Spectroscopic Parameters of the Exotic Helium Atom within the Hyperspheric Adiabatic Approach in One-Dimensional Space

M.I. Haysak^a, I.I. Haysak^b, M. Nagy^c and V.V. Onysko^b

^{a}*Institute of Electron Physics of the National Academy of Sciences of Ukraine, Universitetska 21, 88017 Uzhhorod, Ukraine*
^{b}*Uzhhorod National University, Universitetska 14, 88000 Uzhhorod, Ukraine*
^{c}*Institute of Physics of the Slovak Academy of Sciences, Dúbravská cesta 9, 845 11 Bratislava 45, Slovak Republic*

This paper presents the results of calculations of spectroscopic parameters of three-particle quantum systems, in particular the exotic helium atom $(^3\text{He}^{2+}, e, \overline{^3\text{H}})$. These calculations were made within the framework of a nonrelativistic quantum-mechanical model for the problem of three bodies interacting according to the Coulomb's law.

topics: quantum mechanical model, three-particle system

1. Introduction

The matter and antimatter interaction is one of the most interesting problems of modern quantum physics. This opens up the possibility of observing and theoretically predicting new phenomena, processes, quantum systems, molecules, as well as solving relevant experimental and applied problems. It is known that in 1947 Fermi and Teller [1] considered the role of the dipole interaction of matter and antimatter. After experimentally obtaining the antihydrogen and antihelium atoms, it is of considerable interest to find spectroscopic parameters of quantum systems with antiparticles participation. Such systems in the standard model are described by the nonrelativistic Schrödinger equation [2]. For the two-body problem, this equation can be solved analytically. At the same time, the analytical solution for three bodies exists only for a certain kind of interaction potentials between particles, and in the general case of this problem, the solution can be found only by a numerical method. One of the effective numerical methods is the method of mixing configurations [3].

2. Theoretical approach

Let us consider three-particle molecules (ions), which consist of isotopes of helium atoms (^{3}He, ^{4}He) and isotopes of atomic hydrogen (^{1}H, ^{2}H, ^{3}H) and their antiparticles. In particular, we are talking about an exotic helium atom $(^3\text{He}^{2+}, e, \overline{^3\text{H}})$ — isotope of a 2+ helium ion, electron, and hydrogen isotope (tritium).

The non-relativistic Schrödinger equation for a system of three particle with the arbitrary masses (m_i) and charges (z_i) that interact by a pair Coulomb interaction, has the following form (in the atomic system of units)

$$\left[\frac{1}{2} \left(\frac{\partial^2}{m_1 \partial x_1^2} + \frac{\partial^2}{m_2 \partial x_2^2} + \frac{\partial^2}{m_3 \partial x_3^2} \right) \right.$$
$$\left. + V(x_1, x_2, x_3) - E \right] \Psi(x_1, x_2, x_3) = 0, \quad (1)$$

where x_i is the position of i-th particle, E and $\Psi(x_1, x_2, x_3)$ are the total energy and the total wave function of the system, respectively, $V(x_1, x_2, x_3)$ is the potential energy operator. It has the form

$$V(x_1, x_2, x_3) = \frac{z_1 z_2}{|x_1 - x_2|} + \frac{z_1 z_3}{|x_1 - x_3|} + \frac{z_2 z_3}{|x_2 - x_3|}. \quad (2)$$

Since we consider only a pair interaction of particles, (1) allows the separation of the motion of the center of mass of a system. For this purpose, it is necessary to introduce the relative Jacobi coordinates [4],

$$\rho = x_2 - x_3, \quad \tau = x_1 - \frac{m_2 x_2 + m_3 x_3}{m_2 + m_3},$$

$$\mathfrak{R} = \frac{m_1 x_1 + m_2 x_2 + m_3 x_3}{m_1 + m_2 + m_3}. \quad (3)$$

Entering the relative Jacobi coordinates (3) and separating the variables in (1) is equivalent to the following system of equations

$$\begin{cases} \left[-\frac{1}{2\mu_1}\frac{\partial^2}{\partial\rho^2} - \frac{1}{2\mu_2}\frac{\partial^2}{\partial\tau^2} + V(\rho,\tau) - \varepsilon\right]\psi(\rho,\tau) = 0, \\ -\frac{1}{2M}\frac{\partial^2}{\partial\mathfrak{R}^2}\phi(\mathfrak{R}) = (E-\varepsilon)\phi(\mathfrak{R}), \end{cases}$$
(4)

where $M = m_1 + m_2 + m_3$, $\Psi = \psi(\rho,\tau)\phi(\mathfrak{R})$. The first equation of the system (4) describes the relative motion of the system, and the second one — the motion of the center of mass of the system. The constant ε is the energy of the relative motion of the system, and μ_1 and μ_2 are the relative masses given as, respectively,

$$\mu_1 = \frac{m_1 m_2}{m_1 + m_2} \quad \text{and} \quad \mu_2 = \frac{m_1(m_2 + m_3)}{m_1 + m_2 + m_3}.$$
(5)

By separating the motion of the center of mass of the system in (1), we thus reduced the problem from three to two independent variables that describe the relative motion of the system and the motion of the center of mass of the system. The equation of relative motion in the variables defined in (3) will take the form

$$\left[-\frac{1}{2\mu}\left(\frac{1}{R}\frac{\partial}{\partial R}\left(R\frac{\partial}{\partial R}\right) + \frac{1}{R^2}\frac{\partial^2}{\partial\alpha^2}\right)\right.$$
$$\left. + V(R,\alpha) - \varepsilon\right]\psi(R,\alpha) = 0.$$
(6)

Partial solutions of the relative motion equation (6) are convenient to find in an elliptical coordinate system. In this system, the angular variable α varies in the limited interval $[0,\beta]$, and the radial variable R belongs to the semi-limited interval $[0,\infty)$. These variables are expressed as

$$R = \sqrt{\frac{\mu_1}{\mu}\rho^2 + \frac{\mu_2}{\mu}\tau^2} \quad (0 \le R < \infty)$$

$$\text{with} \quad \mu = \sqrt{\mu_1\mu_2},$$

$$\tan(\alpha) = \frac{\sqrt{\mu_1}\rho}{\sqrt{\mu_2}\tau}, \quad \left(\tan(\beta) = \frac{\sqrt{\mu_1\mu_2}}{m_2}\right). \quad (7)$$

Adiabatic potentials $(U_\nu(R))$ are obtained by solving a generalized boundary value problem on eigenvalues and eigenfunctions $(\chi_\nu(R,\alpha))$ of the operator received from the Hamilton operator for the relative motion of particles at a fixed radial variable. To eliminate the differences in the matrix

TABLE I

Characteristics of the minimum adiabatic potential of the system $(^3\text{He}^{2+}, e, \overline{^3\text{H}})$.

State	Characteristics of the minimum adiabatic potential	
	Energy [a.u.]	Coordinates [a.u.]
$^1S^{oe}$	$-1.038913337 \times 10^{13}$	$5.496447630 \times 10^{-7}$
$^1S^{ee}$	$-5.879911607 \times 10^{13}$	$6.803870053 \times 10^{-8}$

elements of the potential energy operator, the idea of scalable multiplier proposed by Hiroshi Nakatsui was used [5]. The scalable multiplier is a function of only the angular variable α and has the following form

$$g(\alpha) = \left|\sin(\alpha)\sin(\alpha+\beta)\sin(\alpha-\beta)\right|.$$
(8)

Adiabatic potentials and channel functions are obtained by solving the generalized boundary value problem (6) with fixed radial variable

$$\left[\frac{\partial^2}{\partial\alpha^2} - 2\mu R\left(\frac{z_1 z_2 \sin(\beta)}{|\sin(\alpha+\beta)|} + \frac{z_1 z_3 \sin(\beta)}{|\sin(\alpha-\beta)|} + \frac{z_2 z_3}{|\sin(\alpha)|}\right)\right.$$
$$\left. + 2\mu R^2 U_\nu(R)\right]\chi_\nu(R,\alpha) = 0.$$
(9)

In (9), the channel functions $\chi_\nu(R,\alpha)$ are presented as a linear combination of the basic functions $(\varphi_n(R,\alpha))$, which are solutions of the relative motion equation (6) at zero value of the radial variable $(R = 0)$

$$\varphi_n(\alpha) = \begin{cases} \sin((4n-2)\alpha), & n = 1,2,3\ldots \\ \cos(4n\alpha), & n = 0,1,2\ldots \end{cases}$$
(10)

These periodic functions are solutions of the angular equation for the radial variable $R = 0$ that satisfy the Dirichlet and Neumann boundary conditions. Thus, we have two sets of basic functions — odd and even.

The numerical values of the adiabatic potentials $U_\nu(R)$ [6, 7] are obtained for different dimensions of the base (10), by which the channel functions $\chi_\nu(R,\alpha)$ are decomposed, and which parametrically depend on radial variable as

$$\chi_\nu(R,\alpha) = \sum_{n=1}^{N} C_{n\nu}(R)\varphi_n(\alpha).$$
(11)

Using the decomposition (11), from (9) we obtain a system of algebraic homogeneous equations, the solution of which allows to receive the values of the adiabatic potentials $U_\nu(R)$ and the coefficients $C_{n\nu}(R)$, and thus the channel functions (11). Having adiabatic potentials, we can find the energies of the ground and excited quantum states and their radial wave functions that satisfy the equation

$$\left[\frac{1}{R}\frac{\partial}{\partial R}\left(R\frac{\partial}{\partial R}\right) + U_\nu(R) + 2\mu\varepsilon\right]f_\nu(R) = 0.$$
(12)

The spectroscopic parameters of the considered three-particle systems were calculated from the determined adiabatic potentials in the Born–Oppenheimer approximation in the two-channel approximation.

3. Results of numerical calculation

The numerical values of the spectroscopic parameters for two singlet series of an exotic helium atom are obtained using the essential tools for mathematics — MAPPLE (2017). These results are presented in Table I and II. The left column in Table I indicates the odd–even (oe) and the even–even (ee)

TABLE II

The results of numerical calculations: spectral characteristics of the $(^3\text{He}^{2+}, e, \overline{^3\text{H}})$ system.

State	Energy value of the state [GeV]	Interval of radial variable [a.u.]	Mean radius of the state [a.u.]	The average radius of the system [m]
$^1S^{\text{oe}}\varepsilon_{00}$	1395.27479	$[0, 1/200000]$	1×10^{-6}	5.29×10^{-17}
$^1S^{\text{oe}}\varepsilon_{01}$	535.8780388	$[0, 9/1000000]$	2.5×10^{-6}	1.3225×10^{-16}
$^1S^{\text{oe}}\varepsilon_{02}$	244.496226	$[0, 13/1000000]$	5×10^{-6}	2.645×10^{-16}
$^1S^{\text{oe}}\varepsilon_{03}$	124.8114457	$[0, 19/1000000]$	6.05×10^{-6}	3.20045×10^{-16}
$^1S^{\text{ee}}\varepsilon_{00}$	2089.200523	$[0, 1/250000]$	9×10^{-6}	2.116×10^{-17}
$^1S^{\text{ee}}\varepsilon_{01}$	412.3373748	$[0, 1/125000]$	2×10^{-6}	1.058×10^{-16}
$^1S^{\text{ee}}\varepsilon_{02}$	128.7652912	$[0, 9/500000]$	5×10^{-6}	2.645×10^{-16}
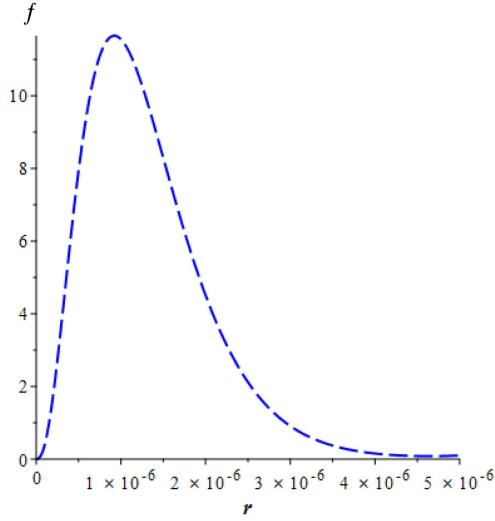
Fig. 1. Radial wave function of the ground state of the antitritium helium $(^3\text{He}^{2+}, e, \overline{^3\text{H}})$.
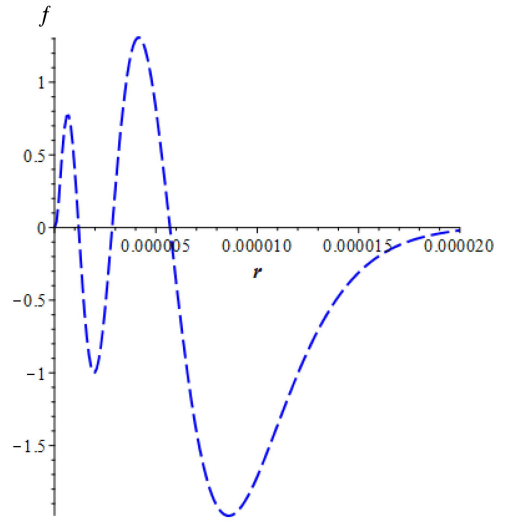
Fig. 2. Radial wave function for the third excited state of the antitritium helium $(^3\text{He}^{2+}, e, \overline{^3\text{H}})$.

series, and the right column shows the characteristics of the minimum adiabatic potential for two series. Parameters of the spectral characteristics for the ground and excited states of the system $(^3\text{He}^{2+}, e, \overline{^3\text{H}})$ are presented in the Table II.

As it follows from the presented data, the energy values for the ground state and for the excited states of the even series (ee) are higher than for the excited states in the odd series (oe). In this case, the energy value for the third excited state of the series (oe) — 124.81 GeV — coincides with the Higgs boson mass obtained experimentally at the Large Hadron Collider in 2012 ($M_\text{H} = 125.09\pm0.24$ GeV). It is also interesting to note that in the $^1S^{\text{ee}}$ singlet series, the second excited state with a relative error of 3% coincides with the Higgs boson mass.

The radial wave functions of the ground and third excited states of $^1S^{\text{oe}}$ antitritium helium are presented in Figs. 1 and 2, respectively.

There are several experimental and other theoretical investigations. For example, A. Arbey et al. [8] used scans of the 19-parameter space of the so-called phenomenological minimal supersymmetric Standard Model. This approach allows the evaluation of different missing parameters of bosons. In other investigation (H.Y. Cheng et al. [9], 2022) the quasi-two-body $D \to SP$ decays and the three-body D decays proceeding through intermediate scalar resonances were studied [9].

4. Conclusions

We have calculated the spectral characteristics for two singlet series ($^1S^{\text{oe}}, ^1S^{\text{ee}}$) of the antitritium helium $(^3\text{He}^{2+}, e, \overline{^3\text{H}})$. Our approach makes it possible to calculate both particles and antiparticles in physical systems, which opens up the possibility of expanding the field of application of the method, for example, to organic molecules.

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