FCI Questions

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$$\langle\Psi|V|\Psi(m\to p)\rangle = (-1)^{\varepsilon(\kappa)}(1/2)*\sum_{PQRS} v^{PQRS}\langle 0|\left(\prod_{\kappa=(\kappa_n\ldots\kappa_2)} a_\kappa\right) a_m a_P^\dagger a_R^\dagger a_S a_Q a_p^\dagger \left(\prod_{\kappa'=(\kappa_2\ldots\kappa_n)} a_{\kappa'}^\dagger\right) \tag{1}$$

$$= \delta_{Pm}\delta_{Qp}\sum_{n=spinIntersection}\delta_{Rn}\delta_{Sn} \tag{2}$$

$$-\delta_{Rm}\delta_{Qp}\sum_{n=spinIntersection}\delta_{Pn}\delta_{Sn} \tag{3}$$

$$-\delta_{Pm}\delta_{Sp}\sum_{n=spinIntersection}\delta_{Rn}\delta_{Qn} \tag{4}$$

$$+\delta_{Rm}\delta_{Sp}\sum_{n=spinIntersection}\delta_{Pn}\delta_{Qn} \tag{5}$$

$$= (1/2)\sum_{n=spinIntersection}\left(v^{mpnn} - v^{npmn} - v^{mnnp} + v^{nnmp}\right) \tag{6}$$

symmetry

$$= (1/2)\sum_{n=spinIntersection}\left(2v^{mpnn} - 2v^{mnnp}\right) \tag{7}$$

$$= \sum_{n=n=spinIntersection}\left(v^{mpnn} - v^{mnnp}\right) \tag{8}$$

$$= \sum_{n=n=spinIntersection}\Big((mp|nn)\delta_{[m][p]}\delta_{[n][n]} - (mn|np)\delta_{[m][n]}\delta_{[n][p]}\Big) \tag{9}$$

$$
\begin{aligned}
= \sum_{n=n=spinIntersection} \Big(\delta_{[m][p]} np.einsum('ijkk \\
- ij', somthingCombined?)[(m),(p)] \\
- \delta_{[m][n]}\delta_{[n][p]} np.einsum('ijjk - ik', somthingCombined?)[(m),(p)]\Big)
\end{aligned} \tag{10}
$$

so, to solve

$$\delta_{[m][n]}\delta_{[n][p]} \tag{11}$$

need to find how many times that spin of m and p equal common orbs in n=spinIntersection
also, need to figure out the instant summation notation for this integral mesh.