Structure of matter: Homework to exercise 12

23/23

ATOMS

Due on January 16th 2024

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

1. Multiple-choice test: Please tick all box(es) with correct answer(s)! 2
(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:	$m = 1$	✓
	$m = 0$	✓
	$l = 0$	
	$n = 1$	
	$n = 5$	✓
The electronic configuration $^2S_{1/2}$ is	possible	✓
	impossible	

2. true or wrong? (tick the appropriate box):

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

Assertion	true	wrong
Fermions obey the Pauli exclusion principle.	✓	
Photons are bosons.	✓	

3. 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 <r> of the distance of the electron from the nucleus, as well as its variance $\langle r^2 \rangle - \langle r \rangle^2$. (8 points)
4. 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)
5. Calculate the angle between orbital and total angular momenta in an atomic $^4D_{3/2}$ state (4points)
6. Calculate the minimum angle formed between the angular momentum vector **L** and the z-axis in a d-state! (3points)

3. $a_0 = \frac{\varepsilon_0 \hbar^2}{e^2 \pi M} \approx 0.53 \times 10^{-10}\,m$

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

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

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

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

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

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

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 $l = 0 \cdots, n-1$ have the same energy and are degenerate. for given value of n and l, the $(2l+1)$ states with $m_l = -l, \cdots l$ are degenerate.

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

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

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

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

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

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

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

$$n^{2S+1}X_j \longrightarrow {}^4D_{\frac{3}{2}} \Rightarrow l = 2 \quad s = \frac{3}{2} \quad j = \frac{3}{2}$$

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

$$\Rightarrow \theta \approx 50.77°$$

(6) d-state $\Rightarrow l = 2 \quad m = 0, 1, -1, 2, -2$

$$\hat{L}^2 \varphi = \hbar^2 l(l+1) \varphi \qquad \hat{L}_z \varphi = m\hbar\varphi \qquad \cos\theta = \frac{m\hbar}{\hbar\sqrt{l(l+1)}} = \frac{m}{\sqrt{6}} \qquad \theta_{min} = \arccos\frac{2}{\sqrt{6}}$$

$$\approx 35.26°$$