TP 4a

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$\Psi_1 \quad \Psi_2 \Rightarrow$ conjunto ortogonal

$$\int \Psi_1^* \Psi_1 \, d\tau = 1 \qquad \int \Psi_2^* \Psi_2 \, d\tau = 1$$

$$\int \Psi_1^* \Psi_2 \, d\tau = 0$$

$$\int \Psi_1^* \Psi_1 \, d\tau = \int \left[2(1+S_{12})\right]^{-1/2} \left[\phi_1^*(\vec{r}) + \phi_2^*(\vec{r})\right] \cdot \left[2(1+S_{12})\right]^{-1/2}$$

$$\left[\phi_1(\vec{r}) + \phi_2(\vec{r})\right] d\tau =$$

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

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

$$\left. + \underbrace{\int \phi_2^* \phi_2 \, d\tau}_{1} \right\}$$

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

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

$$|\Psi_0\rangle = \Psi_0(x_1, x_2) = \frac{1}{\sqrt{2}} \begin{vmatrix} \chi_1(x_1) & \chi_2(x_1) \\ \chi_1(x_2) & \chi_2(x_2) \end{vmatrix} =$$

$$= \frac{1}{\sqrt{2}} \left[\chi_1(x_1)\chi_2(x_2) - \chi_1(x_2)\chi_2(x_1) \right] =$$

$$= \frac{1}{\sqrt{2}} \left[\psi_1(r_1)\alpha(w_1)\psi_1(r_2)\beta(w_2) - \psi_1(r_2)\alpha(w_2)\psi_1(r_1)\beta(w_1) \right]$$

$$= \frac{1}{\sqrt{2}} \Big[\underline{[2(1+S_{12})^{-1/2}]} [\phi_1(r_1)+\phi_2(r_1)] \alpha(w_1) \underline{[2(1+S_{12})^{-1/2}]} \times$$

$$[\phi_1(r_2)+\phi_2(r_2)]\beta(w_2) - \underline{[2(1+S_{12})^{-1/2}]} [\phi_1(r_2)+\phi_2(r_2)] \alpha(w_2)$$

$$\times \underline{[2(1+S_{12})^{-1/2}]} [\phi_1(r_1)+\phi_2(r_1)] \beta(w_1) \Big] =$$

$$= \frac{\overbrace{[2(1+S_{12})^{-1/2}]^2}^{C_1^2}}{\sqrt{2}} \Big\{ [\phi_1(r_1)+\phi_2(r_1)][\phi_1(r_2)+\phi_2(r_2)]\alpha(w_1)\beta(w_2)$$

$$- [\phi_1(r_2)+\phi_2(r_2)][\phi_1(r_1)+\phi_2(r_1)]\alpha(w_2)\beta(w_1) \Big\}$$

$$= \frac{C_1^2}{\sqrt{2}} \Big\{ \big(\phi_1 \underline{(r_1)\phi_1(r_2)} + \phi_1(r_1)\phi_2(r_1) + \underline{\phi_2(r_1)\phi_2(r_2)} + \underline{\phi_2(r_1)\phi_2(r_2)} \big) \alpha(w_1)\beta(w_1)$$

$$- \big(\underline{\phi_1(r_2)\phi_1(r_1)} + \phi_1(r_2)\phi_2(r_1) + \underline{\phi_2(r_2)\phi_1(r_1)} + \underline{\phi_2(r_2)\phi_2(r_1)} \big) \alpha(w_2)\beta(w_1) \Big\}$$

$= C^2 ($ [illegible]

$$= \frac{C_1^2}{\sqrt{2}} \Big\{ \phi_1(r_1)\phi_1(r_2)\alpha(w_1)\beta(w_2) - \phi_1(r_2)\phi_1(r_1)\alpha(w_2)\beta(w_1) +$$

$$\phi_2(r_1)\phi_2(r_2)\alpha(w_1)\beta(w_2) - \phi_2(r_2)\phi_2(r_1)\alpha(w_2)\beta(w_1) +$$

$$\phi_2(r_1)\phi_1(r_2)\alpha(w_1)\beta(w_2) - \phi_2(r_2)\phi_1(r_1)\alpha(w_2)\beta(w_1) +$$

$$\phi_1(r_1)\phi_2(r_2)\alpha(w_1)\beta(w_2) - \phi_1(r_2)\phi_2(r_1)\alpha(w_2)\beta(w_1) \Big\}$$

$$\phi_1(\uparrow)\phi_j(\downarrow) = \begin{vmatrix} \phi_1(\vec{r}_1)\alpha(w_1) & \phi_j(\vec{r}_1)\beta(w_1) \\ \phi_i(\vec{r}_2)\alpha(w_2) & \phi_j(\vec{r}_2)\beta(w_2) \end{vmatrix} =$$

$$= \phi_1(\vec{r}_1)\phi_j(\vec{r}_2)\alpha(w_1)\beta(w_2) - \phi_1(\vec{r}_2)\phi_j(\vec{r}_1)\alpha(w_2)\beta(w_1)$$

$$|\psi_0\rangle = \frac{C_1^2}{\sqrt{2}} \Big[\phi_1(\uparrow)\phi_1(\downarrow) + \phi_2(\uparrow)\phi_2(\downarrow) + \phi_2(\uparrow)\phi_1(\downarrow) + \phi_1(\uparrow)\phi_2(\downarrow) \Big]$$