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The Analytical Modeling of Nuclear Size Effect on Relativistic Electron in Hydrogen Atom

Aliyu Adamu[a*], Adamu Hassan[b], Ahmad Abdulkadir[a] and Adamu Z. Ngari[c]
[a]Department of Physics, Faculty of Science, University of Maiduguri, P. M. B. 1069, Maiduguri – Nigeria
[b]Muhammed Goni College of Legal & Islamic Studies, P.M.B. 1526, Maiduguri – Nigeria
[c]Department of Physics, Nigerian Army University Biu – Nigeria
[*]**Corresponding Author:** aliyuadamu703@gmail.com

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Abstract

The effects of relativistic motion, the spin-orbit interaction and Zitterbewegung of an electron, which are of the same order of magnitude, defined the fine structure correction to hydrogen spectra. In this work, perturbation theory, as an approximation method is applied to examine the effects of finite sized of atomic nucleus on relativistic motion of electron in hydrogen atom. The nuclear finite corrections to 1s, 2s, 3s, 4s and 5s energy states in hydrogen atom due to the finite size of nucleus were computed and the results showed that the nuclear size effects, which is of order of 10^{-6} eV, depends on the size, A(N, Z) of the nucleus and energy states, n of relativistic electron. This suggested that the nuclear size is more effective on relativistic electron in the lower energy levels of heavy nuclei, as the effect varied directly with the nuclear size and inversely with the electron states, n. Thus, the finite size of atomic nucleus has an impact on relativistic motion of an electron. Moreover, a simple model was developed to predict the energy level variation as a function of the size of the nucleus. Therefore, this study justifies the effects of nuclear size on relativistic electron and the measured values are of greatest interest since it will reveal significant changes of the nuclear structure and may also improve the knowledge of fine structure correction.

1. Introduction

The hydrogen atom is the fundamental two-body system and perhaps the most important tool of atomic physics and the challenge is to calculate its properties to the highest accuracy possible. The study of the hydrogen atom has been at the heart of the development of modern physics [1]. The hydrogen atom has been the testing ground for theoretical atomic physics for over a hundred years. The original quantum mechanics was motivated to model the hydrogen atom and explain its spectrum. In 1912, Niels Bohr proposed the first electronic hydrogen atom model which successfully predicted the main energy levels of the hydrogen atom in the framework of a semi-classical theory based on Planck's hypothesis. But the main spectral lines of hydrogen atom can be described by the Schrödinger equation, without using any postulates [2].

It is well known that, when the lone orbiting electron solely subject to the electrostatic influence of the nucleus, the complete solution, $\widehat{H}_0|\psi_n\rangle = E_n|\psi_n\rangle$, of eigenfunctions ψ_n and eigenvalues E_n of the Hamiltonian, $\widehat{H}_0$, give rise to the allowed energies of an electron, which depends exclusively on the principal quantum number, *n* as $E_n = -13.6\ eV(Z/n)^2$[3-8]. It is clearly observed that these allowed energies of an electrondo not give an exact description of the interaction between the fermions and the nucleus. Schrödinger equation was derived based on the assumptions that the atomic nucleus has a point-like charge. The simple point-charge nucleus approximation resulting in a well known *Z*/*r* potential (Bohric and Schrodinger approximation) is no longer completely adequate as nuclear system takes into account in particular the following interactions, ordered according to their importance: *The spin of the electron; Spin-orbit interaction; Relativistic motion of the electron; Hyperfine Structure Correction; Vacuum fluctuations of the electromagnetic fields; Vacuum polarization.* These interactions which are usually incorporated via perturbation theory and quantum electrodynamics, lead to the energy splitting such as fine structure splitting, hyperfine structure splitting and the lamb shift. These splitting have been calculated in many literatures see for example [9 – 18]. The fine structure of hydrogen atom is interpreted as the effects of relativistic motion, the spin-orbit interaction and Zitterbewegung of an electron [19]. These effects, which are always treated together, are of the same order of magnitude when calculated based on point-charge nuclear assumption.

The dependence of the corrections to discrete eigenvalues of the *Z*/*r* potential inside the nucleus necessitates a choice of a model for the nuclear potential that modifies its unphysical infinity at the origin [20-21]. The recent electron scattering experiments at Stanford University have established the finite size of the nucleus and Hofstadter and McAllister were first observed this effect [22,23]. High-energy electron-scattering measurements have demonstrated clearly the existence of deviations from point-nucleon scattering laws [24,25] which attributed entirely to finite structure effects in the nucleons. The nucleus has a finite size charge distribution due to the fact that its nucleons consist of the combination of *u*-quarks and *d*-quarks of charges 2*e*/3 and *e*/3 respectively. The quarks distributions inside nucleons make the charge distribution of nucleus to be finite over a range *R* (Figure 1).

The early theorist uses analytical descriptions of charge distribution and potentials, which enabled series expansions of analytical solutions of the wavefunctions within and close to the nucleus and for finite nuclear distributions, the possible range exceeds much further. If the nucleus is being described as a finite-size source with a uniform distribution of charges of radius *R*, then the relativistic electron wave function can penetrate to $r \leq R$, and thus the electron spends part of its time inside the nuclear charge distribution, there it feels a very different interaction. This idea is considered in this paper to refine the relativistic motion of an electron in finite size charge assumption since it is under the influence of nuclear charge. The time independent perturbation theory, as an approximation method will be applied to examine the effects of finite-size nuclear on relativistic electron of hydrogen atom and compared to the previously calculated values.

2. Methodology

2.1 Nuclear Potential and Wavefunction

One of the simplest models of nucleus is the spherically symmetric charge distribution with the corresponding charge density.

$$\rho(r) = \frac{3Ze}{4\pi R^3} \qquad (1)$$

where *Z* is the nuclear charge, $R = r_0 A^{1/3}$, is the effective radius of nucleus. The experimental data indicates that $r_0 \approx 1.2\ fm$ [20,21]. This simple distribution gives a reasonable approximation for the homogeneous distribution and the correct analytical behavior of the electronic wavefunctions at $r = 0$ and has been used in many early analyses. The effect of the nuclear distribution on atomic properties is proportional to the expectation values of the nuclear distribution.

$$\langle r^2 \rangle = \frac{3}{5} R^2$$

Thus, the nuclear charge *R* is effective radius of nucleus, connected with root-mean-square radius as

$$R = \sqrt{\frac{5}{3}} \langle r^2 \rangle^{1/2} \qquad (2)$$

The root-mean-square nuclear matter radii $\langle r^2 \rangle^{1/2}$ and the density distributions contain an important insight on nuclear potentials and nuclear wavefunctions [26-31]. However, several atomic properties depend directly on the wave function close to the nucleus. This gives a reasonable approximation for the homogeneous distribution.

The simple distribution (1) gives the correct analytical behavior of the electronic wavefunctions at $r = 0$ and has been used in many early analyses. These expansions are also useful for a general understanding of the effects involved [32]. For spherically symmetric charge distribution $\rho(r)$ inside the nucleus, the interaction between fermions and nucleus can best be described by the lepton-nuclear potential energy $U(r)$:

$$U(r) = -ke \left[\frac{4\pi}{r} \int_0^R \rho(r') r'^2 \, dr' + 4\pi \int_R^\infty \frac{1}{r'} \rho(r') r'^2 \, dr' \right] \qquad (3)$$

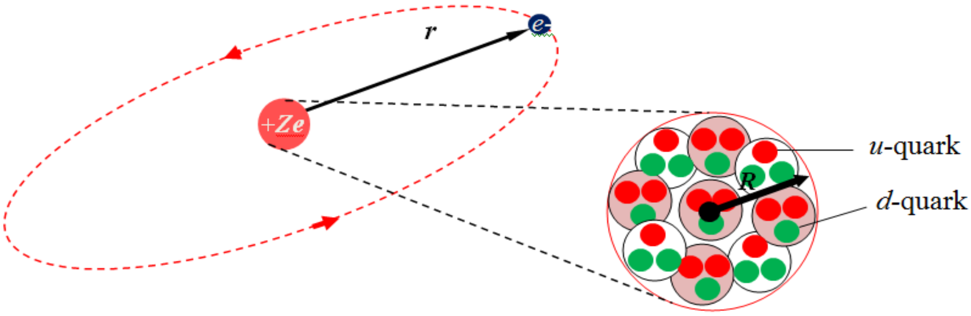

Figure 1: The finite size of atomic nucleus

where outside the nucleus, $r > R$, this expression reduces to a point charge potential

$$U(r) = -\frac{Zke^2}{r} \qquad (4)$$

and within a nuclear radius $r \leq R$, the expression is described by

$$U(r, R) = -\frac{Zke^2}{r} \left(\frac{3r}{2R} - \frac{r^3}{2R^3} \right) \qquad (5)$$

Thus, inside the nucleus of radius *R*, the lepton-nuclearpotential will not have Coulomb form. The constant value of the potential (5) at ($r \sim 0$) very close to the origin, makes the Z/r potential less singular at small distances and extend, the possible range, much further. The magnitude of the nuclear size effects on hydrogen spectra were accurately calculated by the use of first order time independent perturbation theory:

$$\hat{E}_n^{(1)} = \lambda \langle \psi_n^{(0)} \big| \hat{H}' \big| \psi_n^{(0)} \rangle$$

which is the superposition of all unperturbed states, $\psi_n^{(0)}$.

The first order calculation of the effect of finite size of nucleus with potential (5) gives the energy shift [33]:

$$\lambda E_n = \int \psi_n^{(0)*}[U(r,R) - U(r)]\psi_n^{(0)} d\tau = \frac{2Z^4ke^2R^2}{5n^3a_0^3} = -E_n\left(\frac{4Z^2R^2}{5na_0^2}\right) \tag{6}$$

where the use of $d\tau = 4\pi r^2 dr$ and

$$E_n = -\frac{Z^2ke^2}{2n^2a_0} \tag{7}$$

The Bohr radius $a_0 = 5.29 \times 10^{-11}$ m.

2.2 Relativistic Motion of the Electron of Finite-Size Nucleus

In relativistic classical mechanics, the total energy of an electron is

$$E = \sqrt{p_\mu p^\mu} = mc^2 + \frac{\vec{p}^2}{2m} \to \sqrt{(pc)^2 + (mc^2)^2}$$

In the case where the particle is only slightly relativistic ($v \ll c$) the square root can be expanded to obtain

$$E = mc^2\sqrt{1 + \left(\frac{\vec{p}}{mc}\right)^2} = mc^2\left[1 + \frac{1}{2}\left(\frac{\vec{p}}{mc}\right)^2 - \frac{1}{8}\left(\frac{\vec{p}}{mc}\right)^4 + \cdots\right] \tag{8}$$

The first term in (8) is interpreted as the rest energy of the electron; the second term is the non-relativistic kinetic energy. Hence, the third term is used in writing the perturbed Hamiltonian:

$$\lambda\hat{H}' = -\frac{1}{2mc^2}\left(\frac{\vec{p}^2}{2m}\right)^2 \tag{9}$$

The new Hamiltonian of this system in terms of finite-size charge distribution takes the form:

$$\hat{H} = \frac{\vec{p}^2}{2m} - \frac{Zke^2}{r}\left(\frac{3r}{2R} - \frac{r^3}{2R^3}\right)$$

And the perturbed Hamiltonian is given by

$$\lambda\hat{H}' = -\frac{1}{2mc^2}\left(\frac{\vec{p}^2}{2m}\right)^2 = -\frac{1}{2mc^2}\left[\hat{H}' + \frac{Zke^2}{R}\left(\frac{3}{2} - \frac{1}{2}\frac{r^2}{R^2}\right)\right]^2 \tag{10}$$

Thus, the relativistic correction for a new state $|\psi_n\rangle$ of relativistic electron can be expressed as:

$$\Delta E_r = -\frac{1}{2mc^2}\left\langle\psi_n\right|\left[\hat{H}' + \frac{Zke^2}{R}\left(\frac{3}{2} - \frac{1}{2}\frac{r^2}{R^2}\right)\right]^2\left|\psi_n\right\rangle \approx -\frac{9(\lambda E_n)^2}{2mc^2} = -\frac{72E_n^2}{25ma_0^4c^2}\left(\frac{Z^4R^4}{n^2}\right)$$

$$= -\left(\frac{r_0}{a_0}\right)^4\frac{72}{25mc^2}\frac{Z^4E_n^2A^{4/3}}{n^2} \tag{11}$$

where the use of (6) and (7) have been made, $m = 9.1 \times 10^{-31}kg$ is the electron mass and $c = 3.0 \times 10^8 ms^{-1}$ is the speed of light in vacuum. The allowed energies of an electron (7) obtained by solving

Schrödinger equation and the calculated values of finite size nuclear effects to energies (11) obtained from this work are computed for the ground state and first four excited states of relativistic electron in hydrogen atom. Denoting

$$\zeta = \frac{\Delta E_r}{E_n} \quad (12)$$

as the deviation of energy ΔE_r due to finite size of nucleus relative to the energy, E_n.

3. Results and Discussion

Equation (11) gives first order perturbation corrections to energy states of relativistic electron under the influence of finite-size nucleus. The nuclear finite corrections to 1*s*, 2*s*, 3*s*, 4*s* and 5*s* energy states in hydrogen atom due to the finite size of nucleus were computed using the results obtained by Equation (11) and the results obtained are presented in Table 1.

Table 1 showed that the nuclear structure effect on relativistic electron, which is of order of $10^{-6}eV$, depends on the nuclear size, $A(N, Z)$ and the energy states, n of relativistic electron. This suggested that the nuclear size is more effective on relativistic electron in the lower s energy levels of heavy nuclei, as the effect varied directly with the nuclear size and inversely with the quantum number, n.

Table 1: The calculated values of finite size nuclear effects to energies of the ground state and first four excited states of relativistic electron in hydrogen atom

State	$E_n(eV)$	ΔE_r ($10^{-6}eV$)	$\zeta \times 10^{-6}$
1*s*	-13.600	-1703.5	125.25
2*s*	-3.4000	-26.617	7.8285
3*s*	-1.5111	-2.3367	1.5464
4*s*	-0.8500	-0.4158	0.4893
5*s*	-0.5440	-0.1090	0.2004

The information represented in Table 1 is extended further by plotting a graph of log (ΔE_r) as a function of principal quantum number, n (Figure 2).

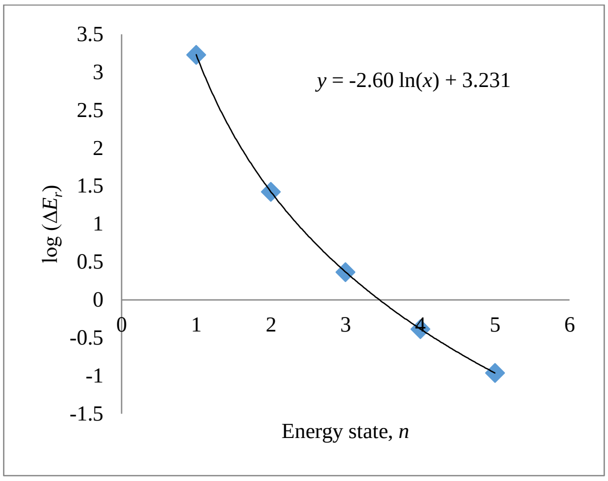

Figure 2: The variation of the magnitude of nuclear finite-size effects, log (**ΔE_r**) on relativistic electron with principal quantum number, n**.**

Figure 2 represents the variation of the magnitude of nuclear finite-size effects, log (**ΔE_r**) on relativistic electron calculated in Table 1, with principal quantum number, n. The figure showed that the relativistic effect due to finite size of nucleus decreases with the principal quantum number, n.Thus, the nuclear size effect depends on the energy states, n of relativistic electron. This suggested that the nuclear size is more effective on relativistic electron in the lower energy levels of heavy nuclei.Figure 2 showed a very clear continuous curve in decreasing order which points out to be non-linear from the plot of relativistic effect of finite size of nucleus log[$\Delta \boldsymbol{E_r}$ (n, j)] as a function of the principal quantum number, n for hydrogen atom that corresponds to those recorded in Table 1 by the use of Equation (11). This data can be modeled and studied using the regression analysis. By applying the regression analysis, a simple model satisfying the relationship in Equation (13):

$$\log \Delta E_r\,(n, j) = -2.60 \ln(n) + 3.231 \qquad (13)$$

was developed and can predicts the nuclear size effect on relativistic electron. The simple model was used and predicts the energy level variation (up to n = 100) as a function of the size of the nucleus in Table 3 (Appendix). The energy level shifts (11) calculated due to the effect of nuclear size on relativistic electron is compared with the relativistic effect of an electron obtained from Ref. [34] based on the point-charge nucleus calculation. As can be seen from Table 2 that the finite-size nuclear corrections do affects the relativistic electron in any states with values 10 times larger than the relativistic corrections to energy levels of point-charge nucleus.

Table 2: The calculated values of finite size nuclear effects to energies, $\Delta \boldsymbol{E_r}$ in the ground state and first four excited states of hydrogen atom obtained from the present work with from point-like nucleus, $\Delta \boldsymbol{E_n}$ in 1s, 2s, 3s, 4s and 5s states obtained from Ref. [34].

Orbitals	$\Delta E_n(eV)$	$\Delta E_r \times 10^{-6}$ (eV)
$1S_{1/2}$	1.8115×10^{-4}	1.7035×10^{-3}
$2S_{1/2}$	2.8305×10^{-6}	2.6617×10^{-5}
$2P_{1/2}$	2.8305×10^{-6}	-
$2P_{3/2}$	8.4898×10^{-6}	-
$3S_{1/2}$	2.4843×10^{-7}	2.3367×10^{-6}
$3P_{1/2}$	2.4843×10^{-7}	-
$3P_{3/2}$	7.4543×10^{-7}	-
$3D_{3/2}$	7.4543×10^{-7}	-
$3D_{5/2}$	1.7393×10^{-6}	-

The nuclear size corrections to relativistic electron, is more effective on the lower s energy levels and in heavy nuclei, as the effect varied directly with the nuclear size and inversely with the principal quantum number, n. A large number of publications (see, for example [21,34-38] showed that the nuclear finite-size effects, which is largest for s levels, are more important for higher atomic nuclei and muonic atoms, since for muon the effects are enhanced by $(m_e/m_\mu)^2 \sim 10^{-5}$.

4. Conclusion

In this study a simple model satisfying the relationship between nuclear size correction to relativistic electron and electron energy state was developed to predict the energy level variation as a function of the size of the nucleus. This suggested application of analytical methods in solving relativistic equation that involved the finite-size nucleus through time independent perturbation theory. This study justifies the effects of nuclear size on relativistic electron and the measured values are of greatest interest since it will reveal significant changes of the nuclear structure and may also improve the knowledge of fine structure effect. The fine structure of hydrogen atom is important in atomic physics as it brings the idea of relativistic quantum mechanics and an important driving force in theoretical developments of atomic physics after it is experimentally discovered.

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Appendix

The predicted Log[$\Delta E_r(n, j)$] for n = 1, 2, …, 100 states of hydrogen

n	**Log ΔE_r (*n, j*)**
001	3.2310
002	1.4288
003	0.3746
004	-0.3734
005	-0.9535
006	-1.4276
007	-1.8284
008	-2.1756
009	-2.4818
010	-2.7557
011	-3.0035
012	-3.2298
013	-3.4379
014	-3.6306
015	-3.8099
016	-3.9777
017	-4.1354
018	-4.2840
019	-4.4245
020	-4.5579
021	-4.6848
022	-4.8057
023	-4.9213
024	-5.0319
025	-5.1381
026	-5.2401
027	-5.3382
028	-5.4327
029	-5.5240
030	-5.6121
031	-5.6974
032	-5.7799
033	-5.8599
034	-5.9375
035	-6.0129
036	-6.0862
037	-6.1574
038	-6.2267
039	-6.2943
040	-6.3601
041	-6.4243
042	-6.4869
043	-6.5481
044	-6.6079
045	-6.6663
046	-6.7235
047	-6.7794
048	-6.8341
049	-6.8877
050	-6.9403
051	-6.9918
052	-7.0422
053	-7.0918
054	-7.1404
055	-7.1881
056	-7.2349
057	-7.2809
058	-7.3262
059	-7.3706
060	-7.4143
061	-7.4573
062	-7.4996
063	-7.5412
064	-7.5821
065	-7.6224
066	-7.6621
067	-7.7012
068	-7.7397
069	-7.7777
070	-7.8151
071	-7.8520
072	-7.8883
073	-7.9242
074	-7.9596
075	-7.9945
076	-8.0289
077	-8.0629
078	-8.0964
079	-8.1296
080	-8.1623
081	-8.1946
082	-8.2265
083	-8.2580
084	-8.2891
085	-8.3199
086	-8.3503
087	-8.3804
088	-8.4101
089	-8.4395
090	-8.4685
091	-8.4972
092	-8.5257
093	-8.5538
094	-8.5816
095	-8.6091
096	-8.6363
097	-8.6633
098	-8.6899
099	-8.7163
100	-8.7424