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Lateral Position Uncertainty of Electrons in Bohr Hydrogen-like Atoms: An Implication of Heisenberg Uncertainty Principle

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Abstract

This paper presents a theoretical investigation on effects of lateral position uncertainty of captivity electrons within spherical electron shells of Bohr hydrogen-like atoms. A captivity electron, which is spatially confined in Bohr orbits, introduces a lateral position uncertainty that can be determined by considering the area of the electron shell. After deriving uncertainty relation for position and kinetic energy, author theoretically demonstrates that, due to the lateral position uncertainties of electrons in spherical shells, Heisenberg uncertainty principle suggests uncertainty bounds in measurement of kinetic energy states of captivity electrons that orbits non-relativistic hydrogen-like Bohr atom. Afterward, these analyses are extended for relativistic hydrogen-like Bohr atom case.

Keywords: Hydrogen-like Bohr atom, Heisenberg uncertainty principle, Position uncertainty, Kinetic energy uncertainty

Bohr Hidrojen Benzeri Atomlarda Elektronların Yanal Konum Belirsizliği: Heisenberg Belirsizlik İlkesinin Uygulanması

Öz

Bu makale, Bohr hidrojen benzeri atomların küresel elektron yörüngelerinde bulunan elektronlarının yanal konum belirsizliğinin etkileri üzerine teorik bir araştırma sunmaktadır. Bohr yörüngelerinde uzamsal olarak hapsolmuş bir elektron, elektron kabuğunun alanı göz önüne alınarak belirlenebilecek bir yanal konum belirsizliği sağlar.

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Konum ve kinetik enerji için belirsizlik ilişkisini türettikten sonra, yazar teorik olarak, küresel kabuklar içindeki elektronların yanal konum belirsizliklerini teorik olarak göstermektedir. Heisenberg belirsizlik ilkesi, göreceli olmayan hidrojen benzeri Bohr atomunun yörüngesinde bulunan esaret elektronlarının kinetik enerji durumlarının ölçümündeki belirsizlik sınırlarını ortaya koymaktadır. Daha sonra, bu analizler göreceli hidrojen benzeri Bohr atomu durumu için genişletilmiştir.

Anahtar Kelimeler: Hidrojen benzeri Bohr atomu, Heisenberg belirsizlik ilkesi, Konum belirsizliği, Kinetik enerji belirsizliği

1. Introduction

Following observations of electromagnetic wave energy quantization in experiments, Niels Henrik David Bohr postulated an atom model, which suggests that mechanical energy related with energy of atomic electrons should be also quantized. Based on findings of experimental observations, Bohr model suggests that electrons orbiting around nucleus of atom can be in explicit states, known as “stationary states”, and therefore it offers an explanation to overcome difficulties associated with the classical collapse of the electron into the nucleus [1]. In those stationary states, it is accepted that there is no electromagnetic radiation, which is emitted from the atom, and angular momentums of electrons should be quantized as $\hbar$, $2\hbar$, $3\hbar$ ... Although, Bohr model has provided an explanation for non-collapsing atom on the bases of experimental data, implication of Heisenberg uncertainty principle for orbiting electrons substantiated explanations that are given for prevention of theoretical collapse of hydrogen atoms, and it confirmed stability of electrons that are orbiting of Bohr’s hydrogen-like atoms.

In literature, prevention of electron collapse on the nucleus of hydrogen atom was explained by using the uncertainty principle as follows [2, 3]: Energy of electron is $E = p^2 / 2m - e^2 / r$ in classical model. It implies that, in order to collapse electron on the nucleus, electron energy should be negative and very large (almost infinitive) because it needs $p = 0$ and $r = 0$ in this case. However, the state of $p = r = 0$ is not valid for an electron according to Heisenberg uncertainty principle. In accordance with the uncertainty principle, electron moment can be taken as $p \approx \hbar / r$, and correspondingly the energy state of electron is written as $E = \hbar^2 / 2mr^2 - e^2 / r$. After solving $dE / dr = 0$ to find minima of energy state, the minimum energy state was found as $E_{\min} = -\frac{me^4}{2\hbar^2}$ for $r_{\min} = \frac{\hbar^2}{me^2}$ [3, 4]. This minimum energy state coincides exactly Rydberg energy, and the minimum orbit radius $r_{\min}$ is correctly Bohr radius denoted by a_0: These results verifies that the collapse of electrons on the nucleus is avoided theoretically and the atom can be stabilized by contribution of Heisenberg uncertainty principle. Later, Heisenberg uncertainty principle has been widely used for explanation of sub-atomic phenomenon in quantum mechanics. To demonstrate gravitational interaction of the photon and the particle being observed [5], generalized uncertainty principle (GUP) was suggested by modifying the uncertainty principle with an additional term. Then, it contributed to discussions on small black hole structuring [3]. This principle was utilized to figure out ground-state energy of the helium-like Hookean atom in a similar manner [6].

Implications of Heisenberg uncertainty principle on Bohr atom model have enhanced the relevance of Bohr model for experimental measurements, and these efforts have significance to cope with some deficiencies of Bohr model. For instance, Bohr model does not foresee the existence of fine structures and broadening effects in spectral lines [1]. On the other hand, it is known that Bohr model cannot predict the correct the value of angular momentum for the electron at ground state: it is found $L = \hbar = h/2\pi$, but experiments show $L = 0$ [1]. Implications of Heisenberg uncertainty principle on Bohr atom model may aid to reduce the gap appearing between experimental observations and theoretical anticipations. A similar point has been already noted by Akhoury et al. in mentioning that the investigation of effects of non-standard 2S–1S energy shift on the bases of uncertainty principle may have implications for the observation of the fine and hyperfine structure according to postulation of Bohr model [7].

Bohr atom model essentially suggests that the electrons are confined in definite orbits, which are known as Bohr orbits, and it gives the atom model a shell structuring of the orbiting captivity electrons. These shells bring out the concept of bounded atomic volumes and finite atomic radii of atoms. This concept was a significant milestone: Many chemical models developed for atoms, molecules, crystal structure require the atomic radii and the bounded (finite) atomic volume parameters in modeling. Atomic radii refer to a measure of radial extent of atom [8]. Definition and value of atomic radius vary depending on model requirements and assumptions. A well-known atomic radii is the Bohr radius. It is obvious that Heisenberg uncertainty principle should have useful suggestions related with observations and experiments of finite volume atom models in quantum mechanics and quantum chemistry.

In the literature, several works have addressed implications of uncertainty principle for hydrogen-like atom: Hydrodynamic uncertainty relations based on Heisenberg uncertainty was illustrated for elementary quantum systems such as the hydrogen-like atom [9]. Minimal length uncertainty relation was discussed for hydrogen atom in [7]. Recently, Bohr's spectrum of quantum states for hydrogen atoms were considered according to the uncertainty principle of energy and time, and then the possible momentary forces taking effect on electron in the case of transition between the orbits were formulized in [10]. Deeney et al. pointed out differences between the values calculated from the Bohr Theory and those found by experiments according to atomic number Z. Author has mentioned a need for additional mechanisms, whose effects should be added to those already present in the Bohr Theory in order to account reductions in the observed ionization energies [11]. Later, Kuo presented analyses for the uncertainties in measurements of the radial position Δr , radial momentum Δp, relative dispersion of radial position, $\Delta r / r$ and the product of both uncertainties, $\Delta r \, \Delta p$ in a non-relativistic hydrogen-like atoms depending on the quantum numbers [12].

In the current work, lateral position uncertainty of captivity electrons that are orbiting in Bohr hydrogen-like atoms are considered for spherical electron shells. Bohr model confines motion of electrons into electron shells in stationary states, and this spatial limitation introduces a lateral position uncertainty for electron motion within shell structuring. In addition to radial position uncertainty of electrons given in [12], we investigate the lateral position uncertainty of electron motion in Bohr orbits to discuss implications on the bases of Heisenberg uncertainty principle. For this purpose, we demonstrate uncertainty relation of lateral position and kinetic energy of electrons in electron shells according to Heisenberg uncertainty principles. Bound of kinetic energy uncertainty is derived for spherical electron shells of Bohr hydrogen-like atoms. Then, the results are extended for the case of relativistic Bohr hydrogen-like atom.

In the following sections, after briefly mentioning Bohr model of hydrogen-like atoms and Heisenberg uncertainty principle, the uncertainty relations between electron position and kinetic energy state of the Bohr orbits are derived and this investigation is extended to the case of relativistic Bohr hydrogen-like atoms.

2. Theoretical Foundations

2.1. Bohr Model of Hydrogen-likes Atoms

Bohr model, which is known as the Rutherford–Bohr model, describes hydrogen atom as the combination of a positively charged nucleus and a captivity electron traveling in certain circular orbits around the nucleus at certain angular momentums [13-15]. The model's key success lays on explaining the Rydberg formula for spectral emission lines of atomic hydrogen. Bohr model has provided a theoretical explanation for the Rydberg structures and accomplished an elaboration of empirical results in terms of fundamental physical constants.

Due to difficulties in prevention of classical collapse of the electron into the nucleus, Bohr proposed electron orbiting at certain stationary states, where no electromagnetic emission takes place. In these states, the angular momentums of electrons take certain values $L = n\hbar = nh/2\pi$ depending on the principal quantum number $n = 1,2,3,...$. The lowest value of n is one, and it refers the smallest possible orbital radius of 0.0529 nm known as also Bohr radius (a_0) and the corresponding minimum energy state of –13.6 eV known as the ground state. As known, Bohr model of hydrogen-like atom has a positive charged nucleus (Ze) that is orbited by an electron. The allowed radii for electrons in circular orbits of the hydrogen atom with Z number of protons in nucleus are given by,

$$r_n = \frac{a_0 n^2}{Z} . \tag{1}$$

The corresponding energy states of an electron in the stationary orbits are given by,

$$E_n = -\frac{Z^2 e^2}{8\pi\varepsilon_0 a_0 n^2} \tag{2}$$

The radiation frequencies (ν) of Bohr Hydrogen-like atoms for a transition from the orbit n to the orbit m are written as,

$$E_f(n,m) = E_n - E_m = h\nu \tag{3}$$

Three deficiencies of the Bohr model, which have widely agreed by Physics community, can be summarized as,

(i) It does not anticipate some spectral features that were observed in experiments with hydrogen-like atoms such as fine structures, broadening and shifting in spectral lines.

(ii) It predicts angular momentum of ground state electrons inconsistent with experimental observations.

(iii) Bohr model does not have any suggestion for Heisenberg uncertainty principle.

2.2. Heisenberg Uncertainty Principle

Heisenberg uncertainty principle fundamentally conjectures bounds of associated uncertainty between states of sub-atomic events when they are observed. Heisenberg reached this conclusion on the bases of general principles of optics and quantization of electromagnetic radiation in the form of photons [5, 16-18]. He suggested position-momentum uncertainty relation of electron as [19],

$$\Delta x \, \Delta p \geq \frac{\hbar}{2}, \tag{4}$$

where Δx is the uncertainty in the position of electron, Δp is the uncertainty in the momentum of electron. Eq. (4) describes the limits that are imposed by nature on the precision of simultaneous measurements [12]. When the position or the momentum of an electron has been independently measured in the specific state, then the uncertainties in the measurements of the other parameter should satisfy Eq. (4) [12]. However, due to very small value of the Plank's constant ($h \cong 6.8\,10^{-34}$ Js), this principle has a significance at the atomic scales [12]. Therefore, Heisenberg's uncertainty principle was used to express the lower bound of state uncertainty in sub-atomic phenomenon [5] and therefore the minimum position and moment uncertainties are commonly treated as,

$$\Delta x_{\min} \approx \frac{\hbar}{2\Delta p} \text{ and } \Delta p_{\min} \approx \frac{\hbar}{2\Delta x}. \tag{5}$$

Also, uncertainty relations are derived for energy and time quantities as follows [19]:

$$\Delta E\, \Delta t \geq \hbar \tag{6}$$

Heisenberg's uncertainty principle is usually utilized to express a limitation of observations, which is imposed by quantum mechanics. The theoretical prospects and experimental findings can be better reconciled when the appropriate trade-off between conjugate quantities is accepted [20]. It produces reasonable explanations between theoretical conjectures and experimental observations, and hence plays a fundamental role in quantum mechanics.

2.3. Implications of Heisenberg Uncertainty Principle for Lateral Electron Position Uncertainty of Non-relativistic Bohr Hydrogen-like Atoms

Bohr atom model suggests that captivity electrons are confined into certain orbits known as Bohr orbits. This model gives the atom a shell structuring of electron orbits around the nucleus, and electron shells were utilized to define atomic radii or finite atomic volumes. This section addresses analysis of the lateral position uncertainty of captivity electrons within shell structuring of Bohr atom model. According to Heisenberg uncertainly principle, the position uncertainty of electrons in the Bohr orbits leads to a momentum uncertainty. This case also suggests an uncertainty for kinetic energy of captivity electrons.

Let us consider an electron, which is confined in a spherical Bohr orbits with radius r as depicted in Fig. 1. In the figure, we consider a simple case that is a single non-relativistic Bohr Hydrogen-like atom at rest in an infinite space volume. Considering Heisenberg uncertainty given by Eq. (4), one can easily express the uncertainty bound for electron's linear momentum Δp while orbiting with Δr position uncertainty in the electron shells as follows:

$$\Delta p \geq \frac{\hbar}{2\Delta r}. \tag{7}$$

Due to the relation of $E_k = \frac{p^2}{2m_e}$ between kinetic energy and linear momentum, the uncertainty in electron momentum causes the kinetic energy uncertainty for the electron as given by

$$\Delta E_k = \frac{\Delta p^2}{2m_e}. \tag{8}$$

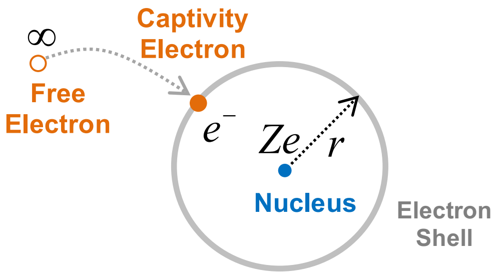

Figure 1. Hydrogen like Bohr atom with a captivity electron in spherical electron shell

Considering Eq. (7) for Δp, association between position uncertainty and kinetic energy uncertainty can be expressed depending on electron mass m_e as,

$$\Delta E_k \Delta r^2 \geq \frac{\hbar^2}{8m_e}. \tag{9}$$

Then, one can easily write an uncertainty bound for the observation of electron's kinetic energy as,

$$\Delta E_k \geq \frac{\hbar^2}{8\Delta r^2 m_e}. \tag{10}$$

As known, non-relativistic Bohr hydrogen-like atom model suggests the allowed energy levels that are complying with Bohr radii as $r_n = a_0 n^2 / Z$ [21]. The lateral positional uncertainty for a captivity electron orbiting in a spherical shell can be expressed as the area of these shells so that we cannot measure exact position electron in the shell.

By taking account the area of a spherical electron shell, the lateral positional uncertainty of electrons in spherical shells can be written by

$$\Delta r = 4\pi \, r_n^{\ 2} = 4\pi \, a_0^{\ 2} \, \frac{n^4}{Z^2} \,. \tag{11}$$

When the lateral positional uncertainty of captivity electrons in spherical shells (Eq. (11)) are used in Eq. (10), the uncertainty in kinetic energy state of electrons for Bohr orbits can be obtained as,

$$\Delta E_k \approx \frac{Z^4 \hbar^2}{128\pi^2 a_0^{\ 4} n^8 m_e} \ . \tag{12}$$

Table 1 lists minimum uncertainty expectations in measurements of kinetic energy states of the captivity electrons versus the principal quantum numbers (n). In measurements, captivity electron position is assumed to be anywhere in the spherical electron shells of Bohr model.

Table 1. Minimum uncertainty bounds for measurements of kinetic energy states of captivity electrons in non-relativistic Bohr Hydrogen-like atom

n	ΔE_k (J)
1	1.2340
2	0.0048
3	1.8809 10^{-4}
4	1.8830 10^{-5}
5	3.1592 10^{-6}
6	7.3472 10^{-7}
7	2.1407 10^{-7}
8	7.3555 10^{-8}

Fig. 2 shows the minimum uncertainty of kinetic energy states in normal scale (a) and the logarithmic scale (b) for large principal quantum numbers. The figure reveals that the uncertainty in kinetic energy state of electrons in Bohr orbits sharply decreases depending on the principle quantum number. The main reason is that increase of quantum numbers causes increase of position uncertainty and it leads to decrease of kinetic energy uncertainty. One can conclude that, for measurements according to Bohr hydrogen-like atom models, electron kinetic energy for higher energy levels (large quantum numbers) can be measured more reliable than those of lower energy levels.

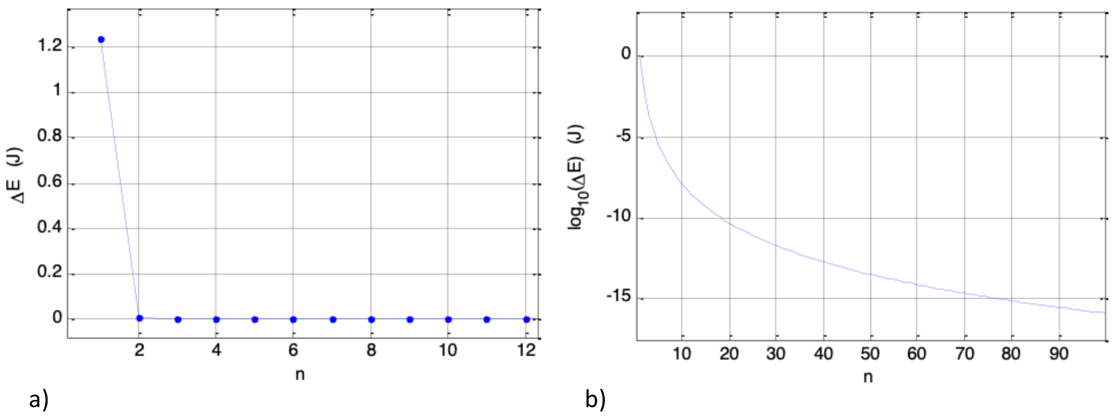

Figure 2. The minimum uncertainty of kinetic energy states of captivity electron in a) linear and b) logarithmic scales

2.4. An Extension of Kinetic Energy Uncertainty Analysis for Relativistic Bohr Hydrogen-like Atoms

In the development of relativistic approach, Terzis et al. expressed relativistic version of the Bohr radii for hydrogen-like atoms with circular orbits as [22],

$$r_n = a_0 n\sqrt{n^2 - Z\alpha^2}\,/\,Z \quad , \tag{13}$$

where α is the fine structure constant. It is also known as electromagnetic coupling constant and characterizes the strength of the electromagnetic interaction [23]. By considering relativistic version of the Bohr radii for hydrogen-like atoms, the lateral positional uncertainty of electron can be written for area of spherical shells by

$$\Delta r = 4\pi\, r_n^{\ 2} = 4\pi\, a_0^{\ 2}\, \frac{n^2(n^2 - Z\alpha^2)}{Z^2} \,. \tag{14}$$

By using Eq. (10), one can write the minimum uncertainty in kinetic energy state of relativistic electrons orbiting in spherical shells as,

$$\Delta E_k \approx \frac{Z^4\hbar^2}{128\pi^2 a_0^{\ 4} n^4 (n^2 - Z\alpha^2)^2 m_e} \tag{15}$$

3. Discussion and Conclusions

This paper presents a theoretical study on implications of lateral position uncertainty of captivity electrons that orbit spherical electron shells of Bohr hydrogen-like atoms for the both non-relativistic and relativistic cases. Findings of the study suggest that lateral position uncertainty of electrons in Bohr orbits leads to an inherent uncertainty in measurement of kinetic energy state of electrons according to Heisenberg uncertainty principle.

Some remarks of this study can be summarized as follows:

(i) The presented uncertainty analysis suggests that lateral position uncertainty of electrons in Bohr orbits leads to an inherent uncertainty in measurements of kinetic energy state of electrons on the bases of Heisenberg uncertainty principle. This uncertainty has dependence for quantum number and the electron mass parameters.

(ii) The lower bounds of uncertainty in kinetic energy state of non-relativistic and relativistic electrons was derived for Bohr hydrogen-like atom considerations. This analysis reveals that increase of principle quantum number sharply decreases the uncertainty in measurements of kinetic energy states of cavity electrons. Therefore, the measurements of kinetic energy at higher principle quantum numbers is expected to be more consistent than those of ground state or the low principle quantum numbers because of sharply decrease of uncertainty bounds. This case is also valid for the linear moment uncertainty of electrons, which can be written by considering the lateral position uncertainty in spherical electron shells (Eq. (11)) in Eq. (7) as follows:

$$\Delta p \geq \frac{Z^2 \hbar}{8\pi a_0^{\,2} n^4} \qquad (16)$$

These analyses are useful to estimate uncertainty limits, that is, the degree of accuracy in the experimental measurements of position and kinetic energy of captivity electrons under the consideration of Bohr atom model. The computational framework of the proposed analyses is summarized in Fig. 3. Results of this study can be beneficial for the assessment of experimental observations and modeling efforts in the fields of quantum chemistry and quantum electronics.

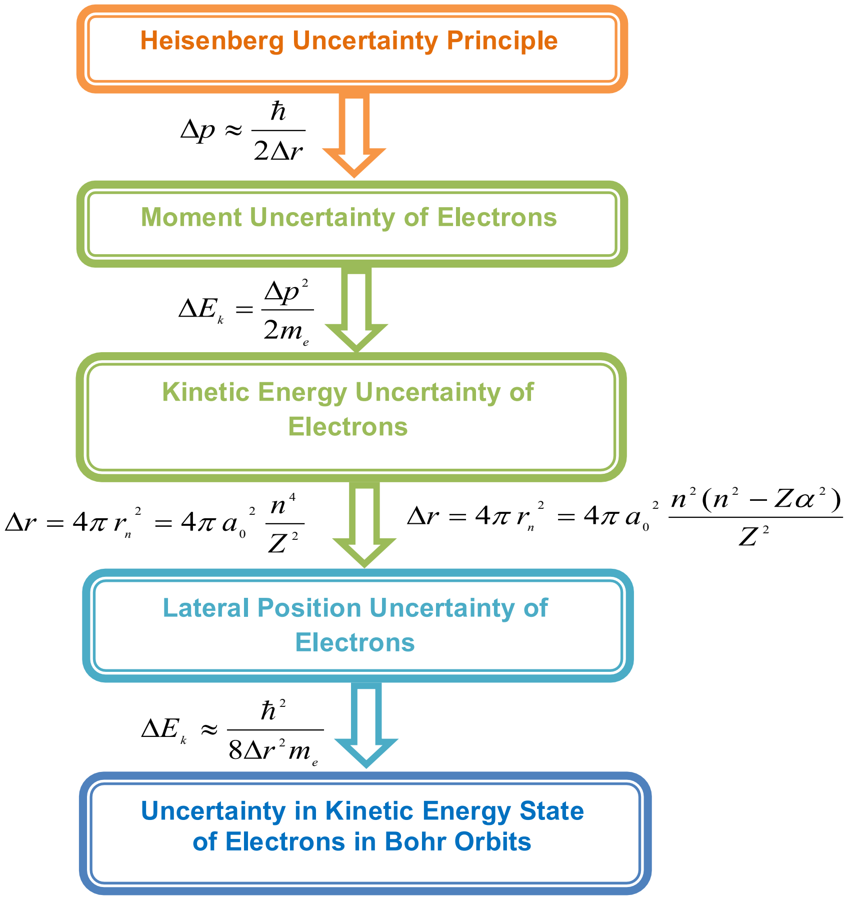

Figure 3. A simplified computational framework of the proposed analyses

We presented implications of lateral position uncertainty of electrons for Bohr hydrogen-like atoms. Also, analysis on geometric representation of uncertainty relation [24] can be derived for orbit geometries different from sphere.

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