

Ex | ①

Contraction is written such that lower case is the target index w/
pair ij while upper case is those that are not such as pair kl
Ex | ②

P2 referring to first line of code w/in count-old for double residual

First term $0.5 * \langle a_{ij} | \bar{a}_{ij} \bar{b}_{ij} \rangle$

Second term $\sum_{\bar{e}_{ij}} T_{\bar{a}_{ij} \bar{e}_{ij}}^m F_{\bar{b}_{ij} \bar{e}_{ij}}$

Third term *contracted in MO basis then transform to semicanonical
local since it involved single amplitude

$\sum_m t_b^m F_{me} \rightarrow x_{b_{ij}}^{e_{ij}}$ placeholder variable

Fourth term $\sum_{\bar{e}_{ij}} T_{\bar{a}_{ij} \bar{e}_{ij}}^{ij} x_{\bar{b}_{ij}}^{e_{ij}}$

Fifth term $\sum_{mj} S_{ij, jm}^{ij, jm} T_{\bar{a}_{jm} \bar{b}_{im}}^{im} S_{ij, im}^{ij, im} F_{mj}$

Sixth Term * same reasoning as third term

$- \sum_e t_e^j F_{me} \rightarrow x_m^j$

Seventh Term $-0.5 S_{ij, am}^{ij, am} T_{\bar{a}_{am} \bar{b}_{im}}^{im} S_{ij, im}^{ij, im} x_m^j$

$$\text{Eight Term} \quad \sum_{mn} S^{ij,mn} \quad \begin{matrix} \textcircled{a} \\ \textcircled{b} \end{matrix} \quad \begin{matrix} \textcircled{A} \\ \textcircled{B} \end{matrix} +$$

$$x^{\frac{mn}{\bar{a}_{mn} \bar{b}_{mn}}} \quad S^{ij,mn} \quad w_{mnij}$$

$$\begin{matrix} \textcircled{a} \\ \textcircled{b} \end{matrix} \quad \begin{matrix} \textcircled{A} \\ \textcircled{B} \end{matrix}$$

$$\text{Ninth Term} \quad \sum_{\bar{e}_{ij} \bar{f}_{ij}} x^{\frac{ij}{\bar{e}_{ij} \bar{f}_{ij}}} \quad \begin{matrix} \textcircled{a} \\ \textcircled{b} \\ \textcircled{c} \\ \textcircled{d} \end{matrix} \quad \begin{matrix} \textcircled{A} \\ \textcircled{B} \\ \textcircled{C} \\ \textcircled{D} \end{matrix}$$

$$w_{\bar{e}_{ij} \bar{f}_{ij}} \bar{b}_{ij} \bar{e}_{ij} \bar{f}_{ij}$$

$$\begin{matrix} \textcircled{e} \\ \textcircled{f} \end{matrix}$$

Still working w/ the rest of the Terms

$\bar{f}_{\bar{a}y \bar{e}y}$

referring to variables in locfun-test which corresponds to cowlfn-old

Fac term

$\bar{f}_{\bar{a}y \bar{e}y}$

$$\text{Fac1 term} - 0.5 \sum_m \bar{s}_{ij,mm}^{\textcircled{E} \textcircled{F}} f_{\bar{e},mm}^m t_{\bar{a},mm}^m \bar{s}_{ij,mm}^{\textcircled{A} \textcircled{B}} +$$

$\textcircled{E} \quad \textcircled{A}$

$$\text{Fac2 term} \sum_{m\bar{f}mm} \bar{t}_{\bar{f}mm}^m - L_{m\bar{a}y} \bar{f}_{\bar{a}y} \bar{s}_{ij,mm}^{\textcircled{A} \textcircled{D} \textcircled{C} \textcircled{E} \textcircled{F}}$$

\textcircled{F}

Fac3 term not working for now, I thought this would work:

$$- \sum_{mn\bar{f}mn} \bar{s}_{ij,mn}^{\textcircled{A} \textcircled{B}} \bar{x}_{\bar{a}mn\bar{f}mn}^{mn} L_{mn\bar{e}y} \bar{f}_{\bar{e}y} \bar{s}_{ij,mn}^{\textcircled{D} \textcircled{F}}$$

$\textcircled{A} \textcircled{F}$

Wm̄b̄ȳēȳj̄

Wm̄b̄ȳj̄ = m̄b̄ȳ | ēȳj̄

Working progress

Wm̄b̄ȳj̄ - $\sum_{f_{jj}} t_{\bar{f}_{jj}}^{\delta} < m̄b̄ȳ | \bar{e}_{yj} f_{yj} > s^{y, jj}$ (b) (e) (f) (F) (E)

Wm̄b̄ȳj̄ - $\sum_n s^{y, nn} t_{\bar{b}_{nn}}^n < m_{nn} | \bar{e}_{yj} j >$ (b) (B) (e)

my issue w/
implementation

Wm̄b̄ȳj̄ - $\sum_{nf_{jn}} \tilde{t}_{\bar{f}_{jn}}^{jn} s^{y, jn} + < m_{jn} | \bar{e}_{jn} \bar{f}_{jn} > s^{y, jn}$ (b) (B) (e) (E) + (F) (B) (D) (F)

Wm̄b̄ȳj̄ 0.5 $\sum_{n\bar{f}_{ay}} \tilde{t}_{\bar{f}_{ay}}^{ny} s^{y, ny} + < m_{ny} | \bar{e}_{ny} \bar{f}_{ny} > s^{y, ny}$ (b) (B) + (F) (B) (e) (E) +