Analytical Derivative

CNDO/2 energy:

$$E = \underbrace{\frac{1}{2}\sum_{\mu\nu} p^{\alpha}_{\mu\nu}\left(h_{\mu\nu} + f^{\alpha}_{\mu\nu}\right)} + \frac{1}{2}\sum_{\mu\nu} p^{\beta}_{\mu\nu}\left(h_{\mu\nu} + f^{\beta}_{\mu\nu}\right) + V_{nuc}$$

tricky component ⇒ find position derivative of this

AO indices

$$E^{\vec{R}_A} = \underbrace{\frac{1}{2}\left(\frac{\partial}{\partial \vec{R}_A}\sum_{\mu\nu} p^{\alpha}_{\mu\nu}\left(h_{\mu\nu} + f^{\alpha}_{\mu\nu}\right)\right)} + \text{other components}$$

derive this, and the β term is the same

$$\frac{\partial p^{\alpha}_{\mu\nu}}{\partial \vec{R}_A} = \vec{0},$$ since we force an "orthonormal" basis w/ $S = \mathbb{1}$

For same AO ($\mu\mu$):

$$h_{\mu\mu} = -\frac{1}{2}\left(I_\mu + A_\mu\right) + \left(Z_A - \frac{1}{2}\right)\gamma_{AA} - \sum_{B\neq A} Z_B \gamma_{AB}$$

$$\frac{\partial}{\partial \vec{R}_A} h_{\mu\mu} = -\frac{1}{2}\cancelto{0}{\frac{\partial}{\partial \vec{R}_A}\left(I_\mu + A_\mu\right)} + \left(Z_A - \frac{1}{2}\right)\cancelto{0}{\frac{\partial}{\partial \vec{R}_A}\gamma_{AA}} - \sum_{B\neq A} Z_B \gamma^{R_A}_{AB}$$

$\therefore$

$$\frac{\partial}{\partial \vec{R}_A} h_{\mu\mu} = -\sum_{B\neq A} Z_B \gamma^{R_A}_{AB}$$

$$f^{\alpha}_{\mu\mu} = -\frac{1}{2}(I_\mu + A_\mu) + \left[(p^{tot}_{AA} - Z_A) - (p^{\alpha}_{\mu\mu} - \tfrac{1}{2})\right]\gamma_{AA}$$

here, $\mu \in A$!!

$$+ \sum_{B \neq A} (p^{tot}_{BB} - Z_B)\gamma_{AB}$$

$$\frac{\partial}{\partial \vec{R}_A} f^{\alpha}_{\mu\mu} = \frac{\partial}{\partial \vec{R}_A}\left(-\frac{1}{2}(I_\mu + A_\mu)\right)^{0} + \frac{\partial}{\partial \vec{R}_A}\left(\left[(p^{tot}_{AA} - Z_A) - (p^{\alpha}_{\mu\mu} - \tfrac{1}{2})\right]\gamma_{AA}\right)^{0}$$

doesn't change when moving atom A

$$+ \frac{\partial}{\partial \vec{R}_A}\left(\sum_{B \neq A} (p^{tot}_{BB} - Z_B)\gamma_{AB}\right)$$

$$\frac{\partial}{\partial \vec{R}_A} f^{\alpha}_{\mu\mu} = \sum_{B \neq A} (p^{tot}_{BB} - Z_B)\underbrace{\gamma^{R_A}_{AB}}_{\text{gamma derivative}}$$

So now,

$$\frac{1}{2}\left(\frac{\partial}{\partial \vec{R}_A}\sum_{\mu\mu} p^{\alpha}_{\mu\mu}\left(h_{\mu\mu} + f^{\alpha}_{\mu\mu}\right)\right) \Rightarrow \text{for the } \mu\mu \text{ elements}$$

$$\Downarrow$$

$$\frac{1}{2}\sum_{\mu} p^{\alpha}_{\mu\mu}\left(-\sum_{B \neq A} Z_B \gamma^{R_A}_{AB} + \sum_{B \neq A}(p^{tot}_{BB} - Z_B)\gamma^{R_A}_{AB}\right)$$

$$= \frac{1}{2}\sum_{\mu \in A} p^{\alpha}_{\mu\mu}\left(\sum_{B \neq A}(p^{tot}_{BB} - 2Z_B)\gamma^{R_A}_{AB}\right)$$

Here, it's important to remember $\mu \in A$!

if $\mu \in B$, it would be flipped $\Rightarrow$ p^{tot}_{AA}, Z_A, & $\gamma^{R_A}_{BA}$

For different AO ($\mu\nu$):

$$h_{\mu\nu} = \frac{1}{2}(\beta_A + \beta_B) S_{\mu\nu}$$

$$f_{\mu\nu}^{\alpha} = \frac{1}{2}(\beta_A + \beta_B) S_{\mu\nu} - P_{\mu\nu}^{\alpha} \gamma_{AB}$$

$$\frac{\partial}{\partial \vec{R}_A} h_{\mu\nu} = \frac{1}{2}(\beta_A + \beta_B) \underbrace{S_{\mu\nu}^{R_A}}_{\text{overlap element derivative}}$$

$$\frac{\partial}{\partial \vec{R}_A} f_{\mu\nu}^{\alpha} = \frac{1}{2}(\beta_A + \beta_B) \underbrace{S_{\mu\nu}^{R_A}}_{\text{overlap element derivative}} - P_{\mu\nu}^{\alpha} \underbrace{\gamma_{AB}^{R_A}}_{\text{gamma derivative}}$$

$\mu \in A$, $\nu \in B$! Key! & $A \neq B$!

Since there are off-diagonal components, $\mu \neq \nu$

So,

$$\frac{1}{2}\left(\frac{\partial}{\partial \vec{R}_A} \sum_{\substack{\cancel{\mu\neq\nu} \\ \mu\in A,\, \nu\in B,\, A\neq B}} P_{\mu\nu}^{\alpha}\left(h_{\mu\nu} + f_{\mu\nu}^{\alpha}\right)\right)$$

$$= \frac{1}{2} \sum_{\mu\neq\nu} P_{\mu\nu}^{\alpha}\left((\beta_A + \beta_B) S_{\mu\nu}^{R_A} - P_{\mu\nu}^{\alpha} \gamma_{AB}^{R_A}\right)$$

$\mu \in A$, $\nu \in B$, $A \neq B$ ⟸ flipped if $\mu \in B$, tho that doesn't affect anything

Altogether, let's look at what we have:

$$E = \frac{1}{2}\sum_{\mu\nu} P_{\mu\nu}^{\alpha}\left(h_{\mu\nu} + f_{\mu\nu}^{\alpha}\right) + \frac{1}{2}\sum_{\mu\nu} P_{\mu\nu}^{\beta}\left(h_{\mu\nu} + f_{\mu\nu}^{\beta}\right)$$

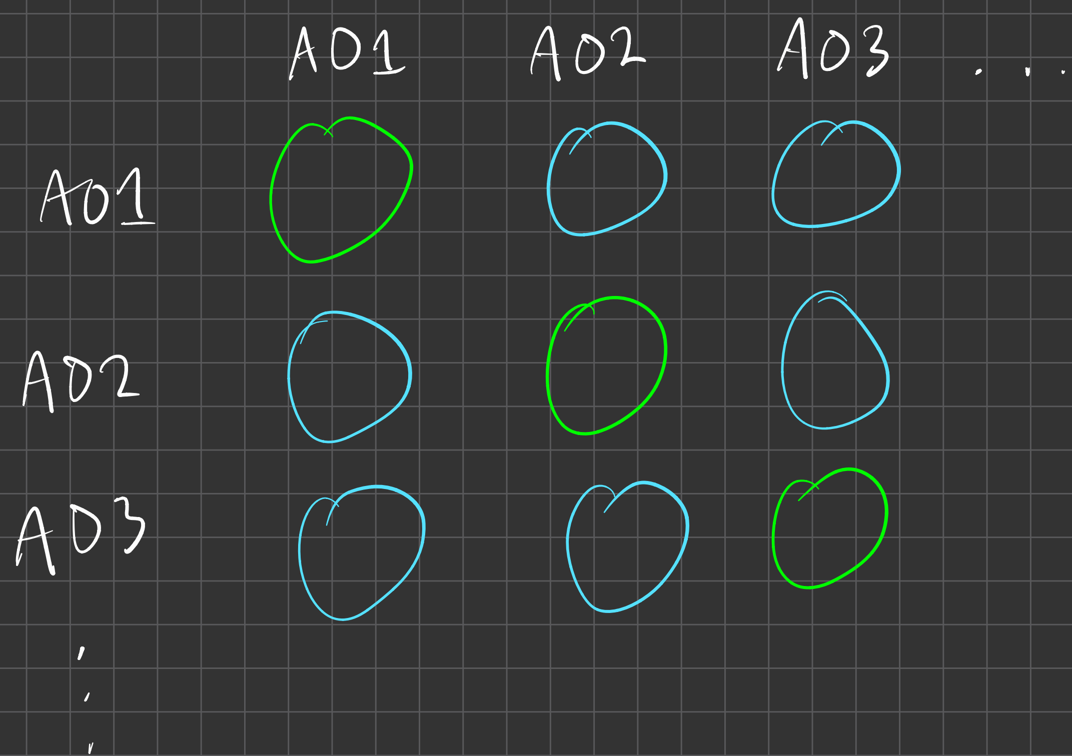
$$+ V_{nuc}$$

The derivative:

$$\frac{\partial}{\partial \vec{R}_A}\left(\frac{1}{2}\sum_{\mu\nu} P^{\alpha}_{\mu\nu}\left(h_{\mu\nu}+f^{\alpha}_{\mu\nu}\right)\right)$$

note it's a summation over all combos of μ, ν

Visualizing the matrices



$\mu\mu$ terms $\Downarrow$ $\sum_{\mu}$

$\mu\nu$ terms $\Downarrow$ $\sum_{\mu\neq\nu}$

so,

$$\frac{\partial}{\partial \vec{R}_A}\left(\frac{1}{2}\sum_{\mu\nu} P^{\alpha}_{\mu\nu}\left(h_{\mu\nu}+f^{\alpha}_{\mu\nu}\right)\right) = \frac{1}{2}\sum_{\mu\nu} P^{\alpha}_{\mu\nu}\overbrace{\left(h^{R_A}_{\mu\nu}+f^{\alpha,R_A}_{\mu\nu}\right)}^{\text{derivatives}}$$

$$= \frac{1}{2}\left(\underbrace{\sum_{\mu\mu}+\sum_{\mu\neq\nu}}\right) P^{\alpha}_{\mu\nu}\left(h^{R_A}_{\mu\nu}+f^{\alpha,R_A}_{\mu\nu}\right)$$

captures unnecessary terms tho!

Note that h^{R_A}, f^{R_A} contain dependence on atoms A, B, so we can split sum differently

$\nu \downarrow$ \ $\mu \rightarrow$	AO1 (On atom A)	AO2 (On atom B)	AO3 (On atom B)
AO1	$\mu \in A, \nu = \mu$	$\nu \in A, \mu \in B \neq A$	
AO2	$\mu \in A, \nu \in B \neq A$	$\mu \in B \neq A, \nu = \mu$	$\varnothing$
AO3		$\varnothing$	$\mu \in B \neq A, \nu = \mu$

for the derivative w/respect to R_A!

affected by R_A b/c diagonal fock & H_core elements include $\sum_{B \neq A}$ component

unaffected by movement of A! (off-diagonals for fock & h_core only depend on A & B (no $\sum_{B\neq A}$))

So really, we can write:

$$= \frac{1}{2}\Big(\underbrace{\overset{①}{\sum_{\substack{\mu\in A,\\ \nu=\mu}}} + \overset{②}{\sum_{\substack{\mu\in B\neq A,\\ \nu=\mu}}}}_{\text{diagonals}} + \underbrace{\overset{③}{\sum_{\substack{\nu\in A,\\ \mu\in B\neq A}}} + \overset{④}{\sum_{\substack{\mu\in A,\\ \nu\in B\neq A}}}}_{\text{nonzero off diagonals}}\Big) P^{\alpha}_{\mu\nu}\left(h^{R_A}_{\mu\nu} + f^{\alpha, R_A}_{\mu\nu}\right)$$

① $$\sum_{\substack{\mu\in A,\\ \nu=\mu}} P^{\alpha}_{\mu\nu}\left(h^{R_A}_{\mu\nu} + f^{\alpha, R_A}_{\mu\nu}\right) = \sum_{\substack{\mu\in A,\\ \nu=\mu}} P^{\alpha}_{\mu\nu}\left(\sum_{B\neq A}\left(P^{tot}_{BB} - 2Z_B\right)\gamma^{R_A}_{AB}\right)$$

Diagonals, $\mu = \nu$

② $$\sum_{\substack{\mu\in B\neq A,\\ \nu=\mu}} P^{\alpha}_{\mu\nu}\left(h^{R_A}_{\mu\nu} + f^{\alpha, R_A}_{\mu\nu}\right) = \sum_{\substack{\mu\in B\neq A,\\ \nu=\mu}} P^{\alpha}_{\mu\nu}\left(\underbrace{\sum_{A\neq B}\left(P^{tot}_{AA} - 2Z_A\right)}\gamma^{R_A}_{BA}\right)$$

Diagonals, $\mu = \nu$

need to flip/sum over atoms $\neq B$, b/c we're on B atom AO diagonal!

from $P_{BB} \rightarrow P_{AA}$

3. $$\sum_{\substack{\nu\in A,\\ \mu\in B\neq A}} p_{\mu\nu}^{\alpha}\left(h_{\mu\nu}^{R_A}+f_{\mu\nu}^{\alpha,R_A}\right) = \sum_{\substack{\nu\in A,\\ \mu\in B\neq A}} p_{\mu\nu}^{\alpha}\left((\beta_A+\beta_B)\,S_{\mu\nu}^{R_A} - p_{\mu\nu}^{\alpha}\gamma_{\underbrace{BA}_{\text{b/c } \mu\in B}}^{R_A}\right)$$

off-diagonals, $\mu\neq\nu$

4. $$\sum_{\substack{\mu\in A,\\ \nu\in B\neq A}} p_{\mu\nu}^{\alpha}\left(h_{\mu\nu}^{R_A}+f_{\mu\nu}^{\alpha,R_A}\right) = \sum_{\substack{\mu\in A,\\ \nu\in B\neq A}} p_{\mu\nu}^{\alpha}\left((\beta_A+\beta_B)\,S_{\mu\nu}^{R_A} - p_{\mu\nu}^{\alpha}\gamma_{AB}^{R_A}\right)$$

off-diagonals, $\mu\neq\nu$

Adding in β elements for each of 1-4:

1. $$\sum_{\substack{\mu\in A,\\ \nu=\mu}} p_{\mu\nu}^{\alpha}\left(\sum_{B\neq A}(p_{BB}^{tot}-2Z_B)\,\gamma_{AB}^{R_A}\right) + \sum_{\substack{\mu\in A,\\ \nu=\mu}} p_{\mu\nu}^{\beta}\left(\sum_{B\neq A}(p_{BB}^{tot}-2Z_B)\,\gamma_{AB}^{R_A}\right)$$

Diagonals, $\mu=\nu$

$p_{\mu\nu}^{\alpha}+p_{\mu\nu}^{\beta}=p_{\mu\nu}^{tot}$

$$= \sum_{\substack{\mu\in A,\\ \nu=\mu}} p_{\mu\nu}^{tot}\left(\sum_{B\neq A}(p_{BB}^{tot}-2Z_B)\,\gamma_{AB}^{R_A}\right)$$

Similarly,

2. $$\sum_{\substack{\mu\in B\neq A,\\ \nu=\mu}} p_{\mu\nu}^{\alpha}\left(h_{\mu\nu}^{R_A}+f_{\mu\nu}^{\alpha,R_A}\right) + \sum_{\substack{\mu\in B\neq A,\\ \nu=\mu}} p_{\mu\nu}^{\beta}\left(h_{\mu\nu}^{R_A}+f_{\mu\nu}^{\beta,R_A}\right)$$

Diagonals, $\mu=\nu$

$$= \sum_{\substack{\mu\in B\neq A,\\ \nu=\mu}} p_{\mu\nu}^{tot}\left(\sum_{A\neq B}(p_{AA}^{tot}-2Z_A)\,\gamma_{AB}^{R_A}\right)$$

$\gamma_{BA}^{R_A}=\gamma_{AB}^{R_A}$
(symmetric matrix)

3

$$\sum_{\substack{\nu\in A,\\ \mu\in B\neq A}} P_{\mu\nu}^{\alpha}\left((\beta_A+\beta_B)\, S_{\mu\nu}^{R_A} - P_{\mu\nu}^{\alpha}\,\gamma_{BA}^{R_A}\right) + \sum_{\substack{\nu\in A,\\ \mu\in B\neq A}} P_{\mu\nu}^{\beta}\left((\beta_A+\beta_B)\, S_{\mu\nu}^{R_A} - P_{\mu\nu}^{\beta}\,\gamma_{BA}^{R_A}\right)$$

off-diagonals, $\mu\neq\nu$

$$= \sum_{\substack{\nu\in A,\\ \mu\in B\neq A}} P_{\mu\nu}^{\alpha}(\beta_A+\beta_B)\, \underline{S_{\mu\nu}}^{R_A} - P_{\mu\nu}^{\alpha}P_{\mu\nu}^{\alpha}\,\gamma_{\underline{BA}}^{R_A} + P_{\mu\nu}^{\beta}(\beta_A+\beta_B)\, \underline{S_{\mu\nu}}^{R_A} - P_{\mu\nu}^{\beta}P_{\mu\nu}^{\beta}\,\gamma_{\underline{BA}}^{R_A}$$

$\gamma_{BA}^{R_A} = \gamma_{AB}^{R_A}$
(symmetric matrix)

$$= \sum_{\substack{\nu\in A,\\ \mu\in B\neq A}} P_{\mu\nu}^{tot}(\beta_A+\beta_B)\, S_{\mu\nu}^{R_A} - \left(P_{\mu\nu}^{\alpha}P_{\mu\nu}^{\alpha} + P_{\mu\nu}^{\beta}P_{\mu\nu}^{\beta}\right)\gamma_{AB}^{R_A}$$

Similarly,

4

$$\sum_{\substack{\mu\in A,\\ \nu\in B\neq A}} P_{\mu\nu}^{\alpha}\left((\beta_A+\beta_B)\, S_{\mu\nu}^{R_A} - P_{\mu\nu}^{\alpha}\,\gamma_{BA}^{R_A}\right) + \sum_{\substack{\mu\in A,\\ \nu\in B\neq A}} P_{\mu\nu}^{\beta}\left((\beta_A+\beta_B)\, S_{\mu\nu}^{R_A} - P_{\mu\nu}^{\beta}\,\gamma_{BA}^{R_A}\right)$$

off-diagonals, $\mu\neq\nu$

$$= \sum_{\substack{\mu\in A,\\ \nu\in B\neq A}} P_{\mu\nu}^{tot}(\beta_A+\beta_B)\, S_{\mu\nu}^{R_A} - \left(P_{\mu\nu}^{\alpha}P_{\mu\nu}^{\alpha} + P_{\mu\nu}^{\beta}P_{\mu\nu}^{\beta}\right)\gamma_{AB}^{R_A}$$

<u>Provided Form:</u>

$$E^{R_A} = \sum_{\mu\neq\nu} X_{\mu\nu}\, \underline{S_{\mu\nu}}^{R_A} + \sum_{B\neq A} Y_{AB}\, \underline{\gamma_{AB}}^{R_A} + V_{nuc}^{R_A}$$

Overall what we have so far:

$$E^{R_A} = \frac{1}{2}\left(1 + 2 + 3 + 4\right) + V_{nuc}^{R_A}$$

$$= \frac{1}{2}\Bigg[\sum_{\substack{\mu\in A,\\ \nu=\mu}} P^{tot}_{\mu\nu}\left(\sum_{B\neq A}\left(P^{tot}_{BB} - 2Z_B\right)\gamma^{R_A}_{AB}\right) + \sum_{\substack{\mu\in B\neq A,\\ \nu=\mu}} P^{tot}_{\mu\nu}\left(\sum_{A\neq B}\left(P^{tot}_{AA} - 2Z_A\right)\gamma^{R_A}_{BA}\right)$$

$$+ \sum_{\substack{\nu\in A,\\ \mu\in B\neq A}} P^{tot}_{\mu\nu}(\beta_A+\beta_B)\, S^{R_A}_{\mu\nu} - \left(P^{\alpha}_{\mu\nu}P^{\alpha}_{\mu\nu} + P^{\beta}_{\mu\nu}P^{\beta}_{\mu\nu}\right)\gamma^{R_A}_{AB}$$

$$+ \sum_{\substack{\mu\in A,\\ \nu\in B\neq A}} P^{tot}_{\mu\nu}(\beta_A+\beta_B)\, S^{R_A}_{\mu\nu} - \left(P^{\alpha}_{\mu\nu}P^{\alpha}_{\mu\nu} + P^{\beta}_{\mu\nu}P^{\beta}_{\mu\nu}\right)\gamma^{R_A}_{AB}\Bigg] + V^{R_A}_{nuc}$$

Deriving $\chi_{\mu\nu}$: Taking just $S^{R_A}_{\mu\nu}$ components

$$\frac{1}{2}\Bigg[\sum_{\substack{\nu\in A,\\ \mu\in B\neq A}} P^{tot}_{\mu\nu}(\beta_A+\beta_B)\, S^{R_A}_{\mu\nu} + \sum_{\substack{\mu\in A,\\ \nu\in B\neq A}} P^{tot}_{\mu\nu}(\beta_A+\beta_B)\, S^{R_A}_{\mu\nu}\Bigg]$$

really just $\mu\neq\nu$, but $S^{R_A}_{\mu\nu} = 0$ for $\mu,\nu \notin A$ ("re-introduce" zero terms for writing it out)

$$= \sum_{\substack{\mu\neq\nu\\ \mu\in A,\, \nu\in B}} \cancel{\tfrac{1}{2}}\left(\cancel{2}\, P^{tot}_{\mu\nu}\,(\beta_A+\beta_B)\right) S^{R_A}_{\mu\nu}$$

$$\therefore\ \boxed{\chi_{\mu\nu} = (\beta_A+\beta_B)\,P^{tot}_{\mu\nu}}$$ in summation s.t. $\mu\in A$, $\nu\in B\neq A$

Deriving y_{AB}: Taking just $\gamma^{R_A}_{AB}$ components

*Remember it's a derivative w/respect to A!

$$\frac{1}{2}\left[\sum_{\substack{\mu\in A\\ \nu=\mu}} P^{tot}_{\mu\nu}\left(\boxed{\sum_{B\neq A}\left(P^{tot}_{BB}-2Z_B\right)\gamma^{R_A}_{AB}}\right) + \sum_{\substack{\mu\in B\neq A,\\ \nu=\mu}} P^{tot}_{\mu\nu}\left(\sum_{A\neq B}\left(P^{tot}_{AA}-2Z_A\right)\gamma^{R_A}_{BA}\right)\right.$$

ind. of μ,ν, can pull out of sum

diagonal components

$$\left.+\sum_{\substack{\nu\in A,\\ \mu\in B\neq A}} -\left(P^{\alpha}_{\mu\nu}P^{\alpha}_{\mu\nu}+P^{\beta}_{\mu\nu}P^{\beta}_{\mu\nu}\right)\gamma^{R_A}_{AB} + \sum_{\substack{\mu\in A,\\ \nu\in B\neq A}} -\left(P^{\alpha}_{\mu\nu}P^{\alpha}_{\mu\nu}+P^{\beta}_{\mu\nu}P^{\beta}_{\mu\nu}\right)\gamma^{R_A}_{AB}\right]$$

off-diagonal components

$$=\frac{1}{2}\left[\sum_{B\neq A}\left(P^{tot}_{BB}-2Z_B\right)\gamma^{R_A}_{AB}\overbrace{\underbrace{\sum_{\substack{\mu\in A\\ \nu=\mu}} P^{tot}_{\mu\nu}}_{P^{tot}_{AA}}}^{\text{total density on atom A}} + \sum_{A\neq B}\left(P^{tot}_{AA}-2Z_A\right)\gamma^{R_A}_{BA}\overbrace{\underbrace{\sum_{\substack{\mu\in B\neq A,\\ \nu=\mu}} P^{tot}_{\mu\nu}}_{P^{tot}_{BB}}}^{\text{total density on atom B}}\right.$$

$$\left.-\underbrace{\left(\sum_{\substack{\nu\in A,\\ \mu\in B\neq A}}+\sum_{\substack{\mu\in A,\\ \nu\in B\neq A}}\right)}_{\text{captures all non-zero off-diagonal elements where } B\neq A}\left(P^{\alpha}_{\mu\nu}P^{\alpha}_{\mu\nu}+P^{\beta}_{\mu\nu}P^{\beta}_{\mu\nu}\right)\gamma^{R_A}_{AB}\right]$$

captures all non-zero off-diagonal elements where $B\neq A$ ⟵ but double counts! ⟶ $\sum_{\substack{\nu\in A,\\ \mu\in B\neq A}} = \sum_{B\neq A}\sum_{\mu\neq\nu}$!

simplify to $2\sum_{B\neq A}\sum_{\mu\neq\nu}$ ($\gamma^{R_A}_{AB}=0$ for zero elements)

$$=\frac{1}{2}\left[\sum_{B\neq A}\left(P^{tot}_{BB}-2Z_B\right)\gamma^{R_A}_{AB}P^{tot}_{AA} + \sum_{A\neq B}\left(P^{tot}_{AA}-2Z_A\right)\gamma^{R_A}_{BA}P^{tot}_{BB}\right.$$

$$\left.-2\sum_{B\neq A}\sum_{\mu\neq\nu}\left(P^{\alpha}_{\mu\nu}P^{\alpha}_{\mu\nu}+P^{\beta}_{\mu\nu}P^{\beta}_{\mu\nu}\right)\gamma^{R_A}_{AB}\right]$$

Combine sums!

$$= \frac{1}{2}\sum_{B\neq A}\left[\left(P_{BB}^{tot} - 2Z_B\right)P_{AA}^{tot} + \left(P_{AA}^{tot} - 2Z_A\right)P_{BB}^{tot} - 2\sum_{\mu\neq\nu}\left(P_{\mu\nu}^{\alpha}P_{\mu\nu}^{\alpha} + P_{\mu\nu}^{\beta}P_{\mu\nu}^{\beta}\right)\right]\gamma_{AB}^{R_A}$$

$$= \frac{1}{2}\sum_{B\neq A}\left[2P_{AA}^{tot}P_{BB}^{tot} - 2P_{AA}^{tot}Z_B - 2P_{BB}^{tot}Z_A - \sum_{\mu\neq\nu}\left(P_{\mu\nu}^{\alpha}P_{\mu\nu}^{\alpha} + P_{\mu\nu}^{\beta}P_{\mu\nu}^{\beta}\right)\right]\gamma_{AB}^{R_A}$$

$$= \sum_{B\neq A}\underbrace{\left[P_{AA}^{tot}P_{BB}^{tot} - P_{AA}^{tot}Z_B - P_{BB}^{tot}Z_A - \sum_{\mu\neq\nu}\left(P_{\mu\nu}^{\alpha}P_{\mu\nu}^{\alpha} + P_{\mu\nu}^{\beta}P_{\mu\nu}^{\beta}\right)\right]}_{Y_{AB}!}\gamma_{AB}^{R_A}$$

$\therefore$

$$Y_{AB} = P_{AA}^{tot}P_{BB}^{tot} - P_{AA}^{tot}Z_B - P_{BB}^{tot}Z_A - \sum_{\mu\neq\nu}\left(P_{\mu\nu}^{\alpha}P_{\mu\nu}^{\alpha} + P_{\mu\nu}^{\beta}P_{\mu\nu}^{\beta}\right)$$