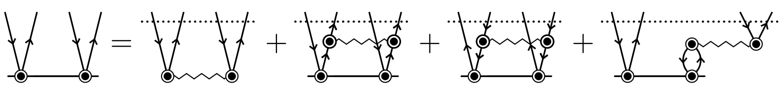
Extra Programming Project Theory
Spin-Integrated UCEPA$_0$

The spin-orbital CEPA0 amplitude equation is:

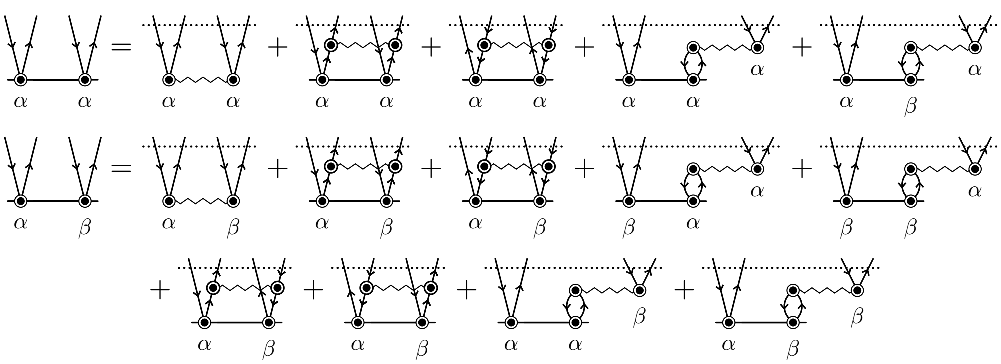
$$t^{ij}_{ab} = \mathcal{E}^{ij}_{ab}\left(\overline{g}^{ij}_{ab} + \tfrac{1}{2}\overline{g}^{cd}_{ab}t^{ij}_{cd} + \tfrac{1}{2}\overline{g}^{ij}_{kl}t^{kl}_{ab} + P^{(i/j)}_{(a/b)}\overline{g}^{ic}_{ak}t^{jk}_{bc}\right)$$



with implicit summation over k,l,c,d. Letting P,Q,R,S denote alpha spin-orbitals and $\overline{P},\overline{Q},\overline{R},\overline{S}$ denote beta spin-orbitals, we spin-integrate by fixing the external indices i,j,a,b to a particular spin block I,J,A,B or $I,\overline{J},A,\overline{B}$ and considering all non-vanishing cases for the remaining internal indices c,d,k,l of each term.

$$\begin{aligned}
t^{IJ}_{AB} &= \mathcal{E}^{IJ}_{AB}\left(\overline{g}^{IJ}_{AB} + \tfrac{1}{2}\overline{g}^{cd}_{AB}t^{IJ}_{cd} + \tfrac{1}{2}\overline{g}^{IJ}_{kl}t^{kl}_{AB} + P^{(I/J)}_{(A/B)}\overline{g}^{Ic}_{Ak}t^{Jk}_{Bc}\right)\\
&= \mathcal{E}^{IJ}_{AB}\left(\overline{g}^{IJ}_{AB} + \tfrac{1}{2}\overline{g}^{CD}_{AB}t^{IJ}_{CD} + \tfrac{1}{2}\overline{g}^{IJ}_{KL}t^{KL}_{AB} + P^{(I/J)}_{(A/B)}\overline{g}^{IC}_{AK}t^{JK}_{BC} + P^{(I/J)}_{(A/B)}\overline{g}^{I\overline{C}}_{A\overline{K}}t^{J\overline{K}}_{B\overline{C}}\right)\\
t^{I\overline{J}}_{A\overline{B}} &= \mathcal{E}^{I\overline{J}}_{A\overline{B}}\left(\overline{g}^{I\overline{J}}_{A\overline{B}} + \tfrac{1}{2}\overline{g}^{cd}_{A\overline{B}}t^{I\overline{J}}_{cd} + \tfrac{1}{2}\overline{g}^{I\overline{J}}_{kl}t^{kl}_{A\overline{B}} + P^{(I/\overline{J})}_{(A/\overline{B})}\overline{g}^{Ic}_{Ak}t^{\overline{J}k}_{\overline{B}c}\right)\\
&= \mathcal{E}^{I\overline{J}}_{A\overline{B}}\left(\overline{g}^{I\overline{J}}_{A\overline{B}} + \tfrac{1}{2}\overline{g}^{cd}_{A\overline{B}}t^{I\overline{J}}_{cd} + \tfrac{1}{2}\overline{g}^{I\overline{J}}_{kl}t^{kl}_{A\overline{B}} + \overline{g}^{Ic}_{Ak}t^{\overline{J}k}_{\overline{B}c} - \overline{g}^{\overline{J}c}_{Ak}t^{Ik}_{\overline{B}c} - \overline{g}^{Ic}_{\overline{B}k}t^{\overline{J}k}_{Ac} + \overline{g}^{\overline{J}c}_{\overline{B}k}t^{Ik}_{Ac}\right)\\
&= \mathcal{E}^{I\overline{J}}_{A\overline{B}}\left(\overline{g}^{I\overline{J}}_{A\overline{B}} + \overline{g}^{C\overline{D}}_{A\overline{B}}t^{I\overline{J}}_{C\overline{D}} + \overline{g}^{I\overline{J}}_{K\overline{L}}t^{K\overline{L}}_{A\overline{B}} + \overline{g}^{IC}_{AK}t^{\overline{J}K}_{\overline{B}C} + \overline{g}^{I\overline{C}}_{A\overline{K}}t^{\overline{JK}}_{\overline{BC}} - \overline{g}^{\overline{J}C}_{AK}t^{I\overline{K}}_{\overline{B}C} - \overline{g}^{I\overline{C}}_{\overline{B}K}t^{\overline{J}K}_{A\overline{C}} + \overline{g}^{\overline{J}C}_{\overline{B}K}t^{IK}_{AC} + \overline{g}^{\overline{JC}}_{\overline{BK}}t^{I\overline{K}}_{A\overline{C}}\right)\\
&= \mathcal{E}^{I\overline{J}}_{A\overline{B}}\left(\overline{g}^{I\overline{J}}_{A\overline{B}} + \overline{g}^{C\overline{D}}_{A\overline{B}}t^{I\overline{J}}_{C\overline{D}} + \overline{g}^{I\overline{J}}_{K\overline{L}}t^{K\overline{L}}_{A\overline{B}} + \overline{g}^{IC}_{AK}t^{\overline{J}K}_{\overline{B}C} + \overline{g}^{I\overline{C}}_{A\overline{K}}t^{\overline{JK}}_{\overline{BC}} - \overline{g}^{C\overline{J}}_{A\overline{K}}t^{I\overline{K}}_{C\overline{B}} - \overline{g}^{I\overline{C}}_{K\overline{B}}t^{K\overline{J}}_{A\overline{C}} + \overline{g}^{\overline{J}C}_{\overline{B}K}t^{IK}_{AC} + \overline{g}^{\overline{JC}}_{\overline{BK}}t^{I\overline{K}}_{A\overline{C}}\right)
\end{aligned}$$

Graphically, these equations can be expressed as follows.



Dropping overbars for the mixed-spin electron repulsion integrals, the final amplitude equations are

$$\begin{aligned}
t^{IJ}_{AB} &= \mathcal{E}^{IJ}_{AB}\left(\overline{g}^{IJ}_{AB} + \tfrac{1}{2}\overline{g}^{CD}_{AB}t^{IJ}_{CD} + \tfrac{1}{2}\overline{g}^{IJ}_{KL}t^{KL}_{AB} + P^{(I/J)}_{(A/B)}\overline{g}^{IC}_{AK}t^{JK}_{BC} + P^{(I/J)}_{(A/B)}g^{I\overline{C}}_{A\overline{K}}t^{J\overline{K}}_{B\overline{C}}\right)\\
t^{I\overline{J}}_{A\overline{B}} &= \mathcal{E}^{I\overline{J}}_{A\overline{B}}\left(g^{I\overline{J}}_{A\overline{B}} + g^{C\overline{D}}_{A\overline{B}}t^{I\overline{J}}_{C\overline{D}} + g^{I\overline{J}}_{K\overline{L}}t^{K\overline{L}}_{A\overline{B}} + \overline{g}^{IC}_{AK}t^{\overline{J}K}_{\overline{B}C} + g^{I\overline{C}}_{A\overline{K}}t^{\overline{JK}}_{\overline{BC}} - g^{C\overline{J}}_{A\overline{K}}t^{I\overline{K}}_{C\overline{B}} - g^{I\overline{C}}_{K\overline{B}}t^{K\overline{J}}_{A\overline{C}} + g^{\overline{J}C}_{\overline{B}K}t^{IK}_{AC} + \overline{g}^{\overline{JC}}_{\overline{BK}}t^{I\overline{K}}_{A\overline{C}}\right)\\
t^{\overline{IJ}}_{\overline{AB}} &= \mathcal{E}^{\overline{IJ}}_{\overline{AB}}\left(\overline{g}^{\overline{IJ}}_{\overline{AB}} + \tfrac{1}{2}\overline{g}^{\overline{CD}}_{\overline{AB}}t^{\overline{IJ}}_{\overline{CD}} + \tfrac{1}{2}\overline{g}^{\overline{IJ}}_{\overline{KL}}t^{\overline{KL}}_{\overline{AB}} + P^{(I/J)}_{(A/B)}\overline{g}^{\overline{IC}}_{\overline{AK}}t^{\overline{JK}}_{\overline{BC}} + P^{(I/J)}_{(A/B)}g^{\overline{I}C}_{\overline{A}K}t^{\overline{J}K}_{\overline{B}C}\right)\ .
\end{aligned}$$

Finally, expanding the energy expression $E_c = \frac{1}{4}\overline{g}^{ab}_{ij}t^{ij}_{ab}$ by spin blocks gives the following.

$$E_c = \tfrac{1}{4}\overline{g}^{AB}_{IJ}t^{IJ}_{AB} + g^{A\overline{B}}_{I\overline{J}}t^{I\overline{J}}_{A\overline{B}} + \tfrac{1}{4}\overline{g}^{\overline{AB}}_{\overline{IJ}}t^{\overline{IJ}}_{\overline{AB}}$$