Metastable states in the antiprotonic helium atom decaying via Auger transitions

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In the present paper, we perform a systematic calculation of the complex resonance energy for metastable states in the antiprotonic helium atoms, which decay predominantly via Auger transitions, by using the complex-coordinate rotation (CCR) method. Special attention is paid to relativistic corrections for the bound electron related to the Breit interaction. These corrections have been calculated using the CCR wave functions, which are square integrable. Some higher-order relativistic and QED effects have been included into consideration to get precise theoretical values for transition frequencies.

I. INTRODUCTION

Metastable states of an exotic atom $He^+\bar{p}$ were of considerable interest in the past years. After first observation at KEK of the delayed annihilation phenomena, when about 3.6% of antiprotons injected into the helium target [1] survived as long as a few microseconds, precise spectroscopic measurements of several transition lines both in ^{4}He and ^{3}He atoms have been performed at CERN [2,3]. It was expected that such longevity could be explained by the stability model suggested by Condo [4]. According to this hypothesis, antiprotons that occupy nearly circular orbits (with $n\sim40$) decay by slow radiative transitions only. Further theoretical calculations of the transition energies [5] that brought agreement between theory and experiment to about 5–10 ppm have rigorously confirmed the Condo model.

In the recent precise measurements [6] carried out at CERN, a daughter state of the measured transition, in general, is a state decaying via Auger channel. That allows to observe a spike in the annihilation time spectra when a laser wavelength is on-resonance. To meet the requirements of these experiments, it is necessary to perform an accurate study of the "Auger states."

Very precise nonrelativistic energies and wave functions have been obtained for the metastable states which decay dominantly via radiative channels [7]. In this case one can effectively apply the Feshbach formalism, when the Hamiltonian is projected onto the subspace of closed channels that still provide a sufficiently accurate zero-order approximation for the wave function. The other advantage is that the standard variational technique may be applied. In case when the Auger decay becomes dominant, the state should be considered as an essentially resonant one, and more sophisticated methods are required.

In a present calculation, we apply the complex-coordinate rotation (CCR) method [8] to this problem.

II. THE FESHBACH FORMALISM

The exotic helium atoms under consideration consist of an electron of mass m_e, a helium nucleus of mass M_{He}, and a negatively charged antiproton $\bar{p}$ of mass $M_{\bar{p}}$. The nonrelativistic Hamiltonian (in atomic units $e=\hbar=m_e=1$) reads

$$H=T+V$$

$$=-\frac{1}{2\mu_1}\nabla_R^2-\frac{1}{2\mu_2}\nabla_r^2-\frac{1}{M_{He}}\nabla_R\cdot\nabla_r-\frac{2}{R}-\frac{2}{r}+\frac{1}{|R-r|},$$

$$\mu_1^{-1}=M_{He}^{-1}+M_X^{-1}, \quad \mu_2^{-1}=M_{He}^{-1}+m_e^{-1}, \quad (1)$$

where R and r are the position vectors of $\bar{p}$ and of the electron relative to the helium nucleus, while T and V denote the operators of kinetic and potential energy.

The wave function of a state of total angular momentum L, its projection M onto z axis of the space-fixed frame, and total spatial parity λ may be written as

$$\Psi_M^{L\lambda}(R,r)=\sum_{l+l_e=L}R^l r^{l_e}\{Y_l\otimes Y_{l_e}\}_{LM}G_{ll_e}^{L\lambda}(R,r,\theta), \quad (2)$$

where the components $G_{ll_e}^{L\lambda}(R,r,\theta)$ are functions of the internal degrees of freedom and are expanded as follows:

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

The complex parameters α_i, β_i, and γ_i are generated in a quasirandom manner [7]:

$$\alpha_i=\left[\left\lfloor\frac{1}{2}i(i+1)\sqrt{p_\alpha}\right\rfloor(A_2-A_1)+A_1\right]$$

$$+i\left[\left\lfloor\frac{1}{2}i(i+1)\sqrt{q_\alpha}\right\rfloor(A_2'-A_1')+A_1'\right], \quad (4)$$

$\lfloor x\rfloor$ designates the fractional part of x, p_α, and q_α are some prime numbers, $[A_1,A_2]$ and $[A_1',A_2']$ are real variational intervals which need to be optimized. Parameters β_i and γ_i are obtained in a similar way.

To get a Feshbach-type closed-channel solution, one needs to retain in expansion (2) components with small l_e (angular momentum of an electron) and if $l_e^{(max)}<\Delta l$, where $\Delta l=l-l'$ is the smallest energetically possible change of the antiproton orbital angular momentum in the Auger transition,

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

TABLE I. Variational parameters and number of basis functions [n_i, where i stands for $l_e = i$ in Eq. (2), and n_{tot} is a sum over components] for different subsets of the variational wave function of the (38,33) state of $^4\text{He}^+\bar{p}$. Intervals $[A_1, A_2]$ and $[A'_1, A'_2]$ correspond to real and imaginary parts of a randomly chosen parameter α_i [see Eq. (4) for details], intervals $[B_1, B_2]$ and $[B'_1, B'_2]$ to β_i, and intervals $[G_1, G_2]$ and $[G'_1, G'_2]$ to γ_i. Prime numbers are $p_\alpha = 2$, $p_\beta = 3$, $p_\gamma = 5$, and $q_\alpha = 7$, $q_\beta = 11$, $q_\gamma = 13$.

	n_{tot}	n_0	n_1	n_2	n_3	A_1	A_2	A'_1	A'_2	B_1	B_2	B'_1	B'_2	G_1	G_2	G'_1	G'_2
$i=1$	500	450	50	0	0	59.0	91.0	1.00	4.50	1.00	5.60	0.00	0.00	0.00	1.50	0.00	0.00
$i=2$	650	450	150	50	0	53.0	84.0	2.00	5.00	0.00	2.20	0.00	0.00	0.00	0.80	0.00	0.00
$i=3$	530	30	270	230	0	60.0	100.0	1.50	4.50	0.00	0.80	0.00	0.00	0.00	0.30	0.00	0.00
$i=4$	820	20	250	420	130	65.0	110.0	1.50	4.50	0.00	0.40	0.00	0.00	0.00	0.15	0.00	0.00

then the subspace spanned over these basis functions is a subspace of closed channels for this resonant state. A detailed discussion can be found in Ref. [7].

As it has been obtained in previous calculations [3,9,10], the radiative width for the metastable antiprotonic helium states is about 10^{-12} a.u. So the states with $\Delta l \leq 3$ predominantly decay via the Auger transition, while states with $\Delta l \geq 4$ have a radiative decay as a dominant channel and the lifetime for these states is about few microseconds. On the other hand, the Auger width of the states with $\Delta l = 3$ is of the order of $10^{-8} - 10^{-9}$ a.u. In this case, the zero-order wave function obtained within the closed-channel approximation only would be of approximate relative accuracy of $\sim 10^{-4}$ that is limiting the relative accuracy of mean values of various operators related to relativistic and QED corrections. Thus this approximation is insufficient for a precise determination of transition energies to compare with experimental measurements.

III. COMPLEX-COORDINATE ROTATION

The Coulomb Hamiltonian is analytic under dilatation transformations,

$$(U(\theta)f)(\mathbf{r}) = e^{m\theta/2}f(e^\theta \mathbf{r}), \quad H(\theta) = U(\theta)HU^{-1}(\theta), \quad (5)$$

for real θ and can be analytically continued to the complex plane. The complex-coordinate rotation method [8] "rotates" the coordinates of the dynamical system ($\theta = i\varphi$), $r_{ij} \rightarrow r_{ij}e^{i\varphi}$, where φ is the parameter of the complex rotation. Under this transformation, the Hamiltonian (1) changes as a function of φ,

$$H_\varphi = Te^{-2i\varphi} + Ve^{-i\varphi}, \quad (6)$$

where T and V are the kinetic energy and Coulomb potential operators. The continuum spectrum of H_φ is rotated on the complex plane around branch points ("thresholds") to "uncover" resonant poles situated on the unphysical sheet of the Reimann surface in accordance with the Augilar-Balslev-Combes theorem [11]. The resonance energy is then determined by solving the complex eigenvalue problem for the rotated Hamiltonian,

$$(H_\varphi - E)\Psi_\varphi = 0. \quad (7)$$

The eigenfunction Ψ_φ obtained from Eq. (7) is square integrable and the corresponding complex eigenvalue $E = E_r$

$-i\Gamma/2$ defines the energy E_r and the width of the resonance, Γ, the latter is being related to the Auger rate as $\lambda_A = \Gamma/\hbar$.

The use of a finite set of N basis functions defined by Eqs. (2) and (3) reduces problem (7) to the generalized algebraic complex eigenvalue problem

$$(A - \lambda B)x = 0, \quad (8)$$

where $A = \langle \Psi_\varphi | H_\varphi | \Psi_\varphi \rangle$ is the finite $N \times N$ matrix of the Hamiltonian in this basis, and B is the matrix of overlap $B = \langle \Psi_\varphi | \Psi_\varphi \rangle$.

It is known that to get an accurate solution for an Auger state of the antiprotonic helium is a rather difficult problem due to a very narrow width of the state and different scales for antiproton and electron orbitals. In our calculations, we use a general strategy of a multilayered variational wave function as is described in Ref. [12]. In the case of antiprotonic helium metastable states, a trial wave function contains four basis sets. First two sets are required for better approximation of the closed-channel solution. Parameters of a third set are adjusted in a way to better represent excited electron intermediate states, and the last set corresponds to electron continuum. An example of a wave-function configuration for the (38,33) state of $^4\text{He}^+\bar{p}$ is presented in Table I. We use conventional atomic notation to identify a state, namely, approximate quantum numbers of the antiprotonic orbital, (n,l) (while an electron for these states is situated roughly in the ground $1s$ state).

The numerical solution of Eq. (8) was obtained using the inverse iteration method. The variational intervals for the nonlinear parameters α, β, γ in Eq. (3) were optimized manually using two components (with $l_e = 0,1$) in the variational expansion (2). Equation (8) was then repeatedly solved with these optimized values for a set of rotational parameters $\varphi = 0, \ldots, 0.20$ and dilatation parameters $a_{dl} = 0.99, 1, 1.01$ using basis sets with $N = 2200-2500$. Here the dilatation is defined as a transformation of all coordinates of the dynamical system: $r_{ij} \rightarrow r_{ij}a_{dl}$. The number of components kept in expansion (2) was taken to be equal to 4, except for the case of the (32,31) state of $^4\text{He}^+\bar{p}$, when $\Delta l = 4$ and the number of components should be equal to 5 in order to include continuum states. Inclusion of higher l_e components in Eq. (2) does not improve the result within achieved accuracy.

The results for the (38,33) state are plotted in Fig. 1, from which one can extract precise parameters for this resonance:
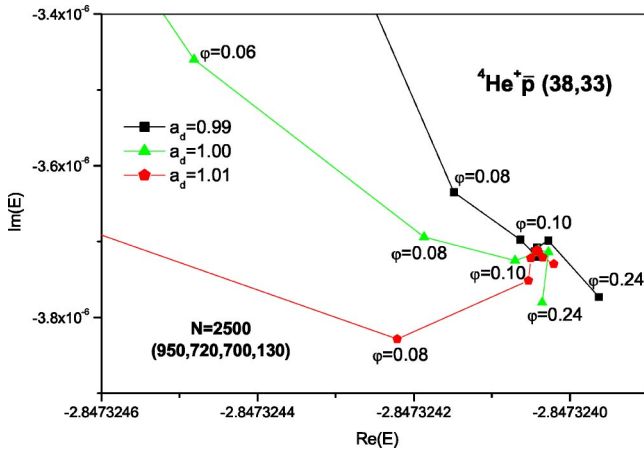
FIG. 1. (Color online) Rotational paths for the (38,33) state of ^{4}He$^+\bar{p}$. The point on the plot where the paths are nearly stationary determines a position of the resonance on the complex plane. Parameters of the resonance for this state derived from the plot are $E_r = -2.847\,324\,042(3)$ a.u. and $\Gamma/2 = 3.714(3) \times 10^{-5}$ a.u.

$$E_r = -2.847\,324\,042(3) \quad \text{a.u.},$$

$$\Gamma/2 = 3.714(3) \times 10^{-5} \quad \text{a.u.}$$

The uncertainty in the calculated parameters of the resonance is about 10^{-9} a.u. That is somewhat less accurate than in a case of states with a dominance of the radiative decay mode. The reason for that is an absence of simple criteria for choosing optimal variational parameters as in case of the standard variational principle for bound states.

From these calculations, the Auger decay rates can be extracted. Table II contains the Auger rates obtained by the approach expounded above, which are compared with experimental measurements and other theoretical calculations. It is required to note that beyond the Auger decay, other effects such as collisional quenching have influence on experimental data. As is seen from the table, our results are in a rather good agreement with previous theoretical calculations. Especially, good agreement is with our previous calculations [14], except for one case of (37,33) state, which has been marked in Ref. [14] as not converging. It is worth saying that in the early calculation, a different type of basis functions has been used and a Feshbach-like formalism has been applied to get the Auger width.

IV. LEADING-ORDER RELATIVISTIC CORRECTIONS FOR THE RESONANT STATES

In this work, we will consider the spin-independent part of a transition energy only. The major contribution beyond the nonrelativistic transition energy comes from the relativistic correction for the bound electron,

$$E_{rc} = \alpha^2 \left\langle -\frac{\mathbf{p}_e^4}{8m_e^3} + \frac{4\pi}{8m_e^2}[Z_{\text{He}}\delta(\mathbf{r}_{\text{He}}) + Z_{\bar{p}}\delta(\mathbf{r}_{\bar{p}})] \right\rangle. \quad (9)$$

The other terms of the Breit Hamiltonian, which have to be considered, are the following: the relativistic correction to the kinetic energy for heavy particles (including the Darwin term for an antiproton),

$$E_{kin} = -\alpha^2 \left\langle \frac{\mathbf{p}_{\text{He}}^4}{8m_{\text{He}}^3} + \frac{\mathbf{p}_{\bar{p}}^4}{8m_{\bar{p}}^3} - \frac{Z_{\bar{p}}}{8m_{\bar{p}}^2}4\pi\delta(\mathbf{r}_{\bar{p}}) \right\rangle; \quad (10)$$

the retardation (or the transverse photon exchange),

$$E_{ret} = -\alpha^2 \sum_{i>j} \frac{Z_i Z_j}{2m_i m_j} \left\langle \frac{\mathbf{p}_i \cdot \mathbf{p}_j}{r_{ij}} + \frac{\mathbf{r}_{ij}(\mathbf{r}_{ij} \cdot \mathbf{p}_i)\mathbf{p}_j}{r_{ij}^3} \right\rangle; \quad (11)$$

and the nuclear finite-size correction,

$$E_{\text{FSC}} = \sum \frac{2\pi Z_i (R_i/a_0)^2}{3} \langle \delta(\mathbf{r}_i) \rangle, \quad (12)$$

where R is the root-mean-square radius of the nuclear charge distribution. The rms radius for the helium nucleus and antiproton is, respectively, $R(^4\text{He}) = 1.673(1)$ fm, $R(\bar{p}) = 0.862(12)$ fm.

The last three contributions are less than the leading contribution from Eq. (9) by three or four orders of magnitude. That means that they can be calculated using the closed-channel zero-order wave function, since a relative accuracy of $\sim 10^{-4}$ is sufficient for these corrections. On the contrary, the leading contribution requires more accurate zero-order approximation, which can be obtained within the framework of the complex-coordinate rotation approach.

In this case a perturbation theory has to be formulated, which can be applied to resonant states. The relevant theory is provided by the theorem proved by Simon [17].

Theorem. Let H be a three-body Hamiltonian with the Coulomb pairwise interaction, and $W(\theta)$ be a dilatation analytic perturbation. Let E_0 be an isolated simple resonance

TABLE II. Comparison of theoretical Auger decay rates λ_A and experimentally measured decay rates (in s^{-1}) for the ^{4}He$^+\bar{p}$ atom.

State	Δl	Expt. [13]	[14]	[15]	[16]	CCR
(38,33)	2	$3.85(26) \times 10^{11}$	3.1×10^{11}	3×10^{11}	3.08×10^{11}	$3.071(3) \times 10^{11}$
(37,33)	3	$1.11(16) \times 10^{11}$	5.7×10^9	3×10^{10}	4.41×10^{10}	$4.21(2) \times 10^{10}$
(38,34)	3	$1.11(7) \times 10^8$	1.3×10^8	1.4×10^8		$1.344(4) \times 10^8$
(34,32)	3	$1.45(16) \times 10^8$	2.2×10^8	2.3×10^8	1.84×10^8	$2.260(3) \times 10^8$

TABLE III. Relativistic corrections to the energy and Auger width of the (38,33) state of the $^4\mathrm{He}^+\bar{p}$ atom.

	Re	Im
E_{NR}	$-2.847324042(3)$	$3.714(3)\times10^{-6}$
$\mathbf{p}_e^4$	$48.7142(4)$	$0.0089(4)$
$\delta(\mathbf{r}_{\mathrm{He}})$	$1.60580(1)$	$0.00029(1)$
$\delta(\mathbf{r}_{\bar{p}})$	0.05392	0.000015
E_{rel}	$-2.847384174(5)$	$3.702(5)\times10^{-6}$

energy [discrete eigenvalue of $H(\theta)$]. Then for small β, there is exactly one resonance of $H+\beta W$ near E_0 and

$$E(\beta)=E_0+a_1\beta+a_2\beta^2+\cdots$$

is analytic near $\beta=0$. In particular,

$$a_1=E'(0)=\langle\Psi_\theta^*|W(\theta)|\Psi_\theta\rangle/\langle\Psi_\theta^*,\Psi_\theta\rangle. \tag{13}$$

Some remarks are necessary.

In the complex scaling theory (such as the CCR approach), a resonance is defined as a complex eigenvalue of $H(\theta)$. Thus one needs to establish a relation between this definition of "resonance" and the one generally used in literature, where resonance is understood as a "pole" of the scattering amplitude on the unphysical sheet of the Reimann surface of energy. This definition of resonance, particularly, is required in QED perturbation theory. For some physical cases, it may be proved [18] that these two definitions coincide.

It is obvious that operators encountered in Eq. (9) are dilatation analytic,

$$\delta_\theta(\mathbf{r})=\delta(\mathbf{r})e^{-3\theta}, \quad \mathbf{p}_\theta^4=\mathbf{p}^4e^{-4\theta}.$$

However, they are not "small" perturbations in a sense of the Simon theorem requirements. It is a general practice in QED to regularize these operators in some or the other way, the only requirement is to preserve a "dilatation analyticity"

property. And then after performing all calculations, regularization should be removed to get finite results.

An example of such calculations is shown in Table III, from which it is seen that relativistic correction to the Auger decay rate is about 0.3% and, probably, can be detected in experiment. The uncertainty in the relativistic correction for the bound electron in this case is about 30% greater than the numerical uncertainty in the nonrelativistic energy. In the case of states with the multipolarity of the Auger transition $\Delta l=3$, the final uncertainty is primarily defined by the uncertainty in the leading term of the relativistic corrections.

V. HIGHER-ORDER CORRECTIONS AND FINAL RESULTS

Beyond the relativistic leading-order corrections described in a previous section there are a few other contributions, which are essential to get reliable theoretical values for transition energies.

The first and the most simple one is the correction due to the anomalous magnetic moment of electron,

$$E_{rc\text{-}QED}=\frac{4\pi\alpha^2}{8m_e^2}2a_e\langle Z_{\mathrm{He}}\delta(\mathbf{r}_{\mathrm{He}})+Z_{\bar{p}}\delta(\mathbf{r}_{\bar{p}})\rangle, \tag{14}$$

where

$$a_e=\frac{\alpha}{\pi}\frac{1}{2}+\left(\frac{\alpha}{\pi}\right)^2\left[\frac{197}{144}+\frac{\pi^2}{12}-\frac{\pi^2}{2}\ln2+\frac{3}{4}\zeta(3)\right]$$

$$=1.1596522\times10^{-3}.$$

It may be included into the Breit Hamiltonian, but we find it convenient to treat it separately.

The next two are the one-loop self-energy contribution in a nonrecoil limit [19,20],

TABLE IV. Multipolarities of the Auger transition Δl, nonrelativistic energies E_{nr} (in atomic units), Auger widths Γ (in atomic units), expectation values of operators $\mathbf{p}_e^4$, $\delta(\mathbf{r}_{\mathrm{He}})$, and $\delta(\mathbf{r}_{\bar{p}})$ for the Auger states of the $^4\mathrm{He}^+\bar{p}$ atom.

State	Δl	E_{nr}	$\Gamma/2$	$\mathbf{p}_e^4$	$\delta(\mathbf{r}_{\mathrm{He}})$	$\delta(\mathbf{r}_{\bar{p}})$	$\beta(n,l)$
(39,34)	3	$-2.77101156918(4)$	0.993×10^{-8}	51.5750	1.69187	0.04717	4.4305
(38,34)	3	$-2.836524596427(4)$	1.626×10^{-9}	48.0002	1.58482	0.05533	4.4440
(38,33)	2	$-2.847324042(3)$	3.714×10^{-6}	48.7142	1.60580	0.05393	4.4386
(37,33)	3	$-2.922449847(2)$	5.09×10^{-7}	44.8819	1.49053	0.06262	4.4554
(36,33)	3	$-3.00797908793(2)$	2.93×10^{-9}	41.2334	1.38199	0.07292	4.4741
(36,32)	2	$-3.019058205(5)$	6.760×10^{-6}	42.1265	1.40809	0.07052	4.4673
(35,32)	3	$-3.1166797896(2)$	6.97×10^{-8}	38.3699	1.29586	0.08121	4.4882
(34,32)	3	$-3.227676372722(3)$	2.733×10^{-9}	34.5306	1.18087	0.09256	4.5127
(34,31)	2	$-3.238577980(1)$	5.896×10^{-6}	35.6145	1.21282	0.08942	4.5023
(33,31)	3	$-3.36465178245(3)$	1.453×10^{-8}	31.9300	1.10252	0.10112	4.5395
(32,31)	4	$-3.50763503077540(4)$	5.1×10^{-13}	28.3087	0.99382	0.11308	4.56020
(31,30)	3	$-3.679774778770(4)$	4.754×10^{-9}	26.0710	0.92622	0.12144	4.57894

TABLE V. Multipolarities of the Auger transition Δl, nonrelativistic energies E_{nr} (in atomic units), Auger widths Γ (in atomic units), expectation values of operators $\mathbf{p}_e^4$, $\delta(\mathbf{r}_{He})$, and $\delta(\mathbf{r}_{\bar{p}})$ for the Auger states of the ^{3}He$^+\bar{p}$ atom.

State	Δl	E_{nr}	$\Gamma/2$	$\mathbf{p}_e^4$	$\delta(\mathbf{r}_{He})$	$\delta(\mathbf{r}_{\bar{p}})$	$\beta(n,l)$
(38,33)	3	$-2.7562177355(3)$	3.38×10^{-8}	52.2796	1.71296	0.04549	4.4279
(37,33)	3	$-2.82196302536(3)$	4.26×10^{-9}	48.6427	1.60404	0.05369	4.4414
(37,32)	2	$-2.83307489(1)$	8.12×10^{-6}	49.2841	1.62261	0.05220	4.4369
(36,32)	3	$-2.9087979751(1)$	5.8×10^{-9}	45.6212	1.51328	0.06138	4.4527
(35,32)	3	$-2.99540435174(2)$	8.17×10^{-9}	41.6764	1.39520	0.07159	4.4712
(35,31)	2	$-3.00689318(1)$	1.767×10^{-5}	42.4005	1.41545	0.06868	4.4648
(34,31)	3	$-3.10612885528(1)$	8.1×10^{-10}	38.6976	1.30553	0.08006	4.4858
(33,31)	3	$-3.21950724327(1)$	8.28×10^{-9}	34.7441	1.18716	0.09174	4.5110
(33,30)	2	$-3.230815869(2)$	1.126×10^{-5}	35.8104	1.21828	0.08832	4.498
(30,29)	3	$-3.685380849484(3)$	1.469×10^{-8}	25.9971	0.92377	0.12145	4.57885

$$E_{se} = \frac{4\alpha^3}{3m_e^2}\left[\ln\frac{1}{\alpha^2} - \ln\frac{k_0}{R_\infty} + \frac{5}{6} - \frac{3}{8}\right]\langle Z_{He}\delta(\mathbf{r}_{He}) + Z_{\bar{p}}\delta(\mathbf{r}_{\bar{p}})\rangle$$

$$+ \frac{4\alpha^4}{3m_e^2}\left[3\pi\left(\frac{139}{128} - \frac{1}{2}\ln 2\right)\right]\langle Z_{He}^2\delta(\mathbf{r}_{He}) + Z_{\bar{p}}^2\delta(\mathbf{r}_{\bar{p}})\rangle$$

$$- \frac{4\alpha^5}{3m_e^2}\left[\frac{3}{4}\right]\langle Z_{He}^3\ln^2(Z_{He}\alpha)^{-2}\delta(\mathbf{r}_{He})$$

$$+ Z_{\bar{p}}^3\ln^2(Z_{\bar{p}}\alpha)^{-2}\delta(\mathbf{r}_{\bar{p}})\rangle, \tag{15}$$

and the one-loop vacuum polarization:

$$E_{vp} = \frac{4\alpha^3}{3}\left[-\frac{1}{5}\right]\langle Z_{He}\delta(\mathbf{r}_{He}) + Z_{\bar{p}}\delta(\mathbf{r}_{\bar{p}})\rangle$$

$$+ \frac{4\alpha^4}{3}\left[\frac{5\pi m_e}{64}\right]\langle Z_{He}^2\delta(\mathbf{r}_{He}) + Z_{\bar{p}}^2\delta(\mathbf{r}_{\bar{p}})\rangle. \tag{16}$$

The only quantity that needs numerical evaluation is the Bethe logarithm, which arises from the ultrasoft photon contribution and can be expressed as [21,22]

$$\ln\frac{k_0}{R_\infty} = \frac{\langle \mathbf{J}(H-E_0)\ln[(H-E_0)/R_\infty]\mathbf{J}\rangle}{\langle \mathbf{J}(H-E_0)\mathbf{J}\rangle},$$

where $\mathbf{J} = \Sigma_i z_i \mathbf{v}_i = \Sigma_i z_i \mathbf{p}_i/m_i$ is a nonrelativistic electric current operator for a dynamical system. The denominator can be easily expanded:

$$\langle 0|\mathbf{J}(E_0-H)\mathbf{J}|0\rangle = -\langle 0|\mathbf{J}[H,\mathbf{J}]|0\rangle/2$$

$$= 2\pi\left[z_1 z_2\left(\frac{z_1}{m_1} - \frac{z_2}{m_2}\right)^2\langle\delta(\mathbf{r}_{12})\rangle\right.$$

$$+ z_1 z_3\left(\frac{z_1}{m_1} - \frac{z_3}{m_3}\right)^2\langle\delta(\mathbf{r}_{13})\rangle$$

$$\left.+ z_2 z_3\left(\frac{z_2}{m_2} - \frac{z_3}{m_3}\right)^2\langle\delta(\mathbf{r}_{23})\rangle\right].$$

The numerical evaluation of the Bethe logarithm was carried out following the scheme used in Ref. [23] and is based on the closed-channel variational approximation for the zero-order wave function.

The $m\alpha^5$ order recoil corrections [20] are smaller than error bars in calculated values of the leading-order terms and have not been included into consideration.

The main results of this work are summarized in Tables IV and V, the nonrelativistic energies and expectation values of various operators required for the determination of transition energies. For the helium-4 case, one state of a multipolarity $\Delta l = 4$ is presented, namely, the (32,31) state. This is because it was suspected that this state has an anomalously small Auger lifetime due to a configuration mixture effect [15], when the closed-channel state (with $l_e = 0$) is strongly coupled with excited electron configurations. As is seen from this calculation, which includes excited electron configurations in the variational trial function, that is not the case. The numerical uncertainty in the nonrelativistic energy is pointed out in parentheses as an uncertainty in the last digit.

Table VI shows contribution of different relativistic and QED corrections to the final energy difference of the $(37,34)\rightarrow(38,33)$ transition. As already mentioned, the leading contribution comes from the relativistic Breit correction for the bound electron. The next to leading is the bound electron self-energy. Recoil and finite size corrections are almost negligible in comparison with uncertainty. It is note-

TABLE VI. Contributions from different relativistic and QED corrections to the energy of the $(37,34)\rightarrow(38,33)$ transition.

E_{nr}	$=$	420 158 166(20)
E_{rc}	$=$	$-43\,753(30)$
$E_{rc\text{-}QED}$	$=$	360
E_{se}	$=$	5 929(5)
E_{vp}	$=$	-189
E_{kin}	$=$	-4
E_{ret}	$=$	-65
E_{fsc}	$=$	4
E_{total}	$=$	420 120 448(40)

TABLE VII. Transition frequencies (in GHz) between metastable states in the antiprotonic helium atom for transitions to the Auger dominant decay states.

	Transition	This work	Experiment [6]	Kino [16]
$^4\mathrm{He}^+\bar{p}$	$(32,31)\rightarrow(31,30)$	1 132 609.218(5)		1 132 609.2(5)
	$(33,32)\rightarrow(32,31)$	1 012 445.630(2)	1 012 445.52(15)	1 012 445.7(4)
	$(35,33)\rightarrow(34,32)$	804 633.053(3)	804 633.11(10)	804 632.385(6)
	$(37,34)\rightarrow(36,33)$	636 878.159(5)		636 878.12(2)
	$(39,35)\rightarrow(38,34)$	501 948.765(5)	501 949.01(10)	501 948.8(1)
	$(40,35)\rightarrow(39,34)$	445 608.57(2)		445 607.7(1.6)
	$(34,33)\rightarrow(35,32)$	655 062.100(5)		
	$(35,34)\rightarrow(36,33)$	562 441.00(1)		
	$(36,34)\rightarrow(37,33)$	486 104.88(3)	486 102.7(5)	486 104.43(7)
	$(37,34)\rightarrow(38,33)$	420 120.45(4)	420 121.9(7)	420 121.53(1)
	$(37,35)\rightarrow(38,34)$	412 885.129(6)	412 885.16(8)	412 885.1(1.9)
$^3\mathrm{He}^+\bar{p}$	$(31,30)\rightarrow(30,29)$	1 171 220.81(1)		
	$(34,32)\rightarrow(33,31)$	822 809.178(6)		822 808.8(1.5)
	$(36,33)\rightarrow(35,32)$	646 180.434(6)		646 180.2(8)
	$(38,34)\rightarrow(37,33)$	505 222.293(5)		505 221.27(1)
	$(39,34)\rightarrow(38,33)$	446 900.43(1)		
	$(33,32)\rightarrow(34,31)$	668 082.055(6)		
	$(34,33)\rightarrow(35,32)$	570 479.583(7)		570 479.7(8)
	$(35,33)\rightarrow(36,32)$	490 639.54(1)		
	$(36,33)\rightarrow(37,32)$	421 834.0(1)		
	$(36,34)\rightarrow(37,33)$	414 147.518(6)		414 148.34(1)

worthy that the final uncertainty in other cases is much smaller and inclusion of these contributions is essential.

Transition energies for some transitions, which end up in a state with a dominance of the Auger decay, are presented in Table VII. Theoretical data include all the relativistic and QED corrections listed in Eqs. (9)–(12), (14)–(16). The numerical uncertainty in theoretical predictions is finally determined by the numerical uncertainty of the daughter state and further improvement requires significant computational efforts to increase substantially an accuracy of the variational wave function for the Auger decaying states.

In conclusion, we would like to say that while the theoretical results presented here are rather accurate, still the accuracy is limited mainly by the numerical uncertainty. Thus, for a precise study of the three-body QED bound states, it seems more preferable to deal with states and transitions, which lay higher in (n,l) region. That corresponds to the states, in which the radiative decay rate exceeds significantly (by some orders of magnitude) the Auger (or resonance) decay rate. Especially, that is concerned with the two-photon Doppler-free high-precision spectroscopy, which may allow us to determine precisely the antiproton mass, and/or to check the higher-order relativistic and QED effects.

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