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Finite nuclear size effect to the fine structure of heavy muonic atoms

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Abstract. The finite-nuclear size correction to the fine structure of muonic atoms is considered. The procedure for the analytical calculation of the energies and wave functions has been derived in a homogeneously charged sphere nuclear charge distribution approximation. The finite-nuclear size effect was calculated in a first few orders of the perturbation energy, with the accurate estimations of the convergence. Finally, we present energies of the low-lying electronic and muonic states with the finite-nuclear size correction, calculated analytically, for $^{185}_{75}$Re ion.

1 Introduction

One of the simplest and at the same time exotic atomic system is the highly charged hydrogen-like muonic atom, where a negative muon μ^- is bound to an atomic nucleus. Having the spin of $1/2$ as an electron does, a muon has a much larger mass, $m_\mu \approx 207 m_e$. Due to this fact, muonic orbits are closer to the nucleus than that of electron, making muonic systems a suitable probe to investigate and extract nuclear parameters, i.e., nuclear size, charge distribution and moments [1].

The study of muonic systems has been started a long time ago [2,3], mostly with heavy systems, where nuclear effects are larger. For the light end of the periodic system, the most important and interesting is muonic hydrogen, where the prediction for the proton radius from the muonic spectroscopy disagree with the prediction based on the spectroscopy of the electronic hydrogen (so-called proton-radius puzzle, see, e.g. [4]).

In the present paper, we incorporate muonic systems into a procedure for analytical calculation of the finite nuclear size (FNS) effect developed for electronic states [5]. The distribution of the nuclear charge is described by a the homogeneously charged sphere. We show, that despite of the fact the FNS correction cannot be considered as small, like it is in the case of an electronic system, the analytical expressions derived from the Taylor expansion are still valid here. The convergence of the series and the applicability limits for the procedure are discussed. The results for the first few orders of the FNS correction to the fine structure for the particular case of muonic $^{185}_{75}$Re are presented. Our scheme can be successfully used for any other muonic atom.

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The paper is organized as follows. In Section 2 we demonstrate a procedure to estimate the FNS correction to the energies of fermionic states using analytically derived wave functions. In Section 3 this procedure is modified to calculate FNS effect on $^{185}_{75}$Re for all the states up to principal quantum number $n = 3$. Relativistic units ($\hbar = c = 1$) and Heaviside charge unit ($\alpha = e^2/4\pi$, where α is the fine structure constant, $e < 0$) are used in the paper.

2 The solution of the Dirac equation for the extended nuclei

One of the simplest models of nucleus is homogeneously charged sphere, with the corresponding charge density of nucleus

$$\rho(r) = \frac{3Ze}{4\pi r_0^3}\theta(r_0 - r). \tag{1}$$

Here Z is the nuclear charge and r_0 is effective radius of nucleus, connected with a root-mean-square (RMS) radius of the nucleus as [6]

$$r_0 = \sqrt{\frac{5}{3}\langle r^2 \rangle}. \tag{2}$$

The interaction between electron and nucleus can be therefore described by the potential

$$V(r) = \begin{cases} -\frac{Z\alpha}{2r_0}(3 - \frac{r^2}{r_0^2}), & \text{while } r \leq r_0 \text{ [Region I]}; \\ -\frac{Z\alpha}{r}, & \text{while } r > r_0 \text{ [Region II]}. \end{cases} \tag{3}$$

The energies E and the wave functions $\psi(\mathbf{r})$ of the bound fermion (electron or muon) are the eigenvalues and eigenfunctions, respectively, of the stationary Dirac equation

$$\left[\boldsymbol{\alpha}\cdot\boldsymbol{p} + m_f\beta + V(r)\right]\psi(\mathbf{r}) = E\psi(\mathbf{r}), \qquad (4)$$

where m_f is the rest mass of fermion under consideration, $\boldsymbol{\alpha}, \beta$ are Dirac matrices, and $V(r)$ is the chosen central nuclear potential, in our case, determined by equation (3). For an arbitrary central potential, the radial and the angular dependence can be separated as

$$\psi(\mathbf{r}) = \begin{pmatrix} \frac{1}{r}G(r)\Omega_{\kappa m}(\theta,\phi) \\ \frac{i}{r}F(r)\Omega_{-\kappa m}(\theta,\phi) \end{pmatrix}, \qquad (5)$$

where $\kappa = (-1)^{j+l+\frac{1}{2}}(j+\frac{1}{2})$ is a relativistic angular quantum number, j and m are total angular momentum of fermion and its projection, respectively, and l is orbital angular momentum. Angular part of the wave functions $\Omega_{\pm\kappa m}$ is the same for any central potential and well known [7]. Substituting expression (5) into equation (4) and simplifying, one can obtain the system of radial equations

$$\frac{dG}{dr} + \frac{\kappa}{r}G(r) - [m_f - V(r)]F(r) = EF(r), \qquad (6)$$

$$-\frac{dF}{dr} + \frac{\kappa}{r}F(r) + [m_f + V(r)]G(r) = EG(r). \qquad (7)$$

For the region I, let us assume that the solution can be a power series of the form

$$\begin{pmatrix} G(r) \\ F(r) \end{pmatrix} = r^s \sum_{i=0}^{\infty} (a_i \pm b_i)r^i.$$

Taking the limit $r \to 0$ of equations (6) and (7), one can find that $s = \pm|\kappa|$. The solution corresponding to $s = -|\kappa|$ should be discarded to account for the regularity of the solution at origin. The remaining regular part is given by the formula

$$\begin{pmatrix} G(r) \\ F(r) \end{pmatrix} = N_1 r^{|\kappa|} \sum_{i=0}^{\infty} \left[a_i \pm (-1)^{i+1}\frac{\kappa}{|\kappa|}a_i\right]r^i, \qquad (8)$$

where N_1 is a free parameter and the coefficients are determined recurrently as

$$a_i = 0 \quad \text{for } i < 0,$$
$$a_0 = 1,$$
$$a_i = \frac{a_{i-1}\left[E + \frac{3Z\alpha}{2r_0} - M(-1)^i\frac{\kappa}{|\kappa|}\right] - \frac{Z\alpha}{2r_0^3}a_{i-3}}{\kappa + (-1)^{i+1}\frac{\kappa}{|\kappa|}(i+|\kappa|)}. \qquad (9)$$

To write a solution in region II, we introduce a non-dimensional variable $\rho = 2r\sqrt{m_f^2 - E^2} \equiv 2\lambda r$.

Representing G, F by the linear combinations of two functions ξ_1, ξ_2 as

$$\begin{pmatrix} G(\rho) \\ F(\rho) \end{pmatrix} = \sqrt{m_f \pm E}\,\rho^{-\frac{1}{2}}\left[\xi_1(\rho) \pm \xi_2(\rho)\right], \qquad (10)$$

one can rewrite Dirac equation to the system of the equations for ξ_1, ξ_2 as

$$\rho\frac{d\xi_1}{d\rho} = \xi_1\left(\frac{\rho}{2} - q\right) - \xi_2\left(\kappa + \frac{m_f Z\alpha}{\lambda}\right), \qquad (11)$$

$$\rho\frac{d\xi_2}{d\rho} = \xi_1\left(-\kappa + \frac{m_f Z\alpha}{\lambda}\right) + \xi_2\left(q + 1 - \frac{\rho}{2}\right), \qquad (12)$$

where $q = Z\alpha E/\lambda - 1/2$.

Using the recursion relations for the Whittaker functions $W_{q,\gamma}(\rho)$ of the second kind [8] one can show that the functions $\xi_1 = W_{q,\gamma}(\rho)$ and $\xi_2 = W_{q+1,\gamma}(\rho)/(\kappa + \frac{m_f Z\alpha}{\lambda})$, where $\gamma = \sqrt{k^2 - (Z\alpha)^2}$, satisfy equations (11) and (12). Similarly, another solution for ξ_1, ξ_2 can be found using recursion relations between $W_{-q,\gamma}(-\rho)$ and $W_{-q-1,\gamma}(-\rho)$. Two linearly independent solution sets allow one to describe any solution for ξ_1, ξ_2. The condition of the regular behavior on infinity discards the divergent solution, leading to the following physical solution outside of the nucleus

$$\begin{pmatrix} G(\rho) \\ F(\rho) \end{pmatrix} = \frac{N_2}{\kappa + \frac{m_f Z\alpha}{\lambda}}\rho^{-\frac{1}{2}}\sqrt{m_f \pm E}$$
$$\times \left[\left(\kappa + \frac{m_f Z\alpha}{\lambda}\right)W_{q,\gamma}(\rho) \pm W_{q+1,\gamma}(\rho)\right], \qquad (13)$$

where N_2 is again free parameter. The expression (13) for the wave functions is in an agreement with [5].

So far, we presented the expressions for the wave function separately in two regions. As it corresponds to a physical state, the wave function should be normalized as

$$\int_0^\infty (G^2 + F^2)dr = 1,$$

and it has be continuous at the boundary of two regions

$$G(r_0 - 0) = G(r_0 + 0), \qquad (14)$$

$$F(r_0 - 0) = F(r_0 + 0). \qquad (15)$$

G and F can be replaced by the explicit expression obtained in equation (8) and (13), forming a homogeneous systems of linear equations on N_1 and N_2. Non-trivial solution can be build only if the determinant of the system is equal to zero, which gives the following

$$\delta E = \frac{\dfrac{\sum\limits_{i=0}^{\infty} a_i(0)r_0^i}{\sum\limits_{i=0}^{\infty}(-1)^{i+1}\dfrac{\kappa}{|\kappa|}a_i(0)r_0^i} - \dfrac{F_1(0)}{F_2(0)}}{\dfrac{F_1'(0)F_2(0)-F_2'(0)F_1(0)}{F_2(0)^2} - \dfrac{\sum\limits_{i,i'=0}^{\infty} a_i'(0)a_{i'}(0)r_0^{i+i'}\dfrac{\kappa}{|\kappa|}\big[(-1)^i-(-1)^{i'}\big]}{\left[\sum\limits_{i=0}^{\infty}(-1)^i\dfrac{\kappa}{|\kappa|}a_i(0)r_0^i\right]^2}} \tag{18}$$

condition for the energy E

$$\frac{A_1\big(\kappa+\frac{m_f Z\alpha}{\lambda}\big)W_{q,\gamma}(2\lambda r_0)+A_2 W_{q+1,\gamma}(2\lambda r_0)}{A_2\big(\kappa+\frac{m_f Z\alpha}{\lambda}\big)W_{q,\gamma}(2\lambda r_0)+A_1 W_{q+1,\gamma}(2\lambda r_0)}$$
$$=\frac{\sum\limits_{i=0}^{\infty} a_i r_0^i}{\sum\limits_{i=0}^{\infty}(-1)^{i+1}\frac{\kappa}{|\kappa|}a_i r_0^i},$$
$$A_{1,2}=\sqrt{m_f+E}\pm\sqrt{m_f-E}. \tag{16}$$

By solving this equation, one can determine the energy of the electronic or muonic states in the field of the extended nuclei.

2.1 Estimation of the energy for electronic systems

Equation (16) cannot be solved analytically. To estimate the energy for the different states, let us assume that:

- Energy shift (ΔE) due to finite size of nucleus is small comparing to point-like-nucleus energy E_0, and second and higher-order terms can be neglected.
- The infinite series in the right hand side (RHS) of equation (16) is convergent.

Determining the finite nuclear size effect as

$$\delta E \equiv \frac{\Delta E}{E_0}=\frac{E-E_0}{E_0}, \tag{17}$$

and applying the Taylor expansion around origin on the both sides of the (16) up to the first order, one can write

see equation (18) *above.*

Here F_1 and F_2 are numerator and denominator, respectively, of the left hand side (LHS) of equation (16), expressed as a function of δE. Primed functions stand for the derivative with respect to δE, and the coefficients $a_n(\delta E)$ have been determined in equation (9).

As it was mentioned before, the formula for the FNS correction to the energy was derived in [5] for electronic systems. In this case, the FNS effects can be considered as a small correction, and therefore the terms of order $r_0^{2\gamma+1}$ has been safely neglected. Terms of all orders in r_0 are included in equation (18). To illustrate our statements, we calculated the energy shifts using formula (18) for several

Table 1. Dirac binding energy E_0^{B}, the relative FNS correction to the energy $\Delta E/E_0^{\mathrm{B}}$, and the corrected binding energy E^{B} in some electronic ions with the uncertainty originated from RMS radius uncertainties.

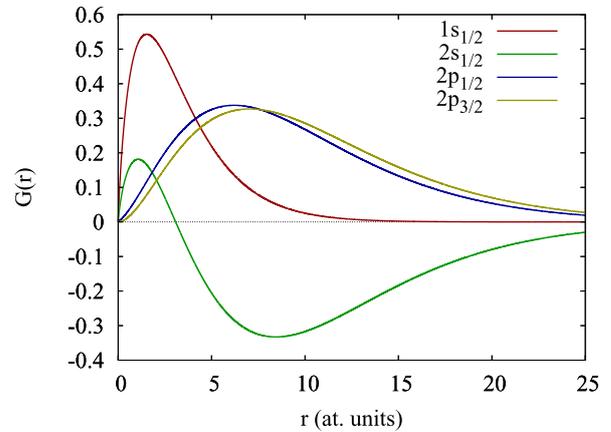| Ion	RMS (fm)	E_0^{B} (eV)	$\Delta E/E_0^{\mathrm{B}}$	E^{B} (eV)
$^{133}_{55}$Cs	4.8041	42986.8	0.000087(1)	42983.1
$^{185}_{75}$Re	5.3596	83373.6	0.000425(3)	83338.2(3)
$^{205}_{81}$Tl	5.4759	98880.6	0.000678(1)	98813.6(1)
$^{208}_{82}$Pb	5.5012	101641.1	0.000735(0)	101566.4(0)
$^{238}_{92}$U	5.8571	132361.3	0.001723(2)	132133.2(3)

Fig. 1. The G component of electronic radial wave function (5) calculated with the homogeneously charged nuclear model is plotted for four lowest lying states for hydrogen-like $^{185}_{75}$Re.

electronic ions and listed the results in Table 1. Nuclear parameters have been taken from [9].

After the calculation of the corrected energy one can use the equations (8) and (13) to build the FNS corrected wave functions. In Figure 1, the upper radial component G of the electronic wave functions (5) for four lowest lying states for $^{185}_{75}$Re are shown. The series provided in equation (8) converges very fast, and after the first few terms the next orders can be neglected.

3 Nuclear size effect on fine structure of muonic atoms

As an example of the muonic ion, let us consider the FNS correction to the fine structure of muonic $^{185}_{75}$Re for the

Table 2. Nuclear size correction factor in fine structure of muonic $^{185}_{75}\mathrm{Re}$ atom for the states up to $n = 3$. E_0^{B} stands for Dirac value of the binding energy, $\Delta E/E_0^{\mathrm{B}}$ is energy shift due to finite nuclear size, E^{B} is the binding energy with FNS corrections. Errors in the first and second order correction are due to the uncertainty in RMS radius. Higher order contributions are listed in the cases when they are bigger than first order uncertainty.

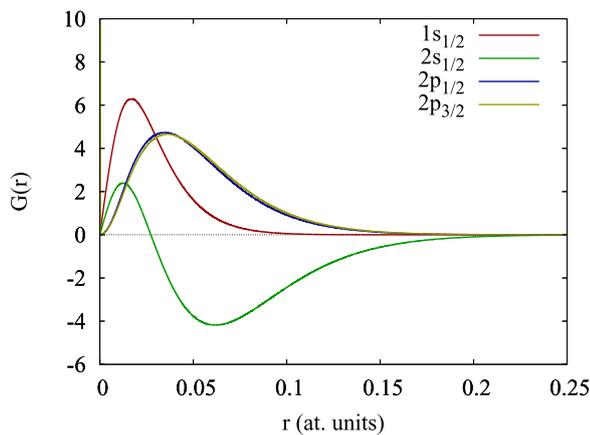| State	E_0^{B} (MeV)	$\Delta E/E_0^{\mathrm{B}}$				E^{B} (MeV)
		1st order	2nd order	3rd order	4th order	
$1s_{1/2}$	17.2286	.4753(10)	$-.0104(1)$	$-.0032$	$-.0006$	9.2845(190)
$2s_{1/2}$	4.3988	.3025(6)	$-.0006$			3.0708(26)
$2p_{1/2}$	4.3988	.0826(4)				4.0355(18)
$2p_{3/2}$	4.0328	.0355(3)				3.8896(12)
$3s_{1/2}$	1.9129	.2194(5)	$-.0001$			1.4934(10)
$3p_{1/2}$	1.9129	.0640(3)				1.7905(6)
$3p_{3/2}$	1.8039	.0285(2)				1.7525(4)
$3d_{3/2}$	1.8039	.0010				1.8021
$3d_{5/2}$	1.7730	.0004				1.7723

Fig. 2. The G component of muonic radial wave function calculated (5) with the homogeneously charged nuclear model is plotted for four lowest lying states for hydrogen-like $^{185}_{75}\mathrm{Re}$.

states up to $n = 3$. Generally, all the formulas presented before for electronic systems can be also used for the muonic systems by replacing electron's mass by muon's mass. However, since the FNS correction is not small anymore, the approximate formula (18) does not necessary provide a reasonable accuracy. Moreover, the analytical inclusion of the higher-order terms can be problematic in terms of convergence. In this case, the Newton's method for the numerical solution of the equation was used. The value δE calculated by the formula (18) can be used normaly as a good initial approximation.

In Table 2, we present FNS correction for $^{185}_{75}\mathrm{Re}$ up to the states with $n = 3$. The first-order-contribution error bar appears due to the RMS uncertainty. In Figure 2, the upper radial component G of the muonic wave functions for four lowest lying states for $^{185}_{75}\mathrm{Re}$ are shown. As it was expected, the FNS correction is more important for the s states. Specifically for $1s_{1/2}$ state the FNS correction is almost 50%, and definitely cannot be considered as a small contribution. However, the high-accuracy results still can

be delivered with the inclusions of the next-order terms. This results could be considered as an excellent basis for further calculations of the fine-structure of highly-charged muonic ions.

Author contribution statement

N.S.O. conceived the presented idea. A.S.M.P. did the calculations. N.S.O. and A.S.M.P. wrote the main manuscript text. All authors contributed to the discussion of the technical aspects and results, and preparation of the manuscript.

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