**Eurasian Journal of Physics and Functional Materials**

**2021, 5(3), 169-173**

# Hyperfine structure S state of muonic helium atom

D.T. Aznabayev[1,2,3], A.K. Bekbaev[*,1,2,4], V.I. Korobov[1]

[1]Joint Institute for Nuclear Research, Dubna, Russia,

[2]The Institute of Nuclear Physics, Ministry of Energy of the Republic of Kazakhstan, Almaty, Kazakhstan

[3]L.N. Gumilyov Eurasian National University, Nur-Sultan, Kazakhstan

[4]Al-Farabi Kazakh National University, Almaty, Kazakhstan

E-mail: aznabaev@theor.jinr.ru, bekbaev-askhat@mail.ru

DOI: **10.32523/ejpfm.2021050301**
Received: 06.07.2021 - after revision

In this work the nonrelativistic ionization energies $^3He^{2+}\mu^-e^-$ and $^4He^{2+}\mu^-e^-$ of helium-muonic atoms are calculated for S states.The estimates are based on the variational principle of exponential expansion. Convergence of the numerical values of variational energies is studied by increasing a number of the basis functions N. That allows to claim that the obtained energy values have 30-33 significant digits for S states

**Keywords:** three-body systems, variational principle, hyperfine structure, muonic helium ions.

## Introduction

Muonic helium ions $^3He^{2+}\mu^-e^-$ and $^4He^{2+}\mu^-e^-$ are simple three-body systems composed of the negative muon and positive nucleus of $^3He$ or $^4He$ and the electron. The lifetime of muonic atoms are determined by the lifetime of muon $\tau_\mu = 2.19703(4) \times 10^{-6}$ sec. The three-body bound states has complicated hyperfine structure which is caused by an interaction of magnetic moments of the electron, the nucles and the muon. Muon systems represent themselves as a unique laboratory for precise determination of nuclei properties such as charge radius [1, 2]. A significant progress in an investigation of energy spectrums of muonic atoms has been achieved by the CREMA group (Charge Radius Experiment with Muonic Atoms). The Lamb shift and hyperfine structure in muonic

hydrogen and muonic deuterium have been measured. Similar experiments are planned for muonic helium. Light muonic atoms are important for testing of the Standard Model, theory of bound states in quantum electrodynamics and for searching of exotic particles and interactions.

Hyperfine splitting of the S state in muonic helium atoms $^3He^{2+}\mu^-e^-$ and $^4He^{2+}\mu^-e^-$ was measured many years ago with high enough accuracy. This measurement is the only experimental result for a three-body muonic atoms. On the other hand, theoretical investigations of the energy spectrum have achieved significant successes in two approaches [3-14]. The first approach, used in [3-5], was based on perturbation theory for the Schrodinger equation. In this case, there exists an analytic form for a three-body wave function in the initial approach. On this basis various corrections of hyperfine splitting were made. The other approach in [6, 11-14] was based on the variational method in quantum mechanics. It allowed to numerically compute bound energy levels of a three-body systems with very high accuracy. To find low-lying energy levels with high accuracy one needs to consider various corrections of an interaction operator of particles. First of all, these corrections are related to the effect of recoil, nuclear structure and vacuum polarization. A program for calculating hyperfine structure in muonic helium, including excited states, was realized in [3-6, 10-12, 15].

In this article we report the results of highly accurate calculations of the $S(L=0)$ -states in the helium-muonic $^3He^{2+}\mu^-e^-$ and $^4He^{2+}\mu^-e^-$ atoms. Our recently improved methods for highly accurate variational computations allow us to construct extremely accurate variational wave functions for these three-body helium-muonic atoms. Such wave functions can be used to obtain essentially exact expectation values of various bound state properties of these systems.

# Variational method

The non-relativistic Hamiltonian for ($^3He^{2+}\mu^-e^-$ or $^4He^{2+}\mu^-e^-$) muonic-helium atom takes the form:

$$H = -\frac{1}{2\mu_1}\bigtriangledown_{r_1}^2 - \frac{1}{2\mu_2}\bigtriangledown_{r_2}^2 - \frac{1}{M}\bigtriangledown_{r_1}\bigtriangledown_{r_2} - \frac{Z}{r_1} - \frac{Z}{r_2} + \frac{1}{r_{12}} \tag{1}$$

where $r_1$ and $r_2$ are position vectors for two negative particles, $r_{12} = r_2 - r_1, \mu_1 = Mm_1/(M+m_1)$ and $\mu_2 = Mm_2/(M+m_2)$ are reduced masses, $M$ is a mass of helium nucleus, and $Z = 2$ is the nuclear charge. We assume that $m_1 = m_\mu$ and $m_2 = 1$, where $m_\mu$ is a mass negative muon (units are atomic units, $\hbar = 1, m_e = 1$, and $e = 1$). Where masses of the muon $m_\mu = 206.768262m_e$ and helium nuclei $M_{^3He} = 5495.8852m_e$ and $M_{^4He} = 7294.2996m_e$ must be expressed in the electron mass $m_e$.

In our calculations we use a variational method based on exponentials with randomly generated parameters. The wave functions:

$$\psi(r_1, r_2, r_{12}) = \sum_i v_i exp\{-\alpha_i r_1 - \beta_i r_2 - \gamma_i r_{12}\} \tag{2}$$

with real $\alpha$, $\beta$, and $\gamma$ chosen randomly and homogeneously between some maximal and minimal values. All these values could be determined by minimization

of the ground-state energy. The convergence of the total energies in atomic units for the $1s\mu 1se$ ground states in the helium-muonic atoms and the convergence of the expectation values for the delta functions for various pairs of particles are shown in Tables 1 and 2

Table 1.
The convergence of the total energies in atomic units for the $1s\mu 1se$ ground states in the helium-muonic atoms. $N$ is the total number of basis functions used in calculations.

| $N$ | $^3He^{2+}\mu^-e^-$ | $^4He^{2+}\mu^-e^-$ |
|---|---|---|
| 10000 | −399.042 336 832 862 534 827 041 568 448 6603 | − 402.637 263 035 135 454 018 974 498 601 4674 |
| 12000 | −399.042 336 832 862 534 827 041 568 448 7145 | − 402.637 263 035 135 454 018 974 498 601 4894 |
| 14000 | −399.042 336 832 862 534 827 041 568 448 7191 | − 402.637 263 035 135 454 018 974 498 601 4911 |
| 16000 | −399.042 336 832 862 534 827 041 568 448 7198 | − 402.637 263 035 135 454 018 974 498 601 4914 |
| 18000 | −399.042 336 832 862 534 827 041 568 448 7192 | − 402.637 263 035 135 454 018 974 498 601 4914 |
| 20000 | −399.042 336 832 862 534 827 041 568 449 8494 | − 402.637 263 035 135 454 018 974 498 601 4914 |

Table 2.
The convergence of the expectation values for the delta functions for various pairs of particles. $N$ is the total number of basis functions used in calculations.

| $N$ | $^3He^{2+}\mu^-e^-$ | | $^4He^{2+}\mu^-e^-$ | |
|---|---|---|---|---|
| | $\langle\delta(\mathbf{r}_{N\mu})\rangle$ | $\langle\delta(\mathbf{r}_{Ne})\rangle$ | $\langle\delta(\mathbf{r}_{\mu e})\rangle$ | $\langle\delta(\mathbf{r}_{\mu e})\rangle$ |
| 10000 | 20 149 938.845 | 0.320 611 551 58 | 0.313 682 319 99 | 0.313 760 536 37 |
| 12000 | 20 149 938.845 | 0.320 611 551 58 | 0.313 682 319 99 | 0.313 760 536 37 |
| 14000 | 20 149 938.845 | 0.320 611 551 58 | 0.313 682 319 99 | 0.313 760 536 37 |
| 16000 | 20 149 938.845 | 0.320 611 551 58 | 0.313 682 319 99 | 0.313 760 536 37 |
| 18000 | 20 149 938.845 | 0.320 611 551 58 | 0.313 682 319 99 | 0.313 760 536 37 |
| 20000 | 20 149 938.845 | 0.320 611 551 58 | 0.313 682 319 99 | 0.313 760 536 37 |

Complex parameters $\alpha_k, \beta_k$, and $\gamma_k$ are generated in a quasirandom manner [16, 17]:

$$\alpha_k = [[1/2k(k+1)\sqrt{p_\alpha}](A_2 - A_1) + A_1] + i[[1/2k(k+1)\sqrt{q_\alpha}](A_2' - A_1') + A_1']$$

where $[x]$ designates the fractional part of $x$, $p_\alpha$ and $q_\alpha$ are some prime numbers, and $[A_1, A_2]$, and $[A_1', A_2']$ are real variational intervals, which need to be optimized. Parameters $\alpha_k, \beta_k$ and $\gamma_k$ are obtained in a similar way. More details may be found in [11].

Computations were performed in the duodecimal arithmetics (about 100 decimal digits). Programs of duodecimal precision were developed by our group in order to overcome the problem of the numerical instability of calculations at large values of $N$. That were developed by one of the authors of the present paper were used in order to remedy the problem of the numerical instability of calculations at large values of $N$. Results of these calculations versus size of the basis set are presented in Table 1.

## Expectation values of the delta function operators

The results of numerical calculations of the ionization energies for ground state of a muonic-helium atom ($^3He^{2+}\mu^-e^-$ and $^4He^{2+}\mu^-e^-$) are listed in Table 1. These calculations were carried out using the inverse iteration method [18]. Variational parameters were optimized manually. It should be noted that the optimum variational parameters for different states differ from each other, and the calculation accuracy depends to a considerable extent on the choice of the optimum variational parameters for the given bound state. Bases with $N = 10000, 12000, 14000, 16000, 18000$ and $20000$ functions were used to optimize the variational parameters. When the states listed in the table were calculated, We used in our calculations 5-7 "layers" of basis functions.

## Hyperfine structure of the $^3He^{2+}\mu^-e^-$ and $^4He^{2+}\mu^-e^-$ atoms

For $S$ states the spin dependent term of the Breit-Pauli Hamiltonian is

$$H_{HFS} = -\frac{8\pi}{3}\mu_N\mu_\mu\delta(\mathbf{r}_{N\mu}) - \frac{8\pi}{3}\mu_e\mu_\mu\delta(\mathbf{r}_{e\mu}) - \frac{8\pi}{3}\mu_N\mu_e\delta(\mathbf{r}_{Ne}) \tag{3}$$

For $^4He$ since the spin of nucleus is zero the Hamiltonian is simplified:

$$H_{HFS} = -\frac{8\pi}{3}\mu_e\mu_\mu\langle\delta(\mathbf{r}_{e\mu})\rangle = E_1(s_e, s_\mu) \tag{4}$$

where $E_1 = -4464.55(60)MHz$

For $^3He$ the effective HFS Hamiltonian has three terms:

$$H_{HFS} = E_1(s_e, s_\mu) + E_2(s_h, s_\mu) + E_3(s_h, s_e), \tag{5}$$

where

$E_1 = -4463.44(24)MHz$, $E_2 = -331846.(16)GHz$, $E_3 = -1091.750(58)MHz$.

The coupling scheme is $\mathbf{F} = \mathbf{s}_h + \mathbf{s}_\mu, \mathbf{J} = \mathbf{F} + \mathbf{s}_e$, and the spin state is denoted as $|FJ\rangle$. Diagonalization of the effective HFS Hamiltonian gives the splitting:

$$\triangle\nu(\chi_{|0,1/2\rangle}) = 248884463.3MHz,$$

$$\triangle\nu(\chi_{|1,1/2\rangle}) = -82962876.6MHz, \quad \triangle\nu(\chi_{|1,3/2\rangle}) = -82958710.2MHz$$

and for the difference of the lower state $(|F = 1\rangle)$:

$$\delta\nu(\chi_{|1,3/2-1/2\rangle}) = 4166.39(58)MHz.$$

## Conclusion

Variational wave functions of bound states were obtained by solving the Schrodinger equation for the quantum three-body problem with Coulomb interaction using a variational approach based on exponential expansion with the parameters of exponents being chosen in a pseudorandom way. The results of calculations of the nonrelativistic energy levels for a helium atom were presented. The numerical calculation results are listed in Table 1. The results of these studies demonstrated that the energy values are as accurate as 30-33 significant digits. This accuracy allows one to obtain reliable theoretical predictions.

## Acknowledgments

This research has been funded by the Science Committee of the Ministry of Education and Science of the Republic of Kazakhstan (Grant No. AP09057862).

## References

[1] R. Pohl et al., Nature **466** (2010) 213-217.
[2] A. Antognini et al., Annals of Physics **331** (2013) 127-145.
[3] S.D. Lakdawala, P.J. Mohr, Phys. Rev. A **22** (1980) 1572-1575.
[4] S.D. Lakdawala, P.J. Mohr, Phys. Rev. A **24** (1981) 2224-2227.
[5] S.D. Lakdawala, P.J. Mohr, Phys. Rev. A **29** (1984) 1047-1054.
[6] E. Borie, Z. Physik A **291** (1979) 107-112.
[7] R.J. Drachman, Phys. Rev. A **22** (1980) 1755-1757.
[8] M.-K. Chen, Phys. Rev. A **45** (1992) 1479-1492.
[9] A.M. Frolov, Phys. Rev. A **61** (2000) 022509.
[10] A.M. Frolov, Phys. Let. A **357** (2006) 334-338.
[11] V.I. Korobov, Phys. Rev. A **61** (2000) 064503.
[12] K. Pachucki, Phys. Rev. A **63** (2001) 032508.
[13] A.A. Krutov, A.P. Martynenko, Phys. Rev. A **78** (2008) 032513.
[14] A.A. Krutov, A.P. Martynenko, Eur. Phys. J. D **62** (2011) 163-175.
[15] A.A. Krutov, A.P. Martynenko, Phys. Rev. A **86** (2012) 052501.
[16] A.M. Frolov, V.H.Jr. Simth, J. Phys. B **28** (1995) L449.
[17] V.I. Korobov D. Bakalov, H.J. Monkhorst, Phys. Rev. A **59** (1999) R919.
[18] D.T. Aznabayev, A.K. Bekbaev, V.I. Korobov, Phys. Rev. A **98** (2018) 012510.