$$\sum_{L}\sum_{M}\sum_{J}\sum_{\substack{abcd\\wxyz}}\langle J|\tilde{c}^{\dagger}_{M,J}T^{\dagger}_{LM,abcd}(\hat{a}_a\hat{a}^{\dagger}_b\hat{a}_c\hat{a}^{\dagger}_d)(\hat{a}^{\dagger}_w\hat{a}_x\hat{a}^{\dagger}_y\hat{a}_z)g(ijkl)|K\rangle$$

where $\{k,l\}\subset\{a,c,w,y\}$ and $\{i,j\}\subset\{b,d,x,z\}$ Define a map between a set of orbital indexes $\{a,b,c,d,w,x,y,z\}$ and a determinant index:

$$\Pi^{MK}:\{a,b,c,d,w,x,y,z\}\rightarrow J \qquad |J\rangle=\hat{a}_a\hat{a}^{\dagger}_b\hat{a}_c\hat{a}^{\dagger}_d\hat{a}^{\dagger}_w\hat{a}_x\hat{a}^{\dagger}_y\hat{a}_z|K\rangle$$

$$\pi^{K}(a,b,c,d,w,x,y,z)=\pi^{K}_{abcdwxyz}=J$$

$$\Theta^{MK}_{abcdwxyz}=c_{M,\pi^{K}_{abcdwxyz}}=c_{M,J}$$

These expressions can be used to rewrite the above expressions without a sum over J:

$$(1)=\sum_{L}\sum_{M}\sum_{\substack{abcd\\wxyz}}\Theta^{MK\dagger}_{abcdwxyz}\langle\pi^{MK}_{abcdwxyz}|T^{*}_{LM,badc}g(ijkl)|K\rangle$$

Note that $|J\rangle$ and $|K\rangle$ are orthogonal to any to determinants with orbitals in the virtual space occupied[1], or orbitals in the inactive space unoccupied. This enables further simplification of the above expressions via grouping together different ranges, i.e., inactive, active, virtual, for the indexes, a,b,c,d, of the MS-CASPT2 amplitudes, $T_{LM,abcd}$:

If $a,b,c,d\notin\{active\}$, then $\{i,j,k,l\}=\{b,a,d,c\}$.

$$\sum_{M}\sum_{J}\sum_{abcd}^{\notin\{act\}}\sum_{wxyz}^{\in\{act\}}c^{\dagger}_{M,J}\langle J|T^{*}_{LM,badc}\hat{a}_a\hat{a}^{\dagger}_b\hat{a}_c\hat{a}^{\dagger}_d\hat{a}^{\dagger}_w\hat{a}_x\hat{a}^{\dagger}_y\hat{a}_z g(ijkl)|K\rangle$$

$$=\sum_{M}\sum_{abcd}^{\notin\{act\}}\sum_{wxyz}^{\in\{act\}}c^{\dagger}_{M,\pi^{K}_{wxyz}}\sum_{abcd}^{\notin\{act\}}\langle K|T^{*}_{LM,badc}g(badc)|K\rangle s(badc,wxyz)$$

$$=\sum_{M}\sum_{wxyz}^{\in\{act\}}c^{\dagger}_{M,\pi^{K}_{wxyz}}A^{(g)}$$

where $s(badc,wxyz)$ is ±1 as determined by the anti-commutation relations of the creation annihilation operators.

If $a,b\notin\{active\}$ and $c,d\in\{active\}$, then

$$\sum_{M}\sum_{ab}^{\notin\{act\}}\sum_{cdwxyz}^{\in\{act\}}c^{\dagger}_{M,J}\langle J|T^{*}_{LM,badc}\hat{a}_a\hat{a}^{\dagger}_b\hat{a}_c\hat{a}^{\dagger}_d\hat{a}^{\dagger}_w\hat{a}_x\hat{a}^{\dagger}_y\hat{a}_z g(ijkl)|K\rangle$$

[1]assuming preservation of the number of electrons

$$= \sum_{M} \sum_{wxyz}^{\in\{act\}} \sum_{cd}^{\in\{act\}} c^{\dagger}_{M,\pi^{K}_{dcwxyz}} \sum_{ab}^{\notin\{act\}} T^{*}_{LM,badc} \sum_{\{v\}}^{\subset\{d,x,z\}} \sum_{\{u\}}^{\subset\{c,w,y\}} \langle K|g(ab,uv)|K\rangle s(badc,wxyz)$$

$$= \sum_{M} \sum_{wxyz}^{\in\{act\}} \sum_{cd}^{\in\{act\}} c^{\dagger}_{M,\pi^{K}_{dcwxyz}} A^{(g)}_{dcwxyz}$$

If $a, b, c, d \in \{active\}$, then

$$\sum_{M} \sum_{abcdwxyz}^{\in\{act\}} c^{\dagger}_{M,J} \langle J|\hat{a}_a \hat{a}^{\dagger}_b \hat{a}_c \hat{a}^{\dagger}_d \hat{a}^{\dagger}_w \hat{a}_x \hat{a}^{\dagger}_y \hat{a}_z g(ijkl)|K\rangle$$

$$= \sum_{M} \sum_{abcdwxyz}^{\in\{act\}} c^{\dagger}_{M,\pi^{K}_{badcwxyz}} \sum_{\{t,v\}}^{\subset\{b,d,x,z\}} \sum_{\{s,u\}}^{\subset\{a,c,w,y\}} \langle K|g(st,uv)|K\rangle s(badc,wxyz)$$

$$= \sum_{M} \sum_{abcdwxyz}^{\in\{act\}} c^{\dagger}_{M,\pi^{K}_{badcwxyz}} T^{*}_{LM,badc} \sum_{\{t,v\}}^{\subset\{b,d,x,z\}} \sum_{\{s,u\}}^{\subset\{a,c,w,y\}} \langle K|\hat{E}_{ba} g(st,uv)|K\rangle s(badc,wxyz)$$

$$= \sum_{M} \sum_{abcdwxyz}^{\in\{act\}} c^{\dagger}_{M,\pi^{K}_{badcwxyz}} A^{(g)}_{badcwxyz}$$