Correlated Trial Wave Function

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Correlated Trial Wave Function

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

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

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

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

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

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.