Trabalho 5a

3 de maio de 2023 10:09

1) $\int \psi_1^* \psi_1 \, d\tau = 1 \qquad \int \psi_2^* \psi_2 \, d\tau = 1 \qquad \int \psi_1^* \psi_2 \, d\tau = 0$

$$\int \psi_1^* \psi_1 \, d\tau = \int [2(1+S_{12})]^{-1/2} [\phi_1^*(\vec{r}) + \phi_2^*(\vec{r})] [2(1+S_{12})]^{-1/2} [\phi_1(\vec{r}) + \phi_2(\vec{r})] \, d\tau =$$

$$= [2(1+S_{12})]^{-1} \int [\phi_1^*(\vec{r}) + \phi_2^*(\vec{r})][\phi_1(\vec{r}) + \phi_2(\vec{r})] \, d\tau =$$

$$= [2(1+S_{12})]^{-1} \left\{ \underbrace{\int \phi_1^*(\vec{r}) \phi_1(\vec{r}) \, d\tau}_{1} + \underbrace{\int \phi_1^*(\vec{r}) \phi_2(\vec{r}) \, d\tau}_{S_{12}} + \underbrace{\int \phi_2^*(\vec{r}) \phi_1(\vec{r}) \, d\tau}_{S_{21}} + \underbrace{\int \phi_2^* \phi_2 \, d\tau}_{1} \right\}$$

$$= [2(1+S_{12})]^{-1} \{ 1 + S_{12} + S_{12} + 1 \} = [2(1+S_{12})^{-1}][2(1+S_{12})] = 1$$

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2) $$|\psi_0\rangle\ \psi_0(x_1, x_2) = \frac{1}{\sqrt{2}} \begin{vmatrix} \chi_1(x_1) & \chi_2(x_1) \\ \chi_1(x_2) & \chi_2(x_2) \end{vmatrix} = \frac{1}{\sqrt{2}} [\chi_1(x_1)\chi_2(x_2) - \chi_1(x_2)\chi_2(x_1)]$$

$$= \frac{1}{\sqrt{2}} \Big\{ [2(1+S_{12})]^{-1/2} [\psi_1(\vec{r}_1) + \psi_2(\vec{r}_1)] \alpha(w_1) [2(1+S_{12})]^{-1/2} [\psi_1(\vec{r}_2) + \psi_2(\vec{r}_2)] \beta(w_2)$$

$$- [2(1+S_{12})]^{-1/2} [\psi_1(\vec{r}_2) + \psi_2(\vec{r}_2)] \alpha(w_2) [2(1+S_{12})]^{-1/2} [\psi_1(\vec{r}_1) + \psi_2(\vec{r}_1)] \beta(w_1) \Big\} =$$

(1) $\{[2(1+S_{12})^{-1/2}]\}^2 \equiv (c_1)^2$

$$= \frac{(c_1)^2}{\ } \{ [\psi_1(\vec{r}_1) + \psi_2(\vec{r}_1)] \alpha(w_1) [\psi_1(\vec{r}_2) + \psi_2(\vec{r}_2)] \beta(w_2)$$

$$= \frac{(C_1)^2}{\sqrt{2}} \Big\{ [\varphi_1(\vec{r_1}) + \varphi_2(\vec{r_1})]\alpha(w_1)[\varphi_1(\vec{r_2}) + \varphi_2(\vec{r_2})]\beta(w_2)$$

$$- [\varphi_1(\vec{r_2}) + \varphi_2(\vec{r_2})]\alpha(w_2)[\varphi_1(\vec{r_1}) + \varphi_2(\vec{r_1})]\beta(w_1) \Big\}$$

$$= \frac{(C_1)^2}{\sqrt{2}} \Big\{ \varphi_1(\vec{r_1})\varphi_1(\vec{r_2})\alpha(w_1)\beta(w_2) + \varphi_1(\vec{r_1})\varphi_2(\vec{r_2})\alpha(w_1)\beta(w_2)$$

$$+ \varphi_2(\vec{r_1})\varphi_1(\vec{r_2})\alpha(w_1)\beta(w_2) + \varphi_2(\vec{r_1})\varphi_2(\vec{r_2})\alpha(w_1)\beta(w_2)$$

$$- \varphi_1(\vec{r_2})\varphi_1(\vec{r_1})\alpha(w_2)\beta(w_1) - \varphi_1(\vec{r_2})\varphi_2(\vec{r_1})\alpha(w_2)\beta(w_1)$$

$$- \varphi_2(\vec{r_2})\varphi_1(\vec{r_1})\alpha(w_2)\beta(w_1) - \varphi_2(\vec{r_2})\varphi_2(\vec{r_1})\alpha(w_2)\beta(w_1) \Big\}$$

$$\phi_i(\uparrow)\phi_j(\downarrow) = \begin{vmatrix} \varphi_i(\vec{r_1})\alpha(w_1) & \varphi_j(\vec{r_1})\beta(w_1) \\ \varphi_i(\vec{r_2})\alpha(w_2) & \varphi_j(\vec{r_2})\beta(w_2) \end{vmatrix} =$$

$$= \varphi_i(\vec{r_1})\varphi_j(\vec{r_2})\alpha(w_1)\beta(w_2) - \varphi_i(\vec{r_2})\varphi_j(\vec{r_1})\alpha(w_2)\beta(w_1)$$

$$|\Psi_0\rangle = \frac{(C_1)^2}{\sqrt{2}} \Big[\phi_1(\uparrow)\phi_1(\downarrow) + \phi_2(\uparrow)\phi_2(\downarrow) + \phi_2(\uparrow)\phi_1(\downarrow) + \phi_1(\uparrow)\phi_2(\downarrow) \Big\}$$