

γ_{AB} Matrix

$$\frac{1}{2} \sum_{\mu\nu} p_{\mu\nu}^{\alpha} (H_{\mu\nu} + F_{\mu\nu}^{\alpha}) + \frac{1}{2} \sum_{\mu\nu} p_{\mu\nu}^{\beta} (H_{\mu\nu} + F_{\mu\nu}^{\beta}) + \text{Nuclear v/t } \gamma \text{ s drop terms}$$

$\downarrow \quad \downarrow$

for off diagonals $H_{\mu\nu}$ doesn't have γ_{AB} component so drops out

$$\rightarrow F_{\mu\nu}^{\alpha} = p_{\mu\nu}^{\alpha} \gamma_{AB}$$

$$\frac{1}{2} \sum_{\mu\nu} p_{\mu\nu}^{\alpha} (p_{\mu\nu}^{\alpha} \gamma_{AB}) + \frac{1}{2} \sum_{\mu\nu} p_{\mu\nu}^{\beta} (p_{\mu\nu}^{\beta} \gamma_{AB})$$

$$\sum_{\mu\nu} p_{\mu\nu}^{\alpha^2} \gamma_{AB} + \sum_{\mu\nu} p_{\mu\nu}^{\beta^2} \gamma_{AB} = \boxed{\sum_{\mu\nu} (p_{\mu\nu}^{\alpha^2} + p_{\mu\nu}^{\beta^2})} \frac{\partial}{\partial \gamma_{AB}}$$

term #1 for γ_{AB}

for on-diagonal terms

$$\frac{1}{2} \sum P^{\alpha} (H + F^{\alpha}) + \frac{1}{2} \sum P^{\beta} (H + F^{\beta})$$

now H and F have γ_{AB} terms

swapped F and H by accident!
drop all γ_{AA} terms too

$$\frac{1}{2} \sum P^{\alpha} (\cancel{H} + \sum_{B \neq A} (P_{BB} - Z_B) \gamma_{AB} + \sum Z_B \gamma_{AB}) + \frac{1}{2} \sum P^{\beta} (\cancel{H} + \sum_{B \neq A} (P_{AA} - Z_A) \gamma_{AB} + \sum Z_A \gamma_{AB})$$

Summing over $\mu \nu$ pair
is equivalent to P_{AA} since it ends
up being the total density of
all N

same for
 $\sum P^{\beta} \rightarrow P_{BB}$

$$P_{AA} (\sum_{A \neq B} (P_{BB} - Z_B) \gamma_{AB} + \sum_{A \neq B} Z_B \gamma_{AB}) + P_{BB} (\sum_{A \neq B} (P_{AA} - Z_A) \gamma_{AB} + \sum_{A \neq B} Z_A \gamma_{AB})$$

change
on atom B
seen by atom A?

reverses?

I'm really
not sure...
guess and
check
from
here...

$$\begin{aligned} & \frac{1}{2} P_{AA} Z_B & \frac{1}{2} P_{AA} P_{BB} & \frac{1}{2} P_{AA} Z_B & \frac{1}{2} P_{BB} P_{AA} & \frac{1}{2} P_{BB} Z_A & \frac{1}{2} P_{BB} Z_A \\ & & & & + P_{BB} P_{AA} & = P_{BB} Z_A & - P_{AA} Z_B & + \text{term \#1} \end{aligned}$$