

Correlated Trial Wave Function

Cody Petrie

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Slater Matrix

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

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

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