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PHYSICS OF ELEMENTARY PARTICLES AND ATOMIC NUCLEI. THEORY

The Hyperfine Structure of the Ground State in the Muonic Helium Atoms[1]

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Abstract—Non-relativistic ionization energies $^3He^{2+}\mu^-e^-$ and $^4He^{2+}\mu^-e^-$ of helium-muonic atoms are calculated for ground states. The calculations are based on the variational method of the exponential expansion. Convergence of the variational energies is studied by an increasing of a number of the basis functions N. This allows to claim that the obtained energy values have 26 significant digits for ground states. With the obtained results we calculate hyperfine splitting of the muonic helium atoms.

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INTRODUCTION

Muonic helium ions $^3He^{2+}\mu^-e^-$ and $^4He^{2+}\mu^-e^-$ are simple three-body systems composed of an electron, a negative muon and positive nucleus of ^3He or ^4He. The lifetime of such atoms are determined by the lifetime of muon, which is $\tau_\mu = 2.19703(4)\times 10^{-6}$ s. Three-body bound states has complicated hyperfine structure which is caused by an interaction of magnetic moments of the electron, the muon and nucles. Muon systems represent themselves as a unique laboratory for precise determination of nuclei properties such as charge radius [1, 2]. Lately, a significant progress in energy spectra investigations of muonic atoms have been achieved by the CREMA collaboration (Charge Radius Experiment with Muonic Atoms). The Lambshift 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 ground 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 three-body muonic atoms. On the other hand, theoretical investigations of the energy spectrum have achieved significant successes in two approaches [3–12, 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. On this basis various corrections of the 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 system 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 of the hyperfine structure in muonic helium, including excited states, was realized in [3–6, 10–12, 15].

In this study we report the results of highly accurate calculations of the ground $S(L = 0)$-states in the helium-muonic $^3He^{2+}\mu^-e^-$ and $^4He^{2+}\mu^-e^-$ atoms. Our recently improved methods [11] 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.

[1] The article is published in the original.

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

N	$^3He^{2+}\mu^-e^-$	$^4He^{2+}\mu^-e^-$
2000	–399.042336832862534827027433	–402.637263035135454018960573
2500	–399.042336832862534827039305	–402.637263035135454018972984
3000	–399.042336832862534827041147	–402.637263035135454018973292
3500	–399.042336832862534827041500	–402.637263035135454018974187
4000	–399.042336832862534827041545	–402.637263035135454018974468
4500	–399.042336832862534827041560	–402.637263035135454018974488

1. THREE-BODY VARIATIONAL WAVE FUNCTION

The non-relativistic Hamiltonian for muonic helium atom ($^3He^{2+}\mu^-e^-$ or $^4He^{2+}\mu^-e^-$) takes the form [11]:

$$H = -\frac{1}{2\mu_1}\nabla^2_{r_1} - \frac{1}{2\mu_2}\nabla^2_{r_2} - \frac{1}{M}\nabla_{r_1}\nabla_{r_2} - \frac{Z}{r_1} - \frac{Z}{r_2} + \frac{1}{r_{12}}, \quad (1)$$

where r_1 and r_2 are position vectors for the 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 the helium nucleus, and $Z = 2$ is the nuclear charge. We assume that $m_1 = m_\mu$ and $m_2 = 1$, where m_μ is a mass of the negative muon (atomic units are used: $\hbar = 1$, $m_e = 1$, and $e = 1$). We use the following values of the particle masses (in terms of the electron mass, m_e): muon $m_\mu = 206.768262 m_e$, helium nuclei $M_{^3He} = 5495.8852 m_e$ and $M_{^4He} = 7294.2996 m_e$.

In our calculations we use a variational expansion based on exponentials with randomly generated parameters [11]. The wave functions are taken in the form:

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

with real α, β, and γ chosen randomly and homogeneously between some minimal and maximal values. All these values could be determined by minimization of the ground state energy.

Complex parameters α_k, β_k, and γ_k are generated in a quasirandom manner [16, 17]:

$$\begin{aligned}\alpha_k &= \left[\left[1/2\, k(k+1)\sqrt{p_\alpha}\right](A_2 - A_1) + A_1\right] \\ &+ i\left[\left[1/2\, k(k+1)\sqrt{q_\alpha}\right]\left(A_2' - A_1'\right) + A_1'\right],\end{aligned} \quad (3)$$

where $[x]$ designates the fractional part of x, p_α and q_α are some prime numbers, and $[A_1, A_2]$, and $[A_1' A_2']$ are real variational intervals, which need to be optimized. Parameters α_k, β_k and γ_k are obtained in a similar way. More details may be found in [11].

Program modules of sextuple and octuple precision (48 and 64 decimal digits, respectively) 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 the size of the basis set are presented in Table 1.

2. NONRELATIVISTIC ENERGIES AND 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 = 2000, 2500, 3000, 3500 and 4000 functions were used to optimize the variational parameters. When the states listed in the table were calculated, 5 "layers" of the basis functions were used.

3. HYPERFINE STRUCTURE OF MUONIC HELIUM ATOM

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

$$\begin{aligned}H_{\mathrm{HFS}} &= -\frac{8\pi}{3}\boldsymbol{\mu}_N\boldsymbol{\mu}_\mu\delta(\mathbf{r}_{N\mu}) - \frac{8\pi}{3}\boldsymbol{\mu}_e\boldsymbol{\mu}_\mu\delta(\mathbf{r}_{e\mu}) \\ &- \frac{8\pi}{3}\boldsymbol{\mu}_N\boldsymbol{\mu}_e\delta(\mathbf{r}_{Ne}).\end{aligned} \quad (4)$$

For ^{4}He, since the spin of nucleus is zero, the Hamiltonian is simplified and we get:

$$\left\langle H_{\mathrm{HFS}}(^4\mathrm{He})\right\rangle = -\frac{8\pi}{3}\boldsymbol{\mu}_e\boldsymbol{\mu}_\mu\left\langle\delta(\mathbf{r}_{e\mu})\right\rangle = E_1(s_e, s_\mu), \quad (5)$$

where $E_1 = -4464.55(60)$ MHz.

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	$^3He^{2+}\mu^- e^-$			$^4He^{2+}\mu^- e^-$
	$\langle\delta(\mathbf{r}_{N\mu})\rangle$	$\langle\delta(\mathbf{r}_{Ne})\rangle$	$\langle\delta(\mathbf{r}_{\mu e})\rangle$	$\langle\delta(\mathbf{r}_{\mu e})\rangle$
2000	20149938.845	0.32061155099	0.31368232001	0.31376053634
2500	20149938.845	0.32061155124	0.31368232001	0.31376053639
3000	20149938.845	0.32061155142	0.31368232000	0.31376053638
3500	20149938.845	0.32061155151	0.31368232000	0.31376053638
4000	20149938.845	0.32061155156	0.31368231999	0.31376053637
4500	20149938.845	0.32061155157	0.31368231999	0.31376053637

For ^{3}He the effective HFS (hyperfine structure) Hamiltonian has three terms:

$$\left\langle H_{\mathrm{HFS}}(^3\mathrm{He})\right\rangle = E_1(s_e, s_\mu) + E_2(s_h, s_\mu) + E_3(s_h, s_e), \quad (6)$$

where

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

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:

$$\begin{aligned}\Delta\nu(\chi_{|0,1/2\rangle}) &= 24\,888\,4463.3\ \mathrm{MHz},\\ \Delta\nu(\chi_{|1,1/2\rangle}) &= -82\,962\,876.6\ \mathrm{MHz},\\ \Delta\nu(\chi_{|1,3/2\rangle}) &= -82\,958\,710.2\ \mathrm{MHz}.\end{aligned} \quad (7)$$

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

$$\delta\nu(\chi_{|1,3/2-1/2\rangle}) = 4166.39(58)\ \mathrm{MHz}. \quad (8)$$

4. CONCLUSIONS

Variational wave functions of bound states were obtained by solving the Schröodinger 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 26 significant digits. This accuracy allows one to obtain reliable theoretical predictions. The calculated wave functions with high precision were used to compute hyperfine structure of the muonic helium atoms.

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