

PHY 491

HW Assignment #1, Sept 2-9, 2011

- Using a hydrogenic model, estimate the 1<sup>st</sup> ionization energy of Li atom, assuming that the two electrons in the 1s state essentially screen the nuclear charge making the effective charge +1e. The actual value of this 1<sup>st</sup> ionization energy is 5.39 eV. Discuss possible physical reasons for this difference.

Answer: 13.6 eV

The actual ionization energy is 5.39 eV which is considerably less than that given by the simple model used. There are two physical effects not included in the simple model. (i) The 2s electron penetrates the core and sees a stronger attractive potential leading to stronger binding (increasing the ionization energy). (ii) The 2s electron wave function must be orthogonal to core 1s wave function. This introduces node in the radial wave function of the 2s thereby increasing its kinetic energy, leading to weaker binding. The combination of (i) and (ii) results in a net increase in energy from that given by the simple hydrogenic model.

There is another way of looking at it. Start from the 2s state energy of the hydrogen atom. It has already nodes in the wave function, taking care of (ii) above). The ionization energy is  $Ryd/4=3.4$  eV. Now introduce effect (i) which will increase attraction and increase the binding energy, from 3.4 eV to 5.39 eV.

- Calculate the 3<sup>rd</sup> ionization energy of the Li atom. Is your answer exact?

$$E_n = -\frac{Z^2}{n^2} Ryd$$

$$\text{Ionization energy} = 9 \times 13.6 \text{ eV} = 122.4 \text{ eV}$$

- What is the probability of finding the 1s electron in  $Pb^{81+}$  inside the Pb nucleus? The nuclear radius  $R = r_0 A^{1/3}$ , where  $r_0=1.2$  fermi and A is the atomic number of Pb.

$Pb^{81+}$  Hydrogenic model with  $Z=82$  with the length scale reduced by Z.

$$\varphi_{1s} = \frac{1}{\sqrt{\pi a_B^3}} e^{-\frac{r}{a_B}}$$

$$a_B = \frac{\hbar^2}{me^2 Z}$$

Probability that the 1s electron is inside the nucleus  $P = \int_0^{R_N} |\phi_{1s}|^2 r^2 dr d\Omega$   
 First assume that the electron wave function decays very little (confirm this approximation later) and use its value at the origin. This gives

$$P = \frac{4}{a_B^3} V_N$$

$V_N$  is the volume of the nucleus. Plugging all the numbers I find (you double check)

$$P = \frac{16\pi}{3} \left(\frac{R_N}{a_B}\right)^3 = 2.3 \times 10^{-5}$$

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

4. Binding energies of excitons in quantum wells can be approximated by a 2-dimensional (2d) hydrogen atom model. Show that the radial part of the Schrodinger equation after separating the radial,  $R(r)$  and angular  $Y(\theta)$  parts is given by (in atomic units)

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

The angular part of the wave functions are  $e^{im\theta}$ ,  $R'$  and  $R''$  are the first and second derivatives of  $R$  with respect to  $r$ . Use the same scaling that was used for the 3d case in defining the variable  $\rho = \kappa r$ ;  $\kappa = \sqrt{-2E}$  to write down a second order differential equation for  $R(\rho)$  in terms of the parameter  $\rho_0 = \frac{2}{\kappa}$

How does  $R(\rho)$  behave as  $\rho \rightarrow 0$  and  $\infty$ ? Define a function  $v(\rho)$  following the same procedure as for the 3d case. Solve this equation for physical solutions and find the spectrum of the 2d hydrogen atom.

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

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

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

The Schrodinger equation becomes

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

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

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

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

To solve 2d case use :

$$\kappa = \sqrt{-2E}; \rho = \kappa r; \rho_0 = \frac{2}{\kappa} \text{ (same as 3d)}$$

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

The spectrum is symmetric under  $m \rightarrow -m$ . So we will choose  $m \geq 0$ . After looking at the small and large  $\rho$  behaviors of  $R(\rho)$  we define  $R(\rho) = \rho^m e^{-\rho} v(\rho)$ ,

where  $v(\rho)$  satisfies the following equation.

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

$$\text{where } v'' = \frac{d^2v}{d\rho^2}; v' = \frac{dv}{d\rho}$$

Now use a power series expansion for  $v(\rho) = \sum_0^{\infty} c_j \rho^j$

Substitute in the above differential equation for  $v(\rho)$  and equate the powers of  $\rho^j$ .

We 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

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

I have used the  $m \rightarrow -m$  symmetry to replace  $m$  by  $|m|$ .

Finally we get

$$\rho_0 = 2k + 1, k = 0, 1, 2, \dots$$

$$\kappa = \frac{2}{\rho_0} = \frac{2}{2k + 1}$$

$$E = -\frac{1}{2}\kappa^2 = -\frac{1}{2} \frac{1}{(n - 1/2)^2}; n = 1, 2, 3, \dots$$

