Average Size of a Hydrogen Atom

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Abstract

In this project we derived the average size of a hydrogen atom in the frameworks of classical and quantum mechanics. From the classical point of view, the motion of an electron in a hydrogen atom is similar to the motion, for example, of the Earth around the Sun: the electron revolves around the nucleus in a plane along an ellipse. To calculate the average size of a hydrogen atom, we applied different theories such as Kepler's problem in classical physics and Schrödinger's equation in quantum mechanics. At first, we derived a formula for average size of hydrogen atom in classical mechanics, then we substituted the energy and angular momentum of the electron in their quantized forms, and finally, we compared the obtained result with the accurate quantum mechanical calculations.

1 Introduction

The main purpose of this project was to investigate the connection between classical and quantum physics. To do so, we calculated the average size of a hydrogen atom from a classical physics point of view and then compared the obtained result to the quantum physics prediction. Such a comparison is a good example to see if these two theories have something in common. For the classical physics approach, we used the Kepler problem to calculate the average size of a hydrogen atom. Due to the similarity between Coulomb's and Newton's forces, the Kepler problem can be used to described the motion of two charged particles. For the quantum mechanical part, we took the expression for the average size of a hydrogen atom from a textbook.

2 Theory Outlines

2.1 General Classical Theory of Orbital Motion

We consider the motion of an electron around a nucleus as a two-dimensional motion along an ellipse. In two dimensions, we introduce two components of the velocity of the electron: one is the radial velocity and the other is the angular velocity. The total velocity of an electron can be written as

$$\vec{v} = \dot{r}\hat{r} + \omega r\hat{\theta}, \tag{1}$$

where $\hat{r}$ and $\hat{\theta}$ are the unit vectors for the radial distance and angular displacement respectively, $\dot{r}$ is radial velocity, ω is the angular velocity, and r is the radius. The kinetic energy of the electron can be presented as a sum of

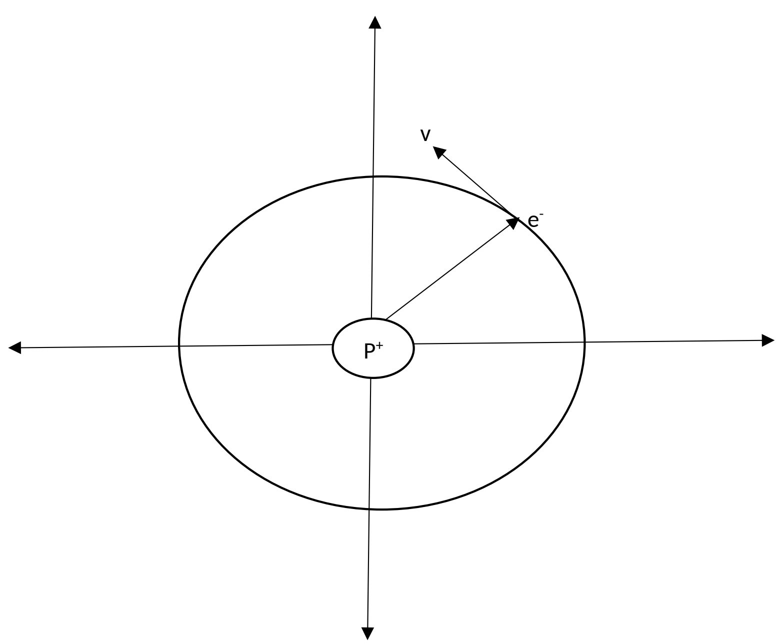

Figure 1: Electron orbiting the nucleus.

the radial and angular parts as

$$\frac{mv^2}{2} = \frac{m\dot{r}^2}{2} + \frac{m\omega^2 r^2}{2}, \tag{2}$$

where m is the mass of electron. If an electron is at a distance r from the proton, then potential energy as a function of r is given by

$$U(r) = -\frac{ke^2}{r}, \tag{3}$$

where e is the elementary charge and k is the Coulomb's constant. The total energy of an electron is the sum of its kinetic and potential energies:

$$E = \frac{m\dot{r}^2}{2} + \frac{m\omega^2 r^2}{2} - \frac{ke^2}{r}. \tag{4}$$

Using the law of conservation of angular momentum we can express the angular part of the kinetic energy through the angular momentum L as

$$E = \frac{m\dot{r}^2}{2} + \frac{L^2}{2mr^2} - \frac{\alpha}{r}, \tag{5}$$

where $\alpha = ke^2$ is a constant and we used $\omega = L/mr^2$. Now we can introduce the effective potential energy which defines the radial motion as

$$E = \frac{m\dot{r}^2}{2} + U_{eff}(r), \tag{6}$$

where

$$U_{eff}(r) = \frac{L^2}{2mr^2} - \frac{\alpha}{r} \tag{7}$$

is the effective potential energy.

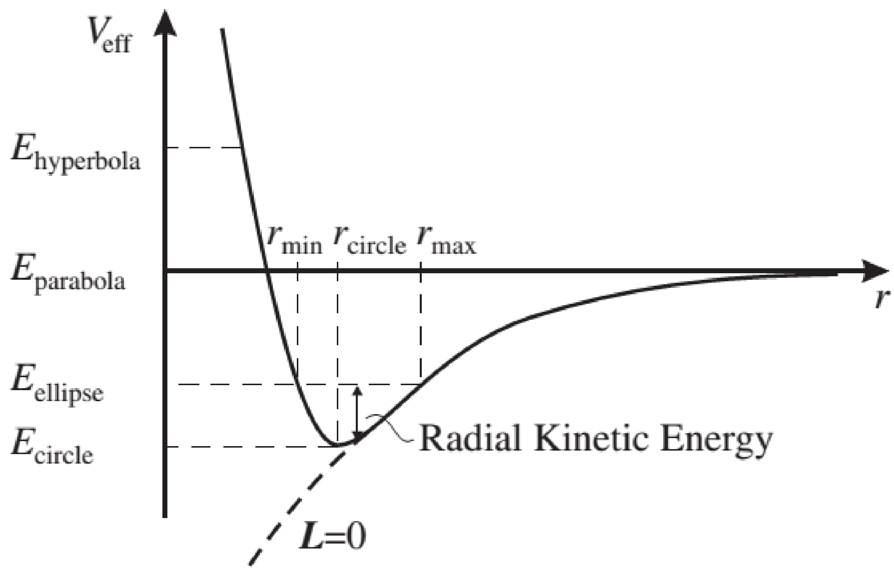

Figure 2: The effective potential energy.

From Fig. 2 we can see that at certain energy E the electron moves from the minimum radius called perihelion to the maximum radius known as aphelion. The nucleus is at its focus of the ellipse.

2.2 Average Size Of a Hydrogen Atom Calculated in Classical Physics

The time period of an electron in a hydrogen atom is the time required for an electron to complete one revolution around a nucleus. To find the average radius of a hydrogen atom we took the integral of the radius as a function of time from 0 to the period T:

$$\langle r \rangle = \frac{1}{T} \int_0^T r(t)\, dt. \tag{8}$$

By the law of conservation of angular momentum we will change the integration variable from the time to angle

$$L = mrv_{\perp} = mr^2\dot{\theta} \text{ and } dt = \frac{mr^2 d\theta}{L}, \tag{9}$$

where $v_\perp = r\dot{\theta} = r\omega$ is the perpendicular component of the velocity. Thus the average radius of a hydrogen atom can be written as:

$$\langle r \rangle = \frac{m}{TL} \int_0^{2\pi} r^3 d\theta. \tag{10}$$

We can find the distance between the central object and the orbiting object as a function of angle by using the Kepler's first law of planetary motion which states that, "The orbit of every planet is an ellipse with the sun at a focus." The mathematical expression for the radius of a hydrogen atom as a function of angle θ has a very well know form:

$$r(\theta) = \frac{p}{1 + e\cos\theta}, \tag{11}$$

where p is the parameter or the semi-latus rectum, e is the eccentricity of the orbit, θ is the angle to the electron's current position from its closest approach, and (r,θ) are polar coordinates. Plugging the expression (11) into the integral (10) we get

$$\langle r \rangle = \frac{mp^3}{LT} \int_0^{2\pi} \frac{d\theta}{(1 + e\cos\theta)^3} = \frac{mp^3}{LT} I_3(1), \tag{12}$$

where it is convenient to introduce the following set of integrals

$$I_n(\lambda) = \int_0^{2\pi} \frac{d\theta}{(\lambda + e\cos\theta)^n}. \tag{13}$$

We can relate the integral we need $I_3(\lambda)$ to a more simple one $I_1(\lambda)$ as follows

$$I_3(\lambda) = \frac{1}{2}\frac{d^2 I_1(\lambda)}{d\lambda^2}. \tag{14}$$

The integral I_1 is well known and its value is

$$I_1(\lambda) = \frac{2\pi}{\sqrt{\lambda^2 - e^2}}. \tag{15}$$

Deriving our integral $I_3(\lambda)$ at $\lambda = 1$ we finally get

$$I_3(1) = \pi \frac{2 + e^2}{(1 - e^2)^{\frac{5}{2}}} \tag{16}$$

and the average radius of a hydrogen atom becomes

$$\langle r\rangle = \frac{mp^3}{LT}\frac{2+e^2}{(1-e^2)^{\frac{5}{2}}}. \tag{17}$$

From the solution of Kepler's problem the eccentricity e, time period T, angular momentum L, energy E, the strength of the interaction α, and parameter p are related to each other as:

$$e^2 = 1 - \frac{2|E|L^2}{\alpha^2 m},\ p = \frac{L^2}{\alpha m},\ T = \pi\alpha\sqrt{\frac{m}{2|E|^3}}. \tag{18}$$

We took these values from the textbook [1]. Hence, the average radius of a hydrogen atom can be expressed only through the energy and angular momentum as:

$$\langle r\rangle = \frac{\alpha}{4|E|}\left(3 - \frac{2|E|L^2}{m\alpha^2}\right), \tag{19}$$

which gives us a correct expression for the average size of a hydrogen atom calculated in the framework of classical physics.

2.3 Average size of a Hydrogen Atom Calculated in Quantum Mechanics

The average radius $\langle r\rangle$ of a hydrogen atom from quantum mechanics is known to be

$$\langle r\rangle = \frac{\hbar^2}{2m\alpha}\left[3n^2 - l(l+1)\right], \tag{20}$$

where $\hbar$ is the reduced Planck constant $\hbar = 1.055\times10^{-34}$ J·s, m is the mass of electron, α is the constant of Coulomb's interaction $\alpha = ke^2$, n is the principal quantum number which represents the atomic energy shells, l is the angular quantum number which describes the shape of the electron orbitals. The result (20) was taken from Vladimir Zelevinsky's textbook [2].

In quantum theory both the angular momentum and energy are quantized. The quantization follows from exact solution of the Schrödinger equation, the corresponding quantization rules are

$$L^2 = \hbar^2 l(l+1), \tag{21}$$

and

$$E = -\frac{m\alpha^2}{2\hbar^2 n^2}. \tag{22}$$

Let's take a closer look at the average radius of a hydrogen atom we derived from the principles of classical mechanics (19)

$$\langle r \rangle = \frac{\alpha}{4|E|}\left(3 - \frac{2|E|L^2}{m\alpha^2}\right). \tag{23}$$

It is easy to notice that if we substitute the quantization rules (21) and (22) into the classical average radius of a hydrogen atom (23), then we will get the exactly quantum expression (20):

$$\langle r \rangle = \frac{\hbar^2}{2m\alpha}\left[3n^2 - l(l+1)\right]. \tag{24}$$

The summary: in this exercise we calculated the average radius of the electron in a hydrogen atom (23); then we replaced the energy of the electron and its angular momentum with its quantized values (21) and (22) (note that these rules can be obtained only through exact quantum mechanical consideration); and as a result we reproduced the exact formula for the average radius of hydrogen atoms calculated in quantum mechanics (24), which is quite remarkable.

3 Conclusion

Are the quantum and classical theories related to each other? If yes, then to which extent? The result we obtained doesn't seem a random coincidence and we cannot ignore this fact. The values we obtained for the radius of a hydrogen atom through classical and quantum mechanics are palatable. It seems as if there is some kind of connection between these two fundamental theories of physics. There are some points in which one of these theories would not be able to explain the other one, but we should not treat these theories as if they are completely unrelated to each other. From the above example, we can conclude that at some point these two theories are interconnected.

References

[1] J.L.Safko, H.Goldstein, C.P.Poole Jr., *Classical Mechanics* (3rd edition)

[2] V.Zelevinsky, *Quantum Physics*, Hoboken, NJ:Wiley