The Nuclear Finite–Size Corrections to Energies of $n = 1$, $n = 2$ AND $n = 3$ States of Hydrogen Atom

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Abstract

The first order perturbative approach has been applied and the finite-size nuclear corrections of order of the scaling factors, , ^{2} and ^{3} for n = 1, n = 2 and n = 3 energy levels respectively for the hydrogen atom, have been computed. Results show that as the energy levels increases, the effects of the finite – size nucleus on the orbiting electron is diminishing. This procedure has shown that the concept of finite nuclear size model has an extremely small impact on the energy spectrum of the hydrogen atom. Electron – nucleus interactions, beyond the coulomb potential, modify the atomic property and due to the change from point-charge to finite-size nuclear model the energy level of nucleus is shifted upwards and thus the atomic spectral line for a finite-size nucleus will not coincide with that of its point-size nucleus. This gives us more information on the nuclear charge distribution. Another observation from this work is that with a higher probability of being farther from the nucleus of finite – size charge, the orbiting electrons feel the same effect as the effects due to the point – charge nucleus. Here the finite – size nuclear model have some relevance with the Schrödinger model of hydrogen atom at large distances from the nucleus.

Keywords: Schrodinger, perturbation, Hamiltonian, wave function, nucleus, point-size, finite–size, potential energy

1.0   Introduction

On the atomic scale, the nucleus of hydrogen atom is a point particle, and the Schrodinger equation becomes a one-particle equation after the center of mass motion is separated out [1].Traditionally, atomic physics could afford to consider the nucleus as a point-like charge without losing accuracy. With increased precision in atomic physics experiments, the nucleus is going through an odyssey from the simplified picture of a point-like charge to its real size and properties [2]. Consequently, the electrostatic nuclear potential is no longer a common coulomb potential[3]. Thus, for finite-size description of nuclei or atoms the introduction of perturbation theory as an approximation method to solving finite – size nuclear potential is necessary[4].

Different nuclear masses, charge distributions or spins do have effects on the electronic levels and transition energies, and the small energy corrections or splitting observed in experiments can give in turn information about the atomic nucleus. Atomic electrons are sensitive to the properties of the nucleus they are bound to, such as nuclear mass, charge distribution, spin, magnetization distribution, or even excited level scheme. These nuclear parameters are reflected in the atomic transition energies. A very precise determination of atomic spectra may thus reveal information about the nucleus, otherwise hardly accessible via nuclear physics experiments [2]. The correct identification of nuclear effects in atomic transitions is very important in connection with accurate theoretical atomic structure calculations involving many-body correlations or quantum electrodynamics corrections, which can be tested in high-precision experiments. The investigation of atomic spectra has given us information about the arrangement and motion (angular momentum) of the electrons in an atom. Furthermore, it had led to the discovery of electron spin and to theoretical understanding of the periodic system of the elements. Splitting of energy level is crucial in understanding certain development of the quantum theory of matter and radiation. The spectra of atoms (and molecules) also play an immensely important role in astronomy [5].

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To determine the significance of a point particle assumption of the nucleus, the correction factors for low energy levels and their corresponding orbital angular momenta are computed using the truncated Taylor's series expansion [8]. In this work, different approach which includes the energy level corresponding to the magnetic quantum number was applied. The wave function for the unperturbed state; n, l and m are used to calculate the energy level correction due to the finite size of hydrogen nucleus.

2.0   Methodology

The energy levels in a hydrogen atom can be obtained by solving non relativistic Schrödinger equation in the three-dimensional potential energy field

$$\hat{H}\Psi(r) = \hat{E}\Psi(r)$$

(1)

where $\hat{H}$ is the Hamiltonian operator. Here the hydrogen electron is treated as a wave, represented by the wave function $_{nlm}$, moving in an electric potential as a function of its distance from the proton:

$$U_0(r) = -\frac{ke^2}{r}$$

(2)

With r, being the distance of electron from the nucleus and $k = 1/4f\vee_0 = 9 \times 10^9 \, mF^{-1}$.

According to equation (1), the allowed energies of an electron in the electrostatic potential of a fixed point charge proton are given by

$$E_n = -\frac{me^4}{2\hbar^2}\frac{1}{n^2} \equiv -\frac{1}{2}\frac{e^2}{a_0 n^2}$$

(3a)

Where $a_0 = \hbar^2/me^2 = 5.29 \times 10^{-11} \, m$ is called the Bohr radius [6]. When we set n = 1, we obtain the binding energy of the hydrogen atom in the ground state,

$$E_1 = -\frac{1}{2}\frac{e^2}{a_0}$$

(3b)

This solves the problem of determining the energy levels of the discrete spectrum in a coulomb field [7]. As with any centrally symmetric potential, the solutions of the Schrodinger equation take the form

$$Œ_{nlm}(r,[,\{) = R_{nl}(r)Y_{lm}([,\{)$$

(4)

Where $Y_{lm}([,\{)$ is the spherical harmonic functions which depend only on spherical polar coordinates, and $R_{nl}(r)$ represents the radial component of the wavefunction. Every state with the eigenfunction $_{nlm}$ is characterized by the three quantum numbers n, l and m: The principal quantum number n characterizes the energy level E_n; the azimuthal quantum number l indicates the magnitude of the angular momentum; and the magnetic quantum number m gives the size of the z component of angular momentum. The electron wave functions however are different for every different set of quantum numbers. For each principal quantum number n, all smaller positive integers are possible values for the quantum number l, i.e., $l = 0, 1, 2,…, n – 1$. The quantum number m can take on all integer values between $- l$ and l. In spectroscopy, it is common to use the notation $s, p, d, f, ...$ for the angular momenta $l = 0, 1, 2, 3, ...$[6].

If the nucleus is being described as a finite-size source with a uniform distribution of charges [8] of radius R_N, then the electron wave function can penetrate to r R_N, and thus the electron spends part of its time inside the nuclear charge distribution, there it feels a very different interaction [9] and the potential inside a spare of radius r due to a point charge

$$q_{inside} = e(r/R_N)^3$$

(5)

located at the origin is from Coulomb's law:

$$U(r \leq R_N) = -\frac{ke^2}{r} \cdot \left(\frac{r}{R_N}\right)^3$$

(6a)

Then the perturbative potential difference between r and R_N is defined by:

$$U'(r \leq R_N) = -\int_r^{R_N} \frac{e4f\ldots r'^2}{r'}dr' = -\frac{3ke^2}{R_N^3}\frac{r'^2}{2}\Big|_r^{R_N} = -\frac{3ke^2}{2R_N^3}(R_N^2 - r^2)$$

(6b)

Where $\ldots = 3q/4f\,R_N^3$ is the nuclear charge distribution and in this case it is constant, $R_N = r_0\sqrt[3]{A}$, A being the mass number, $r_0 = 1.27 \times 10^{-15}\,m$, is the radius parameter [2]. Thus, for $r \leq R_N$ we have the potential:

$$U(R_N) = -\frac{ke^2}{r}\cdot\left(\frac{r}{R_N}\right)^3 - \frac{3ke^2}{2R_N^3}\left(R_N^2 - r^2\right) = -\frac{3ke^2}{2R_N^3}\left(3R_N^2 - r^2\right)$$

(7)

Equation (7) represents the potential for a finite-size nucleus [10]. Therefore, the spherical electrostatic potential function $U(R_N)$, corresponding to a nuclear charge density distribution, will then be used to replace the common Coulomb potential for a point-like nucleus (equation (3)), in numerical atomic structure calculations [3]. To obtain the energy shift of the ground state $\}E_{nlm}^{(1)}$, caused by the finite size of the nucleus, we take

$$\}\hat{H}' = U\left(R_N\right) - U_0\left(r\right) = \begin{cases} -\dfrac{ke^2}{2R_N^3}\left(3R_N^2 - r^2\right) + \dfrac{ke^2}{r}, & 0 < r \leq R_N \\[2mm] 0, & r > R_N \end{cases}$$

(8)

as perturbation [10]. The 1st order time-independent perturbation theory is the expectation value of the perturbation in the unperturbed state [11]:

$$\}E_{nlm}^{(1)} = \left\langle Œ_{nlm}^{(0)}\,\middle|\,\}\hat{H}'\,\middle|\,Œ_{nlm}^{(0)}\right\rangle = \int Œ_{nlm}^{(0)*}\}\hat{H}\,Œ_{nlm}^{(0)}d\ddagger$$

(9)

where $\}\hat{H}'$ is the change in the perturbative Hamiltonian. The wave functions $Œ_{nlm}$ for the lowest (unperturbed) state of the Schrödinger hydrogen atom, are obtain as follows [6]:

$$Œ_{100} = \frac{1}{\sqrt{f\,a_0^3}}e^{-r/a_0}$$

(10)

$$Œ_{200} = \frac{1}{\sqrt{8f\,a_0^3}}\left(1 - \frac{r}{a_0}\right)e^{-r/a_0}$$

(11a)

$$Œ_{210} = \frac{1}{\sqrt{32f\,a_0^5}}r\,e^{-r/2a_0}\cos[$$

(11b)

$$Œ_{211} = \frac{1}{\sqrt{64f\,a_0^5}}r\,e^{-r/2a_0}\sin[\,e^{i\{}$$

(11c)

$$Œ_{21-1} = \frac{1}{\sqrt{64f\,a_0^5}}r\,e^{-r/2a_0}\sin[\,e^{-i\{}$$

(11d)

$$Œ_{300} = \frac{1}{3\sqrt{27f\,a_0^3}}\left(3 - \frac{6r}{a_0} + \frac{2r^2}{a_0^2}\right)e^{-r/3a_0}$$

(12a)

$$Œ_{310} = \frac{2}{27\sqrt{f\,a_0^5}}\left(2 - \frac{r}{a_0}\right)r\,e^{-r/3a_0}\cos[$$

(12b)

$$Œ_{311} = \frac{2}{27\sqrt{f\,a_0^5}}\left(2 - \frac{r}{a_0}\right)r\,e^{-r/3a_0}\sin[\,e^{i\{}$$

(12c)

$$Œ_{31-1} = \frac{2}{27\sqrt{f\,a_0^5}}\left(2 - \frac{r}{a_0}\right)r\,e^{-r/3a_0}\sin[\,e^{-i\{}$$

(12d)

$$Œ_{320} = \frac{1}{3\sqrt{3^7 2f\,a_0^7}}r^2 e^{-r/3a_0}\left(3\cos^2[\,-1\right)$$

(12e)

$$Œ_{321} = \frac{1}{9\sqrt{f\,a_0^7}}r^2 e^{-r/3a_0}\sin[\,\cos[\,e^{i\{}$$

(12f)

$$\text{Œ}_{32-1} = \frac{1}{9\sqrt{f\,a_0^7}}\, r^2 e^{-r/3a_0} \sin[\ \cos[\ e^{-i\{}$$

(12g)

$$\text{Œ}_{322} = \frac{1}{18\sqrt{f\,a_0^7}}\, r^2 e^{-r/3a_0} \sin^2[\ e^{2i\{}$$

(12h)

$$\text{Œ}_{32-2} = \frac{1}{18\sqrt{f\,a_0^7}}\, r^2 e^{-r/3a_0} \sin^2[\ e^{-2i\{}$$

(12i)

The effect of the finite size of the proton in the energy levels in hydrogen can be calculated to obtain the energy shift $\}E^{(1)}_{nlm}$ using (9). Taking the approximation $r \quad _0$, i.e., $e^{-2r/a_0} \approx 1$ and assuming the wave function to remain constant over the region of integration. By letting

$$\text{‹} = \left(R_N / a_0\right)^2$$

(13)

and substituting the wave functions of (10), (11) and (12) in (9), and using (3), the perturbative state corrections of the 1ˢᵗ order in *s, p,* and *d* states are calculated and listed in Table 1.

3.0   Results
The 1ˢᵗ order corrections to energies of *n* = 1, *n* = 2 and *n* = 3 States of hydrogen atom due to finite size of nucleus have been computed and listed in Table 1.

4.0   Discussion
It can be observed from Fig. 1 that the perturbation due to finite – size of nucleus decreases rapidly in significance as the principal quantum number, *n*, or the angular quantum number, *l*, is increased. The correction factors for the 1*s*, 2*s* and 3*s* energy orbital is   and for the 2*p* and 3*p*

Table 1: The values of the 1ˢᵗ and 2ⁿᵈ energy levels of the hydrogen atom

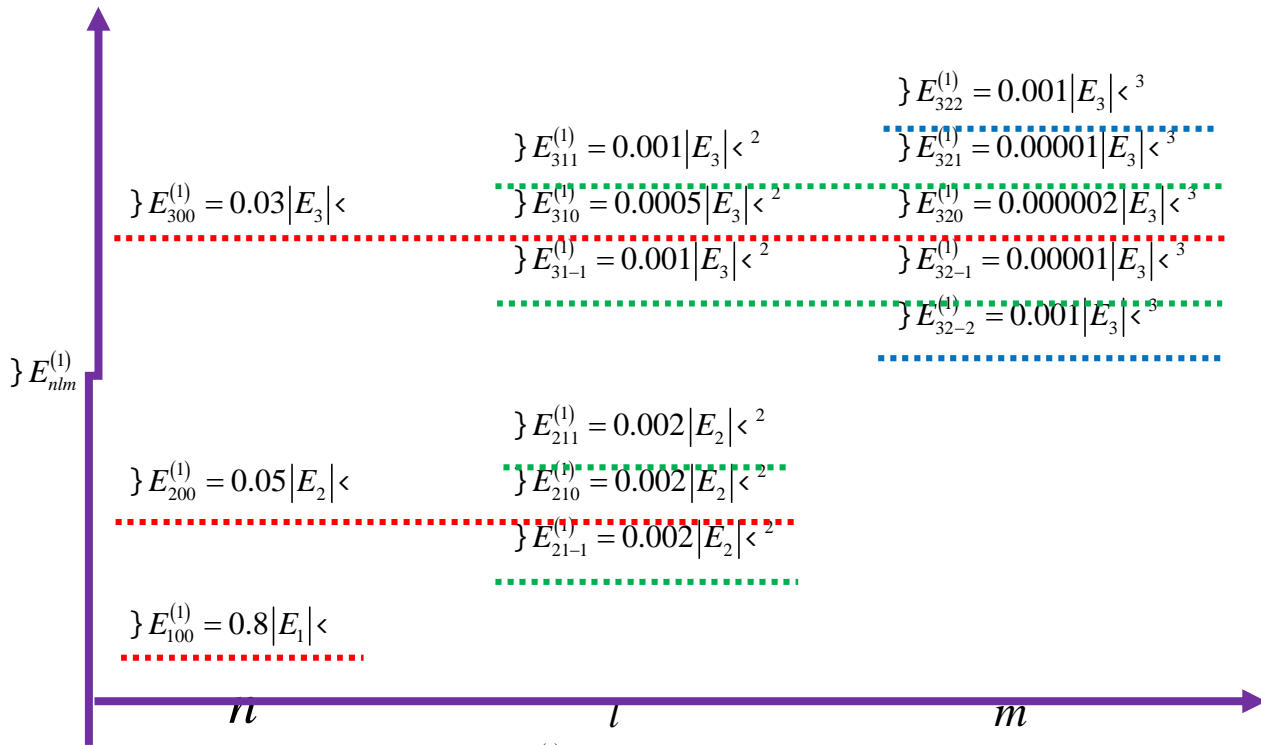| *n*	*L*	*m*	$\}E^{(1)}_{nlm}$		State	$E^{(0)}_n$	$\}E^{(1)}_{nlm}/E^{(0)}_n$
1	0	0	$\}E^{(1)}_{100}$	$0.8\lvert E_1\rvert\text{‹}$	1s	-13.6	0.8‹
2	+1	1	$\}E^{(1)}_{211}$	$0.002\lvert E_2\rvert\text{‹}^2$	2p	-3.4	0.002‹²
		0	$\}E^{(1)}_{210}$	$0.002\lvert E_2\rvert\text{‹}^2$	2p		0.002‹²
		-1	$\}E^{(1)}_{21-1}$	$0.002\lvert E_2\rvert\text{‹}^2$	2p		0.002‹²
	0	0	$\}E^{(1)}_{200}$	$0.05\lvert E_2\rvert\text{‹}$	2s		0.05‹
3	+2	+2	$\}E^{(1)}_{322}$	$0.001\lvert E_3\rvert\text{‹}^3$	3d	-1.51	0.001‹³
		+1	$\}E^{(1)}_{321}$	$0.00001\lvert E_3\rvert\text{‹}^3$	3d		0.00001‹³
		0	$\}E^{(1)}_{320}$	$0.000002\lvert E_3\rvert\text{‹}^3$	3d		0.000002‹³
		-1	$\}E^{(1)}_{32-1}$	$0.00001\lvert E_3\rvert\text{‹}^3$	3d		0.00001‹³
		-2	$\}E^{(1)}_{32-2}$	$0.001\lvert E_3\rvert\text{‹}^3$	3d		0.001‹³
	+1	+1	$\}E^{(1)}_{311}$	$0.001\lvert E_3\rvert\text{‹}^2$	3p		0.001‹²
		0	$\}E^{(1)}_{310}$	$0.0005\lvert E_3\rvert\text{‹}^2$	3p		0.0005‹²
		-1	$\}E^{(1)}_{31-1}$	$0.001\lvert E_3\rvert\text{‹}^2$	3p		0.001‹²
	0		$\}E^{(1)}_{300}$	$0.03\lvert E_3\rvert\text{‹}$	3s		0.03‹

Fig. 1: The finite nuclear size corrections $\} E_{nlm}^{(1)}$ to energies of $n = 1$, $n = 2$ and $n = 3$ states of hydrogen atom with their corresponding values of l and m.

energy orbital is ^{2} while the 3*d*energy orbital has the correction factor of ^{3}. Thus the finite – size nuclear model gives the largest energy correction to the lowest energy orbital. The energy difference between *s, p* and *d* electron states is substantial, comparable to other energy differences between major levels (1*s*, 2*s* or 3*s*). Each increasing orbital angular momentum has a much smaller correction factor. Thus the lowest energy orbitals have the highest energy corrections; 2*s* state is higher in energy than 2*p* states 3*s* state is higher in energy than 3*p* states 3*p* states is higher in energy than 3*d* states this is because the *s* orbitals have higher probability to be closer to the core of nucleus and feels larger attraction than the *p* or *d*orbitals.Non – *s*orbitals have a much smaller fraction inside the nucleus and so cause smaller perturbation, the energy shift is much smaller. The finite-size nucleus gives an extremely small effect on the 3*d*orbitals. On the average an electron closer to the nucleus in its lower energy orbital, experiences the nuclear finite – size charge effect to a larger degree than a more distant electron in the higher orbitals. *d*orbitals are furthest away from the nuclear core therefore have a lower probability to be closer to the nuclear core. The effect of a finite size of the nucleus on hydrogen energy level is larger, in the lowest state(1*s* electron) than in any other state- 2*s*, 3*s*, 2*p*, 3*p*, 3*d*, etc. Thus as the energy levels increase the effects of the finite – size nuclear model have some relevance with the Schrödinger model of hydrogen atom. With a higher probability of being farther from the nucleus, the effects due to the finite size of the nucleus is approaching a point – charge nuclear effect.

5.0   Conclusion
Results show that the quantum number, *m* do contributes to the energy level correction with an amount smaller than the values of quantum number, *l* in the same energy state and that in contrast with energy corrections for *l* state (*p* orbitals), the corrections for *m* states (*d* orbitals) are increasing with the increasing value of the *m*.

In general, the finite size nuclear charge distribution gives the largest energy change to the lowest nuclear charge radius. This is because an electron closer to the finite size nucleus is in the lowest energy orbital and therefore experiences a charge distribution to a larger degree than a more distant electron. At distances farther away from the nucleus, the finite nuclear size effect approaches a point nuclear charge effect in agreement with the Schrödinger's model of the hydrogen atom.

6.0   References
[1].   Gasiorowicz, S., (2003). Quantum Physics, Third Edition. John Wiley & Sons, Inc., U.S.A. pp. 133.

[2]. Adriana, P. (2011). Nuclear effects in atomic transitions. Max Planck Institute for Nuclear Physics in Heidelberg, Germany.

[3]. Andreas D., Reiher M and Hinze J. (2000). A Comparative Study of Finite Nucleus Models for low-lying States of few-electron high-Z Atoms. Chemical Physics Letters 320, pp. 457 - 468.

[4]. Charles, G. T. (2008). Quantum Mechanics. Physics Department, Utah State University, USA. http://ocw.usu.edu/physics/classical-mechanics/pdf_lectures/31.pdf, July, 2014.

[5]. Herzberge, G. and Spink, J.W.T. (1994). Atomic Spectra and Atomic Structure. 2nd Edition. Parentice-Hall, New York. United States of America. pp. 1 and 20.

[6]. Greiner, W. (2001). Quantum Mechanics; An Introduction. Fourth Edition. Springer, Berlin, Germany. pp.181, 220 – 222.

[7]. Landau, L. D. and Lifshitz, E. M., (1991). Quantum Mechanics, Non-relativistic Theory, Volume 3 of Course of Theoretical Physics. Third edition, Pergamon Press, Oxford, England. pp. 119.

[8]. Angelo, J. (2010). Finite Nuclear Size Effect. Physics Department, Drexel University, Philadelphia, Pennsylvania 19104, USA

[9]. Kenneth, S. K. (1988). Introductory Nuclear Physics. John Wiley & Sons, New York. pp. 12.

[10]. Yung-Kuo L., (2000). Problems and Solutions on Atomic, Nuclear and Particle Physics. World Scientific Publishing Co. Pte. Ltd. Singapore. pp. 61.

[11]. Griffiths, D. J., (1995). Introduction to Quantum Mechanics. Prentice Hall, Inc., New Jersey, USA. pp. 222, 248 – 249.