Modern Physics

Instructor: Prof. Bernd Pilawa (bernd.pilawa@kit.edu)

Winter Semester 23/24

Exercise 8

§ Atoms §

Problem 1: Hydrogen atom: Orthogonality of the wave functions

a) The angular components of the wave functions of the electron in a hydrogen atom is given by the spherical harmonic functions. The first few spherical harmonics corresponding to the states with angular momentum quantum numbers $|l, m_l\rangle$ of $|0,0\rangle$, $|1,0\rangle$ and $|1,\pm 1\rangle$ are:

$$Y_{0,0}(\theta,\varphi) = \frac{1}{\sqrt{4\pi}}$$
$$Y_{1,0}(\theta,\varphi) = \sqrt{\frac{3}{4\pi}}\cos\theta$$
$$Y_{1,\pm 1}(\theta,\varphi) = \mp\sqrt{\frac{3}{8\pi}}e^{\pm i\varphi}\sin\theta \tag{1.1}$$

Check that the functions are orthogonal by proving that:

$$\int_{\varphi=0}^{2\pi}\int_{\theta=0}^{\pi} Y*_{l',m'}(\theta,\varphi)\, Y_{l,m}(\theta,\varphi)\sin\theta\, d\theta\, d\varphi = \delta_{l',l}\delta_{m',m}. \tag{1.2}$$

Hint: $\int \sin^3 x dx = \frac{1}{12}(\cos(3x) - 9\cos(x))$.

b) The radial components of the wave function of an electron in the hydrogen atom are constructed from Laguerre polynomials. The first two radial eigenfunctions for the $|n,l\rangle = |1,0\rangle = |1s\rangle$ and $|2,0\rangle = |2s\rangle$ states are:

$$R_{10}(r) = \frac{2}{(a_0)^{\frac{3}{2}}}\cdot e^{-\frac{r}{a_0}},$$
$$R_{20}(r) = \frac{2}{(2a_0)^{\frac{3}{2}}}\cdot\left(1-\frac{r}{2a_0}\right)e^{-\frac{r}{2a_0}}. \tag{1.3}$$

Check that the two functions are orthonormal by calculating:

$$1.\ \int_0^\infty R*_{1,0}(r)R_{1,0}(r)r^2 dr,$$
$$2.\ \int_0^\infty R*_{2,0}(r)R_{2,0}(r)r^2 dr,$$
$$3.\ \int_0^\infty R*_{1,0}(r)R_{2,0}(r)r^2 dr. \tag{1.4}$$

Hint 1: $\int_0^\infty R*_{n,l}(r)R_{n',l'}(r)r^2 dr = \delta_{n,n'}\delta_{l,l'}$

Hint 2: $\int_0^\infty x^n e^{-ax} dx = \frac{n!}{a^{n+1}}$

Problem 2: Hydrogen atom: Probability density

The electron of a hydrogen atom is in the state $|n, l, m_l\rangle = |2, 1, +1\rangle$.
Find the probability that ...:

a) ... the electron is found within $\pm 30°$ of the x-y-plane at any radius.

b) ... the electron is found in the radius interval $2a_0 < r < 6a_0$.

c) ... the electron is found within $\pm 30°$ of the x-y-plane and in the radius interval $2a_0 < r < 6a_0$.

$$\textit{Hint: } R_{21}(r) = \frac{1}{(2a_0)^{\frac{3}{2}}} \cdot \frac{r}{\sqrt{3}a_0} \cdot e^{-\frac{r}{2a_0}}$$

Problem 3: Molecular rotation and oscillation

The atoms of the $C - O$ molecule can oscillate and rotate around the common center of rotation of the molecule ($m_c = 12\,\mathrm{g\,mol^{-1}}$, $m_0 = 16\,\mathrm{g\,mol^{-1}}$).

a) Give the Schrödinger equation for the case that only oscillations of the molecule can be excited.

b) What are the possible energy levels of the oscillating molecule?

c) Calculate the spring constant between the atoms of the molecule, if oscillations can be excited with light of wavelength $\lambda = 4.7 \times 10^{-6}\,\mathrm{m}$.

d) Calculate the excitation energies, if only rotations of the molecule are excited. Calculate the wavelength of the corresponding radiation. Use a bond length of $100\,\mathrm{pm}$ for the $C - O$ molecule.