Calculation of transitions between metastable states of antiprotonic helium including relativistic and radiative corrections of order $R_\infty \alpha^4$

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Precise numerical calculation of transition intervals between metastable states in the antiprotonic helium atom is performed. Theoretical consideration includes a complete account of the relativistic and radiative corrections of order $R_\infty \alpha^4$ in the nonrecoil limit. The final uncertainty is estimated to be about 1–2 MHz.

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I. INTRODUCTION

Antiprotonic helium is a exotic three-body system which is formed when one of the two electrons in a helium atom is replaced by an antiproton. The majority of the antiprotonic helium atoms promptly annihilates, however, some fraction of antiprotons settles on nearly circular orbitals with quantum numbers $n \approx \sqrt{M^*/m_e} \approx 38$ and $l \lesssim n$, here M^* is the reduced mass of an antiproton-nucleus pair. These latter states demonstrate very high longevity of a few microseconds determined by the radiative transition rate between antiprotonic orbitals.

This remarkable feature allows us to perform precision spectroscopy on these exotic atoms [1–3] with few ppm (parts per million) accuracy. During the last decade experimental precision was improved by more than three orders of magnitude [4,5] and became sensitive to the (anti)proton-to-electron mass ratio. This high precision requires serious theoretical improvement in calculation of the transition energies between metastable states of the antiprotonic helium.

The present work is a continuation of [6], where some leading order relativistic and radiative corrections have been obtained. The major advances are the much better numerical accuracy for wave functions and expectation values, and the complete account of $m\alpha^6$ corrections in the nonrecoil limit as well as the recoil corrections of order $m\alpha^5(m/M)$. Here below we calculate only the "diagonal" part of the higher order interactions that contributes to the energy. The spin-dependent terms which lead to a fine or hyperfine splitting will be considered elsewhere. The diagonal part may contain the spin-dependent contribution which results in the energy shift only.

We use atomic units and the CODATA recommended values of the fundamental constants of year 2002 [7] in our calculations (see Table I). Root-mean-square (rms) radii of the electromagnetic charge distribution for helium-4 ($R_{^4\mathrm{He}}$) and helium-3 ($R_{^3\mathrm{He}}$) are taken from [8].

II. WAVE FUNCTION

The wave function of a state of a total angular momentum L, its projection M onto the z axis of the space-fixed frame and a total spatial parity $\lambda=(-1)^L$ may be written as

$$\Psi_M^{L\lambda}(\mathbf{R},\mathbf{r}) = \sum_{l+l_e=L} R^l r^{l_e} \{Y_l \otimes Y_{l_e}\}_{LM} G_{ll_e}^{L\lambda}(R,r,\theta), \qquad (1)$$

where $\mathbf{R}$ and $\mathbf{r}$ are the position vectors of $\bar{p}$ and of an electron relative to the helium nucleus. The functions $G_{ll_e}^{L\lambda}(R,r,\theta)$ of internal degrees of freedom are expanded as follows:

$$G_{ll_e}^{L\lambda}(R,r,\theta) = \sum_{i=1}^{\infty} C_i e^{-\alpha_i R - \beta_i r - \gamma_i |\mathbf{R}-\mathbf{r}|}. \qquad (2)$$

The complex parameters α_i, β_i, and γ_i are generated in a quasirandom manner. Further details may be found in [9,10].

With this choice of the geometry it is easy to get a Feshbach-type closed channel solution. To that end one needs to retain in the expansion (1) 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,

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

then the subspace spanned over these basis functions is a subspace of closed channels for this resonant state.

The radiative width for the metastable antiprotonic helium states is about 10^{-12} a.u. So, the states with $\Delta l \le 3$ predominantly decay via the Auger transition, while the states with $\Delta l \ge 4$ have a radiative decay as a main channel, the lifetime for these states is about few microseconds.

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 would have relative uncertainty of $\sim 10^{-4}$ that sets limits on the accuracy of mean values of various operators related to relativistic and radiative corrections. Thus, this approximation is

TABLE I. Physical constants adopted in this work.

$m_{\bar{p}} = 1836.1526726\, m_e$	$R_{\bar{p}} = 0.8750(68)$ fm
$m_{^4\mathrm{He}} = 7294.299536\, m_e$	$m_{^3\mathrm{He}} = 5495.885269\, m_e$
$R_{^4\mathrm{He}} = 1.6757(26)$ fm	$R_{^3\mathrm{He}} = 1.9448(137)$ fm
$a_e = 0.001159652186$	$\mu_p = 2.792847351$
$\alpha = 7.297352568 \times 10^{-3}$	$a_0 = 52917.72108$ fm
$R_\infty c = 3289841960.360$ MHz	

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TABLE II. Nonrelativistic energies E_{nr}, half-widths $\Gamma/2$, and the expectation values of the most important operators for individual states of $^4He^+\bar{p}$. All quantities are in atomic units.

State	E_{nr}	$\Gamma/2$	$\mathbf{p}_e^4$	$\delta(\mathbf{r}_{He})$	$\delta(\mathbf{r}_{\bar{p}})$	$Q(\mathbf{r}_{He})$	$Q(\mathbf{r}_{\bar{p}})$	$E_{rc}^{(4)}\alpha^{-4}$
(31,30)	−3.6797747876576(1)	4.7602×10^{-9}	26.070956	0.9262219	0.1214405	−1.1942	0.1581	−1.2481
(32,31)	−3.50763503897101(1)	5.4×10^{-13}	28.308649	0.9938238	0.1130804	−1.2919	0.1616	−1.4078
(33,32)	−3.35375787083340(1)	1.07×10^{-12}	30.718285	1.0664983	0.1044583	−1.3964	0.1634	−1.5810
(34,32)	−3.2276763796294(3)	2.7237×10^{-9}	34.530638	1.1808676	0.0925595	−1.5613	0.1597	−1.8530
(35,32)	−3.116679795873(3)	6.9733×10^{-8}	38.370099	1.2958629	0.0812115	−1.7271	0.1538	−2.1171
(34,33)	−3.21624423907002(1)	1.4×10^{-13}	33.304865	1.1443963	0.0956136	−1.5086	0.1641	−1.7670
(35,33)	−3.1053826755489(3)	2.8×10^{-12}	37.278812	1.2635240	0.0838705	−1.6804	0.1583	−2.0442
(36,33)	−3.0079790936832(4)	2.9188×10^{-9}	41.233471	1.3819872	0.0729174	−1.8512	0.1505	−2.3062
(35,34)	−3.09346690791590(1)		36.069959	1.2275613	0.0865934	−1.6284	0.1632	−1.9644
(36,34)	−2.9963354479662700(5)	2.3×10^{-13}	40.168797	1.3503397	0.0751362	−1.8055	0.1554	−2.2415
(37,34)	−2.9111809394697(4)	2.6×10^{-12}	44.174196	1.4702684	0.0646698	−1.9785	0.1458	−2.4961
(38,34)	−2.836524601208(1)	1.604×10^{-9}	48.000329	1.5848219	0.0553288	−2.1439	0.1351	−2.7231
(39,34)	−2.771011573577(1)	9.920×10^{-9}	51.574850	1.6918636	0.0471712	−2.2983	0.1238	−2.9203
(37,35)	−2.89928218336728(1)		43.186470	1.4409042	0.0664487	−1.9361	0.1510	−2.4424
(38,35)	−2.8251468095450(1)		47.185100	1.5605889	0.0566232	−2.1088	0.1398	−2.6839
(39,35)	−2.7602333455733(1)	1.0×10^{-12}	50.925526	1.6725711	0.0480612	−2.2704	0.1279	−2.8932
(40,35)	−2.7032832165135(3)	1.9×10^{-12}	54.349384	1.7751265	0.0407571	−2.4184	0.1159	−3.0701

insufficient for a precise determination of transition energies.

In order to get better accuracy one needs to take into account the resonance nature of the antiprotonic helium states. A powerful tool for that is the complex coordinate rotation (CCR) method [11]. The essence of the method is to transform (rotate) the coordinates of the dynamical system as follows:

$$r_{ij} \to r_{ij}e^{i\varphi},$$

where φ is the parameter of the complex rotation.

Under this transformation the Hamiltonian changes as a function of φ,

$$H_\varphi = Te^{-2i\varphi} + Ve^{-i\varphi}, \tag{3}$$

and the continuum spectrum of H_φ is rotated on the complex plane around branch points ("thresholds") to "uncover" resonant poles situated on the unphysical second sheet of the Riemann surface (see the Augilar-Balslev-Combes theorem [12]).

The resonance energy is then determined by solving the complex eigenvalue problem for the "rotated" Hamiltonian

$$(H_\varphi - E)\Psi_\varphi = 0, \tag{4}$$

The eigenfunction Ψ_φ obtained from Eq. (4) is square integrable and the corresponding complex eigenvalue $E=E_r - i\Gamma/2$ determines the energy E_r and the width of the resonance, Γ.

The use of a finite set of N basis functions reduces the problem (4) to the generalized algebraic complex eigenvalue problem

$$(A - \lambda B)x = 0, \tag{5}$$

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 $B=\langle\Psi_\varphi|\Psi_\varphi\rangle$.

To get an accurate CCR solution for the antiprotonic helium is a numerically difficult problem because antiproton and electron orbitals have different scales. In our calculation we use a general strategy of a multilayered variational approximation as is described in [9]. A trial wave function contains four basis sets. First, two sets are used for better approximation of the closed channel solution. Parameters of a third set are adjusted to approximate excited electron intermediate states, and the last set corresponds to electron continuum configurations.

The numerical solution of Eq. (5) is obtained using the basis sets with $N=4400$ functions, which is 2 times larger than in our previous work [6]. A sextuple precision arithmetic (~48 decimal digits) has been used to avoid round-off errors in calculations. It has been found that for our aims the first five terms in expansion (1) are sufficient. The higher l_e terms in (1) do not improve the result within required accuracy.

III. HIGHER ORDER CORRECTIONS

In this section we will consider only contributions of orders $R_\infty\alpha^3$ and higher. The leading order relativistic corrections, which result from the Breit-Pauli Hamiltonian along with the finite size correction due to the charge distribution of nuclei, and the contribution from the anomalous magnetic moment of an electron, have been discussed in detail in [6]. It is worth mentioning here that the new numerically more accurate values for the most crucial expectation values are

TABLE III. Nonrelativistic energies E_{nr}, half-widths $\Gamma/2$, and the expectation values of the most important operators for individual states of $^3He^+\bar{p}$. All quantities are in atomic units.

State	E_{nr}	$\Gamma/2$	$\mathbf{p}_e^4$	$\delta(\mathbf{r}_{He})$	$\delta(\mathbf{r}_{\bar{p}})$	$Q(\mathbf{r}_{He})$	$Q(\mathbf{r}_{\bar{p}})$	$E_{rc}^{(4)}\alpha^{-4}$
(31,30)	−3.507372719685(1)	3.341×10^{-9}	28.309520	0.9936884	0.1128789	−1.2914	0.1612	−1.4100
(32,31)	−3.34883217260011(1)	5.16×10^{-12}	30.803392	1.0689407	0.1040109	−1.3999	0.1633	−1.5890
(33,31)	−3.2195072511344(2)	8.2761×10^{-9}	34.744072	1.1871601	0.0917424	−1.5703	0.1594	−1.8697
(34,31)	−3.1061288624340(2)	7.935×10^{-9}	38.697601	1.3055346	0.0800594	−1.7411	0.1530	−2.1415
(34,32)	−3.0944509665400(4)	1.72×10^{-11}	37.595356	1.2729449	0.0828113	−1.6939	0.1578	−2.0674
(35,32)	−2.9954043582725(5)	8.1610×10^{-9}	41.676374	1.3951949	0.0715852	−1.8703	0.1496	−2.3363
(35,33)	−2.98337312345513(3)	1.30×10^{-12}	40.593961	1.3630401	0.0738344	−1.8238	0.1546	−2.2713
(36,33)	−2.89719228783746(5)	2.921×10^{-11}	44.720654	1.4866058	0.0631524	−2.0021	0.1445	−2.5314
(37,33)	−2.8219630307782(6)	4.2684×10^{-9}	48.642644	1.6040396	0.0536909	−2.1715	0.1332	−2.7615
(36,34)	−2.88491261933851(4)		43.723769	1.4569802	0.0649187	−1.9593	0.1498	−2.4783
(37,34)	−2.81026108529864(2)	6.8×10^{-13}	47.831114	1.5799276	0.0549480	−2.1367	0.1380	−2.7235
(38,34)	−2.7451741489575(1)	3.9×10^{-12}	51.647727	1.6942063	0.0463399	−2.3016	0.1256	−2.9338
(39,34)	−2.688292963471(2)	1.138×10^{-9}	55.114312	1.7980620	0.0390712	−2.4513	0.1132	−3.1097
(40,35)	−2.62832404729795(4)	7.0×10^{-13}	57.840658	1.8798948	0.0331808	−2.5694	0.1044	−3.2474

presented in Tables II and III. They should be used instead of those given in [6] for evaluation of the leading order relativistic contribution.

A complete set of the $R_\infty\alpha^3$ order QED corrections is determined by the following three equations.

The one-loop self-energy correction $(R_\infty\alpha^3)$,

$$E_{se}^{(3)} = \alpha^3\frac{4}{3}\left(\ln\frac{1}{\alpha^2} - \beta(L,v) + \frac{5}{6} - \frac{3}{8}\right)\langle Z_{He}\delta(\mathbf{r}_{He}) + Z_{\bar{p}}\delta(\mathbf{r}_{\bar{p}})\rangle, \tag{6}$$

where

$$\beta(L,v) = \frac{\langle \mathbf{J}(H_0 - E_0)\ln[(H_0 - E_0)/R_\infty]\mathbf{J}\rangle}{\langle [\mathbf{J},[H_0,\mathbf{J}]]/2\rangle}$$

is the Bethe logarithm [13]of the three-body state (calculated in atomic units scale. The numerical values for $\beta(L,v)$ may be found in [6].

One transverse photon exchange (recoil) correction $[R_\infty\alpha^3(m/M)]$ may be written as [14,15]

$$E_{\text{recoil}}^{(3)} = \sum_{i=1,2}\frac{Z_i^2\alpha^3}{M_i}\left[-\frac{14}{3}Q(r_i) + \frac{2}{3}\left(-\ln\alpha - 4\beta(L,v) + \frac{31}{3}\right)\times\langle\delta(\mathbf{r}_i)\rangle\right], \tag{7}$$

where $Q(r)$ is the so-called Araki-Sucher term [16],

$$Q(r) = \lim_{\rho\to0}\left\langle\frac{\Theta(r-\rho)}{4\pi r^3} + (\ln\rho + \gamma_E)\delta(\mathbf{r})\right\rangle.$$

One-loop vacuum polarization can be written as

$$E_{vp}^{(3)} = \frac{4\alpha^3}{3}\left(-\frac{1}{5}\right)\langle Z_{He}\delta(\mathbf{r}_{He}) + Z_{\bar{p}}\delta(\mathbf{r}_{\bar{p}})\rangle. \tag{8}$$

The recoil correction contribution [Eq. (7)] to the transition energy is of the order of 0.5–0.7 MHz. We expect that the higher order in α recoil contributions are at least an order of magnitude less and may be neglected for the time being. The radiative corrections of the $R_\infty\alpha^4$ and $R_\infty\alpha^5\ln^2\alpha$ in a nonrecoil limit of the adiabatic two-center approximation (or an external field approximation) are known analytically [17,18].

The one-loop self-energy and vacuum polarization contributions $(R_\infty\alpha^4)$ are

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

$$E_{vp}^{(4)} = \alpha^4\left(\frac{5\pi}{48}\right)\langle Z_{He}^2\delta(\mathbf{r}_{He}) + Z_{\bar{p}}^2\delta(\mathbf{r}_{\bar{p}})\rangle. \tag{9}$$

The two-loop QED correction $(R_\infty\alpha^4)$ is

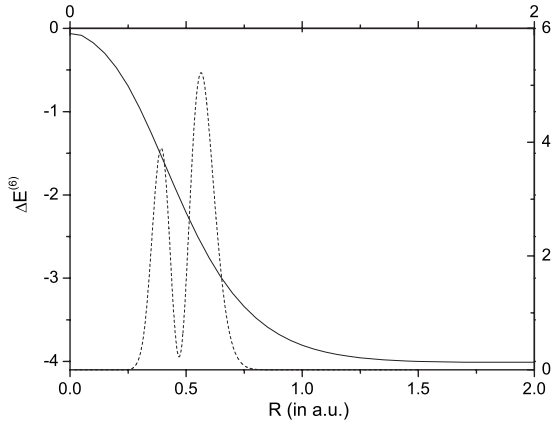

FIG. 1. Adiabatic "effective" potentials for the relativistic $m\alpha^6$ order correction for the antiprotonic helium atom $(Z_1=2, Z_2=-1)$. Dashed line is the radial wave function of the (36,34) state in $^4He^+\bar{p}$ atom. Energies are in (atomic units)$\times\alpha^4$.

TABLE IV. Theoretical predictions to transition frequencies ν (in MHz) between metastable states, and comparison with the latest experiment [5]. Calculations are performed with CODATA02 recommended values.

	Transition	Theory	Experiment
$^4\mathrm{He}^+\bar{p}$	$(32,31)\to(31,30)$	1132609223.5(0.8)(0.2)	1132609209(15)
	$(35,33)\to(34,32)$	804633058.0(1.0)(0.3)	804633059(8)
	$(36,34)\to(35,33)$	717474001.1(1.1)(0.3)	717474004(10)
	$(37,34)\to(36,33)$	636878151.7(1.1)(0.3)	636878139(8)
	$(37,35)\to(38,34)$	412885132.8(1.8)(0.4)	412885132(4)
	$(39,35)\to(38,34)$	501948755.6(1.1)(0.4)	501948752(4)
	$(40,35)\to(39,34)$	445608569.3(1.0)(0.8)	445608558(6)
	$(36,34)\to(34,32)$	1522107059.1(2.1)(0.3)	
$^3\mathrm{He}^+\bar{p}$	$(32,31)\to(31,30)$	1043128579.7(0.9)(0.1)	1043128609(13)
	$(34,32)\to(33,31)$	822809170.9(1.1)(0.2)	822809190(12)
	$(35,33)\to(34,32)$	730833929.9(1.1)(0.2)	
	$(36,33)\to(35,32)$	646180408.2(1.1)(0.4)	646180434(12)
	$(36,34)\to(37,33)$	414147507.8(1.8)(0.3)	414147508(4)
	$(38,34)\to(37,33)$	505222280.9(1.1)(0.3)	505222296(8)
	$(35,33)\to(33,31)$	1553643100.9(2.1)(0.2)	

$$E_{2\ \mathrm{loop}}^{(4)}=\alpha^4\left[\frac{1}{\pi}\left(-\frac{6131}{1296}-\frac{49\pi^2}{108}+2\pi^2\ln 2-3\zeta(3)\right)\right]\times\langle Z_{\mathrm{He}}\delta(\mathbf{r}_{\mathrm{He}})+Z_{\bar{p}}\delta(\mathbf{r}_{\bar{p}})\rangle. \quad (10)$$

It includes both Dirac form factor and polarization operator contributions.

The $R_\infty\alpha^4$ relativistic correction is obtained using the adiabatic "effective" potential for the $m\alpha^6$ order term in the α^2 expansion of the two-center Dirac energy. These effective potentials for the case of the antiprotonic helium ($Z_1=2$, $Z_2=-1$) (see Fig. 1) were calculated in [19]. Averaging them over the squared wave-function density of a state one obtains $E_{rc}^{(4)}$ (see Tables II and III).

The $R_\infty\alpha^5$ order corrections are

$$E_{se}^{(5)}=\alpha^5[-1][Z_{\mathrm{He}}^3\ln^2(Z_{\mathrm{He}}\alpha)^{-2}\langle\delta(\mathbf{r}_{\mathrm{He}})\rangle+Z_{\bar{p}}^3\ln^2(Z_{\bar{p}}\alpha)^{-2}\langle\delta(\mathbf{r}_{\bar{p}})\rangle],$$

$$E_{se}^{(5')}=\alpha^5Z_{\mathrm{He}}^3[A_{61}\ln(Z_{\mathrm{He}}\alpha)^{-2}+A_{60}]\langle\delta(\mathbf{r}_{\mathrm{He}})\rangle,$$

$$E_{2\ \mathrm{loop}}^{(5)}=\frac{\alpha^5}{\pi}Z_{\mathrm{He}}^2[B_{50}]\langle\delta(\mathbf{r}_{\mathrm{He}})\rangle, \quad (11)$$

where the constants A_{61}, A_{60}, and B_{50} are taken equal to the constants of the $1s$ state of the hydrogen atom $A_{61}=5.419$ [20], $A_{60}=-30.924$ [21], and $B_{50}=-21.556$ [22]. The error bars are determined by the total contribution of the terms of the last two equations.

IV. RESULTS AND CONCLUSION

Results of numerical calculation for individual states are summarized in Tables II and III, the nonrelativistic energies are shown with a numerical uncertainty indicated in parentheses. The Auger width of a state has the same error bars as the nonrelativistic energy.

From these tables one may conclude that the numerical accuracy is better for the states with lower Auger width. Thus, from the theoretical point of view transitions between metastable states are preferable for precision spectroscopy.

Table IV presents final results for the transition energies and comparison with the latest experiments [5]. The first error for theoretical values reflects the theoretical uncertainty as it has been defined in the text after Eq. (11). The second one is the numerical uncertainty. As is seen from Table IV, the best candidates for determination of the antiproton mass are the lowest transitions with the smallest principal quantum number n of the antiproton orbital. For these transitions theoretical uncertainty is lower and the transition frequency is larger.

For the two-photon transitions (the last rows for $^4\mathrm{He}^+\bar{p}$ and $^3\mathrm{He}^+\bar{p}$) the numerical uncertainty is an order of magnitude less than the theoretical one. That is because the numerical errors are determined primarily by the less accurate calculation of the daughter state (larger Auger width).

It is important to indicate how the uncertainty in the rms radii of nuclei influences the final value of the transition frequency. A variation of the transition frequency is about 50 kHz due to the uncertainty in the rms radius of the ^{3}He nucleus, less than 10 kHz for ^{4}He, and below 1 kHz for $\bar{p}$.

In conclusion, we want to state that the results obtained here achieve the relative accuracy of 1 ppb (parts per billion). Further improvement may be expected with explicit calculation of the radiative one-loop and two-loop corrections in the $R_\infty\alpha^5$ order. Especially it is important for the two-photon precision spectroscopy, where the numerical error is relatively small. The accomplishing of this task, eventually, will allow for the improved measurement of the (anti)proton-to-electron mass ratio.

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