

Using the anti-commutation relation $\{a_i, a_j\} = 0$, we can write

$$a_{i'}^\dagger a_{j'}^\dagger a_{k'}^\dagger = \epsilon_{i'j'k'} a_i^\dagger a_j^\dagger a_k^\dagger \quad (1)$$

where $\{i', j', k\} = P\{i', j', k\}$, P is some permutation operator, and $\epsilon_{i'j'k'}$ is the Levi-Cevita symbol.

This can then be applied to contributions to the rdm derivatives:

$$\langle I | a_{i'}^\dagger a_{j'}^\dagger a_{k'}^\dagger a_{l'} a_{m'} a_{n'} | J \rangle c_J = \epsilon_{i'j'k'} \epsilon_{l'm'n'} \langle I | a_i^\dagger a_j^\dagger a_k^\dagger a_l a_m a_n | J \rangle c_J \quad (2)$$

Each of the ϵ_{xyz} corresponds exclusively to either creation or annihilation operators, hence the reorderings with which they are associated correspond only to alterations of the phase, and do not affect the total projection.

Recall the identity

$$\epsilon_{ijk} \epsilon_{lmn} = \delta_{il} \delta_{jm} \delta_{kn} - \delta_{im} \delta_{jl} \delta_{kn} + \delta_{in} \delta_{jl} \delta_{km} - \delta_{in} \delta_{jm} \delta_{kl} + \delta_{in} \delta_{jl} \delta_{km} - \delta_{il} \delta_{jn} \delta_{km} = \delta_{ijk}^{lmn} \quad (3)$$

Where is the Kronecker delta. Each of the Dirac delta functions corresponds to a contraction between a creation and annihilation operator. This can be used to rewrite the contraction between the rdm derivative and the "A"-tensor:

$$\sum_{\substack{ijk \\ lmn}} \Gamma_{ijklmn}^I A_{ijklmn} = \quad (4)$$

$$\sum_{\substack{ijk \\ lmn}} \sum_J \langle I | a_i^\dagger a_j^\dagger a_k^\dagger a_l a_m a_n | J \rangle c_J A_{ijklmn} = \quad (5)$$

$$\sum_{\substack{ijk \\ lmn \\ i < j < k \\ l < m < n}} \sum_{\substack{\{i'j'k'\} \\ \{l'm'n'\}}} \sum_J \epsilon_{i'j'k'} \epsilon_{l'm'n'} \langle I | a_i^\dagger a_j^\dagger a_k^\dagger a_l a_m a_n | J \rangle c_J A_{ijklmn} \quad (6)$$

$$\sum_{\substack{ijk \\ lmn \\ i < j < k \\ l < m < n}} \sum_{\substack{\{i'j'k'\} \\ \{l'm'n'\}}} \sum_J \delta_{i'j'k'}^{l'm'n'} \langle I | a_i^\dagger a_j^\dagger a_k^\dagger a_l a_m a_n | J \rangle c_J A_{ijklmn} \quad (7)$$

$$\begin{aligned} & \sum_{\substack{ijk \\ lmn \\ i < j < k \\ l < m < n}} \sum_{\substack{\{i'j'k'\} \\ \{l'm'n'\}}} \sum_J (\delta_{il} \delta_{jm} \delta_{kn} \langle I | a_i^\dagger a_j^\dagger a_k^\dagger a_l a_m a_n | J \rangle c_J A_{ijklmn} \\ & - \delta_{im} \delta_{jl} \delta_{kn} \langle I | a_i^\dagger a_j^\dagger a_k^\dagger a_l a_m a_n | J \rangle c_J A_{ijklmn} \end{aligned}$$

$$\begin{aligned}
& +\delta_{im}\delta_{jn}\delta_{kl}\langle I|a_i^\dagger a_j^\dagger a_k^\dagger a_l a_m a_n|J\rangle c_J A_{ijklmn} \\
& -\delta_{in}\delta_{jm}\delta_{kl}\langle I|a_i^\dagger a_j^\dagger a_k^\dagger a_l a_m a_n|J\rangle c_J A_{ijklmn} \\
& +\delta_{in}\delta_{jl}\delta_{km}\langle I|a_i^\dagger a_j^\dagger a_k^\dagger a_l a_m a_n|J\rangle c_J A_{ijklmn} \\
& -\delta_{il}\delta_{jn}\delta_{km}\langle I|a_i^\dagger a_j^\dagger a_k^\dagger a_l a_m a_n|J\rangle c_J A_{ijklmn} \\
& = \sum_{\substack{ijk \\ lmn \\ i < j < k \\ l < m < n}} \sum_{\substack{\{i'j'k'\} \\ \{l'm'n'\}}} \sum_J \langle I|a_l^\dagger a_m^\dagger a_n^\dagger a_l a_m a_n|J\rangle c_J A_{lmnlmn} \\
& \quad \langle I|a_m^\dagger a_l^\dagger a_n^\dagger a_l a_m a_n|J\rangle c_J A_{mnlmln} \\
& \quad \langle I|a_m^\dagger a_n^\dagger a_l^\dagger a_l a_m a_n|J\rangle c_J A_{mnlmln} \\
& \quad \langle I|a_n^\dagger a_m^\dagger a_l^\dagger a_l a_m a_n|J\rangle c_J A_{nmllmn} \\
& \quad \langle I|a_n^\dagger a_l^\dagger a_m^\dagger a_l a_m a_n|J\rangle c_J A_{nlmlmn} \\
& \quad \langle I|a_l^\dagger a_n^\dagger a_m^\dagger a_l a_m a_n|J\rangle c_J A_{lnmlmn} \\
& = \sum_{\substack{ijk \\ lmn \\ i < j < k \\ l < m < n}} \sum_{\substack{\{i'j'k'\} \\ \{l'm'n'\}}} \sum_J \langle I|a_l^\dagger a_l a_m^\dagger a_m a_n^\dagger a_n|J\rangle c_J A_{lmnlmn} + A_{mnlmln} + A_{mnlmln} + A_{nmllmn} + A_{nlmlmn} + A_{lnmlmn}
\end{aligned}$$

Hence the rdm derivative does not need to be calculated; it's anti-symmetry under permutation of the creation/annihilation indexes means it is possible to rewrite it entirely in terms of delta functions.

It looks as though matrix elements between different determinants vanish, which seems wrong. However, these interactions are still effectively present; elements of A_{ijklmn} corresponding to orbitals not in $|J\rangle$ will be weighted by c_J due to the contractions and nature of the summation.

This will apply to all normal ordered operators:

$$\sum_{\substack{i_1 \dots i_N \\ j_1 \dots j_N \\ i_1 < i_2 < \dots < i_N \\ j_1 < j_2 < \dots < j_N}} \sum_{\substack{\{i'_1 \dots i'_N\} \\ \{j'_1 \dots j'_N\}}} \sum_J \epsilon_{i_1 \dots i_N} \epsilon_{j_1 \dots j_N} \langle I|a_{i_1}^\dagger \dots a_{i_N}^\dagger a_{j_1} \dots a_{j_N}|J\rangle c_J A_{i_1 \dots i_N j_1 \dots j_N} \quad (8)$$