FCI Questions

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April 25, 2023

1 0 differences between two determines

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

$$\ldots \tag{2}$$

$$= \sum_1^N \sum_2^N \left(v^{1221} - v^{2121} - v^{1212} + v^{2112} \right) \tag{3}$$

$$= (1/2) * \sum_{i \neq j} (v^{ijji} - v^{ijij}) \tag{4}$$

$$= (1/2) * \sum_{i \neq j} [ii|jj] - [ij|ji] \tag{5}$$

$$= (1/2) * \sum_{i \neq j} (ii|jj)\delta_{[i][i]}\delta_{[j][j]} - (ij|ji)\delta_{[i][j]} \tag{6}$$

$$= (1/2) * \sum_{i \neq j} (ii|jj) - (1/2) * (ij|ji) \tag{7}$$

$$= (1/2) * (np.einsum('ijij->', v) - (1/2) * np.einsum('ijji->', v)) \tag{8}$$

So, assuming and dealing with something like:

$$v^{\alpha\beta\gamma\delta} = \langle \alpha\beta || \gamma\delta \rangle \tag{9}$$