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Lösungen zur Übungen zur Vorlesung Theoretische Chemie, Teil I: Quantenmechanik

Aufgabe 1

(a)

$$\left\langle \alpha \left| s^2 \right| \alpha \right\rangle = \frac{3}{4}\hbar^2 \left\langle \alpha \mid \alpha \right\rangle = \frac{3}{4}\hbar^2$$

$$\left\langle \beta \left| s^2 \right| \beta \right\rangle = \frac{3}{4}\hbar^2 \left\langle \beta \mid \beta \right\rangle = \frac{3}{4}\hbar^2$$

$$\left\langle \alpha \left| s^2 \right| \beta \right\rangle = \left\langle \beta \left| s^2 \right| \alpha \right\rangle = \frac{3}{4}\hbar^2 \left\langle \beta \mid \alpha \right\rangle = 0$$

$$s^2 = \frac{3}{4}\hbar^2 \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$

$$\left\langle \alpha \left| s_z \right| \alpha \right\rangle = \frac{1}{2}\hbar \left\langle \alpha \mid \alpha \right\rangle = \frac{1}{2}\hbar$$

$$\left\langle \beta \left| s_z \right| \beta \right\rangle = \frac{1}{2}\hbar \left\langle \beta \mid \beta \right\rangle = -\frac{1}{2}\hbar$$

$$\left\langle \alpha \left| s_z \right| \beta \right\rangle = \left\langle \beta \left| s_z \right| \alpha \right\rangle = \frac{1}{2}\hbar \left\langle \beta \mid \alpha \right\rangle = 0$$

$$s_z = \frac{1}{2}\hbar \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

(b)

$$s \pm \left| s, m_s \right\rangle = \hbar \sqrt{s\,(s+1) - m_s\,(m_s \pm 1)}\, \left| s, m_s \pm 1 \right\rangle$$

für $s = \frac{1}{2}, m_s = \frac{1}{2}$

$$s_+ \left| \frac{1}{2}, \frac{1}{2} \right\rangle = \hbar \sqrt{\frac{3}{4} - \frac{3}{4}} \left| \frac{1}{2}, \frac{3}{2} \right\rangle = 0$$

$$s_- \left| \frac{1}{2}, \frac{1}{2} \right\rangle = \hbar \sqrt{\frac{3}{4} - \left(-\frac{1}{4} \right)} \left| \frac{1}{2}, -\frac{1}{2} \right\rangle = \hbar \left| \frac{1}{2}, -\frac{1}{2} \right\rangle$$

$$s_+ \left| \frac{1}{2}, -\frac{1}{2} \right\rangle = \hbar \sqrt{\frac{3}{4} - \left(-\frac{1}{4} \right)} \left| \frac{1}{2}, \frac{1}{2} \right\rangle = \hbar \left| \frac{1}{2}, \frac{1}{2} \right\rangle$$

$$s_- \left| \frac{1}{2}, -\frac{1}{2} \right\rangle = \hbar \sqrt{\frac{3}{4} - \frac{3}{4}} \left| \frac{1}{2}, -\frac{3}{2} \right\rangle = 0$$

$$\Rightarrow$$

$$\left\langle \alpha \left| s_+ \right| \alpha \right\rangle = 0$$

$$\left\langle \alpha \left| s_+ \right| \beta \right\rangle = \hbar \left\langle \alpha \mid \alpha \right\rangle$$

$$\left\langle \beta \left| s_+ \right| \alpha \right\rangle = 0$$

$$\langle \beta | s_+ | \beta \rangle = \hbar \langle \beta \mid \alpha \rangle = 0$$

$$\Rightarrow s_+ = \hbar \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}$$

und

$$\langle \alpha | s_- | \beta \rangle = 0$$

$$\langle \alpha | s_- | \alpha \rangle = \hbar \langle \alpha \mid \beta \rangle = 0$$

$$\langle \beta | s_- | \alpha \rangle = \hbar \langle \beta \mid \beta \rangle$$

$$\langle \beta | s_- | \beta \rangle = 0$$

$$\Rightarrow s_- = \hbar \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}$$

$$s_+ = s_x + \mathrm{i} s_y, s_- = s_x - \mathrm{i} s_y \Rightarrow s_+ + s_- = 2 s_x$$

$$\Rightarrow s_x = \frac{1}{2} (s_+ + s_-) = \frac{\hbar}{2} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$

und

$$s_+ - s_- = 2\mathrm{i} s_y$$

$$\Rightarrow s_y = \frac{1}{2\mathrm{i}} (s_+ - s_-) = \frac{\hbar}{2\mathrm{i}} \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} = \frac{\hbar}{2} \begin{pmatrix} 0 & -\mathrm{i} \\ \mathrm{i} & 0 \end{pmatrix}$$

Pauli'sche Spinmatrizen:

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \sigma_y = \begin{pmatrix} 0 & -\mathrm{i} \\ \mathrm{i} & 0 \end{pmatrix}, \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

(c)

$$s_x^2 |\alpha\rangle = \frac{\hbar^2}{4} \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \begin{pmatrix} 1 \\ 0 \end{pmatrix} = \frac{\hbar^2}{4} \begin{pmatrix} 1 \\ 0 \end{pmatrix} = \frac{\hbar^2}{4} |\alpha\rangle$$

$$s_x^2 |\beta\rangle = \frac{\hbar^2}{4} \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \begin{pmatrix} 0 \\ 1 \end{pmatrix} = \frac{\hbar^2}{4} \begin{pmatrix} 0 \\ 1 \end{pmatrix} = \frac{\hbar^2}{4} |\beta\rangle$$

$$s_x |\alpha\rangle = \frac{\hbar}{2} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} 1 \\ 0 \end{pmatrix} = \frac{\hbar}{2} \begin{pmatrix} 0 \\ 1 \end{pmatrix} = \frac{\hbar}{2} |\beta\rangle$$

$$s_x |\beta\rangle = \frac{\hbar}{2} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} 0 \\ 1 \end{pmatrix} = \frac{\hbar}{2} \begin{pmatrix} 1 \\ 0 \end{pmatrix} = \frac{\hbar}{2} |\alpha\rangle$$

Aufgabe 2

(a)

$$S_z = s_z(1) + s_z(2)$$

$$\begin{aligned} S_z |\alpha_1\rangle |\alpha_2\rangle &= |\alpha_2\rangle s_z(1) |\alpha_1\rangle + |\alpha_1\rangle s_z(2) |\alpha_2\rangle \\ &= \frac{\hbar}{2} |\alpha_1\rangle |\alpha_2\rangle + \frac{\hbar}{2} |\alpha_1\rangle |\alpha_2\rangle \\ &= \hbar |\alpha_1\rangle |\alpha_2\rangle \end{aligned}$$

$\Rightarrow$ EF zu EW $\hbar$

$$\begin{aligned} S_z |\alpha_1\rangle |\beta_2\rangle &= |\beta_2\rangle s_z(1) |\alpha_1\rangle + |\alpha_1\rangle s_z(2) |\beta_2\rangle \\ &= \frac{\hbar}{2} |\alpha_1\rangle |\beta_2\rangle - \frac{\hbar}{2} |\alpha_1\rangle |\beta_2\rangle \\ &= 0 \end{aligned}$$

$\Rightarrow$ EF zu EW 0

$$\begin{aligned} S_z \left|\beta_1\right\rangle \left|\alpha_2\right\rangle &= \left|\alpha_2\right\rangle s_z(1) \left|\beta_1\right\rangle + \left|\beta_1\right\rangle s_z(2) \left|\alpha_2\right\rangle \\ &= -\frac{\hbar}{2} \left|\beta_1\right\rangle \left|\alpha_2\right\rangle + \frac{\hbar}{2} \left|\beta_1\right\rangle \left|\alpha_2\right\rangle \\ &= 0 \end{aligned}$$

$\Rightarrow$ EF zu EW 0

$$\begin{aligned} S_z \left|\beta_1\right\rangle \left|\beta_2\right\rangle &= \left|\beta_2\right\rangle s_z(1) \left|\beta_1\right\rangle + \left|\beta_1\right\rangle s_z(2) \left|\beta_2\right\rangle \\ &= -\frac{\hbar}{2} \left|\beta_1\right\rangle \left|\beta_2\right\rangle - \frac{\hbar}{2} \left|\beta_1\right\rangle \left|\beta_2\right\rangle \\ &= -\hbar \left|\beta_1\right\rangle \left|\beta_2\right\rangle \end{aligned}$$

$\Rightarrow$ EF zu EW $-\hbar$

(b)

$$S_+ = S_x + \mathrm{i}S_y = s_x(1) + \mathrm{i}s_y(1) + s_x(2) + \mathrm{i}s_y(2) = s_+(1) + s_+(2)$$

analog

$$S_- = s_-(1) + s_-(2)$$

$$S_+ \left|\alpha_1\right\rangle \left|\alpha_2\right\rangle = \left|\alpha_2\right\rangle s_+(1) \left|\alpha_1\right\rangle + \left|\alpha_1\right\rangle s_+(2) \left|\alpha_2\right\rangle = 0$$

$$S_- \left|\alpha_1\right\rangle \left|\alpha_2\right\rangle = \left|\alpha_2\right\rangle s_-(1) \left|\alpha_1\right\rangle + \left|\alpha_1\right\rangle s_-(2) \left|\alpha_2\right\rangle = \hbar \left(\left|\beta_1\right\rangle \left|\alpha_2\right\rangle + \left|\alpha_1\right\rangle \left|\beta_2\right\rangle\right)$$

$$S_+ \left|\alpha_1\right\rangle \left|\beta_2\right\rangle = \left|\beta_2\right\rangle s_+(1) \left|\alpha_1\right\rangle + \left|\alpha_1\right\rangle s_+(2) \left|\beta_2\right\rangle = \hbar \left|\alpha_1\right\rangle \left|\alpha_2\right\rangle$$

$$S_- \left|\alpha_1\right\rangle \left|\beta_2\right\rangle = \left|\beta_2\right\rangle s_-(1) \left|\alpha_1\right\rangle + \left|\alpha_1\right\rangle s_-(2) \left|\beta_2\right\rangle = \hbar \left|\beta_1\right\rangle \left|\beta_2\right\rangle$$

$$S_+ \left|\beta_1\right\rangle \left|\alpha_2\right\rangle = \left|\alpha_2\right\rangle s_+(1) \left|\beta_1\right\rangle + \left|\beta_1\right\rangle s_+(2) \left|\alpha_2\right\rangle = \hbar \left|\alpha_1\right\rangle \left|\alpha_2\right\rangle$$

$$S_- \left|\beta_1\right\rangle \left|\alpha_2\right\rangle = \left|\alpha_2\right\rangle s_-(1) \left|\beta_1\right\rangle + \left|\beta_1\right\rangle s_-(2) \left|\alpha_2\right\rangle = \hbar \left|\beta_1\right\rangle \left|\beta_2\right\rangle$$

$$S_+ \left|\beta_1\right\rangle \left|\beta_2\right\rangle = \left|\beta_2\right\rangle s_+(1) \left|\beta_1\right\rangle + \left|\beta_1\right\rangle s_+(2) \left|\beta_2\right\rangle = \hbar \left(\left|\alpha_1\right\rangle \left|\beta_2\right\rangle + \left|\beta_1\right\rangle \left|\alpha_2\right\rangle\right)$$

$$S_- \left|\beta_1\right\rangle \left|\beta_2\right\rangle = 0$$

(c)

$$\begin{aligned} S^2 \left|\alpha_1\right\rangle \left|\alpha_2\right\rangle &= S_z^2 \left|\alpha_1\right\rangle \left|\alpha_2\right\rangle + \frac{1}{2} S_+ S_- \left|\alpha_1\right\rangle \left|\alpha_2\right\rangle + \frac{1}{2} S_- S_+ \left|\alpha_1\right\rangle \left|\alpha_2\right\rangle \\ &= \hbar^2 \left|\alpha_1\right\rangle \left|\alpha_2\right\rangle + \frac{\hbar}{2} s_+ \left(\left|\beta_1\right\rangle \left|\alpha_2\right\rangle + \left|\alpha_1\right\rangle \left|\beta_2\right\rangle\right) + 0 \\ &= \hbar^2 \left|\alpha_1\right\rangle \left|\alpha_2\right\rangle + \frac{\hbar^2}{2} \left(\left|\alpha_1\right\rangle \left|\alpha_2\right\rangle + \left|\alpha_1\right\rangle \left|\alpha_2\right\rangle\right) \\ &= 2\hbar^2 \left|\alpha_1\right\rangle \left|\alpha_2\right\rangle \end{aligned}$$

EF zu EW $2\hbar^2$

$$\begin{aligned} S^2 \left|\alpha_1\right\rangle \left|\beta_2\right\rangle &= S_z^2 \left|\alpha_1\right\rangle \left|\beta_2\right\rangle + \frac{1}{2} S_+ S_- \left|\alpha_1\right\rangle \left|\beta_2\right\rangle + \frac{1}{2} S_- S_+ \left|\alpha_1\right\rangle \left|\beta_2\right\rangle \\ &= 0 + \frac{\hbar}{2} s_+ \left|\beta_1\right\rangle \left|\beta_2\right\rangle + \frac{\hbar}{2} s_- \left|\alpha_1\right\rangle \left|\alpha_2\right\rangle \\ &= \frac{\hbar^2}{2} \left(\left|\beta_1\right\rangle \left|\alpha_2\right\rangle + \left|\alpha_1\right\rangle \left|\beta_2\right\rangle\right) + \frac{\hbar^2}{2} \left(\left|\beta_1\right\rangle \left|\alpha_2\right\rangle + \left|\alpha_1\right\rangle \left|\beta_2\right\rangle\right) \end{aligned}$$

keine EF

$$\begin{aligned} S^2 \left|\beta_1\right\rangle \left|\alpha_2\right\rangle &= S_z^2 \left|\beta_1\right\rangle \left|\alpha_2\right\rangle + \frac{1}{2} S_+ S_- \left|\beta_1\right\rangle \left|\alpha_2\right\rangle + \frac{1}{2} S_- S_+ \left|\beta_1\right\rangle \left|\alpha_2\right\rangle \\ &= 0 + \frac{\hbar}{2} s_+ \left|\beta_1\right\rangle \left|\beta_2\right\rangle + \frac{\hbar}{2} s_- \left|\alpha_1\right\rangle \left|\alpha_2\right\rangle \\ &= \hbar^2 \left(\left|\beta_1\right\rangle \left|\alpha_2\right\rangle + \left|\alpha_1\right\rangle \left|\beta_2\right\rangle\right) \end{aligned}$$

keine EF

$$\begin{aligned} S^2 |\beta_1\rangle |\beta_2\rangle &= S_z^2 |\beta_1\rangle |\beta_2\rangle + \frac{1}{2} S_+ S_- |\beta_1\rangle |\beta_2\rangle + \frac{1}{2} S_- S_+ |\beta_1\rangle |\beta_2\rangle \\ &= \hbar^2 |\beta_1\rangle |\beta_2\rangle + \frac{\hbar}{2} s_- (|\alpha_1\rangle |\beta_2\rangle + |\beta_1\rangle |\alpha_2\rangle) \\ &= \hbar^2 |\beta_1\rangle |\beta_2\rangle + \frac{\hbar}{2} (|\beta_1\rangle |\beta_2\rangle + |\beta_1\rangle |\beta_2\rangle) \\ &= 2\hbar^2 |\beta_1\rangle |\beta_2\rangle \end{aligned}$$

EF zu EW $2\hbar^2$ (d)

$$|\alpha_1\rangle |\alpha_2\rangle : S = 1, M_S = 1$$

$$|\beta_1\rangle |\beta_2\rangle : S = 1, M_S = -1$$

$$|\varphi\rangle = |\alpha_1\rangle |\beta_2\rangle + |\beta_1\rangle |\alpha_2\rangle$$

$$S^2 |\varphi\rangle = \hbar^2 (|\alpha_1\rangle |\beta_2\rangle + |\beta_1\rangle |\alpha_2\rangle + |\alpha_1\rangle |\beta_2\rangle + |\beta_1\rangle |\alpha_2\rangle) = 2\hbar^2 |\varphi\rangle$$

$$S_z |\varphi\rangle = 0$$

$$\Rightarrow |\alpha_1\rangle |\beta_2\rangle + |\beta_1\rangle |\alpha_2\rangle : S = 1, M_S = 0$$

$$|\varphi\rangle = |\alpha_1\rangle |\beta_2\rangle - |\beta_1\rangle |\alpha_2\rangle$$

$$S^2 |\varphi\rangle = \hbar^2 (|\alpha_1\rangle |\beta_2\rangle + |\beta_1\rangle |\alpha_2\rangle - |\alpha_1\rangle |\beta_2\rangle - |\beta_1\rangle |\alpha_2\rangle) = 0$$

$$S_z |\varphi\rangle = \hbar (0 + 0) = 0$$

$$\Rightarrow |\alpha_1\rangle |\beta_2\rangle - |\beta_1\rangle |\alpha_2\rangle : S = 0, M_S = 0$$

Aufgabe 3

(a)

$$\Psi_{1s\alpha} = \Psi_{1s}(\vec{r}) |\alpha\rangle$$

$$\Psi_{2s\alpha} = \Psi_{2s}(\vec{r}) |\alpha\rangle$$

$$\Psi_{1s\beta} = \Psi_{1s}(\vec{r}) |\beta\rangle$$

$$\Psi_{2s\beta} = \Psi_{2s}(\vec{r}) |\beta\rangle$$

Notation für Skalarprodukt:

$$\begin{aligned} \langle \Psi_{a\sigma} \mid \Psi_{a'\sigma'} \rangle &= \int \mathrm{d}\vec{r} \Psi_a^* (\vec{r}) \Psi_{a'} (\vec{r}) \langle \sigma \mid \sigma' \rangle \\ &= \delta_{aa'} \delta_{\sigma\sigma'} \end{aligned} \tag{1}$$

(b)

$$\Psi_a(1,2) = N (\Psi_{1s\alpha}(1) \Psi_{1s\beta}(2) - \Psi_{1s\alpha}(2) \Psi_{1s\beta}(1)) \quad \Rightarrow$$

$$\begin{aligned} 1 &= \langle \Psi_a \mid \Psi_a \rangle \\ &= N^2 [\langle \Psi_{1s\alpha}(1) \Psi_{1s\beta}(2) | \Psi_{1s\alpha}(1) \Psi_{1s\beta}(2) \rangle \\ &\quad + \langle \Psi_{1s\alpha}(2) \Psi_{1s\beta}(1) | \Psi_{1s\alpha}(2) \Psi_{1s\beta}(1) \rangle \\ &\quad - \langle \Psi_{1s\alpha}(1) \Psi_{1s\beta}(2) | \Psi_{1s\alpha}(2) \Psi_{1s\beta}(1) \rangle \\ &\quad - \langle \Psi_{1s\alpha}(2) \Psi_{1s\beta}(1) | \Psi_{1s\alpha}(1) \Psi_{1s\beta}(2) \rangle] \\ &= N^2 [\langle \Psi_{1s\alpha}(1) | \Psi_{1s\alpha}(1) \rangle \langle \Psi_{1s\beta}(2) | \Psi_{1s\beta}(2) \rangle \\ &\quad + \langle \Psi_{1s\beta}(1) | \Psi_{1s\beta}(1) \rangle \langle \Psi_{1s\alpha}(2) | \Psi_{1s\alpha}(2) \rangle \\ &\quad - \langle \Psi_{1s\alpha}(1) | \Psi_{1s\beta}(1) \rangle \langle \Psi_{1s\beta}(2) | \Psi_{1s\alpha}(2) \rangle \\ &\quad - \langle \Psi_{1s\beta}(1) | \Psi_{1s\alpha}(1) \rangle \langle \Psi_{1s\alpha}(2) | \Psi_{1s\beta}(2) \rangle] \\ &= N^2 (1 \cdot 1 + 1 \cdot 1 - 0 \cdot 0 - 0 \cdot 0) \\ &= 2N^2 \end{aligned}$$

$$\Rightarrow \quad N = \frac{1}{\sqrt{2}}$$

analog:

$$\Psi_b = N\left(\Psi_{1s\alpha}(1)\,\Psi_{2s\beta}(2) - \Psi_{1s\alpha}(2)\,\Psi_{2s\beta}(1)\right)$$
$$1 = \langle \Psi_b | \Psi_b \rangle = 2N^2$$
$$\Rightarrow \quad N = \frac{1}{\sqrt{2}}$$

Orthogonalität:

$$\begin{aligned}
& \langle \Psi_a(1,2) | \Psi_b(1,2) \rangle \\
= & \frac{1}{2}\left[\langle \Psi_{1s\alpha}(1) | \Psi_{1s\alpha}(1)\rangle \langle \Psi_{1s\beta}(2) | \Psi_{2s\beta}(2)\rangle\right. \\
& -\langle \Psi_{1s\alpha}(1) | \Psi_{2s\beta}(1)\rangle \langle \Psi_{1s\beta}(2) | \Psi_{1s\alpha}(2)\rangle \\
& -\langle \Psi_{1s\beta}(1) | \Psi_{1s\alpha}(1)\rangle \langle \Psi_{1s\alpha}(2) | \Psi_{2s\beta}(2)\rangle \\
& \left.+\langle \Psi_{1s\beta}(1) | \Psi_{2s\beta}(1)\rangle \langle \Psi_{1s\alpha}(2) | \Psi_{1s\alpha}(2)\rangle\right] \\
= & \frac{1}{2}\left(1\cdot 0 - 0\cdot 0 - 0\cdot 0 + 0\cdot 1\right) \\
= & 0
\end{aligned}$$

(c)

$$\begin{aligned}
\Psi_a(1,2) &= \frac{1}{\sqrt{2}}\left(\Psi_{1s\alpha}(1)\,\Psi_{1s\beta}(2) - \Psi_{1s\alpha}(2)\,\Psi_{1s\beta}(1)\right) \\
&= \frac{1}{\sqrt{2}}\left(\Psi_{1s}(\vec{r}_1)\,|\alpha(1)\rangle\Psi_{1s}(\vec{r}_2)\,|\beta(2)\rangle - \Psi_{1s}(\vec{r}_2)\,|\alpha(2)\rangle\Psi_{1s}(\vec{r}_1)\,|\beta(1)\rangle\right) \\
&= \frac{1}{\sqrt{2}}\Psi_{1s}(\vec{r}_1)\,\Psi_{1s}(\vec{r}_2)\left\{|\alpha(1)\rangle|\beta(2)\rangle - |\beta(1)\rangle|\alpha(2)\rangle\right\}
\end{aligned}$$

Aufgabe 2:

$S_z|\alpha(1)\rangle|\beta(2)\rangle = 0; \quad S_z|\beta(1)\rangle|\alpha(2)\rangle = 0;$

$S^2|\alpha(1)\rangle|\beta(2)\rangle = \hbar^2(|\alpha(1)\rangle|\beta(2)\rangle + |\beta(1)\rangle|\alpha(2)\rangle); \quad S^2|\beta(1)\rangle|\alpha(2)\rangle = \hbar^2(|\alpha(1)\rangle|\beta(2)\rangle + |\beta(1)\rangle|\alpha(2)\rangle)$

$\Rightarrow S_z(|\alpha(1)\rangle|\beta(2)\rangle - |\beta(1)\rangle|\alpha(2)\rangle) = 0; \quad S^2(|\alpha(1)\rangle|\beta(2)\rangle - |\beta(1)\rangle|\alpha(2)\rangle) = 0$

$\Rightarrow \Psi_a(1,2)$ ist Eigenfunktion von S_z und S^2 zum Eigenwert 0.

$$\begin{aligned}
\Psi_b(1,2) &= \frac{1}{\sqrt{2}}\left(\Psi_{1s\alpha}(1)\,\Psi_{2s\beta}(2) - \Psi_{1s\alpha}(2)\,\Psi_{2s\beta}(1)\right) \\
&= \frac{1}{\sqrt{2}}\left(\Psi_{1s}(\vec{r}_1)\,|\alpha(1)\rangle\Psi_{2s}(\vec{r}_2)\,|\beta(2)\rangle - \Psi_{2s}(\vec{r}_1)\,|\alpha(2)\rangle\Psi_{1s}(\vec{r}_2)\,|\beta(1)\rangle\right)
\end{aligned}$$

$S_z\Psi_b(1,2) = 0 \quad \Rightarrow \Psi_b(1,2)$ ist Eigenfunktion von S_z zum Eigenwert 0;

$$\begin{aligned}
S^2\Psi_b(1,2) &= \frac{\hbar^2}{\sqrt{2}}\left(\Psi_{1s}(\vec{r}_1)\,\Psi_{2s}(\vec{r}_2) - \Psi_{2s}(\vec{r}_1)\,\Psi_{1s}(\vec{r}_2)\right)\left(|\alpha(1)\rangle|\beta(2)\rangle + |\beta(1)\rangle|\alpha(2)\rangle\right) \\
&\neq c\Psi_b(1,2)
\end{aligned}$$

$\Rightarrow \Psi_b(1,2)$ ist keine Eigenfunktion von S^2.

(d)

$$\Psi_c(1,2) = \frac{1}{\sqrt{2}}\begin{vmatrix}\Psi_{1s\beta}(1) & \Psi_{2s\alpha}(1) \\ \Psi_{1s\beta}(2) & \Psi_{2s\alpha}(2)\end{vmatrix}$$

$$\Psi_d(1,2) = \frac{1}{\sqrt{2}} \begin{vmatrix} \Psi_{1s\alpha}(1) & \Psi_{2s\alpha}(1) \\ \Psi_{1s\alpha}(2) & \Psi_{2s\alpha}(2) \end{vmatrix}$$

$$\Psi_e(1,2) = \frac{1}{\sqrt{2}} \begin{vmatrix} \Psi_{1s\beta}(1) & \Psi_{2s\beta}(1) \\ \Psi_{1s\beta}(1) & \Psi_{1s\beta}(2) \end{vmatrix}$$

(e)
$1s^2$:

$$\begin{aligned} \Psi &= \frac{1}{\sqrt{2}} \Psi_{1s}(\vec{r}_1)\, \Psi_{1s}(\vec{r}_2)\, (|\alpha(1)\rangle|\beta(2)\rangle - |\beta(1)\rangle|\alpha(2)\rangle) \\ &= \frac{1}{\sqrt{2}} (\Psi_{1s}(\vec{r}_1)\, |\alpha(1)\rangle \Psi_{1s}(\vec{r}_2 |\beta(2)\rangle - \Psi_{1s}(\vec{r}_2)\, |\alpha(2)\rangle \Psi_{1s}(\vec{r}_1)\, |\beta(1)\rangle)) \\ &= \Psi_1(1,2) \end{aligned}$$

$1s2s$:

$$\begin{aligned} \Psi &= \frac{1}{\sqrt{2}} (\Psi_{1s}(\vec{r}_1)\, \Psi_{2s}(\vec{r}_2) + \Psi_{1s}(\vec{r}_2)\, \Psi_{2s}(\vec{r}_1)) \\ &\quad \times (|\alpha(1)\rangle|\beta(2)\rangle - |\alpha(2)\rangle|\beta(1)\rangle) \\ &= \frac{1}{\sqrt{2}} (\Psi_{1s}(\vec{r}_1)\, |\alpha(1)\rangle \Psi_{2s}(\vec{r}_2)\, |\beta(2)\rangle - \Psi_{1s}(\vec{r}_2)\, |\alpha(2)\rangle \Psi_{2s}(\vec{r}_1)\, |\beta(1)\rangle \\ &\quad - \Psi_{1s}(\vec{r}_1)\, |\beta(1)\rangle \Psi_{2s}(\vec{r}_2)\, |\alpha(2)\rangle + \Psi_{1s}(\vec{r}_2)\, |\beta(2)\rangle \Psi_{2s}(\vec{r}_1)\, |\alpha(1)\rangle) \\ &= \frac{1}{\sqrt{2}} (\Psi_{1s\alpha}(1)\, \Psi_{2s\beta}(2) - \Psi_{1s\alpha}(2)\, \Psi_{2s\beta}(1)) \\ &\quad - \frac{1}{\sqrt{2}} (\Psi_{1s\beta}(1)\, \Psi_{2s\alpha}(2) - \Psi_{1s\beta}(2)\, \Psi_{2s\alpha}(1)) \\ &= \Psi_b(1,2) - \Psi_c(1,2) \end{aligned}$$

bei $s = 1, m_s = 1$:

$$\Psi = \frac{1}{\sqrt{2}} (\Psi_{1s}(\vec{r}_1)\, \Psi_{2s}(\vec{r}_2) - \Psi_{1s}(\vec{r}_2)\, \Psi_{2s}(\vec{r}_1))\, |\alpha(1)\rangle|\alpha(2)\rangle = \Psi_d(1,2)$$

bei $s = 1, m_s = -1$:

$$\Psi = \frac{1}{\sqrt{2}} (\Psi_{1s}(\vec{r}_1)\, \Psi_{2s}(\vec{r}_2) - \Psi_{1s}(\vec{r}_2)\, \Psi_{2s}(\vec{r}_1))\, |\beta(1)\rangle|\beta(2)\rangle = \Psi_e(1,2)$$

bei $s = 1, m_s = 0$:

$$\begin{aligned} \Psi &= \frac{1}{\sqrt{2}} (\Psi_{1s}(\vec{r}_1)\, \Psi_{2s}(\vec{r}_2) - \Psi_{1s}(\vec{r}_2)\, \Psi_{2s}(\vec{r}_1))\, (|\alpha(1)\rangle|\beta(2)\rangle + |\alpha(2)\rangle|\beta(1)\rangle) \\ &= \frac{1}{\sqrt{2}} (\Psi_{1s}(\vec{r}_1)\, |\alpha(1)\rangle \Psi_{2s}(\vec{r}_2)\, |\beta(2)\rangle - \Psi_{1s}(\vec{r}_2)\, |\alpha(2)\rangle \Psi_{2s}(\vec{r}_1)\, |\beta(1)\rangle \\ &\quad + \Psi_{1s}(\vec{r}_1)\, |\beta(1)\rangle \Psi_{2s}(\vec{r}_2)\, |\alpha(2)\rangle - \Psi_{1s}(\vec{r}_2)\, |\beta(2)\rangle \Psi_{2s}(\vec{r}_1)\, |\alpha(1)\rangle) \\ &= \frac{1}{\sqrt{2}} (\Psi_{1s\alpha}(1)\, \Psi_{2s\beta}(2) - \Psi_{1s\alpha}(2)\, \Psi_{2s\beta}(1)) \\ &\quad + \frac{1}{\sqrt{2}} (\Psi_{1s\beta}(1)\, \Psi_{2s\alpha}(2) - \Psi_{1s\beta}(2)\, \Psi_{2s\alpha}(1)) \\ &= \Psi_b(1,2) + \Psi_c(1,2) \end{aligned}$$