

Structure of matter: Homework to exercise 12

ATOMS

Due on January 16th 2024

Please indicate your name on the solution sheets and send it to your seminar leader!

- Multiple-choice test: Please tick all **box(es)** with correct answer(s)!
(correctly ticked box: +1/2 point; wrongly ticked box: -1/2 point)

Imagine an electron in a p-orbital in a hydrogen atom. Its state is consistent with the following quantum numbers:	$m = 1$	<input checked="" type="checkbox"/>
	$m = 0$	<input checked="" type="checkbox"/>
	$l = 0$	<input type="checkbox"/>
	$n = 1$	<input type="checkbox"/>
	$n = 5$	<input checked="" type="checkbox"/>
The electronic configuration $^2S_{1/2}$ is	possible	<input checked="" type="checkbox"/>
	impossible	<input type="checkbox"/>

- true or wrong? (tick the appropriate box):

(2 points): 1 point per correct decision, 0 points per wrong or no decision

Assertion	true	wrong
Fermions obey the Pauli exclusion principle.	<input checked="" type="checkbox"/>	<input type="checkbox"/>
Photons are bosons.	<input checked="" type="checkbox"/>	<input type="checkbox"/>

- The electronic ground state of the hydrogen atom is described by the wavefunction

$$\psi(r) = \frac{1}{\sqrt{\pi}} a_0^{-\frac{3}{2}} e^{-\frac{r}{a_0}}$$

where a_0 is Bohr's radius. Please calculate the expectation value $\langle r \rangle$ of the distance of the electron from the nucleus, as well as its variance $\langle r^2 \rangle - \langle r \rangle^2$. (8 points)

- Neglecting any relativistic (i.e. also electron spin) contributions, find an expression for the degree of degeneration of any hydrogen atom energy level defined by the principal quantum number n ! (4 points)
- Calculate the angle between orbital and total angular momenta in an atomic $^4D_{3/2}$ state (4 points)
- Calculate the minimum angle formed between the angular momentum vector \mathbf{L} and the z -axis in a d-state! (3 points)

$$\lambda = a_0 = \frac{2\pi\hbar^2}{e^2\pi m} \approx 0.53 \times 10^{-10} \text{ m}$$

$$\langle r \rangle = \int_V \psi^* r \psi dV = \int_0^{2\pi} d\varphi \int_0^\pi \sin\theta d\theta \int_0^\infty \psi^2 r \cdot r^2 dr$$

$$= 4\pi \cdot \frac{1}{\pi} \frac{1}{a_0^3} \int_0^\infty e^{-\frac{2r}{a_0}} r^3 dr$$

$$\int_0^\infty x^n e^{-px} = \frac{n!}{p^{n+1}} \Rightarrow \int_0^\infty e^{-\frac{2r}{a_0}} r^3 dr = \frac{3!}{\left(\frac{2}{a_0}\right)^4} = \frac{3}{8} a_0^4$$

$$\Rightarrow \langle r \rangle = \frac{3}{2} a_0$$

$$\langle r^2 \rangle = \int_V \psi^* r^2 \psi dV = \frac{4}{a_0^3} \int_0^\infty e^{-\frac{2r}{a_0}} r^4 dr = \frac{4}{a_0^3} \cdot \frac{4!}{\left(\frac{2}{a_0}\right)^5} = 3 a_0^2$$

$$\langle r^2 \rangle - \langle r \rangle^2 = 3a_0^2 - \frac{9}{4}a_0^2 = \frac{3}{4}a_0^2 \approx 0.21 \times 10^{-20} \text{ m}^2$$

4. The energy levels in the hydrogen atom depend only on the principle quantum number n . For a given n , all the states corresponding to $l=0, \dots, n-1$ have the same energy and are degenerate. For given value of n and l , the $(2l+1)$ states with $m_l = -l, \dots, l$ are degenerate.

The degree of degenerate of the energy level E_n is therefore: $\sum_{l=0}^{n-1} (2l+1)$

$$\sum_{l=0}^{n-1} (2l+1) = 1 + 3 + 5 + \dots + 2n-1 = \frac{1}{2}(2n-1+1) = n^2$$

If electron spin is included, it's $2n^2$

$$5. \vec{J} \cdot \vec{L} = |\vec{L}| |\vec{J}| \cos\theta$$

$$\vec{J} = \vec{L} + \vec{S} \Rightarrow \vec{J}^2 = (\vec{J} - \vec{L})^2 = \vec{J}^2 + \vec{L}^2 - 2\vec{J} \cdot \vec{L} \Rightarrow \vec{J} \cdot \vec{L} = \frac{1}{2}(\vec{J}^2 + \vec{L}^2 - \vec{S}^2)$$

$$\vec{J}^2 \rightarrow \hbar^2 j(j+1) \quad \vec{L}^2 \rightarrow \hbar^2 l(l+1) \quad \vec{S}^2 \rightarrow \hbar^2 s(s+1)$$

$$\Rightarrow \vec{J} \cdot \vec{L} = \frac{1}{2} \hbar^2 [j(j+1) + l(l+1) - s(s+1)] \quad |\vec{J}| |\vec{L}| = \hbar^2 \sqrt{j l (j+1)(l+1)}$$

$$n^{2s+1} X_j \rightarrow {}^4D_{3/2} \rightarrow l=2 \quad s=\frac{3}{2} \quad j=\frac{7}{2}$$

$$\cos\theta = \frac{\vec{J} \cdot \vec{L}}{|\vec{J}| |\vec{L}|} = \frac{\frac{1}{2} [j(j+1) + l(l+1) - s(s+1)]}{\sqrt{j l (j+1)(l+1)}} = \frac{1}{2} \frac{6}{\sqrt{3 \cdot 3 \cdot \frac{5}{2}}} = \sqrt{\frac{2}{5}}$$

$$\Rightarrow \theta \approx 50.7^\circ$$

6. d-state $\rightarrow l=2 \quad m_l = 0, 1, -1, 2, -2$

$$\hat{L}^2 \psi = \hbar^2 l(l+1) \psi \quad \hat{L}_z \psi = m_l \hbar \psi \quad \cos\theta = \frac{m_l \hbar}{\hbar \sqrt{l(l+1)}} = \frac{m_l}{\sqrt{6}} \quad \theta_{\min} = \arccos\left(\frac{2}{\sqrt{6}}\right) \approx 35.26^\circ$$