\kappa_2} \delta_{\beta\kappa_1} \delta_{\gamma\kappa_1'} \delta_{\delta\kappa_2} \quad (20)$$

bringing the face falter and the integrals back.

$$= (-1)^{\varepsilon(\kappa_1, \dots, \kappa_i', \dots, \kappa_n)} \sum_{\kappa_2} \left(v^{1221'} - v^{2121'} - v^{121'2} + v^{211'2} \right) \quad (21)$$

$$= (-1)^{\varepsilon(\kappa_1, \dots, \kappa_i', \dots, \kappa_n)} \sum_n^N [mp|nn] - [mn|np] \quad (22)$$

$$= (-1)^{\varepsilon(\kappa_1, \dots, \kappa'_i, \dots, \kappa_n)} \sum_n^N (mp|nn) \delta_{[m][p]} - (mn|np) \delta_{[m][n]} \delta_{[p][n]} \quad (23)$$

$$= (-1)^{\varepsilon(\kappa_1, \dots, \kappa'_i, \dots, \kappa_n)} \sum_n^N (mp|nn) \delta_{[m][p]} - (mn|np) * (1/2) * (1/2) \quad (24)$$