Correlated Trial Wave Function

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Correlated Trial Wave Function

$$\langle \Psi_T | \mathrm{RS} \rangle = \langle \Phi | \prod_{i<j} \left[f_c(r_{ij}) \left[1 + f_p(r_{ij}) \mathcal{O}^p_{ij} \right] \right] | \mathrm{RS} \rangle \tag{1}$$

- This does not obey cluster decomposition because if you exchange two particles it changes who the operators operate on. A fully cluster decomposable correlated wave function could look like an exponential

$$|\Psi\rangle = e^{\mathcal{O}_{corr}} |\Psi_0\rangle \tag{2}$$

where $\mathcal{O}_{corr} = \mathcal{O}_{corr1} + \ldots + \mathcal{O}_{corrA}$.

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$$\langle \Psi_T | \mathrm{RS} \rangle = \langle \Phi | \left[\prod_{i<j} f_c(r_{ij}) \right] \left[1 + \sum_{i<j,p} f_p(r_{ij}) \mathcal{O}^p_{ij} \right] | \mathrm{RS} \rangle \tag{2}$$

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$$\begin{aligned} \langle \Psi_T | \mathrm{RS} \rangle = \langle \Phi | \left[\prod_{i<j} f_c(r_{ij}) \right] & \left[1 + \sum_{i<j,p} f_p(r_{ij}) \mathcal{O}^p_{ij} \right. \\ & \left. + \sum_{i<j,p} \sum_{\substack{k<l \\ \text{indpair?}}} f_p(r_{ij}) \mathcal{O}^p_{ij} f_p(r_{kl}) \mathcal{O}^p_{kl} \right] | \mathrm{RS} \rangle \end{aligned} \tag{3}$$

Independent Pair

- Independent pair sum looks like this.

$$\sum_{\substack{k<l \\ \text{indpair}}} \rightarrow \sum_{\substack{k<l \\ k,l\neq i,j \\ k,l>i,j}} \tag{4}$$

- This will give us insight into how much the correlations from different sets of particle effect the energy.

Method

- Correlation terms are currently calculated in the code as

$$\frac{\langle \Psi_T | \mathrm{RS} \rangle}{\langle \Phi | RS \rangle} = \mathrm{sum}(\mathrm{d2b} * \mathrm{f2b}) \tag{5}$$

where the d2b and f2b look like

$$\mathrm{d2b}(s, s', ij) = \frac{\langle \Phi | R, s_1, \ldots, s_{i-1}, s, s_{i+1}, \ldots, s_{j-1}, s', s_{j+1}, \ldots, s_A \rangle}{\langle \Phi | R, S \rangle} \tag{6}$$

$$\mathrm{f2b}(s, s', ij) = \left\langle s, s' \right| \mathcal{O}^p_{ij} \left| s_i, s_j \right\rangle \tag{7}$$

Method

- Now everywhere that we calculate d2b(s, s', ij) we will need to calculate d2b$(s, s', s'', s''', ij, kl)$ and the corresponding f2b$(s, s', s'', s''', ij, kl)$ for the independent pair terms.