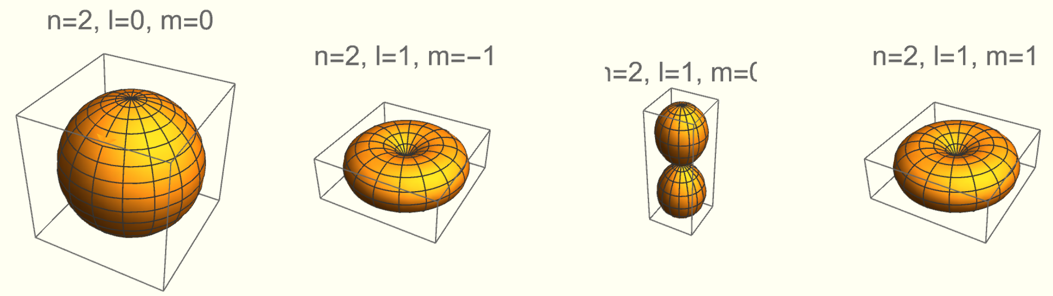
Alexander Helbok

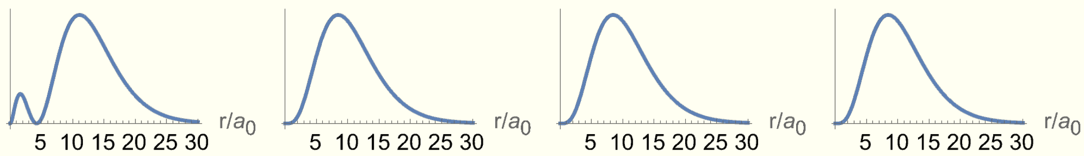
Blatt 9

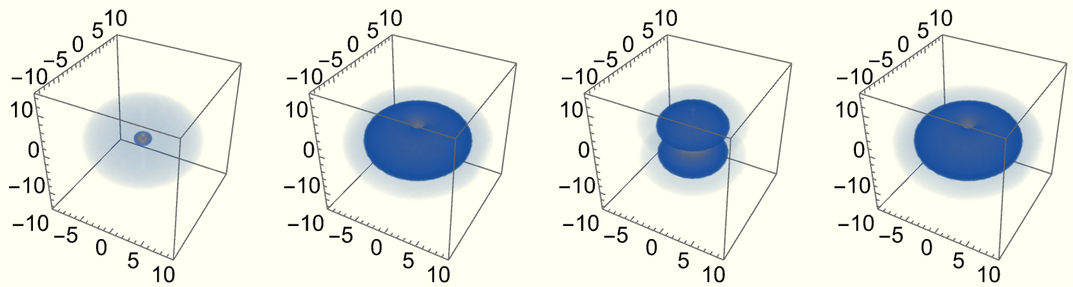
PS Physik
9. Januar 2023

Wasserstoffatom: Aufenthaltswahrscheinlichkeiten



a)





On top you can see the spherical and radial probability of an electron in a hydrogen Atom for different Quantum numbers. Below is a density plot of the square modulus of the whole wave function (as product of the upper 2 plots). If you sum all 4 states up you can kind of recognize a radial symmetry, as the $l = 0, m = 0$ state is already symmetric and the other three apparently add up to a sphere.

b)

$$\langle \hat{r} \rangle = \int_V r|\psi_{2,1,1}|^2 \,\mathrm{d}V = \int_0^{2\pi}\int_0^{\pi}\int_0^{\infty} \frac{1}{24a_0^5}\,\mathrm{e}^{-\frac{r}{a}} r^2 \frac{3}{8\pi}\sin(\theta)^2 r r^2 \sin(\theta)\,\mathrm{d}r\,\mathrm{d}\theta\,\mathrm{d}\phi =$$

$$= \frac{1}{32a_0^5}\int_0^{\infty} r^5\,\mathrm{e}^{-\frac{r}{a_0}}\,\mathrm{d}r \int_0^{\pi}\sin(\theta)^3\,\mathrm{d}\theta = \frac{1}{32a_0^5}\,120a_0^6\,\frac{4}{3} = \underline{\underline{5a_0}}$$

$$\langle \hat{r}^2 \rangle = \int_V r^2|\psi_{2,1,1}|^2 \,\mathrm{d}V = \frac{1}{32a_0^5}\int_0^{\infty} r^6\,\mathrm{e}^{-\frac{r}{a_0}}\,\mathrm{d}r \int_0^{\pi}\sin(\theta)^3\,\mathrm{d}\theta = \underline{\underline{30a_0^2}}$$

$$\langle \Delta\hat{r}^2 \rangle = \langle \hat{r}^2 \rangle - \langle \hat{r} \rangle^2 = 30a_0^2 - 25a_0^2 = \underline{\underline{5a_0^2}}$$

Bohrs model states that $r_n = \frac{n^2}{Z} a_o$ so in the case of a hydrogen atom with $Z = 1$ and an electron described by $\psi_{2,1,1}$ the model predicts a radius of $r_2 = 4a_0$.
Considering (the probabilistic nature of) quantum mechanics one gets a radius of $r_2 = 5a_0$, which clearly contradicts Bohrs model.

c) $d = 1.75$ fm

$$P = \int_V |\psi_{2,0,0}|^2 \,\mathrm{d}V = \int_0^{2\pi}\int_0^{\pi}\int_0^{d} \frac{1}{4a_0^3}\,\mathrm{e}^{-\frac{r}{a}}\left(1 - \frac{r}{a_0} + \frac{r^2}{4a_0^2}\right)\frac{1}{4\pi} r^2 \sin(\theta)\,\mathrm{d}r\,\mathrm{d}\theta\,\mathrm{d}\phi =$$

$$= \frac{1}{2a_0^3}\int_0^{d} \mathrm{e}^{-\frac{r}{a}}\left(1 - \frac{r}{a_0} + \frac{r^2}{4a_0^2}\right) r^2\,\mathrm{d}r = \underline{\underline{6.11\times 10^{-15}}}$$

Drehimpulsquantenzahlen

a) $\hat{L}_z = -i\hbar\frac{\partial}{\partial\phi}; \quad \psi_{n,l,m} = a_m R_{n,l}\cos(\theta)\,\mathrm{e}^{im\phi} P_l^m$

$$\langle \hat{L}_z \rangle = \int_V \psi^* \hat{L}_z \psi \,\mathrm{d}V = -i\hbar \int_V \psi^* \frac{\partial\psi}{\partial\phi}\,\mathrm{d}V = \hbar m \int_V \psi^*\psi\,\mathrm{d}V = \underline{\underline{\hbar m}}$$

b) $\hat{\mathbf{L}}^2 Y_l^m(\theta,\phi) = l(l+1)\hbar^2 Y_l^m(\theta,\phi)$

$$\langle \hat{\mathbf{L}}^2 \rangle = \int_V \psi^* \hat{\mathbf{L}}^2 \psi \,\mathrm{d}V = \int_V \psi^* R_{n,l} \hat{\mathbf{L}}^2 Y_l^m \,\mathrm{d}V = l(l+1)\hbar^2 \int_V \psi^* \psi \,\mathrm{d}V = \underline{\underline{l(l+1)\hbar^2}}$$

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c)

$$\begin{aligned} \left[\hat{\mathbf{L}}^2, \hat{L}_z\right] \psi_{n,l,m} &= \hat{\mathbf{L}}^2(\hat{L}_z \psi_{n,l,m}) - \hat{L}_z(\hat{\mathbf{L}}^2 \psi_{n,l,m}) = \\ &= \hat{\mathbf{L}}^2 \hbar m \psi_{n,l,m} - \hat{L}_z l(l+1)\hbar^2 \psi_{n,l,m} = \\ &= l(l+1)\hbar^3 m \psi_{n,l,m} - l(l+1)\hbar^3 m \psi_{n,l,m} = 0 \end{aligned}$$

Zeeman–Effekt

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a)

$$E = V + T = \underline{\underline{-\vec{\mu} \cdot \vec{B} + \tfrac{1}{2} m (\dot{\vec{r}})^2}}$$

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b) $\vec{B} = B\vec{e}_z; \quad |L_z| = \hbar m; \quad \vec{p}_\mathrm{m} = -\frac{e}{2m_e}\vec{L}$

$$\begin{aligned} E_{\text{pot, B}} &= -\vec{p}_\mathrm{m} \cdot \vec{B} = \tfrac{e}{2m_e} \vec{L} \cdot \vec{B} = \tfrac{e\hbar}{2m_e} m B \\ E_{n,l,m} &= E_{n,l} + \tfrac{e\hbar}{2m_e} m B \\ \Delta E &= \underline{\underline{\tfrac{e\hbar}{2m_e} m B}} \end{aligned}$$

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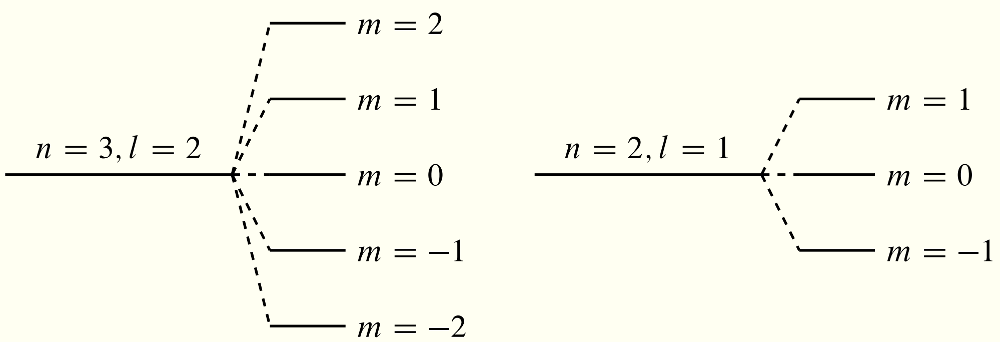
c)



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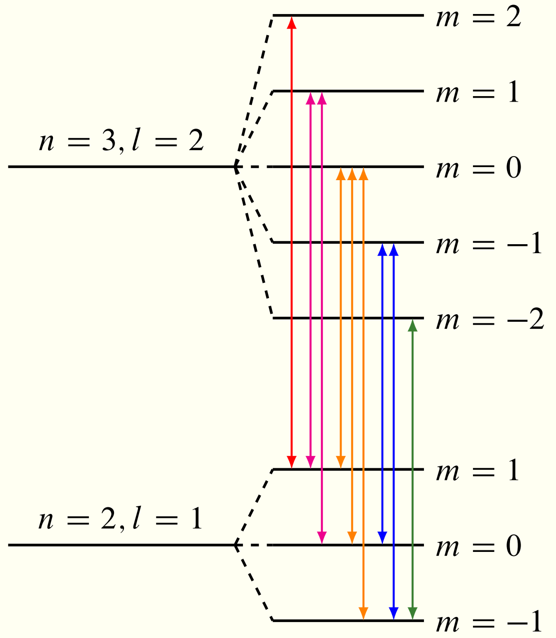
d)



$$1 + 2 + 3 + 2 + 1 = \underline{\underline{9}}$$