Aula 04-05-2022

3 de maio de 2022 18:24

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

$$\int \psi_1^* \psi_1 \, d\tau = \int [2(1+S_{12})]^{-1/2} [\varphi_1^*(\vec{r}) + \varphi_2^*(\vec{r})] \cdot [2(1+S_{12})]^{-1/2} [\varphi_1(\vec{r}) + \varphi_2(\vec{r})] \, d\tau =$$

$$= [2(1+S_{12})]^{-1} \int [\varphi_1^*(\vec{r}) + \varphi_2^*(\vec{r})][\varphi_1(\vec{r}) + \varphi_2(\vec{r})] \, d\tau =$$

$$= [2(1+S_{12})]^{-1} \int \underbrace{\varphi_1^*(\vec{r})\, \varphi_1(\vec{r})}_{1} + \underbrace{\varphi_1^*(\vec{r})\, \varphi_2(\vec{r})}_{S_{12}} + \underbrace{\varphi_2^*(\vec{r})\, \varphi_1(\vec{r})}_{S_{21}} + \underbrace{\varphi_2^*(\vec{r})\, \varphi_2(\vec{r})}_{1} \, d\tau$$

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

2) $$|\Psi_0\rangle = \frac{1}{\sqrt{2}} \begin{vmatrix} \chi_1(x_1) & \chi_2(x_1) \\ \chi_1(x_2) & \chi_2(x_2) \end{vmatrix} = \frac{1}{\sqrt{2}} \left[\chi_1(x_1)\chi_2(x_2) - \chi_1(x_2)\chi_2(x_1) \right] =$$

$$= \frac{1}{\sqrt{2}} \Big\{ \overbrace{[2(1+S_{12})]^{-1/2} [\varphi_1(\vec{r}_1) + \varphi_2(\vec{r}_1)] \alpha(w_1) [2(1+S_{12})]^{-1/2}}^{①} [\varphi_1(\vec{r}_2) + \varphi_2(\vec{r}_2)] \beta(w_2)$$
$$- \underbrace{[2(1+S_{12})]^{-1/2} [\varphi_1(\vec{r}_2) + \varphi_2(\vec{r}_2)] \alpha(w_2) [2(1+S_{12})]^{-1/2}}_{①} [\varphi_1(\vec{r}_1) + \varphi_2(\vec{r}_1)] \beta(w_1) \Big\}$$

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

$$= \frac{(c_1)^2}{\sqrt{2}} \Big\{ [\varphi_1(\vec{r}_1) + \varphi_2(\vec{r}_1)][\varphi_1(\vec{r}_2) + \varphi_2(\vec{r}_2)] \alpha(w_1) \beta(w_2)$$
$$- [\varphi_1(\vec{r}_2) + \varphi_2(\vec{r}_2)] [\varphi_1(\vec{r}_1) + \varphi_2(\vec{r}_1)] \alpha(w_2) \beta(w_1) \Big\} =$$

$\sqrt{2}$ /

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

$$= \frac{(c_1)^2}{\sqrt{2}} \Big\{ \varphi_1(\vec{r_1})\varphi_1(\vec{r_2})\alpha(w_1)\beta(w_2) + \varphi_1(\vec{r_1})\varphi_2(\vec{r_2})\alpha(w_1)\beta(w_2)$$

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

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

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

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

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

$$|\psi_0\rangle = \frac{(c_1)^2}{\sqrt{2}} \Big\{ \phi_1(\uparrow)\phi_1(\downarrow) + \phi_2(\uparrow)\phi_2(\downarrow) + \phi_1(\uparrow)\phi_2(\downarrow) + \phi_2(\uparrow)\phi_1(\downarrow) \Big\}$$

$$= \frac{(c_1)^2}{\sqrt{2}} \Big\{ \phi_1(\uparrow)\phi_2(\downarrow) + \phi_2(\uparrow)\phi_2(\downarrow) + \phi_2(\uparrow)\phi_1(\downarrow) + \phi_1(\uparrow)\phi_2(\downarrow) \Big\}$$

c.q.d.