Few-body model approach to the bound states of helium-like exotic three-body systems

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Abstract. In this paper, calculated energies of the lowest bound S-state of Coulomb three-body systems containing an electron (\(e^-\)), a negatively charged muon (\(\mu^-\)) and a nucleus (\(N^{Z\pm}\)) of charge number Z are reported. The 3-body relative wave function in the resulting Schrödinger equation is expanded in the complete set of hyperspherical harmonics (HH). Use of the orthonormality of HH leads to an infinite set of coupled differential equations (CDE) which are solved numerically to get the energy E.

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1. Introduction

Atoms and ions containing exotic particles like muon, kaon, taon, baryon and their antimatters are of immense have become an interesting research topic in many branches of physics including atomic, nuclear and elementary particle physics, plasma and astrophysics, experimental physics [1, 2]. Apart from being the simplest exotic atom formed by replacing an orbital electron of neutral helium, the muonic helium atom (\(^{4}\text{He}^{2+}\mu^- e^-\)) is an important topic of investigation since its first formation and detection by Souder et al [3]. Muon being about 207 times heavier than an electron, the size of the muonic helium atom is smaller by a factor of about 1/400 of the ordinary electronic helium atom. Muonic helium atoms are the unusual pure atomic three body systems without any restriction due to Pauli exclusion principle for electron and muon being non-identical fermions. These are formed as by-products of the process of muon catalyzed fusion, hence are useful to understand the fusion reactions properly [4, 5]. The electromagnetic interaction between the electron and negatively charged muon can be better understood by this simplest muonic system by precise measurements of hyperfine structure [6, 7].

As exotic particles are mostly unstable, their parent atoms (or ions) are also very short lived. These exotic short-lived atoms or ions can be formed by trapping the accelerated exotic particles inside matter and replacing one or more electron(s) in an ordinary atom by exotic particle(s). The absorbed exotic particle revolves round the...
nucleus of the target atom in orbit of radius equal to that of the electron before its
ejection from the atom, which subsequently cascades down the ladder of resulting
exotic atomic states by the emission of X-rays and Auger transitions before being
lost on its way to the nucleus. If the absorbed exotic particle is a negatively charged
muon, it passes through various intermediate atmospheres before being trapped in
the vicinity of the atomic nucleus [8]. In the course of its journey inside the matter,
it scatters from atom to atom as free electron and gradually loses its energy until
it is captured into an atomic orbit. In the lowest energy level (1S), it experiences
only Coulomb interaction with nuclear protons while it experiences weak interaction
with the rest of the nucleons. As discussed above, exotic muonic atoms (or ions) are
produced by replacing one or more electron(s) of neutral atoms by one or more exotic
particle(s) like muon, pion, kaon, anti-proton having an electric charge equal to that
of the electron [9]. The most studied exotic few-body Coulomb system are the muonic
atoms (or muonic ions) which are formed by removing one or more orbital electron(s)
by one or more negatively charged muon(s). However the present communication we
shall consider only those atoms or ions in which the positively charged nucleus is being
orbited by one electron and one negatively charged muon.

These atoms have been under theoretical scanner of several authors [10, 11, 12,
13, 14, 15, 16, 17, 18, 19, 20, 21, 22, 23, 24, 25, 26] for being investigated. In this
communication, we adopt hyperspherical harmonics expansion (HHE) approach for a
systematic study of the ground state of atoms/ ions containing an orbital electron plus
a negatively charged muon revolving round the positively charged nucleus forming a
three-body system. In our model, we assume that the electromagnetic interaction
of the valence particles with the nucleus is sufficiently weak to influence the internal
structure of the nucleus. Again, the fact that the muon is much lighter than the nucleus
allows us to regard the nucleus to remain a static source of electrostatic interaction.
However, a hydrogen-like two-body model, consisting a quasi-nucleus (µ−N(Z−2)+,
formed by the muon and the nucleus) plus an orbital electron can also be tested due
to much smaller size of muonic orbital than that for an electronic orbital.

In HHE formalism for a general three-body system of three unequal mass particles
the choice of Jacobi coordinates correspond to three different partitions and in the
i-th partition, particle labeled by ‘i’ remains as a spectator while the remaining two
particles labeled ‘j’ and ‘k’ form the interaction pair. So the total potential contains
three binary interaction terms (i.e. $V = V_{jk}(r_{jk}) + V_{ki}(r_{ki}) + V_{ij}(r_{ij})$) and for
computation of matrix element of $V(r_{ij})$, potential of the (ij) pair, the chosen HH is
expanded in the set of HH corresponding to the partition in which $r_{ij}$ is proportional
to the first Jacobi vector [27] by the use of Raynal-Revai coefficients (RRC) [28].
The energies obtained for the lowest bound S-state is compared with the ones of the
literature.

In Section II, we briefly introduce the hyperspherical coordinates and the scheme
of the transformation of HH belonging to two different partitions. Results of
calculation and discussions will be presented in Section III and finally we shall draw
our conclusion in section IV.

2. HHE Method

The choice of Jacobi coordinates for systems of three particles of mass $m_i$, $m_j$, $m_k$ is
shown in Fig.1.
The Jacobi coordinates \([29]\) in the \(i^{th}\) partition can be defined as:

\[
\begin{align*}
\vec{x}_i &= \left[ \frac{m_i m_k}{m_i + m_j + m_k} \right]^{\frac{1}{2}} \left( \vec{r}_j - \vec{r}_k \right) \\
\vec{y}_i &= \left[ \frac{m_i (m_j + m_k)}{m_i + m_j + m_k} \right]^{\frac{1}{2}} \left( \vec{r}_i - \frac{m_j \vec{r}_j + m_k \vec{r}_k}{m_i + m_j + m_k} \right) \\
\vec{R} &= \left( m_i \vec{r}_i + m_j \vec{r}_j + m_k \vec{r}_k \right) / M
\end{align*}
\]

\(1\)

where \(M = m_i + m_j + m_k\) and the sign of \(\vec{x}_i\) is determined by the condition that \((i,j,k)\) should form a cyclic permutation of \((1, 2, 3)\).

The Jacobi coordinates are connected to the hyperspherical coordinates \([30]\) as

\[
\begin{align*}
x_i &= \rho \cos \phi_i; \quad y_i = \rho \sin \phi_i; \\
\rho &= \sqrt{x_i^2 + y_i^2}; \quad \phi_i = \tan^{-1}(\eta_i / \Psi_i)
\end{align*}
\]

\(2\)

The relative three-body Schrödinger's equation in hyperspherical coordinates can be written as

\[
\left[ -\frac{\hbar^2}{2\mu} \left( \frac{\partial^2}{\partial \rho^2} + \frac{5}{\rho} \frac{\partial}{\partial \rho} + \frac{\hat{K}^2(\Omega_i)}{\rho^2} \right) + V(\rho, \Omega_i) - E \right] \Psi(\rho, \Omega_i) = 0
\]

\(3\)

where \(\Omega_i \rightarrow \{\phi_i, \theta_{x_i}, \phi_{x_i}, \theta_{y_i}, \phi_{y_i}\}\), effective mass \(\mu = \left[ \frac{m_i m_j m_k}{m_i + m_j + m_k} \right]^2\), potential \(V(\rho, \Omega_i) = V_{ij} + V_{ki} + V_{ij}\). The square of hyper angular momentum operator \(\hat{K}^2(\Omega_i)\) satisfies the eigenvalue equation \([30]\)

\[
\hat{K}^2(\Omega_i) Y_{K\alpha_i}(\Omega_i) = K(K + 4) Y_{K\alpha_i}(\Omega_i)
\]

\(4\)

where the eigen function \(Y_{K\alpha_i}(\Omega_i)\) is the hyperspherical harmonics (HH). An explicit expression for the HH with specified grand orbital angular momentum \(L(= l_{x_i}^2 + l_{y_i}^2)\) and its projection \(M\) is given by

\[
Y_{K\alpha_i}(\Omega_i) \equiv Y_{Kl_{x_i}l_{y_i}}^{\alpha_i}(\phi_i, \theta_{x_i}, \phi_{x_i}, \theta_{y_i}, \phi_{y_i}) = \left( 2 \right) P_{Kl_{x_i}l_{y_i}}^{\alpha_i} \left[ Y_{l_{x_i}}^{m_{x_i}} (\theta_{x_i}, \phi_{x_i}) Y_{l_{y_i}}^{m_{y_i}} (\theta_{y_i}, \phi_{y_i}) \right]_{LM}
\]

\(5\)

with \(\alpha_i \equiv \{l_{x_i}, l_{y_i}, L, M\}\) and \([_]_{LM}\) denoting angular momentum coupling. The hyper-angular momentum quantum number \(K(= 2n_i + l_{x_i} + l_{y_i}; n_i \rightarrow \text{a non-negative integer})\)
is not a conserved quantity for the three-body system. In a given partition (say partition “i”), the wave-function \( \Psi(\rho, \Omega_i) \) is expanded in the complete set of HH

\[
\Psi(\rho, \Omega_i) = \sum_{K\alpha_i} \rho^{-5/2} U_{K\alpha_i}(\rho) \tilde{Y}_{K\alpha_i}(\Omega_i)
\]  

(6)

Substitution of Eq. (6) in Eq. (3) and use of ortho-normality of HH, leads to a set of coupled differential equations (CDE) in \( \rho \)

\[
-\frac{h^2}{2\mu} \frac{d^2}{d\rho^2} + \left( \frac{(K+3/2)(K+5/2)\hbar^2}{2\mu \rho^2} - E \right) U_{K\alpha_i}(\rho)
+ \sum_{K'\alpha'_i} < K\alpha_i | V(\rho, \Omega_i) | K'\alpha'_i > U_{K'\alpha'_i}(\rho) = 0.
\]  

(7)

where

\[
< K\alpha_i | V(\rho, \Omega_i) | K'\alpha'_i > = \int \tilde{Y}_{K\alpha_i}^*(\Omega_i)V(\rho, \Omega_i)\tilde{Y}_{K'\alpha'_i}^*(\Omega_i) d\Omega_i
\]  

(8)

3. Results and discussions

For the present calculation, we assign the label ‘i’ to the nucleus of mass \( m_i = m_N \) (and charge +Ze), the label ‘j’ to the negatively charged muon of mass \( m_j = m_\mu \) (and charge -e) and the label ‘k’ to the electron of mass \( m_k = m_e \) (and charge -e). Hence, for this particular choice of masses, Jacobi coordinates of Eq. (1) in the partition “i” become

\[
\begin{align*}
\vec{x}_i &= \left[ \frac{m_\mu m_e (m_N + m_\mu + m_e)}{m_N (m_N + m_\mu + m_e)^2} \right]^{1/2} (\vec{r}_j - \vec{r}_k) \\
\vec{y}_i &= \left[ \frac{m_\mu m_e (m_N + m_\mu + m_e)}{m_N (m_N + m_\mu + m_e)^2} \right]^{-1/2} (\vec{r}_j - \frac{m_\mu \vec{r}_j + m_e \vec{r}_k}{m_N + m_\mu + m_e})
\end{align*}
\]  

(9)

and the corresponding Schrödinger equation (Eq. (7)) is

\[
\begin{align*}
-\frac{h^2}{2\mu} &\left\{ \frac{d^2}{d\rho^2} - \frac{(K+3/2)(K+5/2)\hbar^2}{2\mu \rho^2} \right\} - E \right) U_{K\alpha_i}(\rho)
+ \sum_{K'\alpha'_i} < K\alpha_i | \frac{\beta_i}{\rho \cos \phi_i} - \frac{\beta_i \sin \phi_i}{\rho \sin \phi_i} \frac{Z}{\rho} \left[ \frac{\beta_i}{\sin \phi_i} \frac{\vec{y}_i - \frac{\beta_i}{\sin \phi_i} \vec{x}_i}{\cos \phi_i} \right] | K'\alpha'_i > U_{K'\alpha'_i}(\rho) = 0
\end{align*}
\]  

(10)

where \( \beta_i = \left[ \frac{m_\mu m_e (m_N + m_\mu + m_e)}{m_N (m_N + m_\mu + m_e)^2} \right]^{1/2} \) and \( \mu = \left( \frac{m_N m_\mu m_e}{m_N + m_\mu + m_e} \right)^{1/2} \) is the effective mass of the system. In atomic units we take \( \hbar^2 = m_e = e^2 = 1 \). Masses of the particles involved in this work are partly taken from [30, 31, 32, 33].

In the ground state of electron-muon three-body system, the total orbital angular momentum, \( L=0 \) and there is no restriction (on \( l_{x_i} \)) due to Pauli exclusion principle as electron and muon are non-identical fermions. Since \( L = 0 \), \( l_{x_i} = l_{y_i} \), and the set of quantum numbers represented by \( \alpha_i \) is \{\( l_{x_i}, l_{y_i}, 0,0 \)\}. Hence, the quantum numbers \( \{K\alpha_i\} \) can be represented by \( \{Kl_{x_i}\} \) only. Eq. (10) is solved following the method described in our previous work [30] to get the ground state energy \( E \).

One of the major drawbacks of HH expansion method is its slow rate of convergence for Coulomb-type long range interaction potentials, unlike for the Yukawa-type short-range potentials for which the convergence is reasonably fast [29, 34]. Hence, to achieve the desired degree of convergence, sufficiently large \( K_m \) value has to be included in the calculation. But, if all \( K \) values up to a maximum of \( K_m \) are
included in the HH expansion then the number of the basis states can be determined by relation

\[ N_{K_m} = \frac{(K_m + 2)(K_m + 4)}{8} \quad (11) \]

It follows from Eq. (11) that number of basis states and hence the size of coupled differential equations (CDE) (Eq. (7)) increases rapidly with increase in \( K_m \). For the available computer facilities, we are allowed to solve up to \( K_m = 28 \) reliably.

The calculated ground state energies \( (B_{K_m}) \) with increasing \( K_m \) for muonic helium \((\infty He^{2+}\mu^-e^-)\), muonic lithium \((\infty Li^{3+}\mu^-e^-)\) and muonic beryllium \((\infty Be^{4+}\mu^-e^-)\) are presented in columns 2, 4 and 6 of Table 1. Energies for a number of muonic atom/ions of different atomic number (Z) at \( K_m = 28 \) are presented in column 4 of Table 2. The pattern of convergence of the energy of the lowest bound S-state with respect to increasing \( K_m \) can be checked by gradually increasing \( K_m \) values in suitable steps \((dK)\) and comparing the relative energy difference \( \eta = \frac{B_{K_{m+dK}} - B_{K_m}}{B_{K_{m+4}} - B_{K_{m+2}}} \) with that found in the previous step. From Table 1, it can be seen that at \( K_m = 28 \), the energy of the lowest bound S-state of \( e^-\mu^-\infty He^{2+} \) converges up to 3rd decimal places and similar convergence trends are observed in the remaining cases. The pattern of increase in binding energy (B) with respect to increasing \( K_{max} \) is shown in Figure 3 for few representative cases. In Figure 4 the relative energy difference \( \eta \) is plotted against \( K_{max} \) to demonstrate the relative convergence trend in energy. The calculated ground state energies muonic three-body systems of different nuclear charge \( Z \) (and of infinite nuclear mass), have been plotted against \( Z \) as shown in Figure 4 to study the dependence of the bound state energies on the strength of the nuclear charge using data from Table 2. The curve of Figure 4 shows a gradual increase in energy with the increase in the strength nuclear charge \( Z \) approximately following the empirical equation

\[ B(Z) = -154.64851 + 4.47088Z + 131.84786Z^2 \]
\[ -2.79311Z^3 + 0.02174Z^4 \quad (12) \]

Eq. (12) may be used to estimate the ground state energy of muonic atom/ions of given \( Z \) assuming infinite nuclear core. Finally, in Table 2, energies of the lowest bound

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**Figure 2.** Pattern of dependence of the ground-state energy (B) of muonic atom/ions on the increase in \( K_{max} \).

**Figure 3.** Pattern dependence of the ground-state relative energy difference \( \eta = \frac{B_{K_{m+dK}} - B_{K_m}}{B_{K_{m+4}} - B_{K_{m+2}}} \) of muonic helium \((\infty He^{2+}\mu^-e^-)\) on the increase in \( K_{max} \).
Figure 4. Pattern of dependence of the ground-state energy (B) of muonic atom/ions on the increase in nuclear charge Z.

S-state of several muonic three-body systems obtained by numerical solution of the coupled differential equations by the renormalized Numerov method [35] have been compared with the ones of the literature wherever available. Since reference values are not available for systems having nuclear charge $Z > 3$, we made a crude estimation of the ground-state ($1s_e1s_\mu$) energies following the relation

$$B_{est}^{3B} = \frac{A m_N Z^2}{2} \left[ \frac{1}{1 + A m_N} + \frac{m_\mu}{m_\mu + A m_N} \right]$$

(13)

where $m_N = 1836$ , muon mass $m_\mu = 206.762828$ (in atomic unit) and A is mass number of the nucleus. Here we assumed two hydrogen-like subsystems for the muonic atom/ions. This estimate can further be improved by assuming a compact $(A(Z),\mu^-)_1$, positive muonic ion and an electron in the 1s state, "feeling" a $(Z-1)$ charge and an $A m_N + m_\mu$ mass. For this case the estimation formula (Eq. (13)) can be replaced by

$$B_{est}^{2B} = \frac{1}{2} \left[ \frac{A m_N + m_\mu}{1 + A m_N + m_\mu} (Z-1)^2 + \frac{A m_N m_\mu}{m_\mu + A m_N} Z^2 \right]$$

(14)

4. Conclusion

In conclusion, we note that the calculated ground-state energy of muonic helium and muonic lithium at $K_m = 28$ listed in column 4 of Table 2 are greater than the corresponding reference values listed in column 5 of Table 2. This discrepancies may have arose due to the CUSP conditions applicable to Coulomb systems which have not been accommodated in the present calculations. It can be seen that the estimated energies ($B_{est}$) in columns 2 & 3 of Table 2 are less than the corresponding calculated energies ($B_{calc}$) in column 4 of Table 2 for systems having $Z \leq 10$ while the same for $Z > 10$ becomes larger than $B_{calc}$. This may happen due to weaker correlation between electron-muon pair in systems having nuclear charge $Z < 10$ while a stronger correlation in systems having $Z > 10$. It may also be noted that estimated energy listed in column 3 of Table 2 agrees fairly with the reference values.
Table 1. Energy (B) of the lowest bound S-state of electron-muon three-body systems at different $K_{\text{max}}$ along with the corresponding relative energy difference $\eta$.

| System | Binding energies (B) and corresponding relative energy difference ($\eta$) |
|--------|-------------------------------------------------|
| $K_{\text{max}}$ | $\infty \text{He}^3^+ \mu^- e^- \overline{\eta}$ | $\infty \text{Li}^3^+ \mu^- e^- \overline{\eta}$ | $\infty \text{Be}^4^+ \mu^- e^- \overline{\eta}$ |
| 0      | 217.78577 0.552207 490.78036 0.360783 798.35936 0.385798 |
| 4      | 336.19455 0.119097 767.78745 0.116652 1299.82240 0.148813 |
| 8      | 378.13425 0.055125 869.17847 0.052099 1523.49147 0.065150 |
| 12     | 400.19520 0.033222 916.86372 0.029708 1629.66350 0.033758 |
| 16     | 413.94723 0.022228 944.93547 0.019627 1686.59904 0.020329 |
| 20     | 423.35753 0.015913 963.85254 0.014046 1721.59813 0.013800 |
| 24     | 430.20330 0.011949 977.58415 0.010573 1745.68917 0.010153 |
| 28     | 435.40598 0.006945 988.03084 0.005984 1763.59496 0.006227 |

Table 2. Energy (B) of the lowest bound S-state of electron-muon-nucleus three-body systems.

| System | Binding energies expressed in atomic unit (a.u.) |
|--------|-------------------------------------------------|
| $e^- \mu^- \text{He}^3^+$ | Estimated | Calculated | Other Results |
| $e^- \mu^- \text{He}^4^+$ | $B_{\text{est}}^{B[13]} | B_{\text{est}}^{B[14]} | B_{K_{\text{max}}=28}$ |
| $e^- \mu^- \text{Li}^3^+$ | 400.574 399.064 420.424 399.042, 399.043$^b$ |
| $e^- \mu^- \text{Be}^4^+$ | 404.212 402.702 424.017 402.637, 402.641$^d$ |
| $e^- \mu^- \text{B}^5^+$ | 415.537 414.026 435.406 414.036, 414.037$^e$ |
| $e^- \mu^- \text{C}^6^+$ | 917.814 915.291 970.737 915.231, 915.231$^e$ |
| $e^- \mu^- \text{O}^8^+$ | 940.224 941.701 973.166 917.649, 917.650$^f$ |
| $e^- \mu^- \text{Ne}^{10^+}$ | 4154.957 413.423 488.031 932.457$^g$ |
| $e^- \mu^- \text{Ne}^{11^+}$ | 1641.703 1638.181 1745.087 |
| $e^- \mu^- \text{Ne}^{12^+}$ | 1662.146 1658.603 1763.595 |
| $e^- \mu^- \text{Ne}^{13^+}$ | 2568.319 2563.753 2732.374 |
| $e^- \mu^- \text{Ne}^{14^+}$ | 2597.104 2592.535 2761.200 |
| $e^- \mu^- \text{Ne}^{15^+}$ | 3705.224 3699.628 3937.535 |
| $e^- \mu^- \text{Ne}^{16^+}$ | 3739.829 3734.231 3971.528 |
| $e^- \mu^- \text{Ne}^{17^+}$ | 6602.337 6594.666 6907.068 |
| $e^- \mu^- \text{Ne}^{18^+}$ | 6648.585 6640.910 6949.141 |
| $e^- \mu^- \text{Ne}^{19^+}$ | 10330.524 10320.754 10486.654 |
| $e^- \mu^- \text{Ne}^{20^+}$ | 10388.414 10378.841 10534.362 |
| $e^- \mu^- \text{Ne}^{21^+}$ | 14889.783 14877.894 14539.329 |
| $e^- \mu^- \text{Ne}^{22^+}$ | 14959.316 14947.424 14590.826 |
| $e^- \mu^- \text{Ne}^{23^+}$ | 20280.115 20266.085 18956.238 |
| $e^- \mu^- \text{Ne}^{24^+}$ | 20361.291 20347.257 19010.171 |
| $e^- \mu^- \text{Ne}^{25^+}$ | 26501.520 26485.328 23653.644 |
| $e^- \mu^- \text{Ne}^{26^+}$ | 26594.340 26578.142 23709.055 |
| $e^- \mu^- \text{Ne}^{27^+}$ | 33564.416 33546.038 28574.053 |
| $e^- \mu^- \text{Ne}^{28^+}$ | 33564.416 33546.038 28574.053 |
| $e^- \mu^- \text{Ne}^{29^+}$ | 33658.461 33640.078 28624.646 |
| $e^- \mu^- \text{Ne}^{30^+}$ | 33658.461 33640.078 28624.646 |
| $e^- \mu^- \text{Ne}^{31^+}$ | 41473.550 41416.966 31352.978 |
| $e^- \mu^- \text{Ne}^{32^+}$ | 41553.656 41533.966 31379.888 |

$^a$Ref[2, 10, 11, 37], $^b$Ref[38], $^c$Ref[2, 10, 11, 38, 39], $^d$Ref[1, 20, 40], $^e$Ref[2], $^f$Ref[11], $^g$Ref[18]
for $Z=2,3$. Finally, it can also be added that in the cases of highly charged muonic ions relativistic correction together with proper inclusion of Kato’s cusp conditions [36] (in the limit $r_{jk} \to 0$) is important for obtaining improved results.

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