1 Exercise 1 - Bohr Model

a. Radii

Solution: If the electron is moving in circles around a nucleus of charge Ze, with constant tangential velocity v, then in order to stay in any orbit, the centripetal force must be equal to the electric force generated by the electron and the nucleus. Mathematically we can express this as

$$F = \underbrace{\frac{1}{4\pi\epsilon_0}\frac{Ze^2}{r^2}}_{\text{Coulomb force}} = \underbrace{\frac{m_e v^2}{r}}_{\text{Centripetal force}} . \tag{1}$$

For this problem I will assume that the angular momentum can take on values $\hbar$, $2\hbar$, $\ldots$, but never non-integer values. For circular orbits, the position vector of the electron $\vec{r}$ is always perpendicular to the linear momentum of the particle $\vec{p}$. The angular momentum $\vec{L}$ has magnitude $L = rp = m_e vr$ in this case. As a consequence of this and the previously assumed values of the angular momentum we now know that,

$$m_e vr = n\hbar, \qquad n \in \mathbb{Z}, \tag{2}$$

if we isolate the velocity term from equation 2 then we obtain

$$v = \frac{n\hbar}{m_e r}. \tag{3}$$

Now all we need to do is to insert eq. 3 into eq. 1

$$\frac{m_e v^2}{r} = \frac{m_e}{r}\left(\frac{n\hbar}{m_e r}\right)^2 = \frac{1}{4\pi\epsilon_0}\frac{Ze^2}{r^2}, \tag{4}$$

and finally we get

$$\frac{\cancel{m_e} n^2\hbar^2}{r^{\cancel{3}} m_e^{\cancel{2}}} = \frac{Ze^2}{4\pi\epsilon_0 \cancel{r^2}},$$

$$\Rightarrow \frac{n^2\hbar^2}{r m_e} = \frac{Ze^2}{4\pi\epsilon_0},$$

$$r_n = \frac{4\pi\epsilon_0\hbar^2}{m_e e^2}\frac{n^2}{Z} = \boxed{a_0 \frac{n^2}{Z}}, \tag{5}$$

where a_0 is the Bohr radius.

b. Energies

Solution: From eq. 1 we can obtain the kinetic energy K, using r_n

$$\frac{1}{4\pi\epsilon_0}\frac{Ze^2}{r_n^2} = \frac{m_e v^2}{r_n} \Rightarrow m_e v^2 = \frac{1}{4\pi\epsilon_0}\frac{Ze^2}{r_n},$$

$$\Rightarrow K = \frac{m_e v^2}{2} = \frac{1}{8\pi\epsilon_0}\frac{Ze^2}{r_n}. \tag{6}$$

On the other hand, the potential energy U is easy to calculate, since it only comes from the Coulomb forces. U is then

$$U = -\frac{1}{4\pi\epsilon_0}\frac{Ze^2}{r_n}. \tag{7}$$

At this point we use $E = K + U$, therefore

$$E_n = \frac{1}{8\pi\epsilon_0}\frac{Ze^2}{r_n} - \frac{1}{4\pi\epsilon_0}\frac{Ze^2}{r_n} = -\frac{1}{8\pi\epsilon_0}\frac{Ze^2}{r_n}. \tag{8}$$

Finally, we use the value for r_n calculated in the previous section and depicted in eq. 5,

$$E_n = -\frac{1}{8\pi\epsilon_0}\frac{Ze^2}{r_n} = -\frac{1}{8\pi\epsilon_0}\frac{Ze^2}{\left(\frac{a_0 n^2}{Z}\right)} = -\frac{1}{8\pi\epsilon_0}\frac{Z^2e^2}{a_0 n^2} = -\frac{Z^2 E_1}{n^2}, \tag{9}$$

where $E_1 = e^2/(8\pi\epsilon_0 a_0) = 13.6$ eV.

2 Exercise 2 - Hydrogen Atom

a. Solve Schrödinger Equation

Solution: d

b. Quantum numbers

Solution: d

c. Degeneracies

Solution: d

3 Exercise 3 - Real Spherical Harmonics

a. Sketchs

Solution:

By definition, the qubic harmonics for d states are the following.

$$d_{3z^2-1} = Y_{2,0} = \sqrt{\frac{5}{16\pi}}\left(3\cos^2\theta - 1\right) \tag{10}$$

$$d_{zx} = \sqrt{\frac{1}{2}}\left(Y_{2,-1} - Y_{2,1}\right) = \sqrt{\frac{5}{16\pi}}\sin 2\theta\cos\phi \tag{11}$$

$$d_{yz} = \sqrt{\frac{1}{2}}i\left(Y_{2,-1} + Y_{2,1}\right) = \sqrt{\frac{5}{16\pi}}\sin 2\theta\sin\phi \tag{12}$$

$$d_{x^2-y^2} = \sqrt{\frac{1}{2}}\left(Y_{2,-2} + Y_{2,2}\right) = \sqrt{\frac{5}{16\pi}}\sin^2\theta\cos 2\phi \tag{13}$$

$$d_{xy} = \sqrt{\frac{1}{2}}i\left(Y_{2,-2} - Y_{2,2}\right) = \sqrt{\frac{5}{16\pi}}\sin^2\theta\sin 2\phi \tag{14}$$

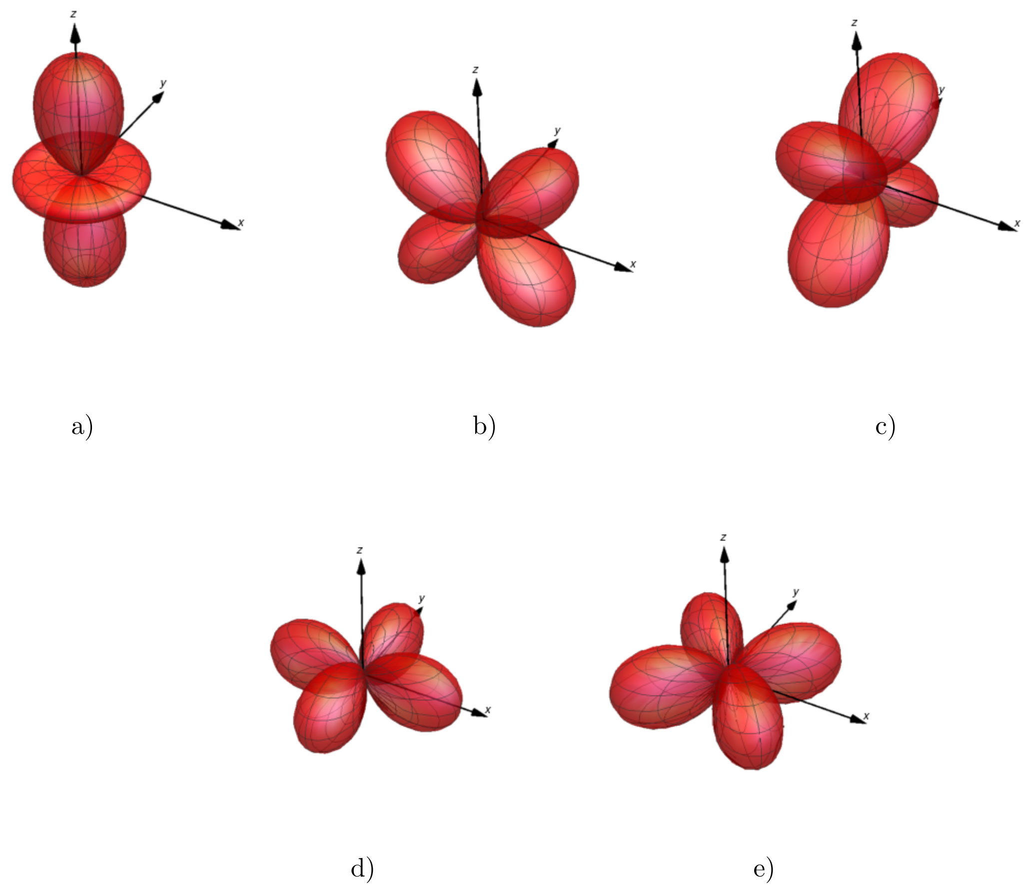

Figure 1: Qubic harmonics, ploted as defined in eqs. 10-14, and organized as follows a) d_{3z^2-1}, b) d_{xz}, c) d_{yz}, d) $d_{x^2-y^2}$, e) d_{xy}

4 Exercise 4 - Crystal Field Splitting

a. Atom in Octahedron

Solution: d