Computing matrix element of the three-body operator for parallel spins

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I. WHAT WE NEED TO COMPUTE

A. General matrix element

We need to compute the matrix elements of this nasty operator

$$O^3 = \frac{1}{6}\sum_{ijm}\sum_{kln}\langle ijm|kln\rangle\, \hat{k}^\dagger\, \hat{l}^\dagger\, \hat{n}^\dagger\, \hat{m}\, \hat{j}\, \hat{i}. \tag{1}$$

Therefore, it is the product of $\hat{k}^\dagger\, \hat{l}^\dagger\, \hat{n}^\dagger$ by $\hat{m}\, \hat{j}\, \hat{i}$, and each term posses a 6-fold permutation symmetry with ± 1 signature. Starting from $\hat{k}^\dagger\, \hat{l}^\dagger\, \hat{n}^\dagger$ there are two symmetric pertumations

$$\hat{k}^\dagger\, \hat{l}^\dagger\, \hat{n}^\dagger = \hat{l}^\dagger\, \hat{n}^\dagger\, \hat{k}^\dagger = \hat{n}^\dagger\, \hat{k}^\dagger\, \hat{l}^\dagger, \tag{2}$$

and three anti-symmetric permutations

$$\hat{l}^\dagger\, \hat{k}^\dagger\, \hat{n}^\dagger = \hat{n}^\dagger\, \hat{l}^\dagger\, \hat{k}^\dagger = \hat{k}^\dagger\, \hat{n}^\dagger\, \hat{l}^\dagger, \tag{3}$$

which fulfill

$$\hat{k}^\dagger\, \hat{l}^\dagger\, \hat{n}^\dagger = -\hat{l}^\dagger\, \hat{k}^\dagger\, \hat{n}^\dagger. \tag{4}$$

Therefore, one can express a 6×6 matrix that is the product all possible permutations for (k,l,n) and (i,j,m), rearrange everything in terms of the original $\hat{k}^\dagger\, \hat{l}^\dagger\, \hat{n}^\dagger\, \hat{m}\, \hat{j}\, \hat{i}$ operator and obtain the following terms

$$\begin{aligned}\frac{1}{6}\mathcal{P}_{ijm}^{kln}\langle ijm|kln\rangle\, \hat{k}^\dagger\, \hat{l}^\dagger\, \hat{n}^\dagger\, \hat{m}\, \hat{j}\, \hat{i} = \qquad & \hat{k}^\dagger\, \hat{l}^\dagger\, \hat{n}^\dagger\, \hat{m}\, \hat{j}\, \hat{i}\Big(\\ + \left(\langle ijm|kln\rangle + \langle ijm|lnk\rangle + \langle ijm|nkl\rangle\right) & \\ - \left(\langle ijm|lkn\rangle + \langle ijm|nlk\rangle + \langle ijm|knl\rangle\right)\Big), &\end{aligned} \tag{5}$$

where $\mathcal{P}_{ijm}^{kln}$ contains the sum over the 36 permutations of the 6 indices with the corresponding signs.

B. Diagonal term

For a diagonal term, one has that

$$\begin{aligned} i &= k \\ j &= l \\ m &= n \end{aligned} \tag{6}$$

and therefore one obtains

$$\begin{aligned}\langle I|\, O^3\, |I\rangle = \sum_{i>j>m\in|I\rangle} & + \left(\langle ijm|ijm\rangle + \langle ijm|jmi\rangle + \langle ijm|mij\rangle\right) \\ & - \left(\langle ijm|jim\rangle + \langle ijm|mji\rangle + \langle ijm|imj\rangle\right)\end{aligned} \tag{7}$$

where the summation $\sum_{i>j>m\in|I\rangle}$ means running over all orbitals occupied in $|I\rangle$ in a unique way.

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C. Single excitation term

For a single excitation term, one has that

$$\begin{aligned} i &\neq k \\ j &= l \\ m &= n \end{aligned} \tag{8}$$

and then

$$\begin{aligned}\langle I|\, O^3\, \hat{k}^\dagger\, \hat{i}\, |I\rangle = (-1)^{\mathcal{P}_{IJ}}\sum_{j>m\in|I\rangle} & + \left(\langle ijm|kjm\rangle + \langle ijm|jmk\rangle + \langle ijm|mkj\rangle\right) \\ & - \left(\langle ijm|jkm\rangle + \langle ijm|mjk\rangle + \langle ijm|kmj\rangle\right)\Big).\end{aligned} \tag{9}$$

D. Double excitation term

For a double excitation term, one has that

$$\begin{aligned} i &\neq k \\ j &\neq l \\ m &= n \end{aligned} \tag{10}$$

and then

$$\begin{aligned}\langle I|\, O^3\, \hat{k}^\dagger\, \hat{l}^\dagger\, \hat{j}\, \hat{i}\, |I\rangle = (-1)^{\mathcal{P}_{IJ}}\sum_{m\in|I\rangle} & + \left(\langle ijm|klm\rangle + \langle ijm|lmk\rangle + \langle ijm|mkl\rangle\right) \\ & - \left(\langle ijm|lkm\rangle + \langle ijm|mlk\rangle + \langle ijm|kml\rangle\right)\Big).\end{aligned} \tag{11}$$