Testing QED and BSM Theories in Purely Leptonic Atoms Through Advanced Solutions of Dirac-Coulomb-Breit Equation

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Abstract. The purpose of this work is to examine the possibilities of solving numerically the relativistic Dirac–Coulomb–Breit equation and provide predictions for some important properties of purely leptonic systems focusing on the Muonium (μ^+e^-) exotic leptonic atom. The investigation of bound-state energies and other properties of this exotic atom, is of fundamental interest in testing the Quantum Electrodynamics (QED) and in probing physics Beyond the Standard Model (BSM). In the next few years, high precision spectroscopy of Mu (Mu-MASS experiment) at PSI combined with ongoing hyper fine measurements of Mu (MUSEUM experiment) at J-PARC will provide one of the most sensitive tests of bound-state QED. These extremely sensitive experiments may probe new regions of the parameter space testing the existence of medium range spin-dependent and spin-independent dark forces between e^- and μ^+ for testing BSM physics. On the other hand, improvement of the accuracy is required for QED calculations in the $1S \to 2S$ transition of Mu by about one order of magnitude as well as for BSM predictions.

INTRODUCTION

The simplest and some of the most extensively studied bound atomic systems are: the Hydrogen atom, (p^+e^-), the muonic-Hydrogen, ($p^+\mu^-$), the positronium, Ps (e^+e^-), and the Muonium, Mu (μ^+e^-) [1]. The simplicity of these atoms allows for the high-precision evaluation of energy corrections arising from the special relativity (relativistic corrections) and from the interactions with the matter and photon fields. The above atoms are very good systems to test QED theory, however, the proton-finite-size reduces the testing accuracy in H and in μ^-H. On the other hand, Mu and Ps are structureless and recently they arose intensive research interests, both theoretical and experimental [2].

The simplest atomic system consisted of a lepton and an antilepton of different flavors is the muonium, (μ^+e^-), which has extensively been investigated in the literature [1]. The predictions of the bound spectra of Coulombic few-body systems including the Mu, requires sophisticated calculations using advanced codes [3]. The difficulty can largely be attributed to the fact that the correlations between leptons are quite different due to the attractive and repulsive interactions. Another factor, which plays a crucial role in the binding of fermions with antifermions, is the Pauli principle. Thus, the main forces determining the stability of the exotic atoms are the Pauli principle, which severely restricts the available configuration space for fermionic systems, and the lepton mass ratios.

In this work, we focus on the two-body leptonic systems for which $m_1 \neq m_2$, as is the case of Muonium, and examine the known as Dirac-Coulomb and Dirac-Coulomb-Breit equations which may be employed for analytic and numerical solutions [3, 4]. In simple systems with $m_1 = m_2$, like the true Muonium ($\mu^+\mu^-$), and Ps (e^+e^-), the Breit interaction is more difficult to treat. Assuming that, the two-body leptonic systems interact only via the Coulombic force, it is possible to solve analytically the fundamental Schrödinger-Coulomb and Dirac-Coulomb equations and find the binding energies of the systems. Such works are many available in the literature. It is not possible, however, to obtain analytical solutions for three- and more-body leptonic atoms, as well as to solve (analytically) even for a two-lepton exotic atom the complete Dirac-Coulomb-Breit equation. In such cases, one needs to perform numerical calculations with advanced and effective algorithms [3].

Recently, authors working in atomic theory, by exploiting the fact that the dominant part of the interaction (Coulomb or Coulomb–Breit) is instantaneous, suggest to re-write the original Bethe-Salpeter equation to an exact equal-time form, which contains the no-pair Dirac–Coulomb or Dirac–Coulomb–Breit Hamiltonian plus a correction term, which carries retardation, pair, and radiative corrections. This correction term is expected to be small so, perturbation treatment is applicable. Due to the close confinement in the bound states, Mu can be used as an ideal probe of electroweak interactions, including particularly QED, and to search for additional yet unknown interactions acting on leptons.

THE TWO-BODY LEPTON-ANTI-LEPTON SYSTEMS

As it is well known, in order to compute the wave functions of the two-particle states, the center-of-mass coordinate system is more convenient [2]. To this end, we start by assuming that $r_i^\mu = (t_i, \mathbf{r}_i)$, with $i = 1,2$ representing the 4-vectors of the particles and m_i being their masses. Subsequently, (i) the relative 4-vector of the system is $r^\mu = r_1^\mu - r_2^\mu \equiv (t, \mathbf{r})$, (ii) the 4-vector center-of-mass $R^\mu \equiv (T, \mathbf{R})$ is defined as

$$R^\mu \equiv (T, \mathbf{R}) = \frac{\sum m_i r_1^\mu}{\sum m_i} = \frac{m_1}{m_1+m_2} r_1^\mu + \frac{m_2}{m_1+m_2} r_2^\mu \,, \tag{1}$$

and (iii) the total 4-momentum is $P^\mu \equiv (E, \mathbf{P}) = p_1^\mu + p_2^\mu$, where E represents the total energy and $\mathbf{P}$ the 3-momentum of the system. Next, the wave function of the two-particle system, $\Phi(r_1^\mu - r_2^\mu)$, by applying the separation of variables method can be written as

$$\Phi(r_1^\mu - r_2^\mu) = e^{-iP_\nu R^\nu} \phi(r^\mu) \tag{2}$$

It is a common practice at this point to choose the so called zero-total-momentum frame of reference, i.e. $\mathbf{P} = \mathbf{0}$, which is equivalent with $\mathbf{p}_1 = -\mathbf{p}_2$. For the corresponding momentum operators we have: $\mathbf{p}_1 = -i\hbar\nabla_1$ and $\mathbf{p}_2 = -i\hbar\nabla_2$. By putting $\mathbf{p}_1 = \mathbf{p} = -i\hbar\nabla$, it follows that $\mathbf{p}_2 = -\mathbf{p} = i\hbar\nabla$, where $\nabla \equiv \nabla_r$ denotes that the partial derivatives are taken with respect to the r, i.e. the components of the relative displacement vector.

The Dirac-Coulomb Equation for two-leptons

For a two-lepton system, the relativistic single-time Dirac equation takes the form

$$[\alpha_1 \cdot \mathbf{p}_1 + m_1\beta_1 + \alpha_2 \cdot \mathbf{p}_i + m_2\beta_2 + V]\,\Psi = E\Psi, \tag{3}$$

where $H_i(\mathbf{p}_i) = \alpha_i \cdot \mathbf{p}_i + m_i\beta_i$ represents the Dirac Hamiltonian and $V = -\alpha_s\hbar c/r$ is a local Coulomb potential ($\alpha_s = e^2/\hbar c$, is the fine structure constant). For the exotic Mu atom, the Dirac-Coulomb equation in matrix form is

$$\begin{bmatrix} (m_1+m_2)c^2 & -c\boldsymbol{\sigma}_2\cdot\mathbf{p} & c\boldsymbol{\sigma}_1\cdot\mathbf{p} & 0 \\ -c\boldsymbol{\sigma}_2\cdot\mathbf{p} & (-m_1+m_2)c^2 & 0 & c\boldsymbol{\sigma}_1\cdot\mathbf{p} \\ c\boldsymbol{\sigma}_1\cdot\mathbf{p} & 0 & (m_1-m_2)c^2 & -c\boldsymbol{\sigma}_2\cdot\mathbf{p} \\ 0 & c\boldsymbol{\sigma}_1\cdot\mathbf{p} & -c\boldsymbol{\sigma}_2\cdot\mathbf{p} & (-m_1-m_2)c^2 \end{bmatrix} \Psi_{n\kappa}(\mathbf{r}) = \left(E + \frac{\alpha_s\hbar c}{r}\right)\Psi_{n\kappa}(\mathbf{r})\,. \tag{4}$$

The latter equation, admits equal-time analytic solutions which are of the form

$$\Psi_{n\kappa}(\mathbf{r}) = \begin{bmatrix} f_{n\kappa}(\mathbf{r}) \\ g_{n\kappa}(\mathbf{r}) \end{bmatrix} = \frac{1}{r}\begin{bmatrix} F_{n\kappa}(r)Y_{jm}^{\ell}(\theta,\phi) \\ G_{n\kappa}(r)Y_{jm}^{\tilde{\ell}}(\theta,\phi) \end{bmatrix} \tag{5}$$

where $f_{n\kappa}(\mathbf{r})$ and $g_{n\kappa}(\mathbf{r})$ are the spatial functions for the upper (large) and the lower (small) components, respectively, $Y_{jm}^{\ell}(\theta,\phi)$ and $Y_{jm}^{\tilde{\ell}}(\theta,\phi)$ are the spin and pseudo-spin (p-spin) spherical harmonics, respectively, while n is the principal quantum number and m is the projection of the angular momentum on the z-axis. The orbital angular momentum quantum numbers ℓ and $\tilde{\ell}$ stand for the spin and p-spin quantum numbers, respectively. For a given spin-orbit coupling term $\kappa = 0, \pm1, \pm2, \ldots$, the total angular momentum, $\mathbf{J}$, the orbital angular momentum and the pseudo orbital angular momentum are given by $j = |\kappa| - 1/2$, $\ell = |\kappa + 1/2| - 1/2$ and $\tilde{\ell} = |\kappa - 1/2| - 1/2$, respectively. We note that, the Dirac equation (unlike the Klein-Gordon equation) admits a conserved 4-current with a non-negative definite time component. So, this current can be interpreted as a probability 4-current.

The no-pair two-lepton Dirac-Coulomb-Breit equation

The relativistic single-time equation for the two-body system developed before the Bethe-Salpeter equation. Soon after the discovery of the Dirac equation, Breit proposed the well known Breit equation. The no-pair Dirac-Coulomb-

Breit (DCB) Hamiltonian, describing the relative motion of a two-fermion system, is written as [2]

$$H_{12}\Psi = \left[\alpha_1 \cdot \mathbf{p}_1 + m_1\beta_1 + \alpha_2 \cdot \mathbf{p}_2 + m_2\beta_2 - \frac{\alpha_s \hbar c}{r_{12}} + B_{12}\right]\Psi \tag{6}$$

where B_{12} represents the known as Breit term which is given by

$$B_{12} = -\frac{1}{r_{12}}\left[a_1 \cdot a_2 + \frac{(a_1 \cdot r_{12})(a_2 \cdot r_{12})}{2r_{12}^2}\right] \tag{7}$$

The DCB equation is difficult to be solved, because among others, it includes separate time-variable for each of the two particles. Equation (6) is known as the 16-component no-pair two-particle Dirac-Coulomb-Breit equation and, in matrix form, it is written as

$$H_{12}\Psi = \begin{bmatrix} V & -c\boldsymbol{\sigma}_2 \cdot \mathbf{p} & c\boldsymbol{\sigma}_1 \cdot \mathbf{p} & B_{12} \\ -c\boldsymbol{\sigma}_2 \cdot \mathbf{p} & V - 2m_2c^2 & B_{12} & c\boldsymbol{\sigma}_1 \cdot \mathbf{p} \\ c\boldsymbol{\sigma}_1 \cdot \mathbf{p} & B & V - 2m_1c^2 & -c\boldsymbol{\sigma}_2 \cdot \mathbf{p} \\ B_{12} & c\boldsymbol{\sigma}_1 \cdot \mathbf{p} & -c\boldsymbol{\sigma}_2 \cdot \mathbf{p} & V - 2m_{12}c^2 \end{bmatrix} \begin{bmatrix} \psi_1 \\ \psi_2 \\ \psi_3 \\ \psi_4 \end{bmatrix} \tag{8}$$

Moreover, because the Dirac-Coulomb-Breit equation includes the Breit term, it provides a more complete relativistic description for the exotic leptonic atoms. The DCB Hamiltonian may, in addition, include the following terms [5]: (i) the terms related to the relativistic velocity of each lepton, (ii) the retardation term, (iii) the known as the Darwin term, (iv) the term containing the spin-orbit interaction of each lepton, and (v) the hyper-fine splitting (hfs) term.

In the quasi-relativistic Hamiltonians, it sounds natural to decouple the positive and negative energy solutions and work on the positive energy solutions only. Notice the presence of some inherently problematic terms as, for example, those with the delta function (Darwin term). Furthermore, by neglecting the Breit term B_{12} (i.e. by putting the anti-diagonal blocks equal to zero) the no-pair Dirac–Coulomb (DC) Hamiltonian of Eq. (4) is obtained.

TESTING QED & BSM THEORIES ON THE EXOTIC MUONIUM ATOM

As stated above, the Mu (μ^+e^-) is a purely leptonic bound system (exotic atom) without internal substructure. For this reason, it qualifies as a potentially well-suited system to probe BSM physics. In our group, we have planned to perform extensive calculations for the bound spectrum of Mu by using the wave functions obtained through solving numerically the Dirac-Coulomb and the Dirac-Coulomb-Breit equations on the basis of the neural networks techniques. Afterwards, we will compare our predictions with the recent data extracted from precision spectroscopy carried out in muon factories as the PSI, the FermiLab, the J-Park, etc.

Initially, we assume a spin-independent dark force between electron-antimuon, mediated either by a new scalar or by a new vector gauge-boson which give rise to a Yukawa-like attractive potential written as [6]

$$V_{SI}^{e\mu}(r) = -\frac{g_e g_\mu}{4\pi}\frac{e^{-m_\phi r}}{r} \tag{9}$$

where g_μ and g_e represent the dimensionless coupling constants to the leptons μ^+ and e^-, while m_ϕ denotes the mass of the scalar/vector mediator. Note that, $V_{SI}^{e\mu}(r)$ reduces to the Coulomb potential on letting $m_\phi = 0$, and $g = 4\pi q$. In this case, the exchanged particle could be a (massless) photon. Such an interaction, leads to modifications of the bound spectrum, i.e. to the atomic energy-levels of Mu as well as to the transition-energy of any transition $|i\rangle \to |f\rangle$, namely, from an initial state $|i\rangle$, of energy $E(n_iL_{J_i})$, to a final state $|f\rangle$, of energy $E(n_fL_{J_f})$.

One of our main goals is to test some new physics scenarios published recently [6]. By taking properly into account existing experimental data, but also astrophysical probes, we may predict specific experimental targets prominent to probe new physics via precise spectroscopy. In the case of Mu, the potential reach of its spectroscopy looks more promising because, in the next few years, experiments like Mu-MASS at PSI will probe new regions of the parameter space testing the existence of spin-dependent and spin-independent dark forces between electrons and muons [6].

The existence of a novel massive pseudoscalar field interacting with μ^+ and e^-, constituent leptons of (μ^+e^-), would lead to lepton-antilepton interactions, e.g., in Refs. [6] authors consider such an interaction of the form

$$V_{ALP}(\mathbf{r}) = \frac{g_e^{ALP} g_\mu^{ALP}}{12\pi m_e m_\mu}\left[\mathbf{S}_1 \cdot \mathbf{S}_2\left(12\pi\delta^3(\mathbf{r}) - \frac{m_{ALP}^2}{r}\right) - \frac{S_{12}(\hat{r})}{4}\left(\frac{m_{ALP}^2}{r} + \frac{3}{r^3} + \frac{m_{ALP}^3}{r^2}\right)\right]e^{-rm_{ALP}} \tag{10}$$

where g_μ^{ALP} and g_e^{ALP} stand for the dimensionless coupling constants to the leptons μ^+ and e^-, while m_{ALP} denotes the mass of the new particle. $\mathbf{S}_1$, $\mathbf{S}_2$ are the spins and m_μ, m_e are the masses of the leptons μ^+ and e^-. Furthermore, $S_{12}(\hat{r})$ denotes the spin-tensor operator given by

$$S_{12}(\hat{r}) = 4\left[3(\mathbf{S}_1 \cdot \hat{r})(\mathbf{S}_2 \cdot \hat{r}) - \mathbf{S}_1 \cdot \mathbf{S}_2\right], \tag{11}$$

which contributes only when $\ell \neq 0$. For arbitrary quantum numbers, the energy levels generated by the above potential produce spin-dependent as well as spin-independent energy shifts of the different states of Mu.

We can estimate the contribution to the hype rfine splitting (hfs) of various states of the Mu exotic atom, focusing on the $1S \to 2S$ transition which is of great importance. Its current experimental measurement is

$$\left[E(2S_{1/2}) - E(1S_{1/2})\right]_{Mu}^{exp} = 2455528941.0\, MHZ, \tag{12}$$

where $E(nL_J)$ is the energy of Mu state described by quantum numbers nL_J. We note that, in the next few years, the planned experiment at PSI, the Mu-MASS, is expected to improve the experimental precision down to the kHz level.

We should also mention that, the latest experimental measurement of the Muonium ground state hfs was performed at the Los Alamos Meson Physics Facility (LAMPF), while in the near future the MuSEUM project at JPARC, with the new and intense muon beam line, is planning to perform a new measurement in order to improve the LAMPF result. Our aim in the present project is to provide accurate prediction for the ground state hfs in Mu and compare it with the aforementioned measurements as well as with recent theoretical values.

CONCLUSIONS AND OUTLOOK

In this paper, we are particularly interested in studying two-body exotic leptonic atoms that contain electrons, muons, and taus (with their corresponding antiparticles). The non-relativistic energies and bound states of these systems have been investigated by several authors and by our research group in previous works. The relativistic or QED corrections of the bound-state energies of such exotic systems have not been considered by many authors and, therefore, they remain a challenging problem. In the near future, one of our goals is to study the sensitivity of the Mu spectroscopy to spin-dependent and spin-independent dark forces between electron and anti-muon. This is because the Mu precision spectroscopy has a more interesting potential to probe new physics since, the planned relevant measurements at PSI and J-PARC have the potential to set stringent bounds for spin-independent interactions between electron and anti-muon in the purely leptonic atom Mu. Finally, regarding the development of advanced computational tools for testing relativistic QED, this is necessary for accurate spectroscopic energy-resolution and for further development of the fundamental Theory of Atomic Matter.

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