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Electron orbits beyond Bohr radius

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ABSTRACT

Starting from the classical energy equation of planetary motion and reviewing the refinement picture of Bohr model of hydrogen atom, the orbits of electron around hydrogen nucleus have been determined. The values of eccentricity of electron orbits fall within the range from 0 to 1, indicating that the path of an electron changes from circular to elliptical orbits, hence it continues toward parabolic orbits.

Keywords: Eccentricity; orbits; central force; Bohr radius; binding energy.

1. Introduction

The classical model of the hydrogen atom [1] representing an electron of charge $-e$ and mass m orbiting an infinitely massive nucleus of charge $+e$. This picture depicts that the electron travels around the nucleus in a similar structure to any solar planet orbiting the sun, with an attraction provided by electrostatic forces [2] rather than the force of gravity, where the motion of electron is governed by a central attraction force [3] Since the central force is conserved [4], the total energy forming a constant [5-7], which resulting the known radial solution [5,8]:

$$r(\theta) = a\frac{1-\varepsilon^2}{1+\varepsilon\cos\theta} \qquad (1.1)$$

This is equivalent to the equation of an elliptical orbit, with θ locates r from one focus with respect to the semi-major axis a, and ε denotes the eccentricity of the orbit [5]

$$\varepsilon = \sqrt{1+\frac{2EL^2}{mK^2}} \qquad (1.2)$$

In what follows, we present our approach in section 2, followed by results of our calculations in section 3, and finally we draw our conclusion in section 4.

2. Ansatz and Approach

We employ Eq. (1.2) in quantum physics by quantizing the energy and angular momentum of orbiting electron [9-10] , where the total energy that binds an electron in the n^{th} orbit of hydrogen atom is given by [11]:

$$E_n = -\frac{me^4}{2(4\pi\epsilon_0)^2 \hbar^2 n^2}\,, \qquad n = 1,\, 2,\, 3,\, \ldots \qquad (2.1)$$

and that the total angular momentum of the corresponding orbiting electron [12] is

$$L^2 = l(l+1)\hbar^2, \quad l \;=\; 0,\; 1,\; 2, \ldots\; n-1 \qquad (2.2)$$

With the help of Eq. (2.1) and Eq. (2.2), one can rewrite Eq. (1.2) in a quantized form, giving the eccentricity of the orbits as

$$\varepsilon_{nl} = \sqrt{1 - \frac{l(l+1)}{n^2}} \qquad (2.3)$$

this Eq. (2.3) can be compared with geometric eccentricity of an ellipse of radii *a* and *b*:

$$\varepsilon = \sqrt{1 - \frac{b^2}{a^2}} \qquad (2.4)$$

The ansatz is to monitor the link between Eq. (2.3) and Eq(2.4), that may reproduce the azimuthal quantum number introduced by Bohr-Sommerfeld in quantization rules [13-14] This can be achieved by imposing the following criterion [13,15]:

$$l(l+1) \to k^2\,, \qquad k = 1,\, 2,\, 3,\, \ldots \qquad (2.5)$$

where k denotes the azimuthal quantum numbers. According to the Bohr-Sommerfeld model of an atom [1], the orbiting electron can have discrete radii

$$a = n^2 a_0 \qquad (2.6)$$

where a_0 is the Bohr radius [16]. Eq. (1.1) to include discrete orbits:

$$r_{nk}(\theta) = a_0 n^2 \frac{1 - \varepsilon_{nk}^2}{1 + \varepsilon_{nk}\cos\theta} \qquad (2.7)$$

This is our fundamental equation, it can be used to describe and to calculate electron orbits around hydrogen nucleus.

3.Results and Discussion

The corresponding values of eccentricity, Eq (2.3) and Eq (2.5), fall within the range $0 \le \varepsilon \le 1$, which describes the change of electron trajectory from a circle ε = 1 to an ellipse 0 < ε < 1, and thereafter when $n \gg k$ it gradually reaches a parabola ε = 1. In such parabolic orbits the electron may continue to lose energy until it becomes unbound. With the aid of Figure 1Figure 1, one can calculate the semi-major axis from Eq. (2.6) and hence the semi-minor axis [15] by using the following relation:

$$b_{nk} = a_0 n k \qquad (3.1)$$

The radial location of electron is calculated from Eq. (2.7). Figure 2, gives an overview of the semi-major and semi-minor axes of electron orbits in hydrogen atom for the first three quantum numbers *n*, *k*. The figure also depicts how rapid is the electron position displaced from the nucleus. Electron location with respect to one focus $r_{nk}(\theta)$ varies with the eccentricity of the orbit. In all cases the electron circles the nucleus a distance coincides with a multiple of Bohr radius, then gradually diverts from a circular orbit depending on the values of *n* and *k*, in accord with Eq. (2.7). As the electron orbits change from circular to elliptical, and thereafter parabolic, it gradually displaced away from nucleus, tending to infinity. In this circumstance, the electron can easily escape from the nuclear potential and hence becomes a free electron. Figure 1Figure 1 shows the calculated parameters with the corresponding numerical values given in Table 1.

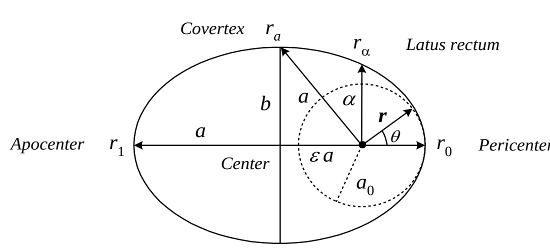

Figure 1. Common parameters used to describe elliptical orbits.

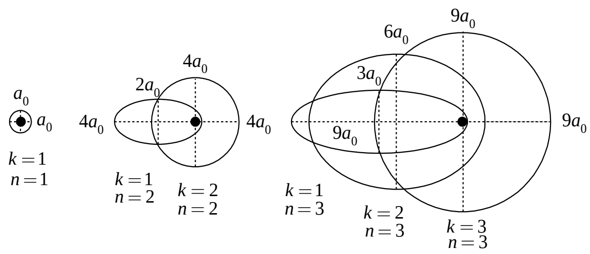

Figure 2. Different sizes of semi-major and semi-minor axes of electron orbits for the first three values of *n* and *k*. The nucleus is denoted by a solid dot to represent the focus of corresponding orbit.

Table 1. Common parameters describe electron route in hydrogen atom

n	E_n [eV]	$k = 1$	$k = 2$	$k = 3$
1	−13.60	$\varepsilon = 0$ $a / b = 1$ $r_0 = 0.53$ $r_\alpha = 0.53$ $r_a = 0.53$ $r_1 = 0.53$		
2	−3.40	$\varepsilon = 0.87$ $a / b = 2$ $r_0 = 0.28$ $r_\alpha = 0.53$ $r_a = 2.12$ $r_1 = 3.95$	$\varepsilon = 0$ $a / b = 1$ $r_0 = 2.12$ $r_\alpha = 2.12$ $r_a = 2.12$ $r_1 = 2.12$	
3	−0.15	$\varepsilon = 0.94$ $a / b = 3$ $r_0 = 0.27$ $r_\alpha = 0.53$ $r_a = 4.76$ $r_1 = 9.25$	$\varepsilon = 0.75$ $a / b = 1.5$ $r_0 = 1.21$ $r_\alpha = 2.12$ $r_a = 4.76$ $r_1 = 8.31$	$\varepsilon = 0$ $a / b = 1$ $r_0 = 4.76$ $r_\alpha = 4.76$ $r_a = 4.76$ $r_1 = 4.76$

4.Conclusion

The followed approach is mainly based on planetary motion of orbits under the action of a central force, where the semi-major and semi-minor axes of orbiting electron in hydrogen atom were obtained by evaluating the corresponding eccentricity in a simple straightforward way. The position of electron at any point of the orbit around the nucleus is precisely located by using the radial equation of planetary motion. The calculations were carried out by employing the total energy that binds electron in the hydrogen atom (the ground state zero point energy of hydrogen atom) and using Bohr radius as the closest approach of electron to the nucleus. It is hoped that this work can be improved and extended to subnuclear scale, to provide a sort of firm understanding.

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