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Nuclear size corrections to the energy levels of single-electron and -muon atoms

R T Deck[1], **Jacques G Amar**[1] **and Gustave Fralick**[2]

[1] Department of Physics and Astronomy, University of Toledo, Toledo, OH 43606, USA
[2] NASA Glenn Research Center, Cleveland, OH 44135, USA

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Abstract

We formulate an analytic method which accounts for the finite size of the nucleus by treating it as a boundary value problem. The method is used to obtain solutions of the Dirac equation for a central potential that is proportional to $1/r$ only for values of the radial coordinate greater than a given value R. Our results are applied to a non-perturbative calculation of the nuclear size corrections to the energy levels of single-electron and single-muon atoms. For values of the nuclear charge number Z greater than 40 in the case of electronic atoms, and greater than 1 in the case of muonic atoms, we find large discrepancies between our results for the atomic energy levels and those obtained from first-order relativistic perturbation theory.

1. Introduction

It is well known that the discrete eigenvalues of the Coulomb potential closely approximate the bound state energies of a single-electron atom. On the other hand, the unphysical infinity in the $1/r$ potential at the origin makes it necessary that this potential be modified for values of r inside a region about the origin that can be identified with the nucleus of the atom. The resulting correction to the energy of the atom due to the finite size of the nucleus leads to the familiar isotope shift between the energy levels of two atoms with nuclei that have the same atomic number Z but different mass numbers A. In the case of electronic atoms, the small magnitude of the nuclear size effect allows the nuclear size correction to the energy levels to be accurately calculated by the use of perturbation theory [1], which is expected to become inaccurate only for large values of Z. Instead, in the case of a muonic atom, in which the inner electron is replaced by a muon with a mass approximately 207 times m_e, because the radius of the muon's orbit is approximately m_e/m_μ times smaller than the radius of the electron's orbit in the electronic atom, perturbation theory becomes invalid for all values of Z greater than 1. This makes it necessary to account for the alteration in the potential at small r without the use of perturbation theory. This problem was recently addressed by Tibarzi and Holstein [2] by constructing a solution to the Schrödinger equation for the muonic atom for

all r, obtained by numerically matching distinct solutions of the equation inside and outside the nuclear radius under the assumption of a uniform nuclear charge density. However, the non-relativistic character of the Schrödinger equation and the importance of relativistic effects on the states of particles close to the nucleus, made it necessary for these authors to make use of perturbation theory to account for the effects of relativistic kinematics and the important spin–orbit and Darwin terms in the complete interaction potential. Here, we instead present a simpler analytic method that accounts for nuclear size effects based on a solution of the Dirac equation for all r, and incorporates (exactly) the effects included in [2] perturbatively. The method reduces the computation of the energies of the electron or muon, in interaction with a finite size nucleus, to a boundary value problem involving a single unknown eigenvalue. The resulting exact energy shifts produced by the nuclear size effect are dependent only on the assumed form for the potential energy inside the nucleus.

A large number of publications exist relating to both nuclear size effects and the isotope shift (see, for example, [3–6]). In the case of hydrogenic atoms with light nuclei, the contribution to the isotope shift produced by the effect of nuclear size is known to be masked by the larger mass-dependent contribution due to nuclear motion. In contrast, in heavy atoms with large Z, the nuclear size effect becomes dominant, but the analysis of the effect is complicated by many-electron effects. The present paper makes no attempt to address the totality of effects on the electronic levels with magnitudes comparable to the nuclear size correction. Instead, the intent is to put forward a method of analysis that correctly accounts for the effect of nuclear size alone. As justification for our analysis, we note that the standard expression for the nuclear size correction to the nth electronic level of a one-electron atom, given by the formula[3] $E_{\text{Finite Size}} = (2(Z\alpha)^4\mu^3)/(3n^2)\langle R^2\rangle\delta_{\ell 0}$, (see [3, 4, 6]), is approximately equal to the correction obtained from non-relativistic perturbation theory, which is shown to be invalid for large Z. In addition, we note that, since a potential that becomes infinite at any point can never be correct everywhere, and the eigenvalues computed from it must therefore be inexact, a non-perturbative method for constructing more exact eigenvalues for such potentials has a significance beyond its use in the description of the nuclear atom.

The structure of this paper is as follows. In section 2 we develop the theory underlying the results we present. We emphasize, in particular, that if the infinity in the Coulomb potential is removed near the origin, the usual series termination condition on the solution of the Dirac equation is invalid, and the energy of the electron is determined by the boundary conditions at the value of the radial coordinate for which the form of the potential is changed. In section 3 we carry out a numerical solution of the resulting boundary equations to obtain the corrections to the energies of both electronic and muonic atoms produced by the finite size of the nucleus. The solutions are based on two commonly used forms for the nuclear potential. Our numerical results are compared with the results obtained from perturbation theory using both relativistic and non-relativistic wavefunctions. In passing, we note that our analysis offers an alternative to a previously proposed theory that predicted the existence of new states of the atom on the basis of the finite size of the nucleus [7].

2. Theory

We focus on single-electron or single-muon atoms for which the potential produced by the nucleus can be well approximated by a central potential $V(r)$. The interest is in large values of the charge number Z for which the tight binding causes the energy of the bound particle to

[3] Here, μ and ℓ are the reduced mass and orbital angular momentum quantum number respectively, α is the fine structure constant and R is the radius of the nucleus. First-order non-relativistic perturbation theory gives the correction to the ground state energy of the hydrogenic atom in equation (40).

be relativistic. In this case, the wavefunction of the particle satisfies the Dirac equation in the form

$$[-i\hbar c\gamma_0\boldsymbol{\gamma}\cdot\nabla + \gamma_0 mc^2 + V(r)]\Psi(\mathbf{r}) = E\Psi(\mathbf{r}) \tag{1}$$

where γ_0 and $\boldsymbol{\gamma}$ represent Dirac γ-matrices, and m and E are the rest mass and total energy of the electron or muon respectively. The solution of equation (1) can, in general, be represented as a four element column matrix dependent on the spherical coordinates, r, θ and ϕ, of the coordinate vector $\mathbf{r}$ as

$$\Psi(\mathbf{r}) = \begin{pmatrix} ig(r)\Omega_{j\ell m_j}(\theta,\phi) \\ f(r)\Omega_{j\ell' m_j}(\theta,\phi) \end{pmatrix} \tag{2}$$

where $\Omega_{j\ell m_j}(\theta,\phi)$ is a two-row spherical spinor, and the quantum numbers ℓ and ℓ' characterize the upper and lower components of the Dirac matrix. What is relevant is the dependence of Ψ on the radial coordinate r, expressed through the radial functions $g(r)$ and $f(r)$, which the Dirac equation connects through the coupled equations

$$\left[\frac{\mathrm{d}}{\mathrm{d}r} + \frac{1+\kappa}{r}\right] g(r) - \frac{1}{\hbar c}[E + mc^2 - V(r)]f(r) = 0 \tag{3a}$$

$$\left[\frac{\mathrm{d}}{\mathrm{d}r} + \frac{1-\kappa}{r}\right] f(r) + \frac{1}{\hbar c}[E - mc^2 - V(r)]g(r) = 0. \tag{3b}$$

Here, for a given value of j, the quantum number κ has the possible values $\pm\left(j+\frac{1}{2}\right)$, corresponding to values of ℓ and ℓ' equal to $j \pm \frac{1}{2}$ and $j \mp \frac{1}{2}$ respectively, with the parity of $\Psi(r)$ given by $(-1)^{\ell}$.

2.1. Solution of the Dirac equation exterior to the nucleus

For values of the radial coordinate r greater than or equal to a value R which defines the nuclear radius, we assume that the central potential has the Coulomb form,

$$V(r) = -Ze^2/r, \qquad (r \geqslant R). \tag{4}$$

As is well known, introduction of the dimensionless coordinate variable $\rho \equiv 2qr$, with

$$q \equiv \sqrt{\frac{(mc^2)^2 - E^2)}{\hbar^2 c^2}}, \tag{5}$$

and use of the sum and difference functions

$$u_{\pm}(\rho) \equiv \rho^{\frac{3}{2}}\left(g \mp \sqrt{\frac{mc^2+E}{mc^2-E}}\,f\right), \tag{6}$$

leads to uncoupled equations for $u_+(\rho)$ and $u_-(\rho)$ in the forms

$$\left\{\frac{\mathrm{d}^2}{\mathrm{d}\rho^2} - \frac{\left[\left(j+\frac{1}{2}\right)^2 - (\alpha Z)^2 - \frac{1}{4}\right]}{\rho^2} + \frac{\left[\alpha Z\frac{E}{\sqrt{(mc^2)^2-E^2}} \pm \frac{1}{2}\right]}{\rho} - \frac{1}{4}\right\} u_{\pm}(\rho) = 0, \tag{7}$$

with $\alpha = e^2/\hbar c$. Equation (7) has the general form of Whittaker's equation

$$\left[\frac{\mathrm{d}^2}{\mathrm{d}\rho^2} - \frac{\gamma^2 - \frac{1}{4}}{\rho^2} + \frac{\beta}{\rho} - \frac{1}{4}\right] M(\rho) = 0, \tag{8}$$

where

$$\gamma^2 = \left(j + \frac{1}{2}\right)^2 - (\alpha Z)^2, \qquad \beta = \beta_\pm = \alpha Z \frac{E}{\sqrt{(mc^2)^2 - E^2}} \pm \frac{1}{2}. \tag{9}$$

Subject to the condition that 2γ is not equal to zero or a positive or negative integer, the general solution of equation (8) is a linear combination of two particular solutions, $M_{\beta,\gamma}(\rho)$ and $M_{\beta,-\gamma}(\rho)$ [8], which differ in the sign of the square root of the parameter γ^2. Explicitly, the particular solutions corresponding to plus and minus γ can be expressed in terms of confluent hypergeometric functions ${}_1F_1$ through the relations

$$M_{\beta,\pm\gamma}(\rho) = \rho^{\pm\gamma+\frac{1}{2}}\, \mathrm{e}^{-\rho/2}\, {}_1F_1\left(\pm\gamma - \beta + \tfrac{1}{2}, \pm 2\gamma + 1, \rho\right), \tag{10}$$

where the function ${}_1F_1$ has the series representation,

$${}_1F_1(a, b; \rho) = 1 + \frac{a}{b}\rho + \frac{1}{2!}\frac{a(a+1)}{b(b+1)}\rho^2 + \cdots. \tag{11}$$

As a consequence of the divergence of the series in equation (11) at $\rho = \infty$ the functions $M_{\beta,\gamma}(\rho)$ and $M_{\beta,-\gamma}(\rho)$ are both divergent for large r unless the series forms of the solutions are terminated by a choice of the parameter β such that the first argument of ${}_1F_1$ is equal to a negative integer.

If the Coulomb potential is assumed to be valid at the origin, the divergence of the function $M_{\beta,-\gamma}(\rho)$ at $\rho = 0$ requires the coefficient of this function in the general solution of equation (8) to be equated to zero. The condition on the parameter β required to terminate the series representation for the solution $M_{\beta,\gamma}(\rho)$ then leads to the familiar formula for the allowed energy eigenvalues of the electron given by

$$E = mc^2 \frac{\left(n' + \sqrt{\left(j + \frac{1}{2}\right)^2 - (\alpha Z)^2}\right)}{\sqrt{\left(n' + \sqrt{\left(j + \frac{1}{2}\right)^2 - (\alpha Z)^2}\right)^2 + (\alpha Z)^2}}, \quad n' = 0, 1, 2, \ldots. \tag{12}$$

Instead, in the case when the finite size of the nucleus restricts the range of ρ in which the Coulomb potential applies, so as to exclude the value zero, the divergence in $M_{\beta,-\gamma}(\rho)$ is removed, and the general solution of Whittaker's equation is a linear combination of both functions $M_{\beta,\gamma}(\rho)$ and $M_{\beta,-\gamma}(\rho)$. Here, however, the relation $2\gamma \neq$ integer makes it impossible to terminate the series forms of both functions for the same value of β. As a result of this, a non-divergent solution of equation (7) can be obtained as a linear combination of $M_{\beta,\gamma}$ and $M_{\beta,-\gamma}$ only if the two functions are combined so that the divergences in the separate functions at $\rho = \infty$ cancel exactly. For this purpose, it is possible to make use of the asymptotic forms of the confluent hypergeometric functions given by the equations

$$\lim_{\rho\to\infty} {}_1F_1\left(\gamma - \beta + \frac{1}{2}, 2\gamma + 1, \rho\right) = \frac{\Gamma(2\gamma+1)}{\Gamma\left(\frac{1}{2} + \gamma - \beta\right)}\, \mathrm{e}^{\rho}\, \rho^{-\frac{1}{2}-\beta-\gamma} + \frac{\Gamma(2\gamma+1)}{\Gamma\left(\frac{1}{2} + \gamma + \beta\right)} (-\rho)^{-\frac{1}{2}+\beta-\gamma} \tag{13a}$$

$$\lim_{\rho\to\infty} {}_1F_1\left(-\gamma - \beta + \frac{1}{2}, -2\gamma + 1, \rho\right) = \frac{\Gamma(-2\gamma+1)}{\Gamma\left(\frac{1}{2} - \gamma - \beta\right)}\, \mathrm{e}^{\rho}\, \rho^{-\frac{1}{2}-\beta+\gamma} + \frac{\Gamma(-2\gamma+1)}{\Gamma\left(\frac{1}{2} - \gamma + \beta\right)} (-\rho)^{-\frac{1}{2}+\beta+\gamma} \tag{13b}$$

to determine the large ρ dependences of $M_{\beta,\gamma}$ and $M_{\beta,-\gamma}$ in the forms

$$\lim_{\rho\to\infty} M_{\beta,\gamma}(\rho) = \frac{\Gamma(2\gamma+1)}{\Gamma\left(\frac{1}{2}+\gamma-\beta\right)}\,\mathrm{e}^{\rho/2}\rho^{-\beta}, \tag{14a}$$

$$\lim_{\rho\to\infty} M_{\beta,-\gamma}(\rho) = \frac{\Gamma(-2\gamma+1)}{\Gamma\left(\frac{1}{2}-\gamma-\beta\right)}\,\mathrm{e}^{\rho/2}\rho^{-\beta}. \tag{14b}$$

These relations allow a 'bound state solution' of Whittaker's equation that vanishes at infinity to be constructed from a linear combination of solutions that are respectively regular and irregular at the origin in the form

$$\begin{aligned} u_{\pm}(\rho) &= N_{\pm}\left[M_{\beta_{\pm},+\gamma}(\rho) - \Delta(\beta_{\pm},\gamma)M_{\beta_{\pm},-\gamma}(\rho)\right] \\ &= N_{\pm}\,\mathrm{e}^{-\rho/2}\left[\rho^{\gamma+\frac{1}{2}}{}_1F_1\left(\gamma-\beta_{\pm}+\tfrac{1}{2},2\gamma+1,\rho\right)\right. \\ &\quad \left.-\Delta(\beta_{\pm},\gamma)\rho^{-\gamma+\frac{1}{2}}{}_1F_1\left(-\gamma-\beta_{\pm}+\tfrac{1}{2},-2\gamma+1,\rho\right)\right], \end{aligned} \tag{15}$$

with

$$\Delta(\beta_{\pm},\gamma) \equiv \frac{\Gamma(2\gamma+1)}{\Gamma(-2\gamma+1)}\,\frac{\Gamma\left(\frac{1}{2}-\gamma-\beta_{\pm}\right)}{\Gamma\left(\frac{1}{2}+\gamma-\beta_{\pm}\right)}. \tag{16}$$

The combination of functions in equation (15) is referred to in the mathematical literature as Whittaker's function [9], and represents the only correct bound state solution of Whittaker's equation in the case of a Coulomb potential terminated at a finite (non-zero) value of r.

We note that the authors of [7] attempted to obtain distinct solutions of equation (7) for a finite nucleus by separately equating the coefficients of the functions $M_{\beta,\gamma}$ and $M_{\beta,-\gamma}$ to zero, and terminating the series form for the remaining function by a choice of a discrete value of β. In this attempt, under the condition that the coefficient of the singular function $M_{\beta,-\gamma}(\rho)$ was set to zero, the termination condition on the series form of the function $M_{\beta,\gamma}$ produced the standard formula for the energy in equation (12), whereas, under the condition that the coefficient of the function $M_{\beta,\gamma}(\rho)$ was set to zero, the condition terminating the function $M_{\beta,-\gamma}(\rho)$ led instead to a formula for the energy expressible as [7]

$$E = mc^2\frac{\left(n'-\sqrt{\left(j+\frac{1}{2}\right)^2-(\alpha Z)^2}\right)}{\sqrt{\left(n'-\sqrt{\left(j+\frac{1}{2}\right)^2-(\alpha Z)^2}\right)^2+(\alpha Z)^2}}, \quad n' = 0,1,2,\ldots. \tag{17}$$

This formula, as a consequence of the negative sign preceding the square root in its numerator, predicts the binding energy of the electron to approach mc^2 for values of n' and j for which $n'-\left(j+\frac{1}{2}\right)=0$, on the basis of which the authors of [7] predicted the existence of new bound states of the hydrogenic atom referred to as 'deep Dirac levels' (DDL). Instead, we point out that both equations (17) and (12) result in inaccurate eigenvalues in the case of an atom with a finite size nucleus. The inaccuracy of the eigenvalues in this case is a consequence of their lack of dependence on either the boundary conditions at the nuclear radius or the form of the potential inside the nucleus[4]. In particular, the lack of dependence on the potential inside the nucleus makes it impossible to match a solution corresponding to either set of energy values to a solution interior to the nucleus.

In the present analysis, the use of the solution in equation (15), in combination with equation (6) and the definition of $u_{\pm}(\rho)$, determines radial functions g and f corresponding to proper bound state solutions of the Dirac equation in the forms

$$g(r) = \tfrac{1}{2}\rho^{-3/2}[u_+(\rho)+u_-(\rho)], \tag{18}$$

[4] This argument was omitted in previous criticisms of [7] by Rice R A, Kim Y E and Rabinowitz M, in 1994 *Fusion Technol.* **26** 110, and 1995 *Fusion Technol.* **27** 348, which were rebutted by Maly J A and Vavra J, in 1994, *Fusion Technol.* **26** 111, and 1996 *Fusion Technol.* **30** 386.

$$f(r) = -\frac{1}{2}\sqrt{\frac{mc^2 - E}{mc^2 + E}}\,\rho^{-3/2}[u_+(\rho) - u_-(\rho)]. \tag{19}$$

Here the coupling between the functions g and f demanded by the Dirac equation connects the coefficients N_+ and N_- in the separate solutions $u_+(\rho)$ and $u_-(\rho)$ through the equality

$$\frac{N_-}{N_+} = -\frac{\gamma - \zeta(E')}{\kappa - \zeta(E')/E'} \equiv -\eta_-(E'), \tag{20}$$

where we use the notation

$$E' \equiv E/mc^2, \quad \zeta(E') \equiv \alpha Z E'/\sqrt{1 - E'^2}, \quad \eta_\pm(E') \equiv \frac{\gamma \pm \zeta(E')}{\kappa - \zeta(E')/E'}. \tag{21}$$

Using equations (15), and (18)–(21), it can be shown that the functions $g(r)$ and $f(r)$ have the explicit forms

$$\begin{aligned} g(r) = \frac{1}{2}N_\beta\, \mathrm{e}^{-\rho/2}\rho^{\gamma-1}[&{}_1F_1(\gamma - \zeta(E'), 2\gamma + 1, \rho) - \eta_-(E')\,{}_1F_1(\gamma + 1 - \zeta(E'), 2\gamma + 1, \rho) \\ &- \triangle(\beta, \gamma)\rho^{-2\gamma}\,{}_1F_1(-\gamma - \zeta(E'), -2\gamma + 1, \rho) \\ &- \triangle(\beta, \gamma)\eta_+(E')\rho^{-2\gamma}\,{}_1F_1(-\gamma + 1 - \zeta(E'), -2\gamma + 1, \rho)] \end{aligned} \tag{22a}$$

$$\begin{aligned} f(r) = \frac{1}{2}N_\beta\sqrt{\frac{1 - E'}{1 + E'}}\,\mathrm{e}^{-\rho/2}\rho^{\gamma-1}[&{}_1F_1(\gamma - \zeta(E'), 2\gamma + 1, \rho) \\ &+ \eta_-(E')\,{}_1F_1(\gamma + 1 - \zeta(E'), 2\gamma + 1, \rho) \\ &- \triangle(\beta, \gamma)\rho^{-2\gamma}\,{}_1F_1(-\gamma - \zeta(E'), -2\gamma + 1, \rho) \\ &+ \triangle(\beta, \gamma)\eta_+(E')\rho^{-2\gamma}\,{}_1F_1(-\gamma + 1 - \zeta(E'), -2\gamma + 1, \rho)] \end{aligned} \tag{22b}$$

where N_β represents a normalization constant, and the energy parameter E' must be derived from the continuity conditions at the value of r for which the Coulomb potential in equation (4) becomes invalid. It should be noted that equations (22) include contributions from solutions of Whittaker's equation corresponding to both positive and negative γ.

2.2. Solution of the Dirac equation inside the nucleus

For values of the radial coordinate less than the nuclear radius the potential energy function $V(r)$ in equation (1) can be assumed to have a finite form different from the Coulomb form in equation (4). In what follows, we adopt two common models for the nuclear potential function, which respectively simulate either a uniform charge distribution or a constant potential for $r < R$. The separate models correspond to functions $V(r)$ of the forms

$$V(r) = -\frac{3}{2}\frac{Ze^2}{R} + \frac{Ze^2}{2R^3}r^2, \quad (r < R) \text{ uniformly charged nucleus}, \tag{23a}$$

$$V(r) = -Ze^2/R, \quad (r < R) \text{ constant potential inside nucleus}, \tag{23b}$$

which can be rescaled for $r < R$ in terms of dimensionless quantities as

$$\frac{V(r)}{mc^2} = -(b' - \xi r'^2), \quad \text{uniformly charged nucleus}, \tag{24a}$$

$$\frac{V(r)}{mc^2} = -\alpha Z/R', \quad \text{constant potential inside nucleus}, \tag{24b}$$

where

$$r' = \left(\frac{mc}{\hbar}\right) r, \quad R' = \left(\frac{mc}{\hbar}\right) R, \quad b' = \frac{3}{2}\frac{\alpha Z}{R'}, \quad \xi = \frac{\alpha Z}{2R'^3}. \tag{25}$$

It is sufficient to construct a series solution of the radial equations (3) for $r < R$. For this purpose, it is useful to assume the forms

$$g(r') = Ar'^{\nu-1}\sum_{n=0}^{\infty} a_n r'^n, \quad f(r') = Br'^{\nu-1}\sum_{n=0}^{\infty} b_n r'^n. \tag{26}$$

Substitution of equations (26) into equations (3) results in recursion relations for the coefficients a_n and b_n that have non-trivial solutions only under either of the two conditions

$$\nu = -\kappa, \quad b_0 = 0, \qquad \kappa < 0 \tag{27a}$$

$$\nu = +\kappa, \quad a_0 = 0, \qquad \kappa > 0. \tag{27b}$$

The two choices result in the separate solutions

$$g(r') = Ar'^{|\kappa|-1}(1 + a_2 r'^2 + a_4 r'^4 + \cdots), \quad f(r') = Ar'^{|\kappa|}(b_1 + b_3 r'^2 + b_5 r'^4 + \cdots), \quad \kappa < 0 \tag{28a}$$

$$g(r') = Br'^{|\kappa|}(a_1 + a_3 r'^2 + a_5 r'^4 + \cdots), \quad f(r') = Br'^{|\kappa|-1}(1 + b_2 r'^2 + b_4 r'^4 + \cdots) \quad \kappa > 0. \tag{28b}$$

For $V(r)$ in the form (24a), the coefficients of the leading terms have the forms

$$\begin{aligned} a_1 &= \frac{Q_+}{2|\kappa|+1}, \quad a_2 = -\frac{Q_+Q_-}{2(2|\kappa|+1)}, \quad a_3 = -\frac{1}{2|\kappa|+3}\left(\frac{Q_+Q_-Q_+}{2(2|\kappa|+1)} + \xi\right), \\ a_4 &= \frac{(Q_+Q_-)^2}{8(2|\kappa|+3)(2|\kappa|+1)} + \frac{\xi}{4}\left[\frac{Q_+}{2|\kappa|+3} + \frac{Q_-}{2|\kappa|+1}\right], \quad a_5 = \frac{1}{2|\kappa|+5}(Q_+b_4 - \xi b_2) \end{aligned} \tag{29}$$

$$\begin{aligned} b_1 &= -\frac{Q_-}{2|\kappa|+1}, \quad b_2 = -\frac{Q_+Q_-}{2(2|\kappa|+1)}, \quad b_3 = \frac{1}{2|\kappa|+3}\left(\frac{Q_-Q_+Q_-}{2(2|\kappa|+1)} + \xi\right), \\ b_4 &= \frac{(Q_+Q_-)^2}{8(2|\kappa|+3)(2|\kappa|+1)} + \frac{\xi}{4}\left[\frac{Q_-}{2|\kappa|+3} + \frac{Q_+}{2|\kappa|+1}\right], \quad b_5 = -\frac{1}{2|\kappa|+5}(Q_-a_4 - \xi a_2), \end{aligned} \tag{30}$$

with

$$Q_\pm \equiv E' + b' \pm 1, \tag{31}$$

whereas, for $V(r)$ in the form (24b), the corresponding coefficients have the above forms with $b' = \alpha Z/R'$ and $\xi = 0$.

2.3. Continuity conditions at the boundary of the nucleus

The solutions of the Dirac equation for values of r exterior and interior to the nucleus derived from the respective equations (22) and (28) need to be made continuous at the boundary of the nucleus defined by $r = R$.[5] To do this, it is necessary to assign a value to the radius of

[5] Because the Dirac equation is first order in the space coordinates, it is sufficient to require only the continuity of $\Psi(r)$ at $r = R$.

the nucleus. Here, we choose to connect the nuclear radius to the mass number A through the empirical relation

$$R \cong r_0 A^{1/3}, \tag{32}$$

where $r_0 = 1.2 \times 10^{-15}$ m. The inaccuracy of this formula for small values of A is made unimportant in the present calculation by the emphasis on large values of both A and Z. The continuity requirement at $r = R$ produces the simultaneous equations

$$g_{\text{interior}}(R) = g_{\text{exterior}}(R), \qquad f_{\text{interior}}(R) = f_{\text{exterior}}(R), \tag{33}$$

which can be conveniently combined into the 'matching equation'

$$\frac{g_{\text{interior}}(R)}{f_{\text{interior}}(R)} = \frac{g_{\text{exterior}}(R)}{f_{\text{exterior}}(R)}. \tag{34}$$

The equation has the effect of reducing the computation of the energies of the atomic electron or muon in the case of a finite size nucleus to a boundary value problem involving a single unknown E', the solution of which determines the allowed energy eigenvalues.

2.4. Derivation of correction to energy by the use of perturbation theory

We can compare the energy eigenvalues derived from equation (34) with the corrected eigenvalues obtained from first-order perturbation theory under the assumption that the change in the Coulomb potential in the interior of the nucleus is treated as a perturbation. Specifically, the perturbation to the Hamiltonian consistent with the expressions for the nuclear potential assumed above has the form

$$\Delta V(r) = \begin{cases} 0, & r > R \\ \Delta(r), & r \leqslant R \end{cases}, \tag{35}$$

with $\Delta(r)$ defined by either of the two formulae

$$\Delta(r) = \frac{Ze^2}{R}\left(\frac{r^2}{2R^2} - \frac{3}{2} + \frac{R}{r}\right), \text{ uniformly charged nucleus,} \tag{36a}$$

$$\Delta(r) = -\frac{Ze^2}{R} + \frac{Ze^2}{r}, \text{ constant potential inside nucleus.} \tag{36b}$$

It is significant that the corrections to the energy, ΔE, obtained from the perturbation theory equation $\Delta E = \langle \Psi^{(o)} | \Delta V(r) | \Psi^{(o)} \rangle$ derive from radial functions g and f representing solutions of the Dirac equation for the case when the Coulomb potential is valid over the entire range of r values from 0 to ∞. For the lowest eigenstates, corresponding to energies defined by equation (12) for n' equal to 0 and 1, the formula for ΔE, along with the form for $\Delta V(r)$ in equation (36*a*), results in corrections to the energy given by the respective formulae[6]

$$(\Delta E)_{n'=0} = \frac{(\alpha Z)^2 (2\alpha Z)^{2\gamma}}{\Gamma(2\gamma+1)} mc^2 R'^2 \left(\frac{1}{2\gamma+3} - \frac{3}{2\gamma+1} + \frac{1}{\gamma}\right), \tag{37}$$

and

$$(\Delta E)_{n'=1} = \frac{(2qR)^{2\gamma+1}(mc^2)}{\Gamma(2\gamma+1)(2\gamma+1+\eta^2)} \frac{\alpha Z}{R'} \{\}, \tag{38}$$

[6] For brevity, we show only the perturbation theory result for ΔE in the case when $\Delta(r)$ has the form in equation (36*a*).

where

$$\{\} \equiv \frac{\eta^2(2qR)^2}{2\gamma+1}\left[\frac{1}{2(2\gamma+5)}-\frac{3}{2(2\gamma+3)}+\frac{1}{2\gamma+2}\right] + (E'-\eta)\eta(2qR)\left[\frac{1}{2\gamma+4}-\frac{3}{2\gamma+2}+\frac{2}{2\gamma+1}\right] + (\eta^2-2\eta E'+1)\left[\frac{(2\gamma+1)}{2(2\gamma+3)}-\frac{3}{2}+\frac{(2\gamma+1)}{2\gamma}\right], \tag{39}$$

with $\eta \equiv -\kappa + \alpha Z/\sqrt{1-E'^2}$. For $n' = 0$, the requirement that the quantum number κ be restricted to the value -1 results in a ground state restricted to the parity $+1$; whereas for $n' = 1$, the two allowed values of κ, equal to $+1$ and -1, result in distinct excited states with odd and even parities, connected, respectively, to the 2p and 2s states of the non-relativistic theory. We note that, in the limit when the quantity γ goes to 1, the perturbation theory corrections to the energy derived here for the ground and even parity excited states reduce (exactly) to the perturbation corrections derived from non-relativistic wavefunctions. Specifically, the ground state correction reduces to

$$(\Delta E)_{\mathrm{NR}} = \tfrac{2}{5}(aZ)^4 R'^2 mc^2. \tag{40}$$

In contrast, because the odd parity state in the non-relativistic theory corresponds to a non-zero orbital angular momentum, for which the non-relativistic wavefunction approaches zero in the vicinity of the nucleus, the correction derived from equation (38) in the limit $\gamma \to 1$, with $\kappa = +1$, exceeds the correction derived from non-relativistic perturbation theory by 6 orders of magnitude! In the non-relativistic limit, the mass m of the electron or muon is properly replaced by the reduced mass of the composite system. The same (less valid) replacement in the relativistic limit has a significant effect on the magnitude of ΔE only in the case of nuclei with small values of A and Z.

3. Numerical results

In this section, we present the results of the solution of the matching equation (34) for the energy eigenvalues of single-electron and single-muon atoms, with the nuclear radius given by equation (32). Specifically, we compare the correction, ΔE, to the eigenvalue produced by the finite size of the nucleus with the 'unperturbed eigenvalue', E_0, of a point nucleus with charge and mass numbers Z and A, computed from equation (12). The dependence of the correction to the energy on the form of the potential energy inside the nucleus necessitates a choice of a model for the nuclear potential. Here we take this potential to have the alternative forms defined by equations (23*a*) and (23*b*), cited as models 1 and 2, respectively. For $Z = 1$, the nuclear size effect is small, as expected, whereas, for high values of Z, the effect becomes large, and can be measured most easily as an isotope shift observed through the splitting of the K x-ray line of an atom with two or more stable isotopes. In electronic atoms with multiple electrons, the effect of nuclear size is in general masked by the (larger) effect of electron screening. On the other hand, because the effect of screening is approximately the same for two isotopes of given Z, the isotope shift is largely unaffected by the screening.

For the two models of the nuclear potential, table 1 lists calculated values of the energy correction to the ground states of single-electron atoms corresponding to stable isotopes of the five elements H, U, Ag, Eu and Tl, the last three of which have isotopes of comparable

Table 1. Values derived from the present calculation and from relativistic and non-relativistic perturbation theory for correction to the ground state energy of an hydrogenic atom produced by the finite size of a nucleus of charge Z. Models 1 and 2 assume (1) a uniformly charged nucleus and (2) a constant potential inside the nucleus, respectively. Ground state: $n' = 0, \kappa = -1$.

Z	E_0 (MeV)	Model 1		Model 2	
1	0.510 9853	$A = 1$	$A = 2$	$A = 1$	$A = 2$
	ΔE (eV)	5.60×10^{-9}	8.89×10^{-9}	9.33×10^{-9}	14.82×10^{-9}
	ΔE_{pert} (eV)	5.60×10^{-9}	8.89×10^{-9}	9.34×10^{-9}	14.82×10^{-9}
	ΔE_{NR} (eV)	5.60×10^{-9}	8.89×10^{-9}	9.33×10^{-9}	14.81×10^{-9}
	ΔE_{code} (eV)	5.60×10^{-9}	8.89×10^{-9}		
47	0.480 0039	$A = 107$	$A = 109$	$A = 107$	$A = 109$
	ΔE (eV)	1.267 55	1.282 28	2.046 64	2.070 40
	ΔE_{pert} (eV)	1.362 65	1.378 54	2.215 98	2.241 82
	ΔE_{NR} (eV)	0.615 58	0.623 23	1.025 97	1.038 72
	ΔE_{code} (eV)	1.267 06	1.281 79		
63	0.453 7962	$A = 151$	$A = 153$	$A = 151$	$A = 153$
	ΔE (eV)	8.609 42	8.676 36	13.5370	13.642 11
	ΔE_{pert} (eV)	9.894 20	9.971 57	15.751 94	15.875 12
	ΔE_{NR} (eV)	2.500 26	2.522 28	4.167 09	4.203 81
	ΔE_{code} (eV)	8.604 38	8.671 24		
81	0.412 176	$A = 203$	$A = 205$	$A = 203$	$A = 205$
	ΔE (eV)	60.383	60.698	91.005	91.478
	ΔE_{pert} (eV)	78.388	78.802	120.540	121.177
	ΔE_{NR} (eV)	8.322	8.377	13.870	13.961
	ΔE_{code} (eV)	60.342	60.658		
92	0.378 719	$A = 235$	$A = 238$	$A = 235$	$A = 238$
	ΔE (eV)	193.180	194.376	281.320	283.047
	ΔE_{pert} (eV)	281.357	283.126	420.373	423.016
	ΔE_{NR} (eV)	15.270	15.400	25.450	25.666
	ΔE_{code} (eV)	193.066	194.260		

abundance with A values that differ by 2. In particular, the table compares the corrections, ΔE, derived from the matching condition in equation (34) with the values of ΔE obtained, for the same model of the nuclear potential, using first-order perturbation theory based on both relativistic, $(\Delta E)_{\text{pert}}$, and non-relativistic wavefunctions, $(\Delta E)_{\text{NR}}$. The significant dependence of ΔE on the model of the nuclear potential is evident from the table. However, the interest here is in the discrepancy between the perturbation theory result and the exact result for a given potential. As expected, the non-relativistic wavefunctions lead to inaccurate values of ΔE for high Z. More significantly, table 1 shows that the values obtained for ΔE from relativistic perturbation theory, for the Z values 47, 63, 81 and 92, exceed the exact values obtained from the continuity conditions by roughly 8, 15, 30 and 45 per cent respectively. Similar calculations, made for higher energy states of the atom, show discrepancies of the same magnitude between the exact theory and perturbation theory for the first two excited states. The relatively weak dependence of ΔE on the mass number A makes it possible to summarize the corrections to the energies of the ground state obtained from the two theories (using model 1) by the graphs of ΔE versus Z shown in figure 1. The inaccuracy of first-order perturbation theory for high Z is made important by the complexity of relativistic second-order perturbation theory.

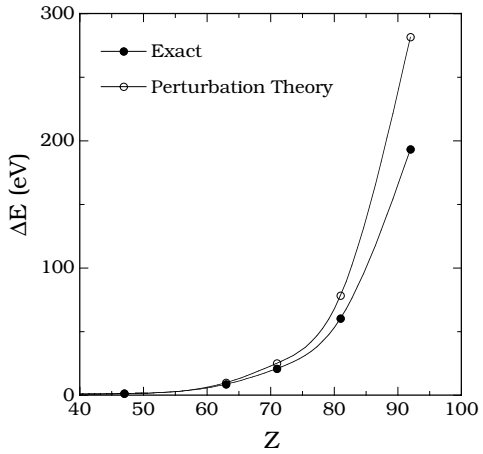

Figure 1. Graphs versus Z of the nuclear size corrections to the ground state energy of a hydrogenic atom obtained from the matching condition in equation (34) (full circles) and relativistic perturbation theory (open circles) using model 1.

Table 2. Isotope shift of the ground state and the first excited state of an hydrogenic atom with charge Z, computed for model 1 by using the matching condition in equation (34) and relativistic perturbation theory.

	Isotope shift in electronic atom $\delta_A E$ (eV) (model 1)			
	Ground state: $n' = 0, \kappa = -1$		First excited state: $n' = 1, \kappa = -1$	
Z	Exact theory	Relativistic perturbation theory	Exact theory	Relativistic perturbation theory
1	3.29×10^{-9}	3.29×10^{-9}	4.11×10^{-10}	4.11×10^{-10}
47	0.0147	0.0159	0.0020	0.0022
63	0.0669	0.0774	0.0101	0.011 65
81	0.315	0.414	0.0537	0.0710
92	1.196	1.769	0.226	0.335

It is useful to compare the results derived from the matching condition in equation (34) with the results extracted from an atomic structure code for the same model and radius of the nucleus. To do this, we include in table 1 the values of ΔE obtained from the general purpose relativistic atomic structure program GRASP [10] for the case of a uniformly charged nucleus. Comparison of these values, denoted by ΔE_{code}, with the values obtained from equation (34) shows that the two sets of values are in excellent agreement.

In general, while the correction to the energy produced by the size of the nucleus is significant for large Z, the isotope shift (defined by the difference between the corrections to the eigenvalues of the (two) isotopes of Z) remains small. Table 2 lists the values obtained for the isotope shift from both the exact theory and perturbation theory. For brevity, we display only the results of model 1, but include the isotope shift for the first excited state of the atom.

In analogy with the results listed in table 1, we list in table 3 the calculated values of E_0 and ΔE for the ground states of muonic atoms with nuclei corresponding to isotopes of the elements H, Ag, Eu, Pb and U. The table shows the inaccuracy of perturbation theory for all values of Z above 1 in the case of muonic atoms (which perturbation theory predicts to be unbound for Z exceeding 47). Table 4 shows the corresponding values of E_0 and ΔE obtained

Table 3. Values derived from the present calculation and relativistic and non-relativistic perturbation theory for corrections to the ground state energy of a muonic atom produced by the finite size of a nucleus of charge Z, using models 1 and 2.

		Ground state of muonic atom: $n' = 0, \kappa = -1$			
		Model 1		Model 2	
Z		$A = 1$	$A = 2$	$A = 1$	$A = 2$
	E_0 (MeV)	105.6555			
1	ΔE (eV)	0.0492	0.0780	0.0819	0.1297
	$(\Delta E)_{\text{pert}}$ (eV)	0.0495	0.0786	0.0825	0.1309
	$(\Delta E)_{\text{NR}}$ (eV)	0.0495	0.0785	0.0825	0.1309
		$A = 107$	$A = 109$	$A = 107$	$A = 109$
	E_0 (MeV)	99.249 58			
47	ΔE (MeV)	1.6605	1.6700	2.0947	2.1053
	$(\Delta E)_{\text{pert}}$ (MeV)	6.3087	6.3823	10.2594	10.3791
	$(\Delta E)_{\text{NR}}$ (MeV)	5.4417	5.5093	9.0695	9.1822
		$A = 151$	$A = 153$	$A = 151$	$A = 153$
	E_0 (MeV)	93.830 65			
63	ΔE (MeV)	4.4832	4.4970	5.3530	5.3671
	$(\Delta E)_{\text{pert}}$ (MeV)	26.5111	26.7184	42.2066	42.5367
	$(\Delta E)_{\text{NR}}$ (MeV)	22.1022	22.2969	36.837	37.162
		$A = 206$	$A = 208$	$A = 206$	$A = 208$
	E_0 (MeV)	84.654 56			
82	ΔE (MeV)	10.5217	10.5395	12.0087	12.0243
	$(\Delta E)_{\text{pert}}$ (MeV)	93.318	93.801	143.163	143.904
	$(\Delta E)_{\text{NR}}$ (MeV)	78.029	78.533	130.048	130.888
		$A = 235$	$A = 238$	$A = 235$	$A = 238$
	E_0 (MeV)	78.307 06			
92	ΔE (MeV)	15.223	15.255	17.063	17.090
	$(\Delta E)_{\text{pert}}$ (MeV)	157.366	158.356	235.119	236.598
	$(\Delta E)_{\text{NR}}$ (MeV)	134.985	136.131	224.975	226.885

from model 1 for the first excited states of the muonic atoms. The different values for the binding energies of the ground states of the muonic atoms as a function of Z predicted by the point nucleus theory and the exact theory (for models 1 and 2) are summarized by the graphs in figure 2. We note that the upper two graphs are in close agreement with the corresponding graphs in [2].

In summary, we develop a general method for the determination of energy eigenvalues of a potential energy function that has separate dependences on the radial coordinate for r greater and less than a given value R, and use this method to calculate the effect of finite nuclear size on the energy levels of single-electron and single-muon atoms in the cases of two commonly used models for the nuclear potential. The method has the advantage of allowing the nuclear size corrections to be derived non-perturbatively in terms of solutions of the Dirac equation. For values of Z greater than 40 in the case of electronic atoms, and greater than 1 in the case of muonic atoms, we find large discrepancies between our results and those obtained from first-order perturbation theory using relativistic wavefunctions. Moreover, we find our method to be considerably simpler and more accurate than higher order perturbation theory.

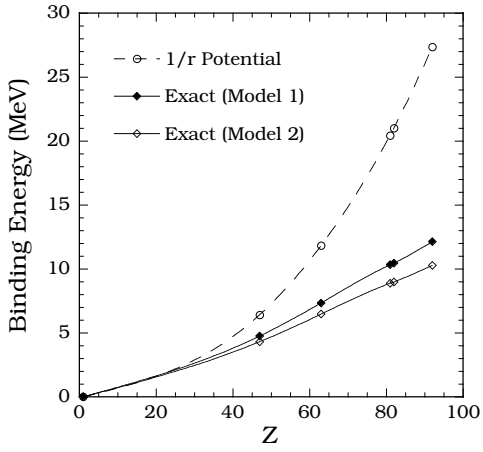

Figure 2. Graphs versus Z of the binding energy of the ground state of a muonic atom, predicted by the point nucleus theory (dashed curve) and the (exact) corrected theory based on the separate models 1 (full squares) and 2 (open squares).

Table 4. Values derived from the present calculation and relativistic and non-relativistic perturbation theory for corrections to the energy of the first excited state of a muonic atom produced by the finite size of a nucleus of charge Z using model 1.

		Excited state of muonic atom: $n' = 1, \kappa = +1$ (Model 1)	
Z		$A = 1$	$A = 2$
	E_0 (MeV)	105.657 66	
1	ΔE (eV)	6.408×10^{-8}	10.390×10^{-8}
	$(\Delta E)_{\rm pert}$ (eV)	6.425×10^{-8}	10.427×10^{-8}
	$(\Delta E)_{\rm NR}$ (eV)	6.410×10^{-8}	10.399×10^{-8}
		$A = 107$	$A = 109$
	E_0 (MeV)	104.043 83	
47	ΔE (MeV)	0.018 09	0.018 31
	$(\Delta E)_{\rm pert}$ (MeV)	0.041 17	0.041 89
		$A = 151$	$A = 153$
	E_0 (MeV)	102.658 86	
63	ΔE (MeV)	0.107 73	0.108 42
	$(\Delta E)_{\rm pert}$ (MeV)	0.4039	0.4089
		$A = 206$	$A = 208$
	E_0 (MeV)	100.270 01	
82	ΔE (MeV)		0.473 37
	$(\Delta E)_{\rm pert}$ (MeV)		3.4209
		$A = 235$	$A = 238$
	E_0 (MeV)	98.583 68	
92	ΔE (MeV)	0.878 08	0.880 55
	$(\Delta E)_{\rm pert}$ (MeV)	8.7805	8.8763

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