

**Exercise Sheet 1** due 16 April

prepare your solutions so you are ready to present them in class  
if you cannot solve a problem, explain where you got stuck.

1. *atomic units*

Express the speed of light and the Bohr magneton in atomic units.

What unit of temperature do we have to choose to also make the numerical value of the Boltzmann constant to equal 1?

2. *magnetic moment*

From classical magnetostatics we know that the magnetic moment due to an electrical current density  $\vec{j}_e$  is given by

$$\vec{m} = \frac{1}{2} \int \vec{r} \times \vec{j}_e d^3r .$$

i. Given the quantum-mechanical probability current density

$$\vec{j} = \frac{\hbar}{2im_e} \left( \overline{\psi(\vec{r})} \vec{\nabla} \psi(\vec{r}) - \psi(\vec{r}) \vec{\nabla} \overline{\psi(\vec{r})} \right) ,$$

calculate the corresponding magnetic moment. Compare to the expectation value of the angular momentum operator  $\vec{L}$ .

ii. What is the z-component of the magnetic moment for the following orbitals of the hydrogen atom  $|n, l, m\rangle$ :  $|1, 0, 0\rangle$ ,  $|2, 0, 0\rangle$ ,  $|2, 1, -1\rangle$ ,  $|2, 1, 0\rangle$ ,  $|2, 1, 1\rangle$ , and  $|5, 3, 2\rangle$ . Express your results using the Bohr-magneton

$$\mu_B = \frac{e\hbar}{2m_e} .$$

3. *charge states*

What formal charge do you expect for the transition metal in  $\text{KCrF}_3$ ? Which for the manganese ions in  $\text{SrMnO}_3$ ?

4. *atomic radii*

Read the article W.L. Bragg, *Phil. Mag.* **40**, 169 (1920) and try to understand how atomic radii are derived from crystal structure data.

Historical notes: First crystal structures were determined 1912 by Max von Laue (Nobel Prize in Physics 1914 *for his discovery of the diffraction of X-rays by crystals*) and by the Braggs (father and son, Nobel Prize 1915 *for their services in the analysis of crystal structure by means of X-rays*). The Schrödinger equation was published 1926 (Nobel Prize 1933). For a readable account of the discoveries, you can browse the Nobel lectures at [http://www.nobelprize.org/nobel\\_prizes/physics/laureates/1914](http://www.nobelprize.org/nobel_prizes/physics/laureates/1914) etc..