$$\sum_{L}\sum_{M}\sum_{J}\sum_{\substack{abcd\\wxyz}}\langle J|\tilde{c}^{\dagger}_{M,J}T^{\dagger}_{LM,abcd}(\hat{E}^{\dagger}_{ab}\hat{E}^{\dagger}_{cd}-\delta_{bc}\hat{E}_{ad})(\hat{E}_{wx}\hat{E}_{yz}-\delta_{xy}\hat{E}_{wz})g(1,2)|K\rangle$$

$$=\sum_{L}\sum_{M}\sum_{J}\sum_{\substack{abcd\\wxyz}}\langle J|\tilde{c}^{\dagger}_{M,J}T^{*}_{LM,badc}\hat{E}_{ba}\hat{E}_{dc}\hat{E}_{wx}\hat{E}_{yz}g(1,2)|K\rangle \tag{1}$$

$$-\sum_{L}\sum_{M}\sum_{J}\sum_{\substack{abcd\\wxyz}}\delta_{xy}\langle J|\tilde{c}^{\dagger}_{M,J}T^{*}_{LM,badc}\hat{E}_{ba}\hat{E}_{dc}\hat{E}_{wz}g(1,2)|K\rangle \tag{2}$$

$$-\sum_{L}\sum_{M}\sum_{J}\sum_{\substack{abcd\\wxyz}}\delta_{bc}\langle J|\tilde{c}^{\dagger}_{M,J}T^{*}_{LM,badc}\hat{E}_{ad}\hat{E}_{wx}\hat{E}_{yz}g(1,2)|K\rangle \tag{3}$$

$$+\sum_{L}\sum_{M}\sum_{J}\sum_{\substack{abcd\\wxyz}}\delta_{bc}\delta_{xy}\langle J|\tilde{c}^{\dagger}_{M,J}T^{*}_{LM,badc}\hat{E}_{ad}\hat{E}_{wz}g(1,2)|K\rangle \tag{4}$$

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

$$\Pi^{MK}:\{a,b,c,d,w,x,y,z\}\rightarrow J \qquad |J\rangle=\hat{E}_{ab}\hat{E}_{cd}\hat{E}_{wx}\hat{E}_{yz}|K\rangle$$

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

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

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

$$(1)=\sum_{L}\sum_{M}\sum_{\substack{abcd\\wxyz}}\Theta^{MK\dagger}_{abcdwxyz}\langle\pi^{MK}_{abcdwxyz}|T^{*}_{LM,badc}g(1,2)|K\rangle$$

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

$$|J\rangle=\begin{cases}\hat{E}_{wx}\hat{E}_{yz}|K\rangle & \text{or}\\ \hat{E}_{uv}|K\rangle & \text{with}\quad \{u\}\in\{w,y\}\quad\text{and}\quad v\in\{x,z\}\quad\text{or}\\ |K\rangle\end{cases} \tag{5}$$

[1] assuming preservation of the number of electrons

$$\sum_{M}\sum_{abcd}^{\notin\{act\}}\sum_{wxyz}^{\in\{act\}} c^{\dagger}_{M,J}\langle J|T^{*}_{LM,badc}\hat{E}_{ba}\hat{E}_{dc}\hat{E}_{wx}\hat{E}_{yz}g(1,2)|K\rangle$$

$$= \sum_{M}\sum_{abcd}^{\notin\{act\}}\Bigg[\sum_{wxyz}^{\in\{act\}}\Bigg(c^{\dagger}_{M,\pi^{K}_{wxyz}}\langle\pi^{K}_{wxyz}|T^{*}_{LM,badc}\hat{E}_{ba}\hat{E}_{dc}g(1,2)|K\rangle$$

$$+\sum_{u}^{\in\{w,y\}}\sum_{v}^{\in\{x,z\}} c^{\dagger}_{M,\pi^{K}_{uv}}\langle\pi^{K}_{uv}|T^{*}_{LM,badc}\hat{E}_{ba}\hat{E}_{dc}g(1,2)|K\rangle\Bigg)$$

$$+c^{\dagger}_{M,K}\langle K|T^{*}_{LM,badc}\hat{E}_{ba}\hat{E}_{dc}g(1,2)|K\rangle\Bigg]$$

$$= \sum_{M}\Bigg[\sum_{wxyz}^{\in\{act\}}\Bigg(c^{\dagger}_{M,\pi^{K}_{wxyz}}+\sum_{u}^{\in\{w,y\}}\sum_{v}^{\in\{x,z\}} c^{\dagger}_{M,\pi^{K}_{uv}}\Bigg)+c^{\dagger}_{M,K}\Bigg]\sum_{abcd}^{\notin\{act\}} T^{*}_{LM,badc}g(ba,cd)$$

$$= \sum_{M}\Bigg[\sum_{wxyz}^{\in\{act\}}\Bigg(\Theta^{MK\dagger}_{wxyz}+\sum_{u}^{\in\{w,y\}}\sum_{v}^{\in\{x,z\}}\Theta^{MK\dagger}_{uv}\Bigg)+\Theta^{MK\dagger}\Bigg]A^{(g)}$$

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

$$|J\rangle = \begin{cases} \hat{E}_{dc}\hat{E}_{wx}\hat{E}_{yz}|K\rangle \quad \text{or} \\ \hat{E}_{st}\hat{E}_{uv}|K\rangle \quad \text{with} \quad \{t,v\}\subset\{c,x,z\} \quad \text{and} \quad \{s,u\}\subset\{d,w,y\} \\ \hat{E}_{qr}|K\rangle \quad \text{with} \quad \{q\}\in\{d,w,y\} \quad \text{and} \quad r\in\{c,x,z\} \quad \text{or} \\ |K\rangle \end{cases} \tag{6}$$

$$= \sum_{M}\sum_{ab}^{\notin\{act\}}\Bigg[\sum_{cdwxyz}^{\in\{act\}}\Bigg(c^{\dagger}_{M,\pi^{K}_{dcwxyz}}\langle\pi^{K}_{dcwxyz}|T^{*}_{LM,badc}\hat{E}_{ba}g(1,2)|K\rangle$$

$$+\sum_{\{t,v\}}^{\subset\{d,x,z\}}\sum_{\{s,u\}}^{\subset\{c,w,y\}} c^{\dagger}_{M,\pi^{K}_{stuv}}\langle\pi^{K}_{stuv}|T^{*}_{LM,badc}\hat{E}_{ba}g(1,2)|K\rangle$$

$$+\sum_{u}^{\in\{w,y\}}\sum_{v}^{\in\{x,z\}} c^{\dagger}_{M,\pi^{K}_{uv}}\langle\pi^{K}_{uv}|T^{*}_{LM,badc}\hat{E}_{ba}g(1,2)|K\rangle\Bigg)$$

$$+c^{\dagger}_{M,K}\langle K|T^{*}_{LM,badc}\hat{E}_{ba}g(1,2)|K\rangle\Bigg]$$

$$= \sum_{M}\sum_{ab}^{\notin\{act\}}\sum_{cd}^{\in\{act\}} T^{*}_{LM,badc}\Bigg[\sum_{cdwxyz}^{\in\{act\}}\Bigg(c^{\dagger}_{M,\pi^{K}_{wxyz}}\langle\pi^{K}_{wxyz}|\hat{E}_{ba}\hat{E}_{dc}g(1,2)|K\rangle$$

$$
+\sum_{\{t,v\}}^{\subset\{d,x,z\}}\sum_{\{s,u\}}^{\subset\{c,w,y\}} c^{\dagger}_{M,\pi^K_{stuv}}\langle\pi^K_{st}|\hat{E}_{ba}\hat{E}_{uv}g(1,2)|K\rangle
$$

$$
\left.\left. +\sum_{u}^{\in\{w,y\}}\sum_{v}^{\in\{x,z\}} c^{\dagger}_{M,\pi^K_{uv}}\langle K|\hat{E}_{ba}\hat{E}_{uv}g(1,2)|K\rangle\right)\right.
$$

$$
\left. +c^{\dagger}_{M,K}\langle K|T^{*}_{LM,badc}\hat{E}_{ba}g(1,2)|K\rangle\right]
$$

$$
=\sum_{M}\sum_{ab}^{\notin\{act\}}\sum_{cd}^{\in\{act\}} T^{*}_{LM,badc}\left[\sum_{cdwxyz}^{\in\{act\}}\left(c^{\dagger}_{M,\pi^K_{wxyz}}\langle\pi^K_{dcwxyz}|\hat{E}_{ba}g(1,2)|K\rangle\right.\right.
$$

$$
+\sum_{\{t,v\}}^{\subset\{d,x,z\}}\sum_{\{s,u\}}^{\subset\{c,w,y\}} c^{\dagger}_{M,\pi^K_{stuv}}\langle\pi^K_{stuv}|\hat{E}_{ba}g(1,2)|K\rangle
$$

$$
\left. +\sum_{u}^{\in\{w,y\}}\sum_{v}^{\in\{x,z\}} c^{\dagger}_{M,\pi^K_{uv}}\langle K|\hat{E}_{ba}g(1,2)|K\rangle\right)
$$

$$
\left. +c^{\dagger}_{M,K}\langle K|T^{*}_{LM,badc}\hat{E}_{ba}g(1,2)|K\rangle\right]
$$

$$
\sum_{L}\sum_{M}\sum_{ab}^{\notin\{act\}}\left[\sum_{cdwxyz}^{\in\{act\}} c^{\dagger}_{M,\pi^K_{dcwxyz}}\langle\pi^K_{dcwxyz}|T^{*}_{LM,badc}\hat{E}_{ba}g(1,2)|K\rangle\right.
$$

$$
\sum_{L}\sum_{M}\sum_{ab}^{\notin\{act\}}\left[\sum_{cdwxyz}^{\in\{act\}} c^{\dagger}_{M,\pi^K_{dcwxyz}}\langle\pi^K_{dcwxyz}|T^{*}_{LM,badc}\hat{E}_{ba}g(1,2)|K\rangle\right.
$$

$$
\left. +\sum_{cdwxyz}^{\in\{act\}}\sum_{\{t,v\}}^{\subset\{d,x,z\}}\sum_{\{s,u\}}^{\subset\{c,w,y\}} c^{\dagger}_{M,\pi^K_{stuv}}\langle K|T^{*}_{LM,badc}\hat{E}_{ba}g(1,2)|K\rangle\right]
$$

$$
=\sum_{L}\sum_{M}\sum_{ab}^{\notin\{act\}}\sum_{cdwxyz}^{\in\{act\}}\sum_{u}^{\in\{d,x,z\}}\sum_{v}^{\in\{c,w,y\}}\Theta^{MK}_{dcwxyz}\langle K|T^{*}_{LM,badc}\hat{E}_{ba}g(1,2)\hat{E}_{uv}|K\rangle
$$

$$
=\sum_{L}\sum_{M}\sum_{cdwxyz}^{\in\{act\}}\Theta^{MK}_{cdwxyz}\sum_{ab}^{\notin\{act\}}\sum_{u}^{\in\{d,x,z\}}\sum_{v}^{\in\{c,w,y\}}\langle K|T^{*}_{LM,badc}\hat{E}_{ba}g(1,2)\hat{E}_{uv}|K\rangle
$$

$$
=\sum_{L}\sum_{M}\sum_{cdwxyz}^{\in\{act\}}\Theta^{MK}_{cdwxyz}\sum_{ab}^{\notin\{act\}}\sum_{u}^{\in\{d,x,z\}}\sum_{v}^{\in\{c,w,y\}} T^{*}_{LM,badc}g(bauv)
$$

$$
=\sum_{L}\sum_{M}\sum_{cdwxyz}^{\in\{act\}}\Theta^{MK}_{cdwxyz}A^{LM}_{cdwxyz}
$$

If $a, b, c, d \in \{active\}$ then $|K\rangle = E_{\gamma\delta\eta\zeta}|J\rangle$ and

$$\sum_L \sum_M \sum_{abcdwxyz}^{\in\{act\}} \Theta^{MK}_{abcdwxyz} \langle \pi^{MK}_{abcdwxyz} | T^*_{LM,badc} \hat{E}_{ba} \hat{E}_{dc} \hat{E}_{wx} \hat{E}_{yz} g(1,2) \hat{E}_{ab} \hat{E}_{cd} \hat{E}_{xw} \hat{E}_{zy} | \pi^{MK}_{abcdwxyz} \rangle$$

$$= \sum_L \sum_M \sum_{abcdwxyz}^{\in\{act\}} \Theta^{MK}_{abcdwxyz} \sum_{\substack{s,u \\ s \neq u}}^{\in\{b,d,x,z\}} \sum_{\substack{t,v \\ t \neq v}}^{\in\{a,c,w,y\}} \langle \pi^{MK}_{abcdwxyz} | T^*_{LM,badc} \hat{E}_{uv} g(1,2) \hat{E}_{tv} | \pi^{MK}_{abcdwxyz} \rangle$$

$$= \sum_L \sum_M \sum_{cdwxyz}^{\in\{act\}} \Theta^{MK}_{cdwxyz} \sum_{ab}^{\notin\{act\}} \sum_{u}^{\in\{d,x,z\}} \sum_{v}^{\in\{c,w,y\}} T^*_{LM,badc} g(stuv)$$

$$= \sum_L \sum_M \sum_{abcdwxyz}^{\in\{act\}} \Theta^{MK}_{abcdwxyz} A^{LM}_{abcdwxyz}$$