

Start with L_{PT2} :

$$\begin{aligned}
L_{PT2} = & \sum_{MN} \langle \tilde{M} | \hat{H} | \tilde{N} \rangle R_{MP}^* R_{NP} + \sum_{LMN} \langle \tilde{M} | \hat{T}_{LM}^\dagger \hat{H} | \tilde{N} \rangle R_{LP}^* R_{NP} - E_s \sum_{LMN} \langle \tilde{M} | \hat{T}_{LM}^\dagger \hat{T}_{LN} | \tilde{N} \rangle R_{LP}^* R_{LP} \\
& + \sum_{LMN} \langle \tilde{M} | \hat{\lambda}_{LM}^\dagger (\hat{f} - \epsilon_L^{(0)} + \epsilon_s) \hat{T}_{LN} | \tilde{N} \rangle + \sum_{LM} \langle \tilde{M} | \hat{\lambda}_{LM}^\dagger \hat{H} | \tilde{L} \rangle
\end{aligned} \tag{1}$$

First Term:

$$\begin{aligned}
& \frac{\partial}{\partial \tilde{c}_{Q,K}} \left[\sum_{MN} \langle \tilde{M} | \hat{H} | \tilde{N} \rangle R_{MP}^* R_{NP} \right] \\
& = \sum_M \langle \tilde{M} | \hat{H} | \tilde{K} \rangle R_{MP}^* R_{QP} + \sum_N \langle \tilde{K} | \hat{H} | \tilde{N} \rangle R_{QP}^* R_{KP} \\
& = R_{QP} \sum_M R_{MP}^* \sum_J \langle \tilde{I} | \tilde{c}_{M,J}^\dagger \hat{H} | \tilde{K} \rangle + R_{QP}^* \sum_N R_{NP} \sum_I \langle \tilde{K} | \hat{H} \tilde{c}_{N,I}^\dagger | \tilde{I} \rangle \\
& = R_{QP} \left[\sum_{wxyz} \sum_M R_{MP}^* \sum_J \langle \tilde{J} | \tilde{c}_{M,J}^\dagger (\hat{E}_{wx} \hat{E}_{yz} - \delta_{xy} \hat{E}_{wz}) g(1,2) | \tilde{K} \rangle \right] \\
& \quad + R_{QP}^* \left[\sum_{wxyz} \sum_N R_{NP} \sum_I \langle \tilde{K} | (\hat{E}_{wx} \hat{E}_{yz} - \delta_{xy} \hat{E}_{wz}) g(1,2) \tilde{c}_{N,I}^\dagger | \tilde{I} \rangle \right] \\
& + R_{QP} \left[\sum_{wx} \sum_M R_{MP}^* \sum_J \langle \tilde{J} | \tilde{c}_{M,J}^\dagger \hat{E}_{wx} h(1) | \tilde{K} \rangle \right] + R_{QP}^* \left[\sum_{wx} \sum_N R_{NP} \sum_I \langle \tilde{K} | \hat{E}_{wx} h(1) \tilde{c}_{N,I}^\dagger | \tilde{I} \rangle \right] \\
& = R_{QP} \left(\sum_M R_{MP}^* \sum_{wxyz} \Theta_{wxyz}^{M,K^\dagger} A^{(g)}(wxyz) + \sum_{wx} \Theta_{wx}^{M,K^\dagger} A^{(h)}(wx) \right) \\
& \quad R_{QP}^* \left(\sum_N R_{NP} \sum_{wxyz} \Theta_{wxyz}^{N,K} A^{(g)}(wxyz) + \sum_{wx} \Theta_{wx}^{N,K} A^{(h)}(wx) \right)
\end{aligned} \tag{2}$$

Second Term:

$$\begin{aligned}
& \frac{\partial}{\partial \tilde{c}_{Q,K}} \left[\sum_{LMN} \langle \tilde{M} | \hat{T}_{LM}^\dagger \hat{H} | \tilde{N} \rangle R_{LP}^* R_{NP} \right] \\
& = \sum_{LM} \langle \tilde{M} | \hat{T}_{LM}^\dagger \hat{H} | \tilde{K} \rangle R_{LP}^* R_{QP} + \sum_{LN} \langle \tilde{K} | \hat{T}_{LQ}^\dagger \hat{H} | \tilde{N} \rangle R_{LP}^* R_{NP} \\
& = \sum_L R_{LP}^* \left(R_{QP} \sum_{M,J} \langle \tilde{J} | \tilde{c}_{M,J}^\dagger \hat{T}_{LM}^\dagger \hat{H} | \tilde{K} \rangle + \sum_N R_{NP} \sum_I \langle \tilde{K} | \hat{T}_{LQ}^\dagger \hat{H} \tilde{c}_{N,I} | \tilde{I} \rangle \right)
\end{aligned} \tag{3}$$

$$\tag{4}$$

Third Term:

$$\begin{aligned}
& \frac{\partial}{\partial \tilde{c}_{Q,K}} \left[-E_s \sum_{LMN} \langle \tilde{M} | \hat{T}_{LM}^\dagger \hat{T}_{LN} | \tilde{N} \rangle R_{LP}^* R_{LP} \right] \\
&= -E_s \left(\sum_{LM} \langle \tilde{M} | \hat{T}_{LM}^\dagger \hat{T}_{LQ} | \tilde{K} \rangle + \sum_{LN} \langle \tilde{K} | \hat{T}_{LQ}^\dagger \hat{T}_{LN} | \tilde{N} \rangle \right) \\
&= -E_s \sum_L |R_{LP}^*|^2 \left(\sum_{M,J} \langle \tilde{J} | \tilde{c}_{M,J}^\dagger \hat{T}_{LM}^\dagger \hat{T}_{LQ} | \tilde{K} \rangle + \sum_{N,I} \langle \tilde{K} | \hat{T}_{LQ}^\dagger \hat{T}_{LN} \tilde{c}_{N,I} | \tilde{I} \rangle \right) \quad (5)
\end{aligned}$$

Fourth Term:

$$\begin{aligned}
& \frac{\partial}{\partial \tilde{c}_{Q,K}} \left[\sum_{LMN} \langle \tilde{M} | \hat{\lambda}_{LM}^\dagger (\hat{f} - \epsilon_L^{(0)} + \epsilon_s) \hat{T}_{LN} | \tilde{N} \rangle \right] \\
&= \sum_{LM} \langle \tilde{M} | \hat{\lambda}_{LM}^\dagger (\hat{f} - \epsilon_L^{(0)} + \epsilon_s) \hat{T}_{LQ} | \tilde{K} \rangle + \sum_{LN} \langle \tilde{K} | \hat{\lambda}_{LQ}^\dagger (\hat{f} - \epsilon_L^{(0)} + \epsilon_s) \hat{T}_{LN} | \tilde{N} \rangle \\
&\quad + \sum_{LMN} \langle \tilde{M} | \hat{\lambda}_{LM}^\dagger \left(\frac{\delta \hat{f}}{\delta \tilde{c}_{Q,K}} \right) \hat{T}_{LN} | \tilde{N} \rangle
\end{aligned}$$

Fifth Term:

$$\frac{\partial}{\partial \tilde{c}_{Q,K}} \left[\sum_{LM} \langle \tilde{M} | \hat{\lambda}_{LM}^\dagger \hat{H} | \tilde{L} \rangle \right] \quad (6)$$

$$\begin{aligned}
&= \sum_M \langle \tilde{M} | \hat{\lambda}_{LM}^\dagger \hat{H} | \tilde{K} \rangle + \sum_L \langle \tilde{K} | \hat{\lambda}_{LQ}^\dagger \hat{H} | \tilde{L} \rangle \\
&= \sum_{M,J} \langle \tilde{J} | \tilde{c}_{M,J}^\dagger \hat{\lambda}_{LM}^\dagger \hat{H} | \tilde{K} \rangle + \sum_{L,I} \langle \tilde{K} | \hat{\lambda}_{LQ}^\dagger \hat{H} \tilde{c}_{L,I} | \tilde{I} \rangle \quad (7)
\end{aligned}$$

$$\begin{aligned}
& \frac{\partial}{\partial \tilde{c}_K^Q} \left[\sum_{LMN} \langle \tilde{M} | \hat{T}_{LM}^\dagger \hat{H} | \tilde{N} \rangle R_{LP}^* R_{NP} \right] \\
&= \sum_L \left[\sum_M \sum_J \langle J | \tilde{c}_J^{M\dagger} \hat{T}_{LM}^\dagger \hat{H} | K \rangle R_{QP} + \sum_N \sum_I \langle K | \hat{T}_{LM}^\dagger \hat{H} \tilde{c}_I^N | I \rangle R_{NP} \right] R_{LP}^* \\
&\sum_L \left[\sum_M \sum_J \left(\langle J | \tilde{c}_J^{M\dagger} T_{LM,abcd}^\dagger (\hat{E}_{ab} \hat{E}_{cd} - \delta_{bc} \hat{E}_{ad}) (\hat{E}_{wx} \hat{E}_{yz} - \delta_{xy} \hat{E}_{wz}) g(1,2) | K \rangle + \right. \quad (8)
\end{aligned}$$

$$\left. \langle J | \tilde{c}_J^{M\dagger} T_{LM,abcd}^\dagger (\hat{E}_{ab} \hat{E}_{cd} - \delta_{bc} \hat{E}_{ad}) \hat{E}_{wx} h(1) | K \rangle \right) R_{QP} + \quad (9)$$

$$\sum_N \sum_I \left(\langle K | T_{LQ,abcd}^\dagger (\hat{E}_{ab} \hat{E}_{cd} - \delta_{bc} \hat{E}_{ad}) (\hat{E}_{wx} \hat{E}_{yz} - \delta_{xy} \hat{E}_{wz}) g(1,2) \tilde{c}_I^N | I \rangle \right. \quad (10)$$

$$\left. \langle K | T_{LQ,abcd}^\dagger (\hat{E}_{ab} \hat{E}_{cd} - \delta_{bc} \hat{E}_{ad}) \hat{E}_{wx} h(1) \tilde{c}_I^N | I \rangle \right) R_{NP} \Bigg] R_{LP}^* \quad (11)$$

$$(1) = \sum_M \sum_J$$