Mathematical formulation of the Dirac, Breit-Darwin equation for purely leptonic atoms

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Abstract. Purely leptonic atoms are ideal in investigating quantum electrodynamics (QED) and beyond the Standard Model theories (BSM). In this work, we initially describe the non-relativistic treatment of purely leptonic atoms. We aim to obtain high-accuracy theoretical predictions for the respective atomic bound states. Towards this purpose, the relativistic treatment of the system is necessary. However, the Dirac equation is often insufficient, especially if the particles have similar masses. For that reason, we will need the energy correction terms of the Breit-Darwin equation that incorporate retardation effects and additional interactions between the system's particles.

INTRODUCTION

Purely leptonic atoms are ideal quantum mechanical systems in order to test beyond the Standard model physics (i.e., BSM) and quantum electrodynamics (i.e., QED) [1, 2]. That is mainly due to their lack of a complex internal structure such as the one existing in a nucleus or even a proton.

One prime example of a leptonic atom thoroughly used in research is the muonium (Mu, μ^+e^-), which consists of an antimuon and an electron in orbit [3, 4]. It is formed when muons are slowed down in matter and capture electrons from nearby atoms. Due to the muon mass being much larger than the electron's, muonium shares many similarities with the hydrogen atom. Furthermore, a possible conversion of a muonium atom to antimuonium ($e^+\mu^-$) [5] has attracted much attention among researchers as it could lead the investigation toward lepton number violation and lepton flavor.

Positronium (Ps, e^+e^-) is a leptonic atom consisting of a positron and an electron [6]. This bound state is unstable as the two particles could engage in annihilation to produce gamma-ray photons. Nonetheless, the atom exhibits substantial deviation in the scaling, polarizability, and binding energy to hydrogen partly due to the similarities between the positron and electron particles. Other two-body leptonic atoms include the true muonium ($\mu^+\mu^-$) and tauonium (τ^+e^-).

In this work, we initially present a non-relativistic description of the studied systems through the solution to the respective Schrödinger equation. Then, we expand to the relativistic treatment of the problem through the Dirac equation, which describes all spin-1/2 particles, and the Breit-Darwin equation for a two-body quantum system.

NON-RELATIVISTIC TREATMENT OF A HYDROGEN-LIKE ATOM

A simplified quantum mechanical description of the respective leptonic bound states is limited in a non-relativistic treatment through the solution of the Schrödinger equation. Moreover, we could also implement the fine-structure terms for more accurate theoretical predictions. Those include the relativistic correction to the kinetic energy of the electron, the electron's spin-orbit coupling, and the Darwin term (i.e., zitterbewegung) related to the trembling movement of the electron due to vacuum energy fluctuations.

The radial part of the wave function of an electron in a leptonic two-body system is given by solving the following differential equation

$$\left[-\frac{\hbar^2}{2\mu}\frac{d^2}{dr^2}+\frac{\hbar^2 l(l+1)}{2\mu r^2}-\frac{e^2}{r}\right]u(r)=Eu(r), \tag{1}$$

where $u(r) = rR_{nl}(r)$ and $\mu = m_i m_j/(m_i+m_j)$ the reduced mass of the two-body system with $i, j = \mu^{+,-}, e^{+,-}, \tau^{+,-}, etc.$ corresponding to the cases of muonium, true muonium, positronium, tauonium, etc.

The well-known analytical solutions of the Schrödinger equation are given by

$$R_{nl}(r) = \sqrt{\left(\frac{\bar{r}}{nr}\right)^3 \frac{(n-l-1)!}{2n(n+l)!}} \left(\frac{\bar{r}}{n}\right)^l e^{-\bar{r}/2n} L_{n-l-1}^{2l+1}\left(\frac{\bar{r}}{n}\right), \tag{2}$$

where $\bar{r} = 2r/\alpha_0^*$. Here, the reduced Bohr radius $\alpha_0^* = (m_e/\mu)\alpha_0$ is implemented.

Moreover, the energy of each bound state is given by

$$E_n = -\frac{\hbar^2}{2\mu\alpha_0^{*2} n^2}. \tag{3}$$

In Fig. 1, we plot the radial part of the wave functions corresponding to the first orbitals of the muonium, positronium, true muonium, and tauonium. The muonium case resembles the hydrogen atom due to the scaling similarities between the two particles. We notice that in heavier systems, such as tauonium, the electron is more likely to be found near the other particle exhibiting restricted relative movement.

THE DIRAC EQUATION FORMALISM

A more realistic quantum mechanical approach requires the solution to the one-body Dirac equation. It considers an electron interacting with a four-vector potential from a point-like source. Notably, the fine-structure correction terms are derived directly through the non-relativistic limit.

By substituting $\psi_A = g(r)\mathscr{Y}_{jlm}$ and $\psi_B = if(r)\mathscr{Y}_{jlm}$, the Dirac equation is written as

$$\begin{aligned}
(E - mc^2 - V(r))g\mathscr{Y}_{jlm} &= \frac{1}{r}\frac{\boldsymbol{\sigma}\cdot\boldsymbol{r}}{r}\left[-ir\frac{\partial}{\partial r} + i\boldsymbol{\sigma}\cdot\boldsymbol{L}\right] if\mathscr{Y}_{jl'm}, \\
(E + mc^2 - V(r))if\mathscr{Y}_{jl'm} &= \frac{1}{r}\frac{\boldsymbol{\sigma}\cdot\boldsymbol{r}}{r}\left[-ir\frac{\partial}{\partial r} + i\boldsymbol{\sigma}\cdot\boldsymbol{L}\right] g\mathscr{Y}_{jlm},
\end{aligned}$$

where $V(r)$ is the Coulomb potential. The operators involving the Pauli matrices act on the angular part of the wave function. The first one acts as a phase shift while the spin-orbit coupling operator acts through a quantum number, namely k, for which it holds $k = -(j+1/2)$ when $j = l+1/2$ (spin-up) and $k = (j+1/2)$ when $j = l-1/2$ (spin-down). Eventually, only the radial part remains that satisfies the following system of differential equations [7, 8]

$$\frac{\partial}{\partial r}\begin{pmatrix} f(r) \\ g(r) \end{pmatrix} = \begin{pmatrix} \frac{k-1}{r} & -\frac{E-V-\mu c^2}{\hbar c} \\ \frac{E-V+\mu c^2}{\hbar c} & -\frac{k+1}{r} \end{pmatrix} \begin{pmatrix} f(r) \\ g(r) \end{pmatrix}, \qquad k = \pm\left(j+\frac{1}{2}\right). \tag{4}$$

Here, k defines the eigenvalues of an operator that commutes with the Hamiltonian (unlike the spin and orbital angular momentum operators) and the total angular momentum operator. Furthermore, this operator, namely K, constitutes a measure of the spin's component along the direction of the total angular momentum. Moreover, the corresponding analytical solutions to the above system are calculated through the confluent hypergeometric functions.

The respective Dirac energy levels are given by

$$E_{nj} = \frac{mc^2}{\sqrt{1 + \frac{\alpha^2}{\left(n-j-\frac{1}{2}+\sqrt{(j+1/2)^2-\alpha^2}\right)^2}}}. \tag{5}$$

The one-body Dirac equation is very effective in describing a two-body system with substantial differences between the particles' masses, as in the case of hydrogen. However, purely leptonic atoms do not always fall under this category, as is evident in the case of positronium. Hence, we need an equation that treats both particles equally and establishes additional interactions and energy corrections for both particles.

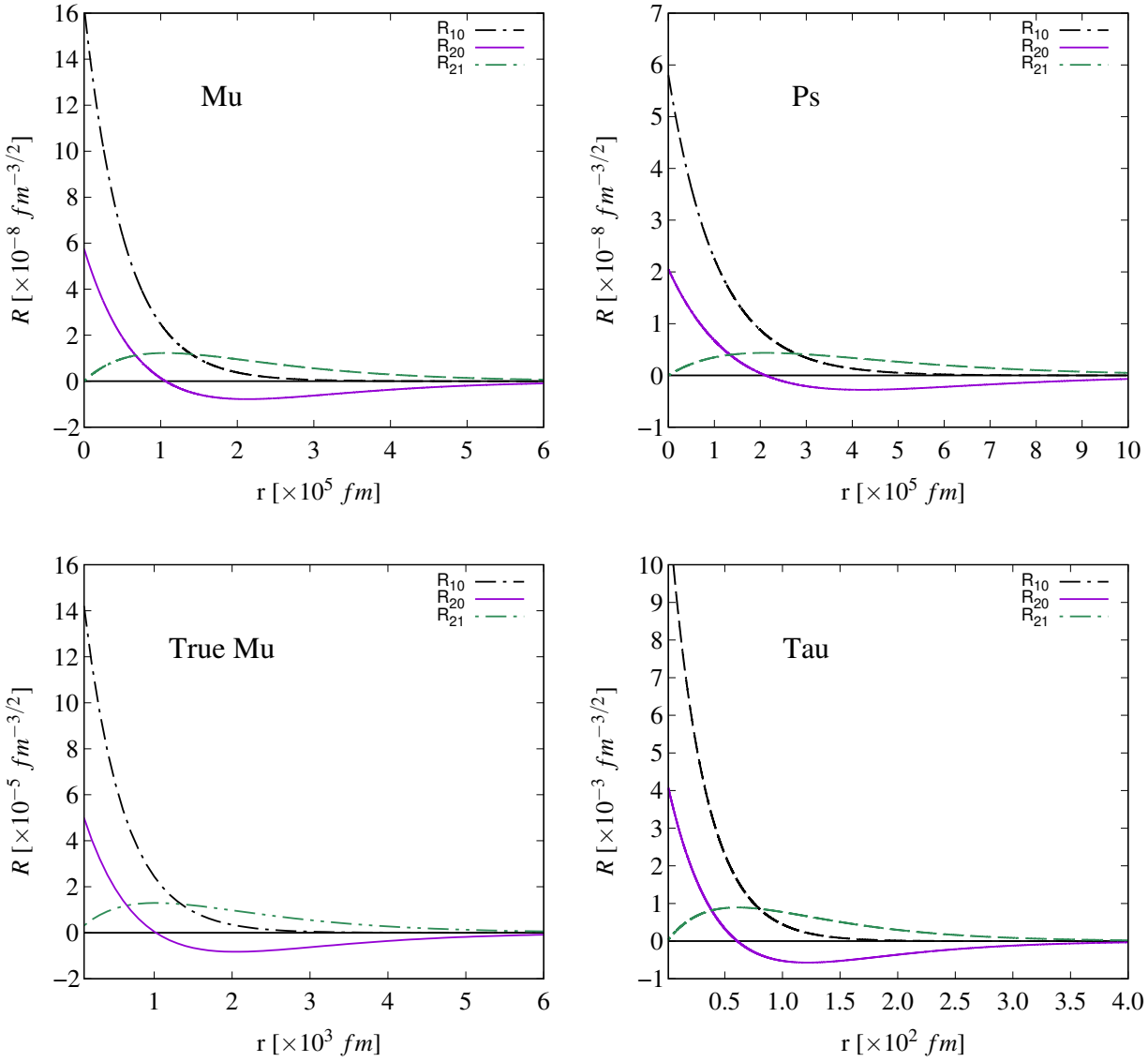

FIGURE 1. The radial wave functions of the first orbitals of the muonium atom (top-left panel), the positronium atom (top-right panel), the true muonium (bottom-left panel), and the tauonium (bottom-right panel). The black dotted-dashed lines correspond to quantum numbers $(n,l) = (1,0)$, the purple solid lines to $(n,l) = (2,0)$, and the green dashed to $(n,l) = (2,1)$.

THE BREIT-DARWIN EQUATION

The Breit equation involves the free-body Dirac Hamiltonians corresponding to each particle, a Coulomb potential, and the Breit interaction. The exchange of a virtual photon between the two particles causes the latter. Thus, we have

$$\left[c\boldsymbol{\alpha_1}\cdot\boldsymbol{p_1}+\beta_1 m_1 c^2 + c\boldsymbol{\alpha_2}\cdot\boldsymbol{p_2}+\beta_2 m_2 c^2 + V_C + B\right]\Psi = E\Psi, \quad B = -\frac{q_1 q_2}{2}\left[\frac{\boldsymbol{\alpha}_1\cdot\boldsymbol{\alpha}_2}{r} + \frac{(\boldsymbol{\alpha}_1\cdot\boldsymbol{r})(\boldsymbol{\alpha}_2\cdot\boldsymbol{r})}{r^3}\right].$$

The Breit operator B compensates for the retardation effects and constitutes a good approximation assuming a weak external field (i.e., non-relativistic atomic states).

However, the Breit equation cannot be solved precisely like the Dirac equation because it is not well-defined and completely Lorentz invariant. The Breit operator has to be treated as a first-order perturbation to the two-body Dirac equation. Otherwise, it would introduce significant higher-order corrections.

In other words, the Breit equation forms a semi-relativistic extension of the Schrödinger treatment. In the Pauli approximation, it breaks down into the relativistic correction terms derived from the Dirac theory and the hyperfine splitting effect [9]. Those include the Darwin and the spin-orbit interaction terms for each particle

$$V_D = \frac{\pi e^2}{2m_i^2 c^2}\delta(\mathbf{r}), \qquad V_{so}^{(1)} = \frac{e^2(\mathbf{r}\times\hat{\mathbf{p}}_i)}{4m_i^2 c^2 r^3}\cdot\boldsymbol{\sigma}_i, \qquad V_{so}^{(2)} = -\frac{e^2(\mathbf{r}\times\hat{\mathbf{p}}_j)}{4m_i m_j c^2 r^3}\cdot\boldsymbol{\sigma}_i. \tag{6}$$

Here, m_i denotes the respective particle mass with $i = 1, 2$. In addition, the following retarded potential is included

$$V_r = \frac{e^2}{2m_1 m_2 c^2 r}\left(\hat{\mathbf{p}}_1\cdot\hat{\mathbf{p}}_2 + \frac{(\mathbf{r}\cdot\hat{\mathbf{p}}_1)(\mathbf{r}\cdot\hat{\mathbf{p}}_2)}{r^2}\right). \tag{7}$$

The energy input coming from the spin-spin interaction between the two particles is given by

$$V_{ss} = \frac{e^2\hbar^2}{4m_1 m_2 c^2}\left(\frac{8\pi}{3}(\boldsymbol{\sigma}_1\cdot\boldsymbol{\sigma}_2)\delta(\mathbf{r}) - \frac{1}{r^3}\left[\boldsymbol{\sigma}_1\cdot\boldsymbol{\sigma}_2 - \frac{3(\boldsymbol{\sigma}_1\cdot\mathbf{r})(\boldsymbol{\sigma}_2\cdot\mathbf{r})}{r^2}\right]\right). \tag{8}$$

Furthermore, the hyperfine structure and the Lamb shift, not predicted by Dirac's theory, are well-investigated in leptonic atoms due to the lack of particle structure complexities.

SUMMARY AND CONCLUSIONS

The simplicity of their internal structure allows us to use the leptonic atoms as examples in examining QED and BSM effects. Such quantum systems include the muonium, positronium, true muonium, tauonium, etc. Several upcoming experiments aim for this purpose, especially concerning muonium and positronium [3, 4, 6].

In this work, we estimate the wave functions of the muonium, positronium, true muonium, and tauonium atoms through the non-relativistic treatment of the Schrödinger equation. We also describe the relativistic treatment through the Dirac equation and the Breit-Darwin equation. The latter incorporates retardation effects as well as spin-orbit and spin-spin interactions between the two particles. We aim to make accurate theoretical predictions for the leptonic atoms' bound states by implementing advanced numerical tools and comparing them to the respective analytical solutions.

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