

Correlated Trial Wave Function

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Slater Matrix

$$S = \begin{pmatrix} \langle \phi_1 | \mathbf{r}_1 s_1 \rangle & \dots & \langle \phi_1 | \mathbf{r}_A s_A \rangle \\ \vdots & \ddots & \vdots \\ \langle \phi_A | \mathbf{r}_1 s_1 \rangle & \dots & \langle \phi_A | \mathbf{r}_A s_A \rangle \end{pmatrix} \quad (1)$$

$$S'' = \begin{pmatrix} \langle \phi_1 | \mathbf{r}_1 s_1 \rangle & \dots & \langle \phi_1 | \mathbf{r}_i s \rangle & \dots & \langle \phi_1 | \mathbf{r}_j s' \rangle & \dots & \langle \phi_1 | \mathbf{r}_A s_A \rangle \\ \vdots & & & \ddots & & & \vdots \\ \langle \phi_A | \mathbf{r}_1 s_1 \rangle & \dots & \langle \phi_A | \mathbf{r}_i s \rangle & \dots & \langle \phi_A | \mathbf{r}_j s' \rangle & \dots & \langle \phi_A | \mathbf{r}_A s_A \rangle \end{pmatrix} \quad (2)$$

Trial Wave Function

$$\begin{aligned} \langle \Psi_T | \text{RS} \rangle = \langle \Phi | & \left[\prod_{i < j} f_c(r_{ij}) \right] \left[1 + \sum_{i < j, p} f_p(r_{ij}) \mathcal{O}_{ij}^p \right. \\ & \left. + \sum_{i < j, p} \sum_{\substack{k < l \\ \text{ip}}} f_p(r_{ij}) \mathcal{O}_{ij}^p f_p(r_{kl}) \mathcal{O}_{kl}^p \right] | \text{RS} \rangle = \psi_T^{(0)} + \psi_T^{(1)} + \psi_T^{(2)} \end{aligned} \quad (3)$$

Trial Wave Function

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$$\psi_T^{(0)} = \det(S) \quad (4)$$

Trial Wave Function

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Trial Wave Function

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$$\psi_T^{(0)} = \det(S) \quad (4)$$

$$\psi_T^{(1)} = \sum \det(S'') = \sum \det(S^{-1} S'') \det(S) \quad (5)$$

$$\psi_T^{(2)} = \sum \det(S''') = \sum \det(S''^{-1} S''') \det(S^{-1} S'') \det(S) \quad (6)$$

Trial Wave Function (look like code)

$$\psi_T^{(0)} = \det(S) \quad (7)$$

$$\psi_T^{(1)} = \sum \det(S^{-1}S'')\det(S) \quad (8)$$

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$$\psi_T^{(0)} = \det(S) \quad (9)$$

$$\psi_T^{(1)} = \sum_{s,s'=1}^4 \sum \det(S^{-1}S''(s,s')) \langle ss' | \mathcal{O}_i \mathcal{O}_j | s_i s_j \rangle \det(S) \quad (10)$$

$$= \sum_{s,s'=1}^4 d2b(s,s',ij) f2b(s,s',ij) \det(S) \quad (11)$$

Trial Wave Function (look like code)

$$\psi_T^{(2)} = \sum \det(S''^{-1}S''''')\det(S^{-1}S'')\det(S) \quad (12)$$

$$\psi_T^{(2)} = \sum_{s,s'=1}^4 \sum \det(S''^{-1}S'''''(s,s')) \langle ss' | \mathcal{O}_k \mathcal{O}_l | s_k s_l \rangle \det(S^{-1}S'')\det(S) \quad (13)$$

$$= \sum_{s,s'=1}^4 d2b(s,s',kl)f2b(s,s',kl)\det(S^{-1}S'')\det(S) \quad (14)$$

Combining $\psi_T^{(1)}$ and $\psi_T^{(2)}$

$$\begin{aligned}
 \psi_T^{(1)} + \psi_T^{(2)} &= \sum_{s,s'=1}^4 \left[\sum \det(S^{-1}S''(s, s')) \right. \\
 &+ \sum \det(S''^{-1}S''''(s, s')) \det(S^{-1}S'') \left. \right] \langle ss' | \mathcal{O}_i \mathcal{O}_j | s_i s_j \rangle \det(S) \quad (15) \\
 &= \sum_{s,s'=1}^4 (d2b(s, s', ij) f2b(s, s', ij)) \det(S)
 \end{aligned}$$