Have multi-configurational wavefunction:

$$|M\rangle = \sum_I c_I|I\rangle \tag{1}$$

$$= |M\rangle = c_{i_1,i_2....i_N} a^\dagger_{i_1} a^\dagger_{i_2}...a^\dagger_{i_N}|0\rangle \tag{2}$$

A second quatized version of a component of an orbital rotation operator is

$$\hat{V}_{ij} = V_{ij} a^\dagger_i a_j \tag{3}$$

A transformations,$\hat{U}$, of the Hamiltonian can be constructed from a rensor product of rotations in reals space, $\hat{S}$, and another in real space $\hat{R}$:

$$\hat{U} = \hat{R} \otimes \hat{S} \tag{4}$$

$\hat{R}$ and $\hat{S}$ can be constructed from transformation of the spatial and spin components of the orbitals. Aa basis formed from configuration state functions can be decomposed into a set subspaces, each of which are invariant under spin transformations $\hat{S}$, e.g.,,

$$[\hat{V}] \begin{bmatrix} [\Phi_{s_{-1}r_1}] \\ [\Phi_{s_0 r_1}] \\ [\Phi_{s_1 r_1}] \\ [\Phi_{s_{-1}r_2}] \\ [\Phi_{s_0 r_2}] \\ [\Phi_{s_1 r_2}] \\ .... \end{bmatrix} = [\hat{R}] \begin{bmatrix} [\hat{S}] \begin{bmatrix} [\Phi_{s_{-1}r_1}] \\ [\Phi_{s_0 r_1}] \\ [\Phi_{s_1 r_1}] \end{bmatrix} \\ [\hat{S}] \begin{bmatrix} [\Phi_{s_{-1}r_2}] \\ [\Phi_{s_0 r_2}] \\ [\Phi_{s_1 r_2}] \\ .... \end{bmatrix} \end{bmatrix} \tag{5}$$

i.e., the rotations $\hat{R}$ only rotate between different CSFs, whilst the rotations, $\hat{S}$, rotate within multiplets. Accordingbly, a roitation in $\hat{R}$ is enough to block diagonalize the Hamiltonian.

The $\gamma^{M,I}_{ij}$ derivatives have matrix elements $\sum_J \langle I|a^\dagger_i a_j|J\rangle c_{M,I}$. It would be nice to find a rotation Q such that

$$\Big[Q\Big] \begin{bmatrix} c_{M,1} \\ c_{M,1} \\ ... \\ ... \\ c_{M,N_{det}} \end{bmatrix} \tag{6}$$