RELATIVISTIC THREE-FERMION WAVE EQUATIONS IN REFORMULATED QED AND RELATIVISTIC EFFECTS IN MUONIUM MINUS

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Abstract

The variational method, within the Hamiltonian formalism of reformulated QED is used to determine relativistic wave equations for a system of three fermions of arbitrary mass interacting electromagnetically. The interaction kernels of the equations are, in essence, the invariant $M$ matrices in lowest order. The equations are used to obtain relativistic $O(\alpha^2)$ corrections to the non-relativistic ground state energy levels of the Muonium negative ion ($\mu^+e^-e^-$) as well as of $\text{Ps}^-$ and $\text{H}^-$, using approximate variational three-body wave functions. The results are compared with other calculations, where available. The relativistic correction for $\text{Mu}^-$ is found to be $-1.0773 \times 10^{-4}$ eV.

1 Introduction

The bound state three-Fermion system, particularly $\text{Ps}^-$, has been the subject of theoretical investigations since the pioneering calculations of Wheeler [1] and Hylleraas [2], who first showed that this system has a single bound state. Although experimental measurements of the binding energy of $\text{Ps}^-$ have not been reported to date, there are preparations to make such measurements [3].

Recently, Drake and Grigorescu reported an essentially exact (converged) variational calculation of the non-relativistic ground state energy of $\text{Ps}^-$ [4]. They also used their very accurate wave function to calculate relativistic and QED corrections to the bound-state energy of this system. Accurate non-relativistic calculations of the Muonium negative ion ($\text{Mu}^- : \mu^+e^-e^-$) have been reported recently by Frolov [5]. Frolov used these to calculate the lowest-order QED $O(\alpha^3)$ corrections to the non-relativistic $\text{Mu}^-$ energy. However, relativistic ($O(\alpha^2)$) corrections to the non-relativistic ground-state energy of $\text{Mu}^-$ seem not to have been calculated.

In the present work, we work out a relativistic wave equation for a system of three fermions of arbitrary mass with electromagnetic interactions. This equation is used to obtain relativistic corrections to the bound-state energy of $\text{Mu}^-$, as well as of $\text{Ps}^-$ in order to compare our results to those of others.

It has been shown in earlier works that a reformulation of various models in Quantum Field Theory (QFT), including QED, allows one to use simple Fock-state trial states to derive relativistic
few-body wave equations by means of the variational method in the Hamiltonian formulation of the theory. An overview of this approach and various results obtained in this way for bosonic and fermionic systems (including Ps and Mu) is given in reference [6] and citations therein. One of the advantages of this approach is that it permits straightforward generalization to relativistic systems of more than two particles.

2 Reformulated Hamiltonian formalism, field operators and variational method

The reformulated QED Hamiltonian density is [7, 6]

\[ \mathcal{H}_R = \sum_{a=1}^{3} \left[ \bar{\psi}_a(x) \left( -i \sum_{j=1}^{3} \gamma^j \frac{\partial}{\partial x^j} + m_a \right) \psi_a(x) - Q_a \bar{\psi}_a(x) \gamma_\mu A_\mu^a(x) \psi_a(x) \right] + \frac{1}{2} \int d^4x' j^\nu(x') D_{\mu\nu}(x-x') j^\nu(x), \]  

(1)

where \( \psi_a(x) \) are Dirac fermion fields of mass \( m_a \) and charge \( Q_a \), \( A_\mu^a \) are free photon fields, \( j^\nu(x) = -\sum_{a=1}^{3} Q_a \bar{\psi}_a(x) \gamma^\nu \psi_a(x) \)

(2)

are the fermionic source currents, and \( D_{\mu\nu}(x-x') = D_{\nu\mu}(x-x') = D_{\mu\nu}(x'-x) \) are symmetric Green functions (photon propagators) defined by

\[ \partial_\alpha \partial^\alpha D_{\mu\nu}(x-x') - \partial_\mu \partial_\nu D_{\alpha\omega}(x-x') = g_{\mu\nu} \delta^4(x-x'). \]  

(3)

In practice, one needs to choose a gauge, however, we do not need to specify one at this point.

The reformulated Hamiltonian (1) is obtained from the usual Lagrangian of QED by using the equations of motion to express the mediating photon field in terms of the fermion fields and photon field Green functions [6], [7]. The reason for using the reformulated Hamiltonian is that it allows one to derive relativistic few-fermion wave equations with the simplest possible Fock-space trial states. Our notation is

\[ \psi_a(x) = \sum_{s=1}^{2} \int \frac{d^3p}{(2\pi)^2} \sqrt{m_a} \left[ b_a(p,s) u_a(p,s) e^{-ip\cdot x} + d_a^\dagger(p,s) v_a(p,s) e^{ip\cdot x} \right], \]  

(4)

where \( p^\nu = (\omega_{ap} = \sqrt{m_a^2 + p^2}, p) \). The mass-\( m_a \) free-particle Dirac spinors \( u_a \) and \( v_a \), where \( (\not{p} - m_a) u_a(p,s) = 0 \) and \( (\not{p} + m_a) v_a(p,s) = 0 \), satisfy the following orthogonality conditions:

\[ u_a^\dagger(p,s) u_a(p,\sigma) = v_a^\dagger(p,s) v_a(p,\sigma) = \frac{\omega_{ap}}{m_a} \delta_{s\sigma} \]  

(5)

\[ u_a^\dagger(p,s) v_a(-p,\sigma) = v_a^\dagger(p,s) u_a(-p,\sigma) = 0. \]  

(6)
The operators $b^\dagger_\alpha$ and $a_{\alpha}$ are the creation and annihilation operators for free particles of mass $m_\alpha$; likewise, $d^\dagger_{\alpha}$ and $d_{\alpha}$ are the corresponding operators for antiparticles of mass $m_\alpha$. These operators satisfy the usual anticommutation relations. The non-vanishing ones are

$$\{b_{\alpha}(p, s), b^\dagger_{\beta}(q, \sigma)\} = \{d_{\alpha}(p, s), d^\dagger_{\beta}(q, \sigma)\} = \delta_{s, \sigma} \delta^3(p - q).$$  \hspace{1cm} (7)

As usual, operators for a given field commute with all the operators corresponding to other fields.

We use the above definitions to express the Hamiltonian operator, $\hat{H}_R = \int d^3x \mathcal{H}_R$, in terms of the fermionic creation and annihilation operators, and we normal order the entire Hamiltonian (thereby denoting it by $:\hat{H}:$) in order to circumvent the need for vacuum and mass renormalization.

We do not exhibit the Fourier decomposition of the photon field, since this is not needed in the present work.

Since exact eigenstates of the Hamiltonian $\hat{H}_R$ (c.f. eq. 1) are not obtainable, we determine approximations using the variational principle

$$\delta \langle \Psi_{\text{tr}} | : \hat{H} : - M | \Psi_{\text{tr}} \rangle_{t=0} = 0.$$  \hspace{1cm} (8)

### 3 Relativistic three-fermion wave equations

For systems of three fermions we use the following simple Fock-space trial state,

$$|\Psi_{\text{tr}}\rangle = \sum_{s_1, s_2, s_3} \int d^3p_1 d^3p_2 d^3p_3 F_{s_1, s_2, s_3}(p_1, p_2, p_3) b^\dagger_1(p_1, s_1)b^\dagger_2(p_2, s_2)d^\dagger_3(p_3, s_3) |0\rangle,$$  \hspace{1cm} (9)

where $F_{s_1, s_2, s_3}(p_1, p_2, p_3)$ are eight adjustable functions, and the vacuum state $|0\rangle$ is defined by $b_j|0\rangle = d_j|0\rangle = 0$ for $j = 1, 2, 3$. We consider three cases for the values of $j$ and $k$: $j = 1$ and $k = 1$, $j = 1$ and $k = 3$, or $j = 2$ and $k = 3$. In the first case, the system consists of three particles of identical mass (e.g. $e^- e^- e^+$). In the second case, the system consists of two identical particles and a different antiparticle (e.g. $e^- e^- \mu^+$). In the third case, the system consists of three distinct particles (e.g. $e^- \tau^- \mu^+$).

Substituting the trial state (9) into (8) we obtain the following relativistic momentum-space wave equations for the states of the three-fermion system:

$$\sum_{n_1} \omega_{q_1} + \omega_{q_2} + \omega_{q_3} - E) F_{r_1, r_2, r_3}(q_1, q_2, q_3) + \frac{i}{2(2\pi)^3} \sum_{s_1, s_2} \int d^3p_1 d^3p_2 F_{s_1, s_2, s_3}(p_1, p_2, q_3) \delta^3(p_1 - q_1 - q_2 + p_2) \mathcal{M}_{r_1, r_2, s_1, s_2}^{d^\dagger}(p_1, p_2, q_1, q_2)$$

$$- \frac{i}{2(2\pi)^3} \sum_{s_1, s_2} \int d^3p_1 d^3p_2 F_{s_1, r_2, s_3}(p_1, q_2, p_2) \delta^3(p_1 - q_1 + p_2 - q_3) \mathcal{M}_{r_1, r_3, s_1, s_2}^{d^\dagger}(p_1, p_2, q_1, q_3)$$

$$- \frac{i}{2(2\pi)^3} \sum_{s_1, s_2} \int d^3p_1 d^3p_2 F_{r_1, s_1, s_3}(q_1, p_1, p_2) \delta^3(p_1 - q_2 + p_2 - q_3) \mathcal{M}_{r_2, r_3, s_1, s_2}^{d^\dagger}(p_1, p_2, q_2, q_3)$$

(10)
\[- \frac{i\delta_{ij}\delta_{k1}}{(2\pi)^3} \sum_{s_1s_2} \int d^3p_1d^3p_2 F_{r_1s_2s_1}(q_1, p_2, p_1) \delta^3(p_1 - q_2 + p_2 - q_3) \mathcal{M}_{r_2r_3s_1s_2}^4(p_1, p_2, q_2, q_3) = 0\]

where

\[
\begin{align*}
\mathcal{M}_{r_1r_2s_1s_2}^1(p_1, p_2, q_1, q_2) &= -iQ_1Q_j \bar{u}_1(q_1, r_1)\gamma^\mu u_1(p_1, s_1)\bar{u}_j(q_2, r_2)\gamma^\nu u_j(p_2, s_2) \\
&\quad \times [D_{\mu\nu}(\omega_{1p_1} - \omega_{1q_1}, p_1 - q_1) + D_{\mu\nu}(\omega_{1p_2} - \omega_{1q_2}, p_2 - q_2)], \\
\mathcal{M}_{r_1r_3s_1s_2}^2(p_1, p_2, q_1, q_3) &= -iQ_1Q_k \bar{u}_1(q_1, r_1)\gamma^\mu u_1(p_1, s_1)\bar{u}_k(q_2, r_2)\gamma^\nu u_k(q_3, r_3) \\
&\quad \times [D_{\mu\nu}(\omega_{1p_1} - \omega_{1q_1}, p_1 - q_1) + D_{\mu\nu}(\omega_{1p_3} - \omega_{1q_3}, p_2 - q_3)], \\
\mathcal{M}_{r_2r_3s_1s_2}^3(p_1, p_2, q_2, q_3) &= -iQ_jQ_k \bar{u}_j(q_2, r_2)\gamma^\mu u_j(p_1, s_1)\bar{u}_k(q_2, r_2)\gamma^\nu u_k(q_3, r_3) \\
&\quad \times [D_{\mu\nu}(\omega_{j_{p_1}} - \omega_{j_{q_2}}, p_1 - q_1) + D_{\mu\nu}(\omega_{k_{p_2}} - \omega_{k_{q_3}}, p_2 - q_3)]
\end{align*}
\]

are matrix elements corresponding to one-photon exchange Feynman diagrams in the particle-particle interaction, and for systems containing particle-antiparticle pairs (e.g. $e^+e^-$).

\[
\begin{align*}
\mathcal{M}_{r_2r_3s_1s_2}^4(p_1, p_2, q_2, q_3) &= iQ_1^2 \bar{u}_1(q_2, r_2)\gamma^\mu v_1(q_3, r_3)\bar{u}(p_2, s_2) \\
&\quad \times [D_{\mu\nu}(\omega_{1p_1} + \omega_{1p_2}, p_1 + p_2) + D_{\mu\nu}(-\omega_{1q_2} - \omega_{1q_3}, -q_2 - q_3)]
\end{align*}
\]

is a matrix element corresponding to Feynman diagrams depicting virtual annihilation. The virtual annihilation matrix elements are obtained along with one-photon exchange terms in the derivation and are not put in “by hand”. Higher order (loop) effects can be included by adding the appropriate $\mathcal{M}$-matrix elements to the kernels in Eq. (10) or, more formally, by generalizing the trial state (9), as was done for Ps [8].

It is straightforward to verify that in the nonrelativistic limit, $(p/m_a)^2 \ll 1$, eq. (10) reduces to the usual three-body Schrödinger equation with Coulombic interparticle interactions. Details of this, as well as of all other calculations presented here, are given in reference [9].

At this point it is worthwhile mentioning that the relativistic three-fermion eq. (10) holds for any values of the masses (i.e. no recoil corrections are necessary) and any strength of the coupling. In addition, this equation, being Salpeter-like rather than Dirac-like, has only positive-energy solutions and is amenable to variational solution without any “negative-energy” difficulties.

It is impossible to solve eq. (10) analytically (even in the nonrelativistic limit). Therefore, approximate (i.e. numerical, variational or perturbative) solutions must be sought for various cases of interest. This is a non-trivial task even in the nonrelativistic case; hence all the more so for the relativistic eq. (10). We shall set up the variational solution of eq. (10), however, in this paper, we will use the resulting matrix elements to calculate perturbatively the (comparatively small) $O(\alpha^2)$ relativistic corrections to the non-relativistic energy eigenvalues for Mu, Ps and H.
4 Variational approximations and relativistic corrections to the bound-state energy of Mu⁻ and Ps⁻

For variational approximations the trial state, eq. (9), can be chosen such that the eight adjustable functions take the following spin and momentum separable form

\[ F_{s_1s_2s_3}(p_1, p_2, p_3) = \Lambda_{s_1s_2s_3} f(p_1, p_2, p_3), \tag{15} \]

where \( f(p_1, p_2, p_3) \) is an adjustable function and \( \Lambda_{s_1s_2s_3} \) are a set of constants. For systems like Ps⁻, Mu⁻ of H⁻ we consider the two cases,

1. \( \Lambda_{111} = \Lambda_{221} = \Lambda_{s_1s_2} = 0, \Lambda_{121} = -\Lambda_{211} = 1/\sqrt{2} \) for all \( s_1, s_2, S = 1/2, m_s = 1/2 \)

2. \( \Lambda_{112} = \Lambda_{222} = \Lambda_{s_1s_1} = 0, \Lambda_{122} = -\Lambda_{212} = 1/\sqrt{2} \) for all \( s_1, s_2, S = 1/2, m_s = -1/2 \)

where \( S \) is the total spin and \( m_s \) is the spin projection of the state. For both cases, the spin part of the adjustable function is normalized such that \( \sum_{s_1s_2s_3} \Lambda^{*}_{s_1s_2s_3} \Lambda_{s_1s_2s_3} = 1 \). Thus, the trial state takes a form in which particles 1 and 2 are described by a spin singlet state; for case one particle 3 is in a spin up state and for case two particle 3 is in a spin down state. We consider the special cases where \( j = 1, k = 1, 2, 3, Q_1 = e, Q_k = Z_n e \) where \( Z_n \) is a positive integer and \( e \) is the elementary charge. The cases with \( Z_n = 1 \) correspond to systems like \( e^- e^- e^+ \), \( e^- e^- \mu^+ \) and \( ^1\text{H}^- \). For the cases where \( Z_n > 1 \), particle 3 may be thought of as the nucleus of a Helium atom (i.e. \( Z_n = 2 \)) or a Helium-like ion (i.e. \( Z_n > 2 \)). For the cases in which the positively charged particle is the nucleus of an atom and not a fundamental fermion the results of the perturbative calculation will apply approximately to these systems if their total nuclear spin is \( 1/2 \), or if the nucleus is very massive and may be treated as a static charge (i.e. the \( m_3 \to \infty \) limit).

Multiplying eq. (10) by \( F^{*}_{r_1r_2r_3}(q_1, q_2, q_3) \) and integrating over all \( q_1, q_2, q_3 \), summing over all \( r_1, r_2, r_3 \) and applying the normalization condition \( \sum_{s_1s_2s_3} \Lambda^{*}_{s_1s_2s_3} \Lambda_{s_1s_2s_3} = 1 \) we obtain the following expression for the energy,

\[ E = \langle \hat{H}_0 \rangle + \langle \hat{H}_{112} \rangle + 2\langle \hat{H}_{113} \rangle, \tag{16} \]

where \( \int d^3q_1d^3q_2d^3q_3 f^*(q_1, q_2, q_3)f(q_1, q_2, q_3) \) is taken to be unity (or, equivalently, the right-hand side of eq. (16) must be divided by this factor). The contributing matrix elements are

\[ \langle \hat{H}_0 \rangle = \int d^3q_1d^3q_2d^3q_3 f^*(q_1, q_2, q_3)f(q_1, q_2, q_3)\left[ \omega_{1q_1} + \omega_{1q_2} + \omega_{3q_3} \right], \tag{17} \]

\[ \langle \hat{H}_{112} \rangle = \frac{e^2}{2(2\pi)^3} \int d^3p_1d^3p_2d^3q_1d^3q_2d^3q_3 f^*(q_1, q_2, q_3)f(p_1, p_2, q_3) \]
\[ \times \delta^3(p_1 - q_1 - q_2 + p_2)K^{\mu\nu}_{12}(p_1, p_2, q_1, q_2) \]
\[ \times \left[ D_{\mu\nu}(\omega_{1p_1} - \omega_{1q_1}, p_1 - q_1) + D_{\mu\nu}(\omega_{1p_2} - \omega_{1q_2}, p_2 - q_2) \right], \tag{18} \]
\[
\langle \hat{H}_{13} \rangle = -\frac{Ze^2}{2(2\pi)^3} \int d^3p_1 d^3p_2 d^3q_1 d^3q_2 d^3q_3 f^*(q_1, q_2, q_3) f(p_1, q_2, p_2) \\
\times \delta^3(p_1 - q_1 + p_2 - q_3) K_{12}^{\mu\nu}(p_1, p_2, q_1, q_2) \\
\times [D_{\mu\nu}(\omega_{1p_1} - \omega_{1q_1}, p_1 - q_1) + D_{\mu\nu}(\omega_{3p_2} - \omega_{3q_3}, p_2 - q_3)], 
\tag{19}
\]

\[
K_{12}^{\mu\nu}(p_1, p_2, q_1, q_2) = B_{12}(p_1, p_2, q_1, q_2) [K_1^{\mu}(q_1, p_1, m_1) K_1^{\nu}(q_2, p_2, m_1) \\
- K_2^{\mu}(q_1, p_1, m_1) K_2^{\nu}(q_2, p_2, m_1) \\
- K_3^{\mu}(q_1, p_1, m_1) K_3^{\nu}(q_2, p_2, m_1) \\
+ K_4^{\mu}(q_1, p_1, m_1) K_4^{\nu}(q_2, p_2, m_1)], 
\tag{20}
\]

\[
B_{12}(p_1, p_2, q_1, q_2) = \frac{1}{4\sqrt{\omega_{1q_1}\omega_{1p_1}\omega_{1q_2}\omega_{1p_2}}} \\
\times \frac{1}{\sqrt{(\omega_{1q_1} + m_1)(\omega_{1p_1} + m_1)(\omega_{1q_2} + m_1)(\omega_{1p_2} + m_1)}}, 
\tag{21}
\]

\[
K_{13}^{\mu\nu}(p_1, p_2, q_1, q_3) = B_{13}(p_1, p_2, q_1, q_3) K_1^{\mu}(q_1, p_1, m_1) [K_1^{\nu}(q_2, p_2, m_1) \\
+ K_2^{\nu}(q_2, q_3, m_3)], 
\tag{22}
\]

\[
B_{13}(p_1, p_2, q_1, q_3) = \frac{1}{4\sqrt{\omega_{1q_1}\omega_{1p_1}\omega_{3p_2}\omega_{3q_3}}} \\
\times \frac{1}{\sqrt{(\omega_{1q_1} + m_1)(\omega_{1p_1} + m_1)(\omega_{3p_2} + m_3)(\omega_{3q_3} + m_3)}}, 
\tag{23}
\]

\[
K_1^{\mu}(p, q, m_a) = g_0^{\mu}(m_a^2 - \omega_{ap}\omega_{aq} + p \cdot q) + p^\mu(m_a + \omega_{ap}) + q^\mu(m_a + \omega_{aq}), 
\tag{24}
\]

\[
K_2^{\mu}(p, q, m_a) = i(g_0^{\mu}(p_1 q_2 - q_1 p_2) + g_1^{\mu}[p_2(m_a + \omega_{aq}) - q_2(m_a + \omega_{ap})] \\
+ g_2^{\mu}[q_1(m_a + \omega_{ap}) - p_1(m_a + \omega_{aq})]), 
\tag{25}
\]

\[
K_3^{\mu}(p, q, m_a) = i(g_0^{\mu}(p_2 q_3 - q_2 p_3) + g_2^{\mu}[p_3(m_a + \omega_{aq}) - q_3(m_a + \omega_{ap})] \\
+ g_3^{\mu}[q_2(m_a + \omega_{ap}) - p_2(m_a + \omega_{aq})]), 
\tag{26}
\]

\[
K_4^{\mu}(p, q, m_a) = g_0^{\mu}(p_1 q_3 - q_1 p_3) + g_1^{\mu}[p_3(m_a + \omega_{aq}) - q_3(m_a + \omega_{ap})] \\
+ g_3^{\mu}[q_1(m_a + \omega_{ap}) - p_1(m_a + \omega_{aq})], 
\tag{27}
\]

\(i = \sqrt{-1}, \ a = 1, 2, \ p^0 = \omega_{ap} \text{ and } p^j = p_j \text{ where } j = 1, 2, 3. \) Note that the subscripts on the vectors in equations (24)-(27), unlike elsewhere, denote the components of the generic vectors \(p\) and \(q\).
The sign \( \mp \) in eq. (22) are taken to be \(-\) if particle 3 has spin projection \( m_s = 1/2 \) (i.e. spin up) or \(+\) if particle 3 has spin projection \( m_s = -1/2 \) (i.e. spin down). Also note that the matrix element corresponding to the interaction between particles 1 and 3 is identical to the matrix element corresponding to the interaction between particles 2 and 3 (particles 1 and 2 are identical so that their respective interactions with particle 3 provide identical contributions to the energy); hence the factor 2 in front of \( \langle H_{13} \rangle \) in eq. (16).

In practice, calculations are done in the rest frame, for which \( f(p_1, p_2, p_3) = \delta^3(p_1 + p_2 + p_3)f(p_1, p_2) \) where \( f(p_1, p_2) \) is an adjustable function (normalized to unity). So far no assumptions about the adjustable function \( f(q_1, q_2, q_3) \), or \( f(p_1, p_2) \) in the rest frame, have been made. For relativistic variational approximations valid at arbitrary strength of the coupling, \( f \) would be expressed by analytic forms with adjustable features (parameters), which would be chosen to minimize the expectation value of the Hamiltonian (eq. (16)). However, as already stated, we shall not pursue such a variational approach in this work. Instead, we shall obtain perturbative solutions which are valid for weak coupling.

To obtain the order \( \alpha^4 \) contributions to the three-fermion energy we expand \( \omega_{ij} \) and all kernels in the above equations to lowest order beyond their non-relativistic limit (the explicit forms are given in ref. [9]). We use the Coulomb gauge. The resulting expression for the energy is

\[
E = 2m_1 + m_3 + E_0 + \Delta E
\]  

(28)

where

\[
E_0 = \int d^3q_1 d^3q_2 \left[ \frac{q_1^2}{2m_1} + \frac{q_2^2}{2m_1} + \frac{|q_1 + q_2|^2}{2m_3} \right] |f(q_1, q_2)|^2
- \frac{2Z ne^2}{(2\pi)^3} \int d^3p_1 d^3q_1 d^3q_2 \frac{f^*(q_1, q_2) f(p_1, q_2)}{|p_1 - q_1|^2}
+ \frac{e^2}{(2\pi)^3} \int d^3p_1 d^3q_1 d^3q_2 \frac{f^*(q_1, q_2) f(p_1, q_1 + q_2 - p_1)}{|p_1 - q_1|^2}
\]  

(29)

and

\[
\Delta E = \Delta KE + \sum_{i=1}^3 \Delta PE_{12i} + 2 \sum_{i=1}^4 \Delta PE_{13i},
\]  

(30)

where

\[
\Delta KE = -\frac{1}{8} \int d^3q_1 d^3q_2 \left[ \frac{q_1^4}{m_1^4} + \frac{q_2^4}{m_1^4} + \frac{|q_1 + q_2|^4}{m_3^4} \right] |f(q_1, q_2)|^2,
\]  

(31)

\[
\Delta PE_{131} = \frac{Z_ne^2}{8(2\pi)^3} \left( \frac{1}{m_1^4} + \frac{1}{m_3^4} \right) \int d^3p_1 d^3q_1 d^3q_2 f^*(q_1, q_2) f(p_1, q_2),
\]  

(32)

\[
\Delta PE_{132} = -\frac{Z_ne^2}{m_1 m_3 (2\pi)^3} \int d^3p_1 d^3q_1 d^3q_2 f^*(q_1, q_2) f(p_1, q_2) \frac{|p_1 \times q_1|^2}{|p_1 - q_1|^4},
\]  

(33)
\[ \Delta PE_{133} = -\frac{Z_n e^2}{2m_1 m_3 (2\pi)^3} \int d^3 p_1 d^3 q_1 d^3 q_2 f^*(q_1, q_2) f(p_1, q_2) \frac{(p_1 + q_1) \cdot q_2}{|p_1 - q_1|^2}, \]  
\[ \Delta PE_{134} = -\frac{Z_n e^2}{2m_1 m_3 (2\pi)^3} \int d^3 p_1 d^3 q_1 d^3 q_2 f^*(q_1, q_2) f(p_1, q_2) \frac{(p_1^2 - q_1^2)(p_1 - q_1) \cdot q_2}{|p_1 - q_1|^4}, \]
\[ \Delta PE_{121} = \frac{e^2}{4m_1^2 (2\pi)^3} \int d^3 p_1 d^3 q_1 d^3 q_2 f^*(q_1, q_2) f(p_1, q_1 + q_2 - p_1), \]
\[ \Delta PE_{122} = -\frac{e^2}{2m_1^2 (2\pi)^3} \int d^3 p_1 d^3 q_1 d^3 q_2 f^*(q_1, q_2) f(p_1, q_1 + q_2 - p_1) \frac{(p_1 + q_1) \cdot q_2}{|p_1 - q_1|^2}, \]
\[ \Delta PE_{123} = -\frac{e^2}{2m_1^2 (2\pi)^3} \int d^3 p_1 d^3 q_1 d^3 q_2 f^*(q_1, q_2) f(p_1, q_1 + q_2 - p_1) \times \frac{(p_1^2 - q_1^2)(p_1 - q_1) \cdot q_2}{|p_1 - q_1|^4}. \]

Note that the expressions for the energy in equations (28)-(38) do not depend on the spin projection of particle 3; therefore, both trial states yield the same kinetic, potential and total energy.

In order to evaluate perturbatively the relativistic corrections, \( \Delta E \), from equations (31), (32)-(38), \( f(p_1, p_2) \) should be a solution of the three-body Schrödinger equation. However, exact solutions of this equation are not available; therefore, we shall use simple variational wave functions that will allow for the approximate evaluation of the non-relativistic expression \( E_0 \) for the energy in eq. (29) and the relativistic correction terms in equations (31), (32)-(38).

The \( \mu^+e^-e^- \), Ps\(^-\) and \( \text{H}^- \) ions have only one bound state, namely the ground state, which we shall represent by the simple (but sufficient for our purposes) wave function with two distance-scale parameters. In coordinate representation this wave function is

\[ \psi(x_1, x_2) = \frac{1}{\sqrt{N}} \phi_{100}(x_1, Z_1) \phi_{100}(x_2, Z_2) + \phi_{100}(x_1, Z_2) \phi_{100}(x_2, Z_1), \]  
\[ \phi_{100}(x_i, Z_j) = R_{10}(x_i, Z_j) Y_0^0(\theta_i, \phi_i), \]
\[ R_{10}(x_i, Z_j) = 2\sqrt{a_j^2 e^{-a_j x_i}}, \]

\( (i, j = 1, 2), a_j = Z_j \alpha \) and \( N \) is the normalization factor. The wave function, Eq. (39), consists of hydrogenic 1s forms for the two electrons but with two different distance scale parameters \( Z_1 \) and \( Z_2 \). The explicit expressions for \( E_0 \) and \( \Delta E \) as functions of the parameters \( Z_1 \) and \( Z_2 \) are given in the Appendix.

5 Numerical results and discussion

The minimum value of \( E_0(Z_1, Z_2) \) and corresponding values of the variational parameters for Mu\(^-\), as well as for Ps\(^-\) and \( \text{H}^- \) are given in Table 1. We use the values \( m_e = 510999.137 \) eV and \( \alpha = 1/137.03599911 \) and the conversion factors 1 au = 27.2113962 eV and 1 Ry = 13.6056981 eV. The
Table 1: Non-relativistic variational energies $E_0$ and the corresponding optimum values for $Z_1$, $Z_2$, along with very accurate values obtained from the literature, for the ground states of Ps$^-$, Mu$^-$ and $^1$H$^-$. $E_0$ is expressed in eV and converted to atomic units ($1 \text{ au} = 27.2113962 \text{ eV}$) or Rydbergs ($1 \text{ Ry} = 13.6056981 \text{ eV}$). The terms in brackets for $^1$H$^-$ are results obtained for the case where the mass of the nucleus is assumed to be infinite.

| System          | Description                              | Value                  |
|-----------------|------------------------------------------|------------------------|
| **Ps$^-$ ground state** | $m_3$ (rest mass energy of a positron) | 510999.137 eV          |
|                 | $Z_1$                                    | 1.03922997             |
|                 | $Z_2$                                    | 0.283221430            |
|                 | $E_0$ energy from Drake and Grigorescu [4] | -6.98384409 eV=-0.513302885 Ry |
|                 | binding energy of $e^+e^-$               | -0.52401014046596021539 Ry |
| **Mu$^-$ ground state** | $m_3$ (rest mass energy of $\mu^+$) | 105658403 eV           |
|                 | $Z_1$                                    | 1.03922997             |
|                 | $Z_2$                                    | 0.283221432            |
|                 | $E_0$ energy from Frolov [5]             | -13.9004610 eV=-0.510832331 au |
|                 | binding energy of $\mu^+e^-$             | -0.5250548062435263292914 au |
| **$^1$H$^-$ ground state** | $m_3$ (rest mass energy of $^1$H$^-$ nucleus) | 938272446 eV          |
|                 | $Z_1$                                    | 1.03922997             |
|                 | $Z_2$                                    | 0.283221432            |
|                 | $E_0$ energy from Frolov [5]             | -13.9600853 eV=-0.513023483 au |
|                 | binding energy of $^1$H                  | -13.5402131 eV         |
|                 | binding energy of $^1$H                  | -0.527445881141788934109 au |

values of the scale parameters, which are $Z_1 \simeq 1$ and $Z_2 \simeq 0.28$ for all three systems, indicate that each can be pictured as an electron orbiting a neutral atom. We also list very accurate variational energies obtained with many parameter wave functions by Drake and Grigorescu [4] for Ps$^-$ and by Frolov [5] for Mu$^-$ and H$^-$. 

Note that the simple variational predictions of the non-relativistic ground state energies differ from the very accurate values by 2.04%, 2.71% and 2.74% for Ps$^-$, Mu$^-$ and H$^-$ respectively. This implies that the relativistic $O(\alpha^4)$ corrections calculated with the simple wave function Eq. (39) will be uncertain by a corresponding amount. The values of the relativistic $O(\alpha^4)$ contributions to the energy, $\Delta E(Z_1, Z_2)$ (cf. Eq.(30)) for the three systems, Ps$^-$, Muonium$^-$ and H$^-$, evaluated by using the wave function (39), with the $Z_1, Z_2$ values of Table 1, are exhibited in Table 2. For Ps$^-$, we also list the results obtained by Drake and Grigorescu [4], Frolov [10] and Bhatia and Drachman.
Table 2: Non-relativistic values for $Z_1$, $Z_2$ and $E_0$ (cf. Table 1) and the corresponding $O(\alpha^4)$ energy corrections $\Delta E$ (in eV), obtained by using these $Z_1$, $Z_2$ values, for the ground state of $\text{Ps}^-$, $\text{Mu}^-$ and $^1\text{H}^-$. Results for $\Delta E$ for $\text{Ps}^-$ obtained by other workers are included for comparison.

| Term          | System      |             |             |             |
|---------------|-------------|-------------|-------------|-------------|
|               | $\text{Ps}^-$ | $\text{Mu}^-$ | $^1\text{H}^-$ |
| $Z_1$         | 1.03922997  | 1.03922997  | 1.03922997  |
| $Z_2$         | 2.83221430 × 10^{-1} | 2.83221432 × 10^{-1} | 2.83221432 × 10^{-1} |
| $E_0$         | -6.98384409 | -13.9004610 | -13.9600853 |
| $\Delta KE$   | -1.11369869 × 10^{-4} | -8.48276777 × 10^{-4} | -8.62924906 × 10^{-4} |
| $\Delta PE$   | 0.11061221 × 10^{-4} | 7.40544121 × 10^{-4} | 7.56110074 × 10^{-4} |
| $\Delta E$    | -1.00308648 × 10^{-4} | -1.07732656 × 10^{-4} | -1.06814831 × 10^{-4} |
| $\Delta E^{\text{Drake,Grigorescu}}$ | -1.05400674 × 10^{-4} |               |             |
| $\Delta E^{\text{Frolov}}$ | -0.914436125 × 10^{-4} |               |             |
| $\Delta E^{\text{Bhatia,Drachman}}$ | -0.91702290 × 10^{-4} |               |             |

Examine the results presented in Table 2, we note that the $O(\alpha^4)$ corrections for each of $\text{Ps}^-$, $\text{Mu}^-$ and $^1\text{H}^-$, are smaller in magnitude by a factor of the order of $\alpha^2$ in comparison to the non-relativistic energies $E_0$, as is to be expected and as happens also in the two-fermion systems $\text{Ps}$, $\text{Mu}$ ($\mu^+e^-$) and $\text{H}$.

We note that the entries in Table 2 for $\text{Mu}^-$ and $^1\text{H}^-$ are quite similar, as one might expect, since $m_e/m_\mu$ and $m_e/m_p$ are both much less than 1, so that recoil effects are small. It is interesting to note, however, that $\Delta E$ is very similar for all three systems, $\text{Ps}^-$, Muonium$^-$ and $^1\text{H}^-$ even though kinetic and potential energy contributions differ substantially between $\text{Ps}^-$ on the one hand, and $\text{Mu}^-$ and $^1\text{H}^-$ on the other.

Our results for $\Delta E$ for $\text{Ps}^-$ agree quite well with the corresponding results obtained by Drake and Grigorescu [4], Frolov [10] and Bhatia and Drachman [11]. This suggests that our results for $\Delta E$ for $\text{Mu}^-$ are of reasonable accuracy as well. As far as we know no previous calculations of $\Delta E$ for $\text{Mu}^-$ have been reported in the literature.

At this time experimental measurements of the $\text{Ps}^-$ and $\text{Mu}^-$ binding energy are not available, although plans to make such measurements for $\text{Ps}^-$ are being considered [3]. We expect that measurements for $\text{Mu}^-$ will also be forthcoming in the future.

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APPENDIX

Expectation values for the non-relativistic ground state energy:

\( (m_1 = m_2 = m, \ m_3 = M, \ \mu = mM/(m + M)) \)

\[
E_0(Z_1, Z_2) = \langle \hat{K} \rangle + \langle \hat{V}_{13} \rangle + \langle \hat{V}_{23} \rangle + \langle \hat{V}_{12} \rangle
\]

\[
\langle \hat{K} \rangle = \frac{\mu \alpha^2}{N} \left( \frac{26Z_1^6Z_2^3 + 158Z_1^4Z_2^2 + 16Z_1^2Z_2 + 16Z_1^2Z_2}{Z_2 + Z_1} \right) + \frac{26Z_1Z_2^6 + 6Z_1Z_2 + Z_2^6 + 6Z_2Z_1}{(Z_2 + Z_1)^6},
\]

\[
\langle \hat{V}_{13} \rangle = \langle \hat{V}_{23} \rangle = -\frac{1}{2}Z_n \mu \alpha^2(Z_1 + Z_2).
\]
\begin{align*}
\langle \hat{V}_{12} \rangle &= 2\mu \alpha^2 \frac{Z_1 Z_2}{N(Z_2 + Z_1)^3} 28\frac{Z_1^2 Z_2^2}{Z_2} + 5\frac{Z_1 Z_2}{Z_2} + \frac{Z_1^2}{Z_2} + 5\frac{Z_1}{Z_2}.
\end{align*}

\(N = 2 \left[ 1 + \frac{64Z_1^3 Z_2^3}{(Z_1 + Z_2)^6} \right] = 2 \frac{15Z_1^3 Z_2^2 + 15Z_1 Z_2^2 + Z_1^2 + 84Z_1 Z_2^2 + Z_1^2 + 6Z_1^3 Z_2 + 6Z_2^2 Z_1}{(Z_2 + Z_1)^6}.\)

The minimum values of \(E_0(Z_1, Z_2)\) and the corresponding values of \(Z_1\) and \(Z_2\) are given in Table 1.

Expectation values for the relativistic corrections:

\begin{align*}
\Delta KE &= -\frac{\mu^4 \alpha^4}{4N(Z_2 + Z_1)^6} \left( \frac{1}{m^3} + \frac{1}{M^3} \right) (5Z_1^{10} + 30Z_2 Z_1^9 + 75Z_1^7 Z_2^2 \\
&+ 100Z_2^2 Z_1^7 + 208Z_2^4 Z_1^5 + 444Z_2^5 Z_1^6 + 208Z_2^6 Z_1^5 + 100Z_2^8 Z_1^3 \\
&+ 75Z_1^2 Z_2 + 30Z_2 Z_1 + 5Z_1^{10} ) - \frac{5\mu^4 \alpha^4 Z_1^2 Z_2^2}{6M^4N(Z_2 + Z_1)^6} (15Z_1^2 Z_2 \\
&+ 15Z_2 Z_1^2 + Z_2^2 + 84Z_1 Z_2^2 + Z_1^2 + 6Z_1^3 Z_2 + 6Z_2^2 Z_1),
\end{align*}

\begin{align*}
\Delta PE_{131} &= \frac{\mu^3 \alpha^4 Z_1^2 (M^2 + m^2)}{2M_2 m^2 N(Z_2 + Z_1)^3} (Z_1^6 + 3Z_1^5 Z_2 + 3Z_1^4 Z_2^2 \\
&+ 18Z_1^3 Z_2^3 + 3Z_1^2 Z_2^4 + 3Z_2 Z_1 + Z_2^3),
\end{align*}

\begin{align*}
\Delta PE_{132} &= -\frac{Z_1^2 m \mu^3 \alpha^4}{m M N(Z_2 + Z_1)^3} \left( 5Z_1^7 Z_1 + 10Z_1^6 Z_2 + Z_2^6 + 11Z_1^5 Z_2 \\
&+ 5Z_1^2 Z_2 + 74Z_1 Z_2^2 + 11Z_1^3 Z_2^5 + 10Z_2^2 Z_2 + Z_1^5 \right),
\end{align*}

\begin{align*}
\Delta PE_{133} = \Delta PE_{134} &= 0,
\end{align*}

\begin{align*}
\Delta PE_{121} &= \frac{4\mu^3 \alpha^4 Z_1 Z_2^2}{m^2 N(Z_2 + Z_1)^3},
\end{align*}

\begin{align*}
\Delta PE_{122} = -\Delta PE_{123} &= -\frac{2\mu^3 \alpha^4 Z_1 Z_2^3 (Z_2 - Z_1)^2}{m^2 N(Z_2 + Z_1)^3},
\end{align*}

where \(N\) is given in eq. (45).

\begin{align*}
\Delta E = \Delta KE + \Delta PE &= \Delta KE + \Delta PE_{12} + 2\Delta PE_{13},
\end{align*}

\begin{align*}
\Delta PE_{13} &= \sum_{i=1}^{4} \Delta PE_{13i},
\end{align*}

\begin{align*}
\Delta PE_{12} &= \sum_{i=1}^{3} \Delta PE_{12i}.
\end{align*}

These expressions for \(\Delta E = \Delta KE + \Delta PE\), evaluated using the parameters given in Table 1, are listed in Table 2.

Analogous expressions for the first two excited states (relevant for \(Z_n > 1\), \textit{i.e.} He-like systems) are given in ref. [9].