Correlated Trial Wave Function

Cody Petrie

October 27, 2015

Slater Matrix

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

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

Trial Wave Function

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

Trial Wave Function

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

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

Trial Wave Function

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

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

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

Trial Wave Function

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

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

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

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

Trial Wave Function (look like code)

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

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

Trial Wave Function (look like code)

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

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

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

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

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

Trial Wave Function (look like code)

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

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

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

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

$$\psi_T^{(1)} + \psi_T^{(2)} = \sum_{s,s'=1}^{4} \Big[\sum \det(S^{-1} S''(s,s')) + \sum \det(S''^{-1} S''''(s,s')) \det(S^{-1} S'') \Big] \langle ss' | \mathcal{O}_i \mathcal{O}_j | s_i s_j \rangle \det(S) \quad (15)$$

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