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The Effect of 1st Order Time Independent Perturbation on the Finite Size of the Nuclei of Atoms

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Abstract

In solving Schrödinger's equation for the hydrogen atom, one assumes the nucleus to be a point charge. The nucleus has a finite-size with some shape over which the proton charge is distributed. In this work, we first showed that the nucleus of atoms have finite size, and then examined the potential energy for both the point-like and the finite-size nucleus of hydrogen atom. The results obtained revealed the finite size charge distribution of nucleus which is not only spherical but also assumes a cigar-like or oblate (discuss) shape. The point-like and the finite-size nucleus of hydrogen atom potentials are plotted against the radius of the nucleus. The time-independent perturbation method was applied to calculate energy shift due to finite-size nature of the nucleus of hydrogen atom. The relative energy change calculated from the 1st order correction in the ground state of hydrogen atom was extended for light, medium and large nuclei and the results were plotted graphically as function of radius. The plots have shown that, due to the finite-size nature, the energy level of a nucleus is shifted upwards and its magnitude depends on the size (nucleon distribution) of the nucleus. Thus, for isotopes of a given element where the proton number is the same but the mass number and therefore the nuclear radii are different, the energy correction will be different and due to this the spectral lines will not coincide completely.This correction is one of many corrections that need to be added to the atomic model.

Keywords: Schrödinger's equation, hydrogen atom, point nucleus, finite size nucleus, potential energy, Hamiltonian, perturbation, relative energy change, nuclear radius

1.0 Introduction

The energy of the atomic levels can be obtained in the first approximation by solving the Schrodinger equation for the electrons in the central potential of the nuclear charge $+Ze$, where Z is the atomic number. In order to take into account the spin of the electron, the Dirac equation is introduced. However, in the first approximation, both equations describe the nucleus as a point-like charge of infinite mass. One improvement on the simple particle-in-a-potential model of an atom takes account of the fact that the atomic nucleus is not truly point-like, but instead exhibits finite-size structure in both its mass and charge distribution [1]. Consequently, the electrostatic nuclear potential is no longer a common coulomb potential[2]. Thus, for finite-size description of nuclei or atoms the introduction of perturbation theory is necessary[3].

Also compared to a point-like nucleus, the extended nuclear charge distribution leads to a shift of the nuclear energy levels and this correction of the nuclear model will reflects on the nature of the atomic spectra of the nuclei of atoms [2].

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) play an immensely important role in astronomy[4].

2.0 Theory

To understand completely the finite size of nuclei, we here calculate the volume of nucleus to see its deviation from point size.Assuming uniform charge distribution with density ρ. We have for a nucleus of charge $+Ze$, the volume

$$V = \int_0^b \sqrt{1-\frac{z'^2}{a^2}}\, \rho' d\rho' \int_0^z dz' \int_0^{2\pi} d\varphi' = 4/3\, \pi a b^2 \qquad (1)$$

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And hence the nucleus will have a density given by

$$\rho = \frac{3Ze}{4\pi ab^2} \tag{2}$$

The shape of a nucleus depends mainly on its charge distribution. The intrinsic quadrupole moment of a symmerty charged distribution is defined by the relation

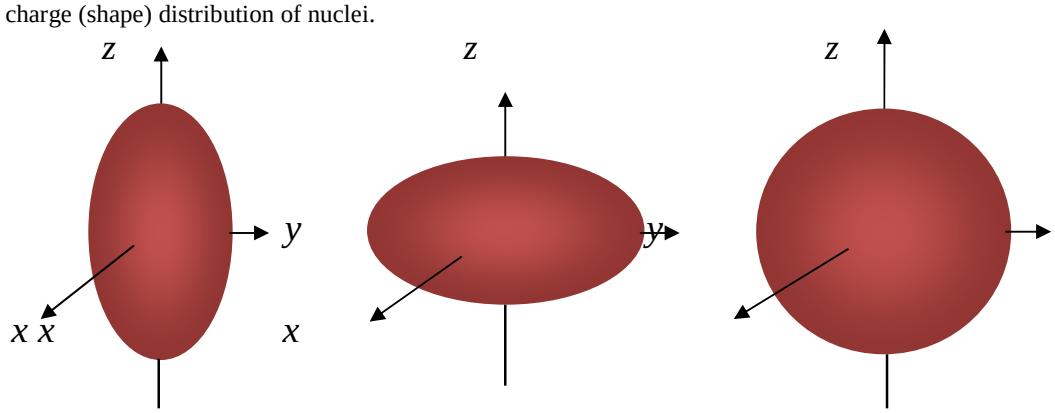
$$Q_0 = \frac{1}{e}Q_{33} = \frac{1}{e}\int \rho\,(r')\left[3(z')^2 - (r')^2\right]dv' \tag{3}$$

Where the integration is carried over the whole volume of the nucleus. $r'(x', y', z')$ is measured from the centre of mass of the nucleus. The nucleus is assumed to have asymmetry axis along z': e is the charge on each proton [5].

Using the fact that $r'^2 = x'^2 + y'^2 + z'^2 = \rho'^2 + z'^2$ and $dv' = \rho' d\rho' d\varphi' dz'$ we find:

$$Q_0 = \frac{ze}{4/3\,\pi ab^2 e}\iiint\left(3z'^2 - z'^2 - \rho'^2\right)dv' = Z\,\frac{2}{5}\left(a^2 - b^2\right) \tag{4}$$

The quadrupole moment is connected to nuclear deformation. A non-zero quadrupole moment Q_0 indicates that the charge distribution is not spherically symmetric. Non-spherical nuclei able to rotate about axes other than the axis of the symmetry: this rotation gives rise to characteristic spectral feature which permits the quadrupole moment to be measured. By convection, the value of Q_0 is taken to be positive (i.e. when $a > b$) if the ellipsoid is prolate and negative (i.e. when $a < b$) if the ellipsoid is oblate and zero (i.e. when $a = b$) if the ellipsoid is a sphere. Fig.1 depicts the possible charge (shape) distribution of nuclei.



Prolate(cigar-shape); **Oblate** (discuss); **Sphere** (protants)**;**
Fig. 1: Electric quadrupole moments for different charge distribution

The Mathematical aspects of nonrelativistic Quantum Mechanics are determined by the solutions to the Schrödinger's. The energy of the atomic levels can be obtained in the first approximation by solving the Schrodinger equation (5) for the electrons in the central potential energy $V(r)$ of nucleus with charge $+Ze$, where Z is the atomic number.

$$-\frac{\hbar^2}{2m}\frac{\mathrm{d}^2\phi(r)}{\mathrm{d}r^2} + V(r)\phi(r) = E\phi(r) \tag{5}$$

Where $\phi(r)$ is the Schrodinger's wave function. The complete solution including the time dependence is

$$\Psi(x,t) = \phi(x)e^{\frac{-iEt}{\hbar}} \tag{6}$$

If $\hat{E}$ is real then the wave function has an amplitude $\phi(x)$ and a phase $e^{-iEt/\hbar}$ [6].

In solving the Schrödinger equation for the case of the atom with a single electron, it is always assumed that the electron feels the coulomb attraction of a point nucleus,

$$V(r) = -k\frac{Ze^2}{r}, \quad r \geq R_N \tag{7}$$

Where $k = (4\pi\varepsilon_0)^{-1} = 9\times10^9\, mF^{-1}$ is the proportionality constant, $\varepsilon_0 \approx 8.854\times10^{-12}\, Fm^{-1}$ is the permittivity in free space, $e = 1.6\times10^{-19}\, C$, is the electronic charge.

As a more realistic assumption, the nucleus was instead being described as a finite-size source with a uniform distribution of charges[7]. Since real nuclei are not points, 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[6]. As an approximation, we can assume the nucleus to be a uniformly charged sphere with a radius R_N for which the potential energy of the electron for $r \leq R_N$ is given by;

$$V(R_N) = \frac{ke^2}{2R_N}\left[\left(\frac{r}{R_N}\right)^2 - 3\right] \tag{8}$$

where $R_N = r_0 A^{1/3}$, A being the mass number, $r_0 = 1.27\times10^{-15}\, m$, is the radius parameter

Schrodinger's equation (5) or its solution (6) applied only to point sources (charges). Thus the introduction of an approximation method is necessary for finite-size nuclei or atoms [3]. It is possible to use the perturbation theory to see the effect of the finite-size by observing the atomic spectra.

By adding the perturbative electric potential (8) to the quantum mechanical model of hydrogen atom, we can calculate the shift in the spectral line of hydrogen atom caused by the presence of an electric field [7].

The 1st order time independent perturbation theory is given as:

$$\lambda E_n^{(1)} = \left\langle \phi_n^{(0)} \middle| \lambda\hat{H}' \middle| \phi_n^{(0)} \right\rangle \tag{9}$$

It says that, the perturbative energy corrections of 1st order are given by the expectation value of the perturbing Hamiltonian in the unperturbed states.

Therefore, the spherical electrostatic potential function $V(R_N)$, corresponding to a nuclear charge density distribution (2), will then used to replace the common Coulomb potential for a point-like nucleus, (7), in numerical atomic structure calculations [1].

Even though the potential (7) diverges at $r = 0$, it does provide an analytic solution to the Hamiltonian given by

$$\hat{H}_0 = -\frac{\hbar^2\nabla^2}{2m} - k\frac{Ze^2}{r} \tag{10}$$

The Hamiltonian is formed by the addition the kinetic energy term.

After producing the new potential due to finite size nucleus of radius R_N as the perturbation of the common Coulomb potential (8), we also developed to a new Hamiltonian equation;

$$\hat{H} = -\frac{\hbar^2\nabla^2}{2m} + V(R_N) = -\frac{\hbar^2\nabla^2}{2m} + k\frac{Zke^2}{2R_N}\left[\left(\frac{r}{R_N}\right)^2 - 3\right] = \hat{H}_0 + \lambda\hat{H}', \quad r \leq R_N$$

Where
$$\lambda\hat{H}' = k\frac{Ze^2}{R_N}\left[\frac{R_N}{r} - \frac{3}{2} + \left(\frac{r}{R_N}\right)^2\right], \; r \leq R_N \tag{11}$$

The effect of the finite size of the proton in the energy levels in hydrogen can be calculated to obtain the energy shift $\lambda E_1^{(1)}$ using the 1st order time independent perturbation theory. The perturbative state correction of the 1st order is given by:

$$\lambda E_n^{(1)} = \left\langle \phi_n^{(0)} \middle| \lambda \hat{H}' \middle| \phi_n^{(0)} \right\rangle = \int \phi^{(0)*} \lambda \hat{H}' \phi^{(0)} d\tau = \int \phi_{100} \lambda \hat{H}' \phi_{100} d\tau \quad (12)$$

$\lambda \hat{H}'$ is the change in the Hamiltonian resulting from the difference between a point charge and some spherical distribution, either over the surface or volume of a sphere.
The ground state wave function of the hydrogen atom is

$$\phi_{100} = \left(\frac{Z^3}{\pi a_0^3} \right)^{\frac{1}{2}} e^{-\frac{Zr}{a_0}} \quad (13)$$

Where a_0 is the Bohr radius and $R_N \ll a_0$. We choose the ground state for simplicity and since the ground state energy is non-degenerate. The 1st order correction in the ground state energy of the hydrogen atom would be

$$\lambda \hat{E}_1^{(1)} = 4k \frac{Z^4 e^2}{a_0^3 R_N} \int_0^{R_N} \left(\frac{R_N}{r} - \frac{3}{2} + \frac{r^2}{2R_N^2} \right) e^{-2Zr/a_0} r^2 dr = \frac{2}{5} k \frac{Z^4 e^2 R_N^2}{a_0^3} \quad (14)$$

Where the use of equations (11) and (13) have been made Since $R_N \ll a_0$, we assume the wave function to remain constant over the region of integration. Hence we replace $\phi^{(0)}$ by its value at $r = 0$
But the unperturbed energy of an electron moving in the 1st orbit around the nucleus (point-like) is

$$E_1^{(0)} = -k \frac{Z^2 e^2}{2a_0} \quad (15)$$

Thus, we can calculate the relative energy change η, due to finite size of the proton as:

$$\eta = \frac{\lambda E_1^{(1)}}{E_1^{(0)}} = \frac{4}{5} \left(\frac{ZR_N}{a_0} \right)^2 \quad (16)$$

where $a_0 = 5.29 \times 10^{-11} m$, is the Bohr's radius

3.0 Results

Here we compute numerical results from equations (8) and (16). From equation (8) we obtain Table 1 which gives detailed information on potential energy differences between a point-like and finite-size nuclear assumption. The relative energy changes have been calculated from equation (16) and are displayed in Table 2.

Table 1: The values of potential energies for a point-like and finite-size nucleus of hydrogen atom

	Potential Energies	
r / R_N	$V(r)$	$V(R_N)$
0.0	0.0000	-2.7213
0.2	-9.4425	-2.6850
0.4	-4.7213	-2.5761
0.6	-3.1475	-2.3947
0.8	-2.3606	-2.1407
1.0	-1.8885	-1.8142
1.2	-1.5737	-1.4151
1.4	-1.3489	-0.9434
1.6	-1.1803	-0.3991
1.8	-1.0492	0.2177
2.0	-0.9443	0.9071
2.2	-0.8584	1.6691
2.4	-0.7869	2.5036

This information is extended further by plotting a graph of two potentials against the radius of the nucleus, r (Fig. 1).

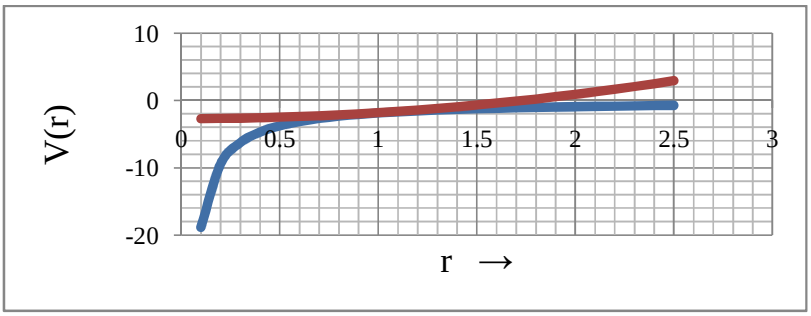


Fig. 1: The potential curves for a point-like and a finite-size nucleus

The potential curve for finite-size nuclear can be seen in Fig. 1, represented by the red line. While the point-like potential curve can be seen by the blue line, falling to $-\infty$ as r approaches 0. We can notice how the finite-size nuclear potential and the point-like potential curves coincide only at $r \approx R_N$. The potential curve for finite-size nuclear can be seen in Fig. 1, represented by the red line. While the point-like potential curve can be seen by the blue line, falling to $-\infty$ as r approaches 0. It is observed that the finite-size potential is finite (with magnitude 2.7213 eV)when $r = 0$. This shows that the size of the nucleus is not in fact zero. The positive charge of the nucleus is spread out over a distance of about 10^{-15}m. At this distance the coulomb potential is no longer r dependence. Thus nucleus is a spherical shell of charge of non-zero or finite size radius.. This shows quite evidence for a finite size nature of a nucleus. We can also notice how the finite-size nuclear potential and the point-like potential curves coincide only at $r \approx R_N$. The difference observed is due to the finite-size structure of nucleus. This shows quite evidence for a finite size nature of a nucleus. Compared to a point-like nucleus, the extended nuclear charge distribution leads to a shift of the nuclear energy levels and this correction of the nuclear model will reflects on the nature of the atomic spectra of the nuclei of atoms. The consequence of finite nucleus size can be estimated. For hydrogen atom itself they are extremely small, but become more important for heavier atoms.

The relative energy change calculated for light, medium and heavy nuclei have been computed using the result obtained by equation (16) in order to see the deviation from point-like nucleus to finite-size nucleus (see Table 2).

Table 2: The relative energy change for light nuclei

Elements	Symbols	Proton no. (Z)	Mass no. (A)	$R_N\left(\times 10^{-15}\,m\right)$	$\eta\left(\times 10^{-6}\right)$
Hydrogen	H	1	1	1.2700	0.0005
Boron	B	5	11	2.8244	0.0570
Neon	Ne	10	20	3.4473	0.3397
Phosphorus	P	15	31	3.9895	1.0237
Calcium	Ca	20	40	4.3433	2.1571
Rhodium	Rh	45	103	5.9531	20.5159
Tin	Sn	50	118	6.2391	27.7312
Caesium	Cs	55	133	6.4827	36.3426
Neodymium	Nd	60	142	6.6257	45.1798
Astatine	At	85	218	7.6434	120.6863
Thorium	Th	90	232	7.8032	141.0483
Americium	Am	95	243	7.9251	162.0449
Fermium	Fm	100	257	8.0744	186.3799

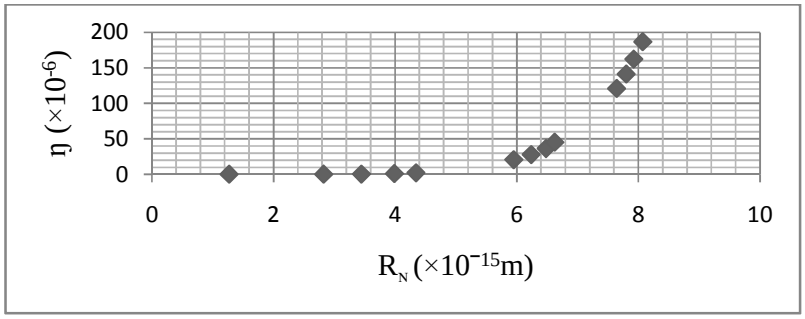


Fig. 2: A Graph of Relative Energy Change against the Nuclear Radius for Various Nuclei

It is observed from Fig. 2 that with the increase of Z from $Z \approx 2$ to $Z \approx 20$,The change due to variation of finite-size nuclear model is very small and is fairly constant. Thus small effects are observed for few-electron atoms with a small nuclear charge distribution. But for medium nuclei when the number of nucleon Z increases from 40 to about 60, a moderate increase is to be sure.In this case the relative energy changes are increasingly small due to change from point-like to finite-size nucleus.Fig. 2 also showed a rapid incline of the relative energy changes in heavy nuclei. This is due to their large number of nucleons in their nucleus. Higher nuclear charges up to $Z \approx 103$ were considered for a particular case of highly charged because of the uniform distribution of charge assumption gives the largest energy correction to the heavy nuclei, because of the contribution of charges by each of their proton.

The magnitude of the point-charge nuclear to finite nuclear size shift behaves quite different in the small, medium and heavy nuclei cases, when considered as a function of Z (Fig. 2). Thus, the total energy shifts reflect the sequence of the finite nuclear size potentials over the full range of Z covered by this study, i.e., every state is found to be shifted upward, due to the change from the point-like to the finite-size source. It is observed from Fig. 2, that the relative energy change increases with the nuclear radius and thus, it depends on the size (nucleon distribution) of the nucleus. For light nucleus the relative energy change is very small, but become more important for heavier atoms. The difference observed is due to the finite-size structure of nucleus.Therefore, for isotopes of a given element where the proton number is the same but the mass number and therefore the nuclear radii are different, the energy correction will be different and due to this the spectral lines will not coincide completely.

4.0 Conclusion

Since different isotopes of the same element with nuclear charge +Ze have different numbers of neutrons, their charge distribution will not coincide, leading to a small shift in their electronic level energies. This difference of an electronic transition is usually described separately as due to the finite mass of the nucleus and to the size of the nuclear charge distribution. In order to extract information about the nuclear properties, a proper interpretation of the measured isotope shifts based on theoretical calculations is necessary. Since often nuclei with the same Z but different mass number A also have different nuclear spins, spectra of different isotopes may also have a completely different hyperfine structure [2].

The history of isotope shifts goes back to 1931, when experiments by Schuler and Keyston on the hyperfine structure of thallium and later on mercury led to the discovery of a structure which was not due to the nuclear spin but to a displacement of the atomic levels in different isotopes. The authors pointed out that their observations have to be explained by some differences in the nuclear fields of the isotopes. Several models for the nuclear charge distributions have been used in the literature. This effect can be explained if the approximation of an infinitely heavy and point-like nucleus is abandoned [8]. One of the obvious choices is to consider the nucleus as a homogeneously charged sphere of radius R_N [2].At this point we can draw the conclusion that the atomic nucleus is not truly point-like, but instead exhibits finite-size structure in both its mass and charge distribution. This finite-size charge distribution of nucleus is not only spherical but may also be a cigar-like or oblate (discuss) in shape. And due to the change of nuclear model from point-like to finite-size nature of nucleus the energy level of nucleus is shifted upwards and thus the atomic spectral line will not coincide completely.In order to extract information about the nuclear properties, a proper interpretation of the measured isotope shifts based on theoretical calculations is necessary. This correction of nuclear model is one of many corrections that need to be added to the atomic model.

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