Übungsaufgaben XII, von 28.01.2002
Musterlösungen

1.

Die Wahrscheinlichkeit ist proportionell zu $|\psi_{1s}|^2$

r_0 = Abstand wo die Aufenthaltswahrscheinlichkeit des Elektrons 10% des Maximums beträgt

$$\psi_{1s} = \frac{1}{\sqrt{\pi a_0^3}} e^{-r/a_0}$$

$$|\psi_{1s}|^2 = \underbrace{\frac{1}{\pi a_0^3}}_{\text{konstante}} e^{-2r/a_0}$$

$$|\psi_{1s}|^2_{r=r_0} = 0.1 |\psi_{1s}|^2_{max}$$

wobei $|\psi_{1s}|_{max} = |\psi_{1s}|_{r=0}$

$$\frac{1}{\pi a_0^3} e^{-2r_0/a_0} = 0.1 \frac{1}{\pi a_0^3} e^0$$

$$\Rightarrow e^{-2r_0/a_0} = 0.1$$

$$\Rightarrow r_0 = -\frac{1}{2} a_0 \ln 0.1$$

$$\Rightarrow r_0 = 1.15 a_0$$

2.

$$\iiint \psi_{1s}\psi_{2s} d\tau \overset{?}{=} 0 \Leftrightarrow \psi_{1s}\psi_{2s} \text{orthogonal}$$

$$\psi_{1s} = R_{10} Y_{00} \qquad R_{10} = 2\left(\frac{Z}{a_0}\right)^{3/2} e^{-Zr/a_0} \qquad Y_{0,0} = \sqrt{\frac{1}{4\pi}}$$

$$\psi_{2s} = R_{20} Y_{00} \qquad R_{20} = \frac{1}{2\sqrt{2}}\left(\frac{Z}{a_0}\right)^{3/2}\left(2 - \frac{Zr}{a_0}\right) e^{-Zr/2a_0}$$

Vorlesung :

$$\iiint \psi^*_{nlm}\psi_{nlm} r^2 \cdot dr \cdot \sin\theta \cdot d\theta \cdot d\phi = \int_0^\infty R^*_{nl}(r) R_{nl}(r) r^2 \cdot dr \underbrace{\int_0^\pi \int_0^{2\pi} Y^*_{lm}(\theta,\phi) Y_{lm}(\theta,\phi) \cdot \sin\theta \cdot d\theta \cdot d\phi}_{=1}$$

$$\Rightarrow \int_0^\infty R_{10} R_{20} r^2 \cdot dr \overset{?}{=} 0$$

$$\int_0^\infty R_{10} R_{20} r^2 \cdot dr = \int_0^\infty \left(2\left(\frac{Z}{a_0}\right)^{3/2} e^{-Zr/a_0}\right) \cdot \left(\frac{1}{2\sqrt{2}}\left(\frac{Z}{a_0}\right)^{3/2}\left(2 - \frac{Zr}{a_0}\right) e^{-Zr/2a_0}\right) \cdot r^2 \cdot dr =$$

$$= \frac{1}{\sqrt{2}}\left(\frac{Z}{a_0}\right)^3 \int_0^\infty e^{-Zr/a_0} \cdot \left(2 - \frac{Zr}{a_0}\right) e^{-Zr/2a_0} \cdot r^2 \cdot dr = \frac{1}{\sqrt{2}}\left(\frac{Z}{a_0}\right)^3 \int_0^\infty \left(2e^{-(3/2)Zr/a_0} - \frac{Zr}{a_0} e^{-(3/2)Zr/a_0}\right) \cdot r^2 \cdot$$

$$\int_0^\infty \left(2e^{-(3/2)Zr/a_0} - \frac{Zr}{a_0} e^{-(3/2)Zr/a_0} \right) \cdot r^2 \cdot dr = \int_0^\infty 2e^{-(3/2)Zr/a_0} \cdot r^2 \cdot dr - \int_0^\infty \frac{Z}{a_0} e^{-(3/2)Zr/a_0} \cdot r^3 \cdot dr =$$

$$= 2 \cdot \frac{2!}{27Z^3} 8a_0^3 - \frac{Z}{a_0} \cdot \frac{3!}{81Z^4} 16a_0^4 = \frac{32a_0^3}{27Z^3} - \frac{96a_0^3}{81Z^3} = 0$$

$\Rightarrow \psi_{1s}\psi_{2s}$ orthogonal

3

$$\psi_1 = \frac{1}{\sqrt{3}} s + \sqrt{\frac{2}{3}} p_y$$

$$\psi_2 = \frac{1}{\sqrt{3}} s + \frac{1}{\sqrt{2}} p_x - \frac{1}{\sqrt{6}} p_y$$

$$\psi_3 = as + bp_x + cp_y$$

$$\int \psi_1 \psi_3 d\tau = 0 \quad \Rightarrow \quad \frac{1}{\sqrt{3}} a + \sqrt{\frac{2}{3}} c = 0$$

$$\int \psi_2 \psi_3 d\tau = 0 \quad \Rightarrow \quad \frac{1}{\sqrt{3}} a + \frac{1}{\sqrt{2}} b - \frac{1}{\sqrt{6}} c = 0$$

$$\int \psi_3 \psi_3 d\tau = 1 \quad \Rightarrow \quad a^2 + b^2 + c^2 = 1$$

$$/ \int s^2 d\tau = 1, \int p^2{}_x d\tau = 1, \int p^2{}_y d\tau = 1, \int p_x\, p_y d\tau = 0, \int s p_y d\tau = 0, \int s p_x d\tau = 0 /$$

$$\Rightarrow a = -\sqrt{2} c$$

$$\frac{1}{\sqrt{2}} b - \frac{1}{\sqrt{6}} c - \sqrt{\frac{2}{3}} c = 0$$

$$\frac{1}{\sqrt{2}} b = \frac{3}{\sqrt{6}} c$$

$$\Rightarrow b = \frac{3}{\sqrt{3}} c$$

$$2c^2 + \frac{9}{3} c^2 + c^2 = 6c^2 = 1$$

$$\Rightarrow c = \pm \frac{1}{\sqrt{6}}$$

$$\Rightarrow b = \frac{3}{\sqrt{3}} c = \frac{3}{\sqrt{3}} \left(\pm \frac{1}{\sqrt{6}} \right) = \pm \frac{1}{\sqrt{2}}$$

$$\Rightarrow a = -\sqrt{2} c = -\sqrt{2} \left(\pm \frac{1}{\sqrt{6}} \right) = \mp \frac{1}{\sqrt{3}}$$

$$\Rightarrow \psi_3 = \mp \frac{1}{\sqrt{3}} s \pm \frac{1}{\sqrt{2}} p_x \pm \frac{1}{\sqrt{6}} p_y$$

4.

$$\hat{L}_z = -i\hbar \frac{\partial}{\partial\phi}$$

für $\quad Y_{1,0} = \sqrt{\frac{3}{4\pi}} \cos\theta$

$$\hat{L}_z Y_{1,0} = -i\hbar \frac{\partial}{\partial\phi}\left(\sqrt{\frac{3}{4\pi}} \cos\theta\right) = 0\hbar Y_{1,0}$$

für $\quad Y_{1,1} = -\sqrt{\frac{3}{8\pi}} \sin\theta e^{i\phi}$

$$\hat{L}_z Y_{1,1} = -i\hbar \frac{\partial}{\partial\phi}\left(-\sqrt{\frac{3}{8\pi}} \sin\theta e^{i\phi}\right) = i^2\hbar\sqrt{\frac{3}{8\pi}} \sin\theta e^{i\phi} = \hbar\left(-\sqrt{\frac{3}{8\pi}} \sin\theta e^{i\phi}\right) = \hbar Y_{1,1}$$

für $\quad Y_{1,-1} = \sqrt{\frac{3}{8\pi}} \sin\theta e^{-i\phi}$

$$\hat{L}_z Y_{1,-1} = -i\hbar \frac{\partial}{\partial\phi}\left(\sqrt{\frac{3}{8\pi}} \sin\theta e^{-i\phi}\right) = i^2\hbar\sqrt{\frac{3}{8\pi}} \sin\theta e^{-i\phi} = -\hbar\left(\sqrt{\frac{3}{8\pi}} \sin\theta e^{-i\phi}\right) = -\hbar Y_{1,-1}$$