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Research paper

Variational calculation of energy levels for metastable states of antiprotonic helium

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ABSTRACT

We apply the variational method in Hylleraas coordinates to solve the energy eigenvalue problem for antiprotonic helium molecular systems including $\bar{p}^3He^+$ and $\bar{p}^4He^+$. The numerical accuracy on the non-relativistic energies is shown to reach 10^{-17}, thus the precision of our results is only limited by the width of the metastable states. Expectation values of the Dirac delta operators for these states are also calculated.

1. Introduction

The existence of metastable antiprotonic helium ($\bar{p}He^+$) was verified experimentally at KEK in 1991 [1]. Soon after its discovery, this Coulomb three-body exotic system $\bar{p}He^+$ has been studied by laser spectroscopy [2–5] to investigate properties of antiprotonic helium atoms. Meanwhile, precise data on antiproton can be extracted by combining experimental and theoretical spectroscopic results of $\bar{p}He^+$ that provides a stringent test of CPT invariance in baryon sector [6,7]. In 2006, the accuracy of $\bar{p}He^+$ spectroscopy was measured to $(9–16)\times10^{-9}$ which yielded a value of (anti) proton-to-electron mass ratio with a relative uncertainty of 2.7×10^{-9} [8]. In 2011, two-photon transitions of $\bar{p}^{3,4}He^+$ were measured to $(2.3–5)\times10^{-9}$ and the accuracy of the mass ratio was derived to be 1.3×10^{-9} [9]. These values of the mass ratio have been adopted in the Committee on Data for Science and Technology (CODATA) adjustment of fundamental physical constants in 2006 [10] and 2010 [11].

For light systems, a bound state energy can be expanded in powers of the fine-structure constant $\alpha\approx1/137$ in the framework of the nonrelativistic quantum electrodynamics (NRQED) [12,13]. Therefore, the theoretical study of these systems can be carried out by first solving the time-independent Schrödinger equation. Then the leading order relativistic and radiative corrections of $R_\infty\alpha^2$ and $R_\infty\alpha^3$, as well as higher order corrections, can be calculated perturbatively using the nonrelativistic energy eigenfunctions, where R_∞ is the Rydberg constant.

Antiprotonic helium atom is composed of a helium nucleus, an electron e^- in the $1s$ ground state, and an antiproton $\bar{p}$ in a Rydberg state with principal quantum number $n\sim38$ and angular momentum quantum number $l\leqslant n-1$ [6,7]. Therefore, a state of $\bar{p}He^+$ can be designated as (n,l) using the quantum numbers of the antiproton. At first glance, $\bar{p}He^+$ is a neutral atom where a helium nucleus attracts an electron and an antiproton. On the other hand, $\bar{p}He^+$ can be seen as a diatomic molecule where an electron moves around massive helium nucleus and the antiproton. This dual nature of the antiprotonic helium was confirmed theoretically based on a simple atomic [14] and Born–Oppenheimer adiabatic approximation [15,16] of the wavefunction. Therefore, a molecular-type variational expansion was introduced to calculate nonrelativistic energies [17,18] in late 1990s and a precision of $\sim10^{-8}$ a.u. was achieved. At that time, some other methods were introduced to calculate nonrelativistic energies of $\bar{p}He^+$ such as variational method [19] and finite-element method [20].

In 1999 nonrelativistic energies of $\bar{p}He^+$ were calculated by Korobov, Bakalov, and Monkhorst [21] using a variational expansion. The radiative dominated states of the antiprotonic helium were calculated to an accuracy of better than 10^{-10} a.u., while the Auger dominated states were remained to be solved. Subsequently, an improved variational basis set was developed by Korobov [22]

$$\exp(-\alpha r_{12}-\beta r_{23}-\gamma r_{31}), \tag{1}$$

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where $r_{ij} = |\boldsymbol{r}_i - \boldsymbol{r}_j|$ is the distance between two particles and α, β, and γ are nonlinear parameters generated quasirandomly. This type of basis set was used to study various Coulomb three-body bound state problems, such as helium, hydrogen molecular ions, positronium ion and antiprotonic helium. The most accurate results, at that time, for the ground states of these systems were reported in [22]. In combination with the complex coordinate rotation (CCR) method [23], nonrelativistic energies for the Auger dominated states were calculated [24] in 2003. Based on the nonrelativistic energies [21,22,24], it was Korobov who performed systematic calculations for $\bar{p}He^+$ including relativistic and radiative corrections of orders $R_\infty\alpha^2$ [24], $R_\infty\alpha^3$ [25], $R_\infty\alpha^4$ [26], and $R_\infty\alpha^5$ [27,28]. While the transition frequencies are calculated to an accuracy of about 10^{-10} [27,28], independent calculations are desirable.

In order to provide an independent verification for Korobov's calculations mentioned above, the first step is to solve the three-body Schrödinger equation variationally. The basis set used in the variational calculation should be simple and efficient. Besides Eq. (1), there have been a number of high-precision works for three-body systems using the following correlated Hylleraas basis set

$$r_1^i r_2^j r_{12}^k \exp(-\alpha r_1 - \beta r_2), \tag{2}$$

where r_1 and r_2 are the distances of particle 1 and particle 2 relative to particle 0. This type of basis set was used to calculate s states of helium atoms [29,30]. It was applied to study nonrelativistic energies for simple molecular ion H_2^+ and its isotopes [31] as well. A precision of 10^{-30} was achieved for low-L states of H_2^+ [32] and HD^+ [33]. In particular, the validity of this basis set for higher angular momentum states of hydrogen molecular ions is confirmed [34], where nonrelativistic energies for states with $L = 2$–12 were calculated to an accuracy of 10^{-17} or better. Moreover, this wavefunction was extended successfully to study four-body systems such as lithium and lithium-like ions [35,36].

The purpose of this paper is to demonstrate that the basis set of Eq. (2) can also be applied to antiprotonic helium metastable states with high angular momentum. Consequently, independent calculations of nonrelativistic energies together with expectation values of the Dirac delta operators for $\bar{p}^{3,4}He^+$ metastable states are carried out in this paper. Atomic units ($m_e = e = \hbar = 1$) are used throughout.

2. Computational method

The exotic helium atom studied here is a three-body system that consists of an electron of mass m_e, a helium nucleus of mass M_{He}, and a negatively charged antiproton $\bar{p}$ of mass $M_{\bar{p}}$. Fig. 1 shows the geometrical configuration of the system, where $\boldsymbol{r}_1$ and $\boldsymbol{r}_2$ are, respectively, the position vectors for the electron and the antiproton, relative to the helium nucleus situated at the origin, and $\boldsymbol{r}_{12} = \boldsymbol{r}_1 - \boldsymbol{r}_2$. Thus, the Hamiltonian of $\bar{p}He^+$ can be expressed in the center-of-mass frame

$$H = -\frac{1}{2\mu_1}\nabla_{r_1}^2 - \frac{1}{2\mu_2}\nabla_{r_2}^2 - \frac{1}{M_{He}}\nabla_{r_1}\cdot\nabla_{r_2} - \frac{2}{r_1} - \frac{2}{r_2} + \frac{1}{r_{12}}, \tag{3}$$

$$\mu_1^{-1} = M_{He}^{-1} + m_e^{-1},\ \mu_2^{-1} = M_{He}^{-1} + M_{\bar{p}}^{-1}. \tag{4}$$

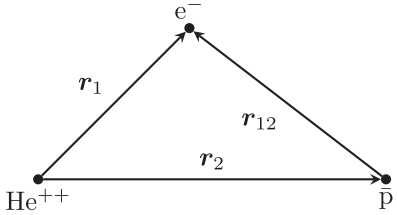

Fig. 1. Coordinate scheme for antiprotonic helium.

In order to compare with the previous calculations [26–28], the masses of the helium nucleus and the antiproton are chosen as the values adopted in [26–28]

$$M_{^3He} = 5495.885269\ m_e, \tag{5}$$

$$M_{^4He} = 7294.299536\ m_e, \tag{6}$$

$$M_{\bar{p}} = 1836.1526726\ m_e. \tag{7}$$

The energy eigenvalue problem for H is solved variationally using the following basis function

$$\phi_{ijk} = r_1^{l_1+i} r_2^{l_2+j} r_{12}^k e^{-\alpha r_1 - \beta r_2} Y_{l_1 l_2}^{LM}(\hat{\boldsymbol{r}}_1, \hat{\boldsymbol{r}}_2), \tag{8}$$

where

$$Y_{l_1 l_2}^{LM}(\hat{\boldsymbol{r}}_1, \hat{\boldsymbol{r}}_2) = \sum_{m_1 m_2} \langle l_1 l_2 m_1 m_2 | LM\rangle Y_{l_1 m_1}(\hat{\boldsymbol{r}}_1) Y_{l_2 m_2}(\hat{\boldsymbol{r}}_2) \tag{9}$$

is the vector coupled product of spherical harmonics for the electron and the antiproton, forming a common eigenstate of $\boldsymbol{L}^2, L_z$, and Π with the corresponding eigenvalues of $L(L+1), M$, and $(-1)^{l_1+l_2}$, respectively.

For a state with total angular momentum L, its wave function consists of angular momentum components fulfilling $l_1 + l_2 = L$

$$(l_1, l_2) = (0, L), (1, L-1), (2, L-2), \ldots, (L, 0). \tag{10}$$

Each configuration (l_1, l_2) has its own nonlinear parameters α and β. Since the electron is in the 1s state and the antiproton is in a Rydberg state, the leading angular momentum component $(0, L)$ has a primary contribution and contributions from the subsequent configurations become smaller. Thus, it is sufficient to consider only first few angular momentum components. In order to enhance rate of convergence and numerical stability, the leading angular momentum component is divided into N_L sub-blocks where each block has its nonlinear parameters (α, β), according to the following scheme [31]: the nth block in $(0, L)$ contains all the terms satisfying the following relations for the power j_n of r_2:

$$g_n < j_n \leqslant g_{n+1}, n = 1, 2, \ldots, N_L, \tag{11}$$

where

$$g_n = \mathrm{int}\left[\frac{\Omega}{N_L}(n-1)\right], \tag{12}$$

int[x] stands for the integer part of x, and Ω is an integer controlling the size of each block. The basis set is generated by including all terms such that

$$i + j + k \leqslant \Omega. \tag{13}$$

The vibrational motion between the helium nucleus and the antiproton should be sufficiently represented in the basis set as suggested by Bhatia and Drachman [37]. It was pointed out that function $\rho^N e^{-b\rho}$ can be used to simulate the vibrational modes, where ρ is the distance between the two nuclei, and N and b are two big numbers satisfying $b \approx N/2$. For the case of hydrogen

Table 1
Convergence study of the energy eigenvalue for the $\bar{p}^4He^+$ state (36,35). N_c is the number of angular momentum components. In atomic units.

N_c	E_{nr}
1	−2.98340755581832400(3)
2	−2.98402088240739306)
3	−2.98402095977657130(2)
4	−2.98402095978355102(2)
5	−2.98402095978355375)
6	−2.98402095978355327(1)
Korobov [40]	−2.98402095978355180