Exercise Sheet 1 due 16 April 2018

1. *atomic units*

Express

- the speed of light
- the Bohr magneton

in atomic units.

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 $KCrF_3$? Which for the manganese ions in $SrMnO_3$?

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` etc..