2 Elektronen in 2 verschiedenen räumlichen Orbitalen

$$\Psi_1(1,2) = \frac{1}{\sqrt{2}} \begin{vmatrix} \psi_a(1)\alpha(1) & \psi_a(2)\alpha(2) \\ \psi_b(1)\alpha(1) & \psi_b(2)\alpha(2) \end{vmatrix}$$

$$= \frac{\alpha(1)\alpha(2)}{\sqrt{2}} \begin{vmatrix} \psi_a(1) & \psi_a(2) \\ \psi_b(1) & \psi_b(2) \end{vmatrix}$$

$$\Rightarrow \quad \hat{s}_z \Psi_1(1,2) = \hbar \Psi_1(1,2)$$

und analog mit $\beta(1)\beta(2)$: $\quad \hat{s}_z \Psi_{-1}(1,2) = -\hbar \Psi_{-1}(1,2).$

$$\Psi_0(1,2) = \frac{1}{\sqrt{2}} \begin{vmatrix} \psi_a(1)\alpha(1) & \psi_a(2)\alpha(2) \\ \psi_b(1)\beta(1) & \psi_b(2)\beta(2) \end{vmatrix}, \qquad \hat{s}_z \Psi_0(1,2) = 0$$

$$\Psi_0'(1,2) = \frac{1}{\sqrt{2}} \begin{vmatrix} \psi_a(1)\beta(1) & \psi_a(2)\beta(2) \\ \psi_b(1)\alpha(1) & \psi_b(2)\alpha(2) \end{vmatrix}, \qquad \hat{s}_z \Psi_0'(1,2) = 0$$

$$\Rightarrow \frac{1}{\sqrt{2}} [\Psi_0(1,2) + \Psi_0'(1,2)] = \frac{1}{2} [\psi_a(1)\alpha(1)\psi_b(2)\beta(2) - \psi_a(2)\alpha(2)\psi_b(1)\beta(1)$$
$$+ \; \psi_a(1)\beta(1)\psi_b(2)\alpha(2) - \psi_b(1)\alpha(1)\psi_a(2)\beta(2)]$$

$$= \frac{1}{2} [\psi_a(1)\psi_b(2) - \psi_a(2)\psi_b(1)] [\alpha(1)\beta(2) + \alpha(2)\beta(1)]$$