PHY801: Survey of Atomic and Condensed Matter Physics
Michigan State University

Homework 1 – Solution

1.1. Using a hydrogenic model, estimate the 1st ionization energy of a Li atom, assuming that the two electrons in the 1s state essentially screen the nuclear charge, thus making its effective charge $+1e$. The observed value of the 1st ionization energy is 5.39 eV. Discuss possible physical reasons for the difference between the estimated and the observed value.

Solution:

Assuming naively that the nuclear charge is screened by the $1s$ core electrons, we may consider this to be close to a hydrogen atom with the ionization potential of $I = 13.6$ eV. This is significantly more than the observed value.

Now, the valence electron is in the $2s$, not $1s$ state of the hydrogen atom. The ionization energy is much smaller, $I = Rydberg/n^2 = 13.6/4$ eV=3.4 eV.

Next, consider the fact that the $2s$ electron penetrates the core region, where screening by the $1s$ electrons is not that effective. This increase the attraction, thus increasing the binding energy from 3.4 eV to 5.39 eV.

1.2. Calculate the 3rd ionization energy of the Li atom. Is your answer exact?

Solution:

The binding energy of the n^{th} state is given by $E_n = -\frac{Z^2}{n^2}$ Ry. With $Z = 3$ and $n = 1$, the 3rd ionization energy of the Li atom is $I = 9{\times}13.6$ eV=122.4 eV. This value is exact, since no other electrons are present.

1.3. What is the probability of finding the $1s$ electron in Pb^{81+} inside the Pb nucleus? Assume that the nuclear radius $R = r_0 A^{1/3}$, where $r_0 = 1.2$ fermi and A is the atomic mass number (which differs from the atomic number Z!) of Pb.

Solution:

Since the atomic number of Pb is $Z = 82$, Pb^{81+} contains only one electron and can be treated by the hydrogenic model with the length scale reduced by $Z = 82$. The normalized wave function is given by

$$\varphi_{1s} = \frac{1}{\sqrt{\pi \tilde{a}_B^3}} e^{-\frac{r}{\tilde{a}_B}} \ ,$$

where we define a reduced Bohr radius by

$$\tilde{a}_B = \frac{\hbar^2}{me^2 Z} \ .$$

The probability to find the $1s$ electron inside the nucleus of radius R is

$$P = \int_0^R |\varphi_{1s}|^2 r^2 dr d\Omega \ .$$

First assume that the electron wave function decays very little (confirm this approximation later) and use its value at the origin. This gives

$$P = \frac{1}{\pi \tilde{a}_B^3} V ,$$

where V is the volume of the nucleus. The mass number of Pb, which you can look up, is $A = 207.19$ (this is an average over most abundant isotopes). Plugging in all the numbers you should find

$$P = \frac{4}{3} \left(\frac{R}{\tilde{a}_B} \right)^3 = 2.1 \times 10^{-6} .$$

This probability is quite small. The assumption of replacing the wave function by its value at the origin in the integral for P should thus be quite good.

1.4. Excitons in quantum wells and their binding energies can be approximated by a 2-dimensional (2D) hydrogen atom model. To use this description, first separate the radial part $R(r)$ and the angular part $Y(\theta)$ of the wavefunctions in the Schrödinger equation. Show that the radial part of the wavefunctions is the solution of (in atomic units)

$$\frac{1}{2}(R'' + \frac{1}{r}R') - \frac{m^2}{2r^2}R + (E + \frac{1}{r})R = 0 .$$

The angular part of the wave functions is given by $e^{im\theta}$. R' is the first and R" the second derivative of $R(r)$ with respect to r. Use the same scaling that was used in the 3D case in defining the variable $\rho = \kappa r$. Use $\kappa = (-2E)^{1/2}$ when writing down the second order differential equation for $R(\rho)$ in terms of the parameter $\rho_0 = 2/\kappa$. How does $R(\rho)$ behave as $\rho \to 0$ and $\rho \to \infty$? Define a function $v(\rho)$ following the same procedure as in the 3D case. Solve this equation and identify physical solutions, which provide the spectrum of the 2D hydrogen atom.

Solution:

$$\left[-\frac{1}{2}\nabla^2 - \frac{1}{r} \right] \phi(\vec{r}) = E\phi(\vec{r}) , \text{ where } \vec{r} = (r, \theta) .$$

Then separate

$$\phi(\vec{r}) = R(r)Y(\theta)$$

and use the expression

$$\nabla^2 = \left(\frac{\partial^2}{\partial r^2} + \frac{1}{r}\frac{\partial}{\partial r} + \frac{1}{r^2}\frac{\partial^2}{\partial \theta^2} \right)$$

in 2D. The Schrödinger equation then becomes

$$\frac{2r^2}{2R}\left(\frac{d^2R}{dr^2} + \frac{1}{r}\frac{dR}{dr} \right) + \frac{1}{Y}\frac{d^2Y}{d\theta^2} + 2r^2\left(\frac{1}{r} + E \right) = 0 \text{ for all } r \text{ and } \theta ;$$

$$\frac{1}{Y}\frac{d^2Y}{d\theta^2} = -m^2 ;$$

$$\frac{1}{2}\left(\frac{d^2R}{dr^2} + \frac{1}{r}\frac{dR}{dr} \right) - \frac{m^2}{2r^2}R + \left(\frac{1}{r} + E \right) R = 0 .$$

In 3D this becomes

$$\frac{1}{2}\left(\frac{d^2R}{dr^2} + \frac{1}{r}\frac{dR}{dr} \right) - \frac{l(l+1)}{2r^2}R + \left(\frac{1}{r} + E \right) R = 0 .$$

To solve the 2D case, same as in 3D, use $\kappa = \sqrt{-2E}$, $\rho = \kappa r$, and $\rho_0 = 2/\kappa$. Then,

$$\frac{d^2R}{d\rho^2} + \frac{1}{\rho}\frac{dR}{d\rho} - \frac{m^2}{\rho^2}R + \left(\frac{\rho_0}{\rho} - 1 \right) R = 0 .$$

The spectrum is symmetric under $m \to -m$. So we can choose $m \geq 0$. After looking at the $\rho \to 0$ and $\rho \to \infty$ behavior of $R(\rho)$, we define $R(\rho) = \rho^m e^{-\rho} v(\rho)$, where $v(\rho)$ satisfies

$$\rho v''(\rho) + (2m + 1 - 2\rho)v' - (2m + 1 - \rho_0)v = 0$$

with

$$v'' = \frac{d^2 v}{d\rho^2} \quad \text{and} \quad v' = \frac{dv}{d\rho} \; .$$

Now use a power series expansion for

$$v(\rho) = \sum_0^\infty c_j \rho^j \; .$$

Substitute $v(\rho)$ in the above differential equation for $v(\rho)$ and equate terms with the same power of ρ^j. Then you get

$$c_{j+1} = \frac{2j + 2m + 1 - \rho_0}{j(j+1) + (j+1)(2m+1)} c_j \; .$$

For bound-state solutions, as in the 3D case, the power series for $v(\rho)$ must terminate. This gives

$$\rho_0 = 2j_{max} + 2|m| + 1 \text{ for } \; j_{max} \geq 0 \; ,$$

where we have used the $m = -m$ symmetry to replace m by $|m|$. Finally we get

$$\begin{aligned} \rho_0 = 2k + 1 \text{ with } \; k = 0, 1, 2, \ldots \; ; \\ \kappa = \frac{2}{\rho_0} = \frac{2}{2k+1} \; ; \\ E = -\frac{1}{2}\kappa^2 = -\frac{1}{2}\frac{1}{(k + 1/2)^2} \text{ with } \; k = 0, 1, 2, \ldots \; ; \end{aligned}$$

Using

$$n = k + 1$$

we get

$$E = -\frac{1}{2}\frac{1}{(n - 1/2)^2} \quad \text{with} \; n = 1, 2, 3, \ldots \; .$$
