

Correlated Trial Wave Function

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Correlated Trial Wave Function

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

- 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

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

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

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

Independent Pair

- Independent pair sum looks like this.

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

- 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

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

where the d2b and f2b look like

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

$$\text{f2b}(s, s', ij) = \langle s, s' | \mathcal{O}_{ij}^p | s_i, s_j \rangle \quad (7)$$

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.