

Variational expansion for antiprotonic helium atoms

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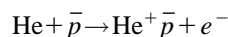
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A very accurate variational expansion is suggested for calculation of nonrelativistic energies of the metastable antiprotonic helium atoms $\text{He}^+\bar{p}$. This expansion reflects the dual atomic-molecular nature of the system. Convergence of the results as a function of the increasing sets of basis functions shows an accuracy better than 10^{-10} a.u., two orders of magnitude better than in our previous calculations.

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The discovery of long-lived antiprotonic states in helium [1], and subsequent precise measurements of some transitions between these states [2,3], presented a new, very interesting exotic atomic physics system. When stopped in helium, an antiproton replaces an electron in the reaction



taking up the space of the released electron. The majority of atoms formed decays promptly due to the emission of Auger electron and in collisions with ambient He atoms. However, about 3% of stopped \bar{p} settle into nearly circular orbits ($l \approx n-1$) and live as long as a few microseconds. This is because the system becomes stable against (internal) Auger transitions: to remove the ≈ 25 eV binding energy of the electron requires a \bar{p} transition with $\Delta l \geq 3$. In Table I the lifetime of the metastable $\text{He}^+\bar{p}$ atom is compared with those of other well-known atomic systems.

The first theoretical predictions, based on rather simple atomic [4] and Born-Oppenheimer adiabatic [5] approximations of the wave function, provided a good qualitative description of the energy-level structure for the $\text{He}^+\bar{p}$, but approached the experimental values with a large dispersion of 1000 ppm. These calculations confirmed the dual nature of the antiprotonic helium atoms as exotic systems exhibiting features of both atoms and molecules.

Substantial progress in calculating nonrelativistic energies has been achieved in [6,7] by using a molecular-type variational expansion. An accuracy of $\sim 10^{-8}$ a.u. has been reached, which improves on the previous level of precision by four orders of magnitude. Recently, finite-element [8], hyperspherical [9], and variational [10] calculations of nonrelativistic energies have become available. All of these calculations support the results of [6].

The theoretical study of three-body systems is usually carried out in several stages. Since the system no longer has an analytical solution the first stage presents the calculation of nonrelativistic energies with the Schrödinger equation. Fur-

ther stages are relativistic and QED corrections of first, second, and higher orders to the nonrelativistic Hamiltonian. Therefore, the accuracy of the nonrelativistic calculations determines the overall precision.

The purpose of this work is to increase the numerical accuracy of the nonrelativistic energies to 10^{-10} a.u. Such an effort is of manifold interest. First, the radiative corrections for a bound electron and vacuum polarization must be taken into account [7]. Recent calculations of the fine and hyperfine structures of the antiprotonic helium energy levels show a slow convergence of numerical results, which sets the limit on the relative accuracy of the hyperfine splitting to 10^{-4} [11] with our previous basis [6]. Therefore, a more accurate numerical method is extremely desirable.

The states considered have very high values of the total angular momentum ($L \sim 35$) and have an adiabatic behavior ($v_{\bar{p}} \ll v_e$). The high L leads to a system of a large number of equations ($L+1$ equations) that couple components of internal degrees of freedom [Eq. (1)]. This makes the numerical treatment of the system difficult. On the other hand, the adiabaticity enables the number of components in this equation to be reduced to a reasonable number.

We could perform a separation of rotational variables by using the molecular expansion based on the symmetrized Wigner D functions [6]

$$\Psi_M^{L\lambda}(\mathbf{R}, \mathbf{r}) = \sum_{m=0}^L \mathcal{D}_{Mm}^{L\lambda}(\Phi, \Theta, \varphi) F_m^{L\lambda}(R, r, \theta). \quad (1)$$

In the case of a semiadiabatic three-body system the above method converges quickly with respect to $m_{\max} \leq L$, where

TABLE I. Comparison of the lifetimes of the hydrogen $2P$ state, the helium 2^3P state, and the antiprotonic helium metastable states.

H($2P$)	He(2^3P)	He $^+\bar{p}$
1.6×10^{-9} s	3.3×10^{-8} s	1.7×10^{-6} s

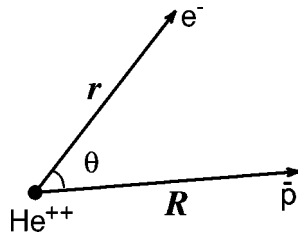


FIG. 1. Coordinate system for the variational wave function.

m_{max} is the number of components kept in expansion (1). If m_{max} is smaller than the $\Delta l = l - l'$ of the Auger transition,

$$[\text{He}^+ \bar{p}]_{(n,l)} \rightarrow [\text{He}^{2+} \bar{p}]_{(n',l')} + e^-,$$

the Hamiltonian projected onto this subspace has a purely discrete spectrum. Expansion (1) was the basis for our previous calculation [6].

Since the antiprotonic helium resembles the atomic system as well, one may construct the wave function as a combination that inherits some features of atomic systems as well as of molecular systems. Thus, the bipolar harmonic expansion [12] (coordinates are shown in Fig. 1),

$$\Psi_M^{L\lambda}(\mathbf{R}, \mathbf{r}) = \sum_{l_1+l_2=L} R^{l_1} r^{l_2} \{Y_{l_1} \otimes Y_{l_2}\}_{LM} G_{l_1 l_2}^{L\lambda}(R, r, \theta), \quad (2)$$

could be chosen for the angular part of the wave function and exponential expansion [13,14],

$$G_{l_1 l_2}^{L\lambda}(R, r, \theta) = \sum_{i=1}^{\infty} C_i e^{-\alpha_i R - \beta_i r - \gamma_i |\mathbf{R}-\mathbf{r}|}, \quad (3)$$

for the description of components of internal degrees of freedom. Here α_i , β_i , and γ_i are generated in a quasirandom manner. To meet the requirements of the molecular nature of this system the functions of type $\cos(\nu_i R) e^{-\alpha_i R}$ should be introduced for the antiprotonic orbital instead of $e^{-\alpha_i R}$. Then it can be proven that the subspace,

$$\mathcal{H}_m = \sum_{m'=0}^m \mathcal{D}_{Mm'}^{L\lambda}(\Phi, \Theta, \varphi) F_{m'}^{L\lambda}(R, r, \theta),$$

coincides with the subspace spanned by the functions,

TABLE II. Convergence of the new variational expansion with the number of basis functions. ${}^4\text{He}^+ \bar{p}$ (37,34).

N	E_{nr}
400	-2.911 180 654 8
600	-2.911 180 925 0
800	-2.911 180 932 1
1000	-2.911 180 933 3
1200	-2.911 180 933 86
1400	-2.911 180 934 02

$$\bar{\mathcal{H}}_m = \sum_{l_2=0}^m R^{l_1} r^{l_2} \{Y_{l_1} \otimes Y_{l_2}\}_{LM} G_{l_1 l_2}^{L\lambda}(R, r, \theta),$$

and we can retain in expansion (2) the components with $l_2 \leq l_{max}$.

Finally we get

$$\Psi_M^{L\lambda}(\mathbf{R}, \mathbf{r}) = \sum_{l_2=0}^{l_{max}} R^{l_1} r^{l_2} \{Y_{l_1} \otimes Y_{l_2}\}_{LM} G_{l_1 l_2}^{L\lambda}(R, r, \theta),$$

$$G_{l_1 l_2}^{L\lambda}(R, r, \theta) = \sum_{i=1}^{\infty} [C_i \cos(\nu_i R) + D_i \sin(\nu_i R)] e^{-\alpha_i R - \beta_i r - \gamma_i |\mathbf{R}-\mathbf{r}|}. \quad (4)$$

This expansion is reminiscent of that used in [15], where the complex exponents $e^{-(\alpha_i + i\nu_i)R}$ have been introduced into Eq. (3). In both cases the problem is reduced to the equation of type

$$A - \lambda B = 0,$$

with real $(2n \times 2n)$ matrices A and B . In our case we get $2n$ different eigenvalues, whereas in [15] only the n twofold eigenvalues can be obtained, and the wave function of the studied state is complex.

The convergence of this variational method is demonstrated in Table II. At present the major limitation is the computational time, which is about 20 h on an IBM RS/6000 workstation for a basis set of $N=1400$. Table II shows that the achieved precision is about 10^{-10} a.u.

TABLE III. Nonrelativistic energies of the states in the $\bar{p} {}^4\text{He}^+$ atom. $N=1200$.

	$v=0$	$v=1$	$v=2$	$v=3$	$v=4$	$v=5$
$L=32$	-3.353 757 863 4					
$L=33$	-3.216 244 232 3	-3.105 382 669 3				
$L=34$	-3.093 466 901 6	-2.996 335 441 9	-2.911 180 933 9			
$L=35$	-2.984 020 954 3	-2.899 282 178 3	-2.825 146 804 3	-2.760 233 341 2	-2.703 283 213 0	
$L=36$	-2.886 682 390 2	-2.813 115 395 6	-2.748 859 922 9	-2.692 624 845 9	-2.643 248 902 9	-2.599 707 672 2
$L=37$	-2.800 372 315 5	-2.736 841 191 6	-2.681 394 129 3	-2.632 832 902 6	-2.590 101 200 1	
$L=38$	-2.724 124 791 9	-2.669 551 749 1	-2.621 891 875 7	-2.580 051 405 5		
$L=39$	-2.657 056 943 1	-2.610 401 281 8	-2.569 547 479 9			
$L=40$	-2.598 340 648 3	-2.558 586 074 3				
$L=41$	-2.547 176 612 9					

close to the natural width 10^{-11} a.u. of these states defined by the radiative lifetime. This method improves upon our previous molecular-type variational calculations [6] and more recent calculations [8–10] by more than two orders of magnitude.

Results of numerical calculations are presented in Table III. Only the radiative dominated decay states are retained, since the Auger dominated states are short-lived and possess a width that is greater than 10^{-10} a.u., and these states should

be treated in a way that is similar to what is described in [16]. The masses of particles adopted for numerical calculations are $m_\alpha = 7294.299$, $m_{\bar{p}} = 1836.1527$.

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