

Approximate Solution to the Schrödinger Equation of Exotic Doubly Muonic Helium-like Systems Using Hydrogenic-based Matrix Mechanics

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ABSTRACT. The approximate solution to the Schrödinger equation of exotic doubly muonic helium-like systems has been obtained using a simple matrix method based on hydrogenic *s*-states. Each system considered consists of a positively charged nucleus surrounded by 2 negatively charged muons $X^{Z+}_{\mu\mu}$ ($2 \leq Z \leq 36$). The present work aims to obtain approximate ground-state energies of the systems and to decompose the energies in terms of the basis states used. Here, the wave function was expressed as a linear combination of 15 eigenfunctions, each written as the product of two hydrogenic *s*-states. The elements of the Hamiltonian matrix were calculated and finally, the energy eigenvalue equation was numerically solved to obtain the ground-state energies of the systems with their corresponding eigenvectors. From the results, ground-state energies of all systems were in agreement with others from the literature, with percentage differences between 0.03% and 2.05%. The analysis of the probability amplitudes from the eigenvectors showed that the $1s1s$ state made the largest contribution to the ground state energies of the systems, approaching 90.99%, 96.98% and 98.54% for $\text{He}^{2+}_{\mu\mu}$, $\text{Li}^{3+}_{\mu\mu}$, and $\text{Be}^{4+}_{\mu\mu}$, respectively.

Keywords: Doubly muonic helium-like systems, ground state energy, hydrogenic basis states, matrix mechanics, Schrödinger equation

INTRODUCTION

A large number of theoretical and computational studies in chemistry has been applied to study various quantum systems ranging from atoms to materials. Some of such studies included the application of QCOMP 116 program in studying interactions of NH_3 molecule on the surface of chromium (Banon, 2010), Quantitative Structure-Activity Relationships (QSAR) analysis to obtain a design of calanone derivatives (Iswanto et al., 2011), Quantitative Structure-Property Relationships (QSPR) models (Delsy et al., 2017; Iswanto et al., 2019; Setiawan et al., 2020), and sparkle RM_1 method to perform a theoretical study on the electronic structure and spectrum of $[\text{Ln}(\text{pytpy})(\text{NO}_3)_3]$ complex ($\text{Ln}=\text{Eu}, \text{Tb}$, $\text{pytpy}=4'-(2\text{-pyrrolyl})-2,2':6',2''\text{-terpyridine}$) (Setiawan & Zulys, 2015). In addition, several recent studies using Density Functional Theory (DFT) were performed for various systems such as Cathinone imprinted polymer (Saputra et al., 2017), surfaces of pure and Sc-incorporated $\text{Mg}(0001)$ (Sutapa et al., 2010), nitrogen-doped diamond (Sholihun et al., 2018), and leuco-indigo and indigo (Maahury et al., 2020).

Among systems studied, quantum three-body systems play a crucial role in theoretical quantum

chemistry and physics as approximations proposed to solve the Schrödinger equation for these systems can be tested before being applied in studying more complex quantum systems. There has been a large number of theoretical investigations conducted for such systems. Some of the recent studies include the energy determination of the Helium atom using the shooting method (Hall & Siegel, 2015), Hartree-Fock method (Young et al., 2016), Laguerre-based functions (Kartono et al., 2005; Livertz & Barnea, 2012; Livertz & Barnea, 2014; King et al., 2018; Baskerville & Cox, 2019), variational method (Purwaningsih et al., 2019) and Rayleigh-Schrödinger perturbation theory (Montgomery et al., 2010). Similar studies have also been carried out such as those for helium-like ions (Mccarthy & Thakkar, 2011; Montgomery & Pupyshev, 2014; Montgomery et al., 2019) and positively charged molecular hydrogen (Pingak & Johannes, 2020).

In addition to helium atom and he-like ions, exotic muonic helium-like systems have been the focus of recent research. Muonic atoms or ions, which are formed by replacing one (or more) orbital electron(s) with one (or more) negatively charged muon(s), are the most studied exotic few-body Coulomb systems

(Khan, 2014). They have attracted researchers in both theoretical chemistry and physics because their physical and chemical properties have not been fully understood. More in-depth and comprehensive studies on these systems using various theoretical approaches are expected to enrich the understanding of the properties of these systems from the fundamental levels to the application levels (Putlitz, 1992). Furthermore, exotic three-body systems have become more significant in the field of physics and chemistry including atomic spectroscopy and quantum electrodynamics (Khan, 2014). Such systems include the muonic helium $\text{He}_{\mu^-e^-}$ which has been intensively investigated such as in (Bailey & Frolov, 2002; Eskandari & Rezaie, 2005; Frolov & Wardlaw, 2012; Frolov, 2012; Khan, 2016; Karshenboim et al., 2018; Aznabayev et al., 2018).

In contrast to the muonic helium $\text{He}_{\mu^-e^-}$ systems which are intensively studied and reported in the literature, only a few reports were found in the literature on exotic doubly muonic helium-like systems of the form $X^{Z+}_{\mu^-\mu^-}$, i.e. a core which is surrounded by two negatively charged valence muons. Theoretical and computational studies on the systems using different methods have been reported, including the use of boundary condition on the wavefunction (Eskandari & Rezaie, 2004), the application of an angular correlated configuration interaction method (Ancarani et al., 2010; Ancarani et al., 2011), hyperspherical harmonics (HH) expansion method involving the Raynal-Revai Coefficients (RRC) (Khan, 2012; Khan, 2014). Recently, the ground-state energy of the $\text{He}_{\mu^-\mu^-}$ was also calculated using the variational approach as presented in (Boimau et al., 2017). The application of other methods in studying these systems is therefore important to gain a much better understanding of the properties of these systems.

An alternative numerical method to solve the Schrödinger equation for two-electron systems was presented by Massé (Massé & Walker, 2015), who expanded the wavefunction of the helium atom in terms of hydrogenic basis states. Despite being simple and straightforward, the method yielded accurate low-lying state energies of the helium atom. The analytical solution to the Schrödinger equation using this method was also presented in (Pingak et al., 2019) and was proven accurate in obtaining energies of $1s^2$, $1s2s$ triplet and $1s2s$ singlet states. Besides, the extension of the method to determine the low-lying energies of helium-like ions was already performed in (Pingak & Deta, 2020; Pingak et al., 2021). The method, however, has not been applied to exotic three-body systems including the doubly exotic muonic helium-like systems $X^{Z+}_{\mu^-\mu^-}$ which should have similar properties to the helium atom and helium-like ions.

The present study focuses on exotic doubly muonic helium-like systems $X^{Z+}_{\mu^-\mu^-}$ ($2 \leq Z \leq 36$), which

consisted of a positively charged $+Ze$ core surrounded by two negatively charged valence muons. This work aims at obtaining an approximate solution to the Schrödinger equation for these systems using the matrix method based on hydrogenic s-states. From the solution, the ground state energies of the systems are determined with their corresponding energy eigenvectors. The spectral decomposition of the energies is also presented to investigate the composition of each hydrogenic basis state used to obtain the ground state energies of the systems. The comparisons to results from other calculations in the literature are also presented and discussed. The results of the present study will make a significant contribution to the field of doubly muonic systems as the majority of the systems studied here have not been investigated in previous studies both theoretically and experimentally. Moreover, this study demonstrates that with this method, reasonably accurate energies of quantum systems can be obtained, consistent with some recent studies using the matrix method on different systems, including anharmonic oscillators (Pingak et al., 2021) and the Morse oscillator (Pingak et al., 2023).

EXPERIMENTAL SECTION

Computational Details

Wave Function Expansion

The time-independent Schrödinger solved in this work is shown in equation (1).

$$\hat{H}\Psi(\mathbf{r}) = E\Psi(\mathbf{r}) \quad (1)$$

Equation (1) is an energy eigenvalue equation whose solutions are energy eigenvalues and eigenfunctions of quantum systems considered, which in this research is the doubly muonic helium-like systems $X^{Z+}_{\mu^-\mu^-}$. Here, \hat{H} is the Hamiltonian operator, E is the energy eigenvalue and $\Psi(\mathbf{r})$ is the wave function.

One of the quantum mechanics postulates is that the wavefunction $\Psi(\mathbf{r})$ can be written as a linear combination of eigenfunctions $\psi_k(\mathbf{r})$ (Bransden & Joachain, 2000), shown in equation (2), where c_k is the probability amplitudes.

$$\Psi(\mathbf{r}) = \sum_{k=1}^{\infty} c_k \psi_k(\mathbf{r}) \quad (2)$$

To solve the Schrödinger equation using the matrix mechanics, the wave function has to be of finite dimension, N . As a result, equation (2) could be written:

$$\Psi(\mathbf{r}) = \sum_{k=1}^N c_k \psi_k(\mathbf{r}) \quad (3)$$

Furthermore, in the matrix method applied by Massé (Massé & Walker, 2015), eigenfunctions $\psi_k(\mathbf{r})$ were formed by taking the product of two wave functions of hydrogenic ions. Within this approach, the correlation function was neglected in the wave function. Therefore, equation (3) can be written in

the form presented in equation (4), where $\phi_{k_n,l,m_l}(\mathbf{r}_1)$ and $\phi_{k_n,l,m_l}(\mathbf{r}_2)$ represent hydrogenic wave function for muon 1 dan muon 2 in a particular $|n, l, m_l\rangle$ state, respectively.

$$\Psi(\mathbf{r}) = \sum_{k=1}^N c_k \phi_{k_n,l,m_l}(\mathbf{r}_1) \phi_{k_n,l,m_l}(\mathbf{r}_2) \quad (4)$$

In this research, 15 unsymmetrized hydrogenic basis s-states are used which took the form of equation (5), adopted from (Pingak & Deta, 2020).

$$\Psi(\mathbf{r}) = \sum_{n=2}^8 c_{11} \phi_{100}(\mathbf{r}_1) \phi_{100}(\mathbf{r}_2) + c_{1n} \phi_{100}(\mathbf{r}_1) \phi_{n00}(\mathbf{r}_2) + c_{n1} \phi_{n00}(\mathbf{r}_1) \phi_{100}(\mathbf{r}_2) \quad (5)$$

The projected Schrödinger equation and its approximate solution

Expressing the wavefunction in the form shown in equation (5) means that the Hamiltonian operator in equation (1) is in the matrix form of size 15x15. Therefore, equation (1) became the projected Schrödinger equation as presented in equation (6).

$$\begin{bmatrix} H_{1,1} & \cdots & H_{1,15} \\ \vdots & \ddots & \vdots \\ H_{15,1} & \cdots & H_{15,15} \end{bmatrix} \begin{pmatrix} c_{1,1} \\ \vdots \\ c_{15,1} \end{pmatrix} = E \begin{pmatrix} c_{1,1} \\ \vdots \\ c_{15,1} \end{pmatrix} \quad (6)$$

To obtain the ground state energy of a quantum system, equation (6) was solved by first calculating the Hamiltonian matrix elements using equation (7).

$$H_{i,j} = \iint \phi_i(\mathbf{r}_1) \phi_i(\mathbf{r}_2) \hat{H} \phi_j(\mathbf{r}_1) \phi_j(\mathbf{r}_2) d\mathbf{r}_1 d\mathbf{r}_2 \quad (7)$$

Where the non-relativistic Hamiltonian operator \hat{H} is calculated using equation (8), where Hartree muon atomic units (*m.a.u*) are used in which the muon mass $m_\mu=1$,

$$\hat{H} = -\frac{\nabla_1^2}{2} - \frac{\nabla_2^2}{2} - \frac{Z_1}{r_1} - \frac{Z_2}{r_2} + \frac{1}{r_{12}} \quad (8)$$

And the hydrogenic wave function was the product of the radial function $R(r)$ and the angular $Y(\theta, \phi)$ as follows

$$\phi_i(\mathbf{r}_1) = R_{nl}(r) Y_l^m(\theta, \varphi) \quad (9)$$

where $R_{nl}(r)$ can be written in terms of associated Laguerre polynomial as shown in equation (10) and $Y_l^m(\theta, \varphi)$ is the spherical harmonics.

$$R_{nl}(r) = \left(\frac{Z(n-l-1)!}{a_\mu(n+l)!n^2} \right)^{\frac{1}{2}} \left(\frac{2Z}{na_\mu} \right) \left(\frac{2Zr}{na_\mu} \right)^l e^{-\frac{Zr}{na_\mu}} L_{n-l-1}^{2l+1} \left(\frac{2Zr}{na_\mu} \right) \quad (10)$$

It is important to notice that a_μ in equation (10) is the modified Bohr radius due to the difference between the muon mass and the electron mass. The radial function as shown in equation (10) could be further written in muon atomic unit (*m.a.u*) using only s-orbitals ($l=0$) as follows:

$$R_{n0}(r) = \left(\frac{Z(n-1)!}{n!n^2} \right)^{\frac{1}{2}} \left(\frac{2Z}{n} \right) e^{-\frac{Zr}{n}} L_{n-1}^1 \left(\frac{2Zr}{n} \right) \quad (11)$$

After Hamiltonian matrix elements were obtained using equation (7), they were then substituted into

equation (6) which was then numerically solved using a Mathematica code modified from (Massé & Walker, 2015). The solution of the equation includes the energy eigenvalues with their corresponding eigenvectors.

RESULTS AND DISCUSSION

Ground State Energies of $X^{Z+}_{\mu\mu^-}$ ($2 \leq Z \leq 36$)

The lowest energy eigenvalues resulted from solving equation (6) numerically for $X^{Z+}_{\mu\mu^-}$ systems with $2 \leq Z \leq 36$ represent their ground state energies. Results are shown in **Table 1**, where comparisons with previous calculations using the hyperspherical harmonics method (Khan, 2014) are also presented wherever available. The percentage differences are also presented in **Table 1**.

It is evident from **Table 1** that the ground state energies 1^1S obtained using the matrix method in this work are in very good agreement with those reported in Khan (2014). Percentage differences in energies ranged from 0.095 % for $\text{Si}^{14+}_{\mu\mu^-}$ to 2.05% for $\text{He}^{2+}_{\mu\mu^-}$. This shows that even though the approximation applied in this study was simple, results were reasonably accurate. A more obvious comparison of our results with those presented in (Khan, 2014) is shown in **Figure 1**.

In addition to the results of Khan (2014), following discussions present the comparisons of our results with other results in the literature using different approaches. Before his recent work in (Khan, 2014), Khan had actually calculated the ground state energies of some of exotic doubly muonic systems in (Khan, 2012), where the ground state energies of $\text{He}^{2+}_{\mu\mu^-}$, $\text{Li}^{3+}_{\mu\mu^-}$, $\text{Be}^{4+}_{\mu\mu^-}$, $\text{B}^{5+}_{\mu\mu^-}$, $\text{C}^{6+}_{\mu\mu^-}$, $\text{O}^{8+}_{\mu\mu^-}$, $\text{Ne}^{10+}_{\mu\mu^-}$, $\text{Si}^{14+}_{\mu\mu^-}$, and $\text{Ar}^{18+}_{\mu\mu^-}$ were -2.8990 m.a.u, -7.2714 m.a.u, -13.6418 m.a.u, -22.0106 m.a.u, -32.3781 m.a.u, -59.1104 m.a.u, -93.8422 m.a.u, -187.3400 m.a.u and -312.1292 m.a.u, respectively. % differences of these results with our results are very small (below 1 %), i.e. 0.055%, 0.067%, 0.069%, 0.066%, 0.061%, 0.046%, 0.029%, 0.028% and 0.682%, for the respective systems. Additionally, results in this study are also in agreement with those reported by others. For instance, ground-state energies reported in (Ancarani et al., 2010; Ancarani et al., 2011) for $\text{He}^{2+}_{\mu\mu^-}$ and $\text{Li}^{3+}_{\mu\mu^-}$ were -2.90107 m.a.u and -7.27660 m.a.u for the respective systems, which are also in agreement with our results with percentage differences of 1.965% and 0.989% respectively. Moreover, excellent agreement with our results was also found in the ground state energy of $\text{He}^{2+}_{\mu\mu^-}$ reported in (Boimau et al., 2017) where the energies were -2.8476 m.a.u (percentage difference of 0.124%). Finally, Eskandari (Eskandari & Rezaie, 2004) also calculated the ground state energy of $\text{He}^{2+}_{\mu\mu^-}$ a system using three different correlation functions, the last of which yielded energy of -2.8206 m.a.u (percentage difference of

0.832%). The agreement with other reports in the literature as discussed above shows that despite being simple, hydrogenic wave functions used in this work yielded reasonably accurate ground-state energies of the exotic doubly muonic helium systems $X^{Z+}_{\mu\mu^-}$. One of the factors leading to the difference between our results and previous study by Eskandari (Eskandari & Rezaie, 2004) is that in the present work, the correlation function in the wave function is neglected. The absence of the correlation function means that some important short-range and long-

range correlation effects are not included in the calculation and therefore it will affect the accuracy of the calculation. Recently, other simple methods neglecting the correlation function were also developed including the semi-classical approximation (Pingak et al., 2021; Pingak et al., 2021), where it was reported that the accuracy in the energy of diatomic molecules are affected by the absence of the correlation function. Hence, in order to improve the accuracy, correlation function should be taken into account in the calculation.

Table 1. Ground state energy 1^1S of exotic doubly muonic helium-like system $X^{Z+}_{\mu\mu^-}$ ($2 \leq Z \leq 36$). All are presented in muon atomic unit (*m.a.u.*).

Z	Atom/ ion	This work (A)	Khan (2014) (B)	Percentage Difference ($ A-B *100/ B $)
2	He $^{2+}_{\mu\mu^-}$	-2.84406	-2.90358	2.04988
3	Li $^{3+}_{\mu\mu^-}$	-7.20461	-7.28028	1.03938
4	Be $^{4+}_{\mu\mu^-}$	-13.57320	-13.65664	0.61098
5	B $^{5+}_{\mu\mu^-}$	-21.94470	-22.03227	0.39746
6	C $^{6+}_{\mu\mu^-}$	-32.31750	-32.40836	0.28036
7	N $^{7+}_{\mu\mu^-}$	-44.69100		
8	O $^{8+}_{\mu\mu^-}$	-59.06490	-59.16209	0.16428
9	F $^{9+}_{\mu\mu^-}$	-75.43910		
10	Ne $^{10+}_{\mu\mu^-}$	-93.81340	-93.92118	0.11476
11	Na $^{11+}_{\mu\mu^-}$	-114.18800		
12	Mg $^{12+}_{\mu\mu^-}$	-136.56200		
13	Al $^{13+}_{\mu\mu^-}$	-160.93700		
14	Si $^{14+}_{\mu\mu^-}$	-187.31200	-187.49066	0.09529
15	P $^{15+}_{\mu\mu^-}$	-215.68600		
16	S $^{16+}_{\mu\mu^-}$	-246.06100		
17	Cl $^{17+}_{\mu\mu^-}$	-278.43600		
18	Ar $^{18+}_{\mu\mu^-}$	-312.81100	-313.2629	0.14426
19	K $^{19+}_{\mu\mu^-}$	-349.18600		
20	Ca $^{20+}_{\mu\mu^-}$	-387.56100		
21	Sc $^{21+}_{\mu\mu^-}$	-427.93500		
22	Ti $^{22+}_{\mu\mu^-}$	-470.31000		
23	V $^{23+}_{\mu\mu^-}$	-514.68500		
24	Cr $^{24+}_{\mu\mu^-}$	-561.06000		
25	Mn $^{25+}_{\mu\mu^-}$	-609.43500		
26	Fe $^{26+}_{\mu\mu^-}$	-659.81000		
27	Co $^{27+}_{\mu\mu^-}$	-712.18500		
28	Ni $^{28+}_{\mu\mu^-}$	-766.56000		
29	Cu $^{29+}_{\mu\mu^-}$	-822.93500		
30	Zn $^{30+}_{\mu\mu^-}$	-881.31000		
31	Ga $^{31+}_{\mu\mu^-}$	-941.68500		
32	Ge $^{32+}_{\mu\mu^-}$	-1004.06000	-1014.84508	1.06273
33	As $^{33+}_{\mu\mu^-}$	-1068.43000		
34	Se $^{34+}_{\mu\mu^-}$	-1134.81000		
35	Br $^{35+}_{\mu\mu^-}$	-1203.18000		
36	Kr $^{36+}_{\mu\mu^-}$	-1273.56000		

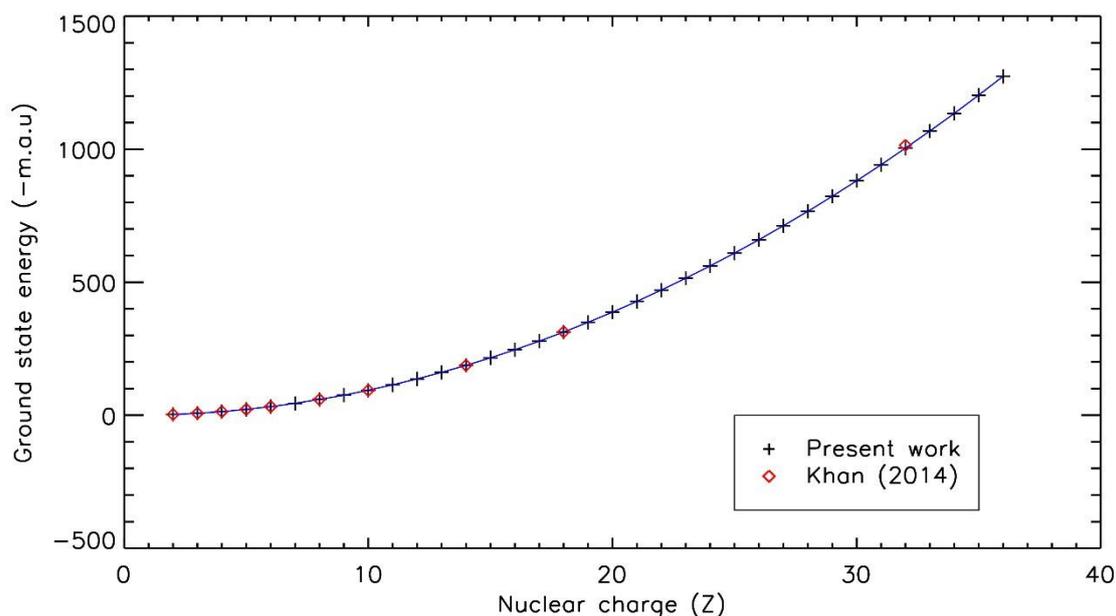


Figure 1. Ground state energies of exotic doubly helium like-ions $XZ^{2+}_{\mu\mu^-}$ are plotted against Z . Corresponding energies presented in (Khan, 2014) are also shown.

It can be seen from **Figure 1** that the ground state energies reported in (Khan, 2014) agree well with our results across all nuclear charge Z considered in this study. Furthermore, Khan (2014) only calculated the ground state energies for some selected ions and therefore there are some gaps in the figure for some ions. The gaps were filled very well by our results, as can be seen by the smooth curve connecting the energies of the ions for the whole range of Z considered. This also indicates that energies resulted from our calculations are accurate for all systems considered in this study.

With the absence of experimental ground state energies for these systems, an agreement between results of a new theoretical or computational study with older ones using different methods can be used to investigate whether a new proposed theoretical approach is 'accurate' or not. As discussed above, ground state energies available in the literature for the exotic doubly muonic helium-like ions calculated using other methods have been proven to be in very good agreement with our results in the present study, with percentage differences below 2 %. This clearly indicates that projecting the Schrödinger equation to a finite dimension space, in which the wave function was expressed as a finite linear combination of product of hydrogenic states and Hamiltonian is in matrix form, and solving it using matrix mechanics is a reasonably accurate method which can be further extended to study other three-body quantum systems.

There are a number of methods that can be used to further study these systems including the Monte Carlo (Metropolis & Ulam, 1949) and the Density Matrix Renormalization Group (DMRG) (White, 1992). The two methods have been successfully applied to calculate the energy of the helium atom.

For instance, Morcillo-Arencibia and co-workers (Morcillo-Arencibia et al., 2023) recently used the configuration interaction and the diffusion Monte Carlo to solve the Schrödinger equation of the helium atom. Furthermore, Snajberk (2017) applied the Density Matrix Renormalization Group to calculate energies of some quantum systems including the ground state energy of the helium atom. One of the advantages of using the proposed method in this manuscript is that it does not require any variational parameter and therefore it is more effective computationally. In addition, there is no need to include the momentum space truncation in the proposed method in contrast to the Density Matrix Renormalization Group which uses the momentum space expansion to reduce the computational cost. Nevertheless, with the absence of experimental data of these systems, theoretical studies are of great importance and therefore the use of different theoretical methods to investigate these systems is highly recommended. As another example, Dar and co-workers (Dar et al., 2021) recently applied the time-dependent density functional theory to accurately study the helium atom.

Spectral Decomposition of the Ground State Energies

In addition to ground state energies obtained from solving the time-independent Schrödinger, the eigenvectors corresponding to the energies were also investigated in the present work. This was performed to analyse the contribution of each basis state on the ground state energies of the systems, the probability amplitudes c_i of the states with their square values c_i^2 are calculated and presented in **Table 2**. The probabilities are only shown for three systems namely $\text{He}^{2+}_{\mu\mu^-}$, $\text{Li}^{3+}_{\mu\mu^-}$, and $\text{Be}^{4+}_{\mu\mu^-}$, since the patterns are the same for other systems.

Table 2 Probability amplitudes of the states used in the wave function expansion for $\text{He}^{2+}_{\mu\mu^-}$, $\text{Li}^{3+}_{\mu\mu^-}$ and $\text{Be}^{4+}_{\mu\mu^-}$.

State Label	State	$\text{He}^{2+}_{\mu\mu^-}$		$\text{Li}^{3+}_{\mu\mu^-}$		$\text{Be}^{4+}_{\mu\mu^-}$	
		c_i	c_i^2 (%)	c_i	c_i^2 (%)	c_i	c_i^2 (%)
1	1s1s	-0.954	90.990	0.985	96.979	0.993	98.543
2	1s2s	0.194	3.766	-0.110	1.217	-0.076	0.579
3	2s1s	0.194	3.766	-0.110	1.217	-0.076	0.579
4	1s3s	0.066	0.439	-0.042	0.173	-0.030	0.088
5	3s1s	0.066	0.439	-0.042	0.173	-0.030	0.088
6	1s4s	0.039	0.149	-0.024	0.060	-0.017	0.031
7	4s1s	0.039	0.149	-0.024	0.060	-0.017	0.031
8	1s5s	0.027	0.070	-0.017	0.028	-0.012	0.014
9	5s1s	0.027	0.070	-0.017	0.028	-0.012	0.014
10	1s6s	0.020	0.040	-0.013	0.016	-0.009	0.008
11	6s1s	0.020	0.040	-0.013	0.016	-0.009	0.008
12	1s7s	0.016	0.025	-0.010	0.010	-0.007	0.005
13	7s1s	0.016	0.025	-0.010	0.010	-0.007	0.005
14	1s8s	0.013	0.017	-0.008	0.006	-0.006	0.003
15	8s1s	0.013	0.017	-0.008	0.006	-0.006	0.003

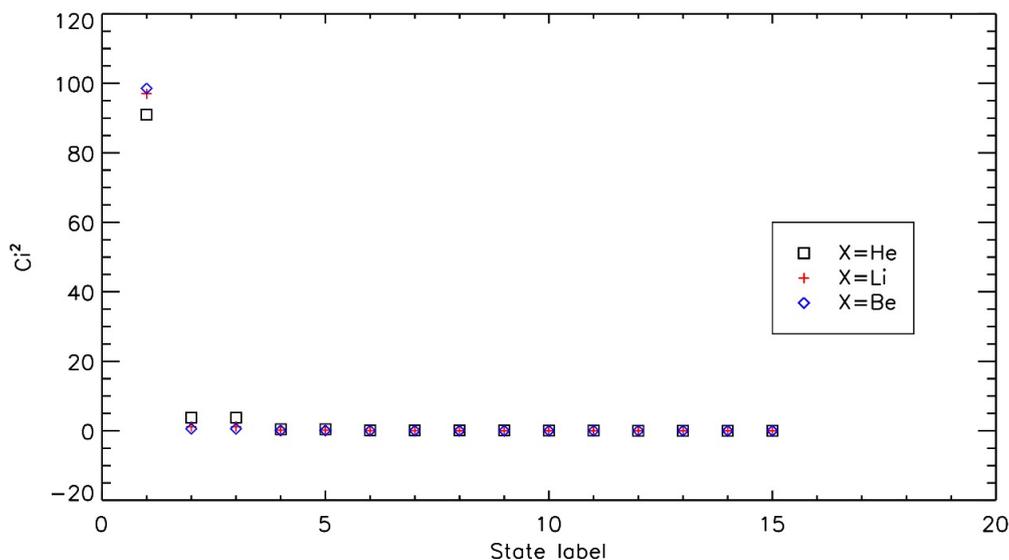


Figure 2. Probabilities of basis states used in obtaining ground state energies of $X^{Z+}_{\mu\mu^-}$ (with $X=\text{He, Li and Be}$) are plotted against state labels defined in **Table 2**.

Table 2 clearly indicates that the 1s1s state makes the largest contribution to the ground state energy of $\text{He}^{2+}_{\mu\mu^-}$ atom (about 91%), while the contribution from higher states is significantly lower with a minimum of about 0.017% for 1s8s state. The results were the same as those presented in (Hutchinson, Baker, & Marsiglio, 2013) who obtained around 91% contribution to the ground state of the helium atom arising from the 1s1s state. This indicates that around 9% contribution should come from higher bound states as well as the unbound states.

It can also be seen from **Table 2** that the state with the largest proportion in the ground state of $\text{Li}^{3+}_{\mu\mu^-}$ and $\text{Be}^{4+}_{\mu\mu^-}$ systems were also the 1s1s state but with larger proportion compared to its proportion in the ground state energy of $\text{He}^{2+}_{\mu\mu^-}$. The

compositions of the 1s1s state in the ground state energy of the $\text{Li}^{3+}_{\mu\mu^-}$ and $\text{Be}^{4+}_{\mu\mu^-}$ were about 96.98% and 98.54%, respectively. When one muon is in higher quantum states (1sns or ns1s where $n>1$), the contribution to the ground state energy decreases significantly reaching 0.006% and 0.003% for the respective systems.

In addition to the above observations found in **Table 2**, it is also clear that the probabilities of 1sns states were the same as those of ns1s states. This indicates that a state in which the first muon is in the $|1,0,0\rangle$ state and the second one in the $|n,0,0\rangle$ state is equivalent to a state in which the first muon is in the $|n,0,0\rangle$ state and the second one is in the $|1,0,0\rangle$ state. A more obvious visualisation of the properties of the states based on data in **Table 2** is shown in **Figure 2**.

It is clear from **Figure 2** that the higher the states used (larger state labels), the less the contribution they made to the ground state energy of the systems. This is true for all systems especially for $X=He$, Li and Be as shown in **Figure 2**. It can also be seen that the larger the nuclear charge, the higher the contribution made by the $1s1s$ state (a state with label 1) to the ground state energy. This can be seen in **Figure 2** for state label 1 ($1s1s$ state), where the highest proportion of this state on the ground state energies is for the $X=Be$ ($Z=4$), followed by $X=Li$ ($Z=3$) and finally $X=He$ ($Z=2$). These observations indicate that including higher bound states and unbound states would not significantly improve the accuracy of the calculations using this method.

CONCLUSIONS

In summary, the Schrödinger equation of exotic doubly muonic helium-like systems of the form $XZ^{2+}_{\mu\mu}$ has been solved with the matrix method using 15 unsymmetrized hydrogenic basis s-states. Accurate ground state energies of the systems with nuclear charge $2 \leq Z \leq 36$ were obtained from the solution to the Schrödinger equation. It was found that the ground state energies were in very good agreement with those reported in the literature using other methods. The analysis of the probability amplitudes from the eigenvectors of the ground state energies was also performed. The analysis indicated that the $1s1s$ state had the highest proportion among all states used in the wave function expansion.

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