Exercise Sheet 1

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

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

i. Given the quantum-mechanical probability current density

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

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

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

3. *charge states*

What formal charge do you expect for the transition metal in $KCrF_3$? Which for the manganese ions in $SrMnO_3$?

4. *lattice structures*

Use the Inorganic Crystal Structure Database `http://icsd.fiz-karlsruhe.de` (accessible from inside the RWTH network) to find the lattice constant of sodium chloride (NaCl) at room temperature and ambient pressure.