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Bethe logarithm for resonant states: Antiprotonic helium

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We develop a numerical method to calculate the Bethe logarithm for resonant states. We use the complex coordinate rotation (CCR) formalism to describe resonances as time-independent Schrödinger solutions. To get a proper expression for the Bethe logarithm we apply the generalization of the second order perturbation theory to an isolated CCR eigenstate. Using the developed method we perform a systematic calculation of the Bethe logarithm for metastable states in the antiprotonic helium $\mathrm{He}^+\bar{p}$ atoms with a precision of 7–8 significant digits. We also recalculate the nonrelativistic energies with improved precision using CODATA10 recommended values of masses. Along with a complete set of corrections of $m\alpha^7$ order and the leading contributions of $m\alpha^8$ order, that has allowed us to get theoretical values for ro-vibrational transition frequencies for the $\mathrm{He}^+\bar{p}$ atoms with an uncertainty of 0.1–0.3 MHz.

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I. INTRODUCTION

Precision spectroscopy of the antiprotonic helium is considered as one of the possible ways to improve the CODATA value for the atomic mass of an electron [1,2] assuming the validity of the CPT symmetry at this level of accuracy. Since the discovery of a long-lived fraction of antiprotons in helium [3] and the first laser experiments [4] a great progress in precision from ppm to ppb level has been achieved [5,6]. More details on this exotic system may be found in Refs. [7] and [8].

On the other hand, it was shown that individual states of the antiprotonic helium may be treated numerically with high precision [9]. Despite the fact that these states appear in the continuum of the nonrelativistic Hamiltonian operator as resonances having antiprotons in nearly circular orbitals with total orbital angular momentum of an atom $L \sim 30$–36, they allow us to calculate very precisely taking into account their resonant nature [10] together with many higher order (in powers of the fine structure constant α) relativistic and radiative corrections [11].

The major goal of the present paper is to get a fractional precision of one part in 10^{10} for the theoretical transition frequencies, which should be compared with the CODATA10 [1] uncertainty limits for the atomic mass 4.1×10^{-10}. To achieve that we need to solve two problems. The first one is to calculate the nonrelativistic Bethe logarithm for individual metastable states with an accuracy of seven significant digits going beyond the usual bound state formalism [10]. The second is to obtain the complete set of contributions of various corrections of $m\alpha^7$ order. The latter was carried out recently in Refs. [12,13]. The former will be considered here below.

In our derivation of the Bethe logarithm formalism for the resonant states we utilize the quantum numbers generally used in the few-body calculations, namely, the total orbital angular momentum L and the vibrational (or excitation) quantum number. When we turn to the antiprotonic helium specifically, we switch to more conventional for this system notation: the principal quantum number n and orbital angular momentum l of an antiprotonic orbital. These two sets of quantum numbers are related as follows: $L = l$, $v = n - l - 1$.

II. RESONANCES AND THE COMPLEX COORDINATE ROTATION APPROACH

To have a rigorous background for our calculations we need to give a brief outline of the complex coordinate rotation (CCR) method [14] along with some basics for the perturbation theory for isolated resonant states. The Coulomb Hamiltonian for a system of pointlike particles is analytic under dilatation transformations

$$[U(\theta)f](\mathbf{r}) = e^{m\theta/2} f(e^{\theta}\mathbf{r}), \qquad H(\theta) = U(\theta)HU^{-1}(\theta), \tag{1}$$

for real θ and can be analytically continued to the complex plane. The complex coordinate rotation method [14] "rotates" the coordinates of the dynamical system ($\theta = i\varphi$), $r_{ij} \to r_{ij}e^{i\varphi}$, where φ is the parameter of the complex rotation. Under this transformation the Hamiltonian changes as a function of φ

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

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

$$(H_\varphi - E)\Psi_\varphi = 0. \tag{3}$$

The eigenfunction Ψ_φ obtained from Eq. (3) 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 being related to the Auger rate as $\lambda_A = \Gamma/\hbar$.

The use of a finite set of N basis functions reduces the problem (3) to the generalized algebraic complex eigenvalue problem

$$(A - \lambda B)x = 0, \tag{4}$$

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 evaluate the nonrelativistic Bethe logarithm for the CCR states a second-order perturbation theory is necessary. The relevant background is provided by the theorem [16].

Theorem. Let H be a three-body Hamiltonian with Coulomb pairwise interaction, and $W(\theta)$ be a dilatation analytic perturbation. Let E_0 be an isolated simple resonance energy [discrete eigenvalue of $H(\theta)$]. Then for β small, there is exactly one eigenstate of $H(\theta)+\beta W(\theta)$ near E_0 and

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

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

$$\begin{aligned} a_1 &= E'(0) = \langle \Psi_0^*(\theta)|W(\theta)|\Psi_0(\theta)\rangle, \\ a_2 &= \sum_{n\neq 0} \frac{\langle \Psi_0^*(\theta)|W(\theta)|\Psi_n(\theta)\rangle\langle \Psi_n^*(\theta)|W(\theta)|\Psi_0(\theta)\rangle}{E_0 - E_n(\theta)}. \end{aligned} \tag{5}$$

It is assumed that the wave functions are normalized as $\langle \Psi_\theta^*, \Psi_\theta\rangle = 1$. Coefficients a_1, a_2, etc. do not depend on θ if only branches uncover E_0 and its vicinity on the complex plane.

III. LEADING ORDER RADIATIVE CORRECTIONS AND THE BETHE LOGARITHM

The complete spin-independent contribution of orders $m\alpha^5$ and $m\alpha^5(m/M)$ for a one electron molecular-type system may be expressed by three terms: the one-loop self-energy correction, the transverse photon exchange term, and the vacuum polarization [17,18].

The one-loop self-energy correction ($R_\infty\alpha^3$) has the following form:

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

where

$$\beta(L,v) = \frac{\langle \mathbf{J}(H-E_0)\ln[(H-E_0)/R_\infty]\mathbf{J}\rangle}{\langle [\mathbf{J},[H,\mathbf{J}]]/2\rangle} \tag{7}$$

is the nonrelativistic Bethe logarithm [19] for a bound state of the three-body system. Here $\mathbf{J} = \sum_a Z_a\mathbf{p}_a/m_a$ is the electric current density operator of the whole system. It is known that the Bethe logarithm is one of the most difficult quantities to evaluate numerically in atomic physics. So far, for the case of the antiprotonic helium it was calculated based on the closed-channel variational approximation for the initial wave function [10]. In this case a state may be considered as a "true" bound state. This approximation was limited in accuracy by four to six significant digits, and become unsatisfactory for present level theoretical estimates.

The next term is the recoil correction of order $R_\infty\alpha^3(m/M)$ [17,18]:

$$\begin{aligned} E_{\rm recoil}^{(3)} = \sum_{i=1,2}\frac{Z_i\alpha^3}{M_i}\left\{\frac{2}{3}\left(-\ln\alpha - 4\beta(L,v) + \frac{31}{3}\right)\langle\delta(\mathbf{r}_i)\rangle \right. \\ \left. - \frac{14}{3}Q(r_i)\right\}, \end{aligned} \tag{8}$$

where $\beta(L,v)$ is the same Bethe logarithm quantity as in Eq. (6), $Q(r)$ is the so-called Araki-Sucher term [20]:

$$Q(r) = \lim_{\rho\to 0}\left\langle \frac{\Theta(r-\rho)}{4\pi r^3} + (\ln\rho + \gamma_E)\delta(\mathbf{r})\right\rangle.$$

The last term is the one-loop vacuum polarization:

$$E_{vp}^{(3)} = \frac{4\alpha^3}{3}\left[-\frac{1}{5}\right]\langle Z_{\rm He}\delta(\mathbf{r}_{\rm He}) + Z_{\bar p}\delta(\mathbf{r}_{\bar p})\rangle. \tag{9}$$

The two quantities, the $Q(r)$ term and the mean value the δ-function operator, which appear in Eqs. (8) and (9), can be easily evaluated for a CCR wave function of a stationary

TABLE I. Multipolarities of the Auger transition Δl, nonrelativistic energies E_{nr} (in a.u.), Auger widths Γ (in a.u.), expectation values of operators: $\mathbf{p}_e^4$, $\delta(\mathbf{r}_{\rm He})$, and $\delta(\mathbf{r}_{\bar p})$, and the Bethe logarithm values, $\beta(n,l)$, for the Auger states of $^4{\rm He}^+\bar p$ atom.

(n,l)	Δl	E_{nr}	$\Gamma/2$	$\mathbf{p}_e^4$	$\delta(\mathbf{r}_{\rm He})$	$\delta(\mathbf{r}_{\bar p})$	$\beta(n,l)$
(31,30)	3	−3.67977478748142(4)	4.76010×10^{-9}	26.070960	0.92622196	0.12144043	4.578969(1)
(32,31)	4	−3.507635038808513(2)	5.36×10^{-13}	28.308650	0.99382380	0.11308041	4.560196(1)
(33,32)	4	−3.353757870683624(4)	1.060×10^{-12}	30.718284	1.0664983	0.10445828	4.5416885(4)
(34,32)	3	−3.2276763794925(1)	2.7236×10^{-9}	34.530626	1.1808674	0.09255952	4.512829(1)
(34,33)	4	−3.216244238932181(1)	1.38×10^{-13}	33.304865	1.1443963	0.09561357	4.523626(1)
(35,32)	3	−3.1166797957470(5)	6.97306×10^{-8}	38.370061	1.2958621	0.08121154	4.488492(4)
(35,33)	4	−3.10538267542400(5)	2.67×10^{-12}	37.278814	1.2635240	0.08387045	4.496653(1)
(35,34)	5	−3.0934669077893306	—	36.069959	1.2275614	0.08659337	4.5061577(4)
(36,33)	3	−3.0079790935681(3)	2.9186×10^{-9}	41.233444	1.3819867	0.07291740	4.474194(2)
(36,34)	4	−2.996335447851055(3)	2.66×10^{-13}	40.168790	1.3503395	0.07513623	4.4812666(4)
(37,34)	4	−2.91118093936496(5)	2.60×10^{-12}	44.174191	1.4702684	0.06466985	4.4608414(4)
(37,35)	5	−2.8992821832621387(5)	1.2×10^{-15}	43.186472	1.4409042	0.06644874	4.4667491(3)
(38,34)	3	−2.8365246011112(6)	1.6029×10^{-9}	48.000302	1.5848214	0.05532901	4.4441865(5)
(38,35)	4	−2.825146809449515(3)	1.64×10^{-13}	47.185112	1.5605892	0.05662323	4.4484354(3)
(39,34)	3	−2.771011573490(1)	0.9920×10^{-8}	51.574881	1.6918639	0.04717053	4.430698(3)
(39,35)	4	−2.76023334548707(3)	0.93×10^{-12}	50.925521	1.6725710	0.04806117	4.433733(1)
(40,35)	4	−2.70328321643503(5)	1.91×10^{-12}	54.349323	1.7751252	0.04075701	4.421998(5)
(40,36)	4	−2.69262484981043(3)	2.02×10^{-12}	53.823828	1.7594940	0.04122551	4.424271(1)
(41,35)	3	−2.6531667754306(4)	1.4400×10^{-9}	57.423461	1.8672689	0.03463431	4.412720(3)

TABLE II. Multipolarities of the Auger transition Δl, nonrelativistic energies E_{nr} (in a.u.), Auger widths Γ (in a.u.), expectation values of operators: $\mathbf{p}_e^4$, $\delta(\mathbf{r}_{\rm He})$, and $\delta(\mathbf{r}_{\bar p})$, and the Bethe logarithm values, $\beta(n,l)$, for the Auger states of $^3{\rm He}^+\bar p$ atom.

(n,l)	Δl	E_{nr}	$\Gamma/2$	$\mathbf{p}_e^4$	$\delta(\mathbf{r}_{\rm He})$	$\delta(\mathbf{r}_{\bar p})$	$\beta(n,l)$
(31,30)	3	−3.5073727202819(5)	3.3424×10^{-9}	28.309519	0.99368837	0.11287882	4.559722(1)
(32,31)	4	−3.348832173150003(2)	5.169×10^{-12}	30.803393	1.0689407	0.10401090	4.540686(1)
(33,31)	3	−3.2195072516355(1)	8.2761×10^{-9}	34.744079	1.1871602	0.09174227	4.511062(1)
(33,32)	4	−3.20767231244689(1)	7.8×10^{-13}	33.484950	1.1497243	0.09489883	4.522121(1)
(34,31)	3	−3.1061288628903(2)	7.925×10^{-10}	38.697601	1.3055346	0.08005938	4.486207(2)
(34,32)	4	−3.09445096699891(2)	1.709×10^{-11}	37.595341	1.2729446	0.08281128	4.4945424(5)
(34,33)	5	−3.082114107332030(1)	—	36.355772	1.2360854	0.08559822	4.5041924(5)
(35,32)	3	−2.9954043586889(1)	8.1608×10^{-9}	41.676373	1.3951949	0.07158519	4.471761(1)
(35,33)	4	−2.983373123874257(5)	1.303×10^{-12}	40.593960	1.3630401	0.07383439	4.4788451(4)
(36,32)	3	−2.9087979813554(5)	5.7466×10^{-9}	45.621175	1.5132762	0.06138275	4.452989(2)
(36,33)	4	−2.89719228821683(3)	2.915×10^{-10}	44.720654	1.4866058	0.06315237	4.4582350(5)
(36,34)	5	−2.88491261972020(1)	—	43.723769	1.4569802	0.06491865	4.4640761(4)
(37,33)	3	−2.8219630311214(2)	4.2678×10^{-9}	48.642644	1.6040396	0.05369086	4.441533(3)
(37,34)	4	−2.81026108564305(5)	7.6×10^{-13}	47.831121	1.5799277	0.05494800	4.4456893(6)
(38,33)	3	−2.756217741055(2)	3.4239×10^{-8}	52.279701	1.7129557	0.04549272	4.428246(1)
(38,34)	4	−2.74517414926844(2)	3.90×10^{-12}	51.647733	1.6942064	0.04633993	4.4310677(4)
(39,34)	4	−2.688292963759(2)	1.130×10^{-9}	55.114275	1.7980611	0.03907099	4.419510(4)
(40,35)	4	−2.62832405152957(1)	6.7×10^{-13}	57.840699	1.8798956	0.03318082	4.4118712(5)

solution for a metastable state. In what follows in this section we explain how calculation of the nonrelativistic Bethe logarithm for a bound state may be extended to resonant states using the complex coordinate rotation formalism.

The Bethe logarithm for a "rotated" state in the coordinate system rotated by the same angle φ ($r_{ij} \to r_{ij}e^{i\varphi}$) is expressed:

$$\beta(L,v) = \frac{\langle \mathbf{J}_\varphi (H_\varphi - E_0) \ln[(H_\varphi - E_0)/R_\infty] \mathbf{J}_\varphi \rangle}{\langle [\mathbf{J}_\varphi, [H_\varphi, \mathbf{J}_\varphi]]/2 \rangle}, \qquad (10)$$

where H_φ and $\mathbf{J}_\varphi$ are the rotated operators of the Hamiltonian and the charge current density. It is better to rewrite this quantity in an equivalent form as an integration over the virtual photon energy k:

$$\beta(L,v) = \frac{\int_0^{E_h} k dk \big\langle \mathbf{J}_\varphi \big(\frac{1}{E_0 - H_\varphi - k} + \frac{1}{k} \big) \mathbf{J}_\varphi \big\rangle + \int_{E_h}^{\infty} \frac{dk}{k} \big\langle \mathbf{J}_\varphi \frac{(E_0 - H_\varphi)^2}{E_0 - H_\varphi - k} \mathbf{J}_\varphi \big\rangle}{\langle [\mathbf{J}_\varphi, [H_\varphi, \mathbf{J}_\varphi]] \rangle / 2}. \qquad (11)$$

Its integrand may be expressed via a basic function $J(k)$, the contribution of the second order perturbation of a virtual

TABLE III. Theoretical predictions to transition frequencies, $(n,l) \to (n',l')$, (in MHz) between metastable states and comparison with the latest experiment [6]. Calculations are performed with CODATA10 recommended values.

	Transition	Theory	Experiment
$^4{\rm He}^+\bar p$	(32,31) → (31,30)	1 132 609 223.8(2)	1 132 609 209(15)
	(34,33) → (35,32)	655 062 102.2(2)	
	(35,33) → (34,32)	804 633 058.3(1)	804 633 059(8)
	(36,34) → (35,33)	717 474 002.0(2)	717 474 004(10)
	(37,34) → (36,33)	636 878 152.1(1)	636 878 139(8)
	(37,35) → (38,34)	412 885 132.7(2)	412 885 132(4)
	(38,35) → (39,34)	356 155 990.8(4)	
	(39,35) → (38,34)	501 948 755.1(2)	501 948 752(4)
	(40,35) → (39,34)	445 608 572.4(4)	445 608 558(6)
	(33,32) → (31,30)	2 145 054 858.1(2)	2 145 054 858(5)
	(36,34) → (34,32)	1 522 107 060.3(2)	1 522 107 062(4)
$^3{\rm He}^+\bar p$	(32,31) → (31,30)	1 043 128 580.4(2)	1 043 128 609(13)
	(34,32) → (33,31)	822 809 172.2(3)	822 809 190(12)
	(35,33) → (34,32)	730 833 930.2(1)	
	(36,33) → (35,32)	646 180 412.6(2)	646 180 434(12)
	(36,34) → (37,33)	414 147 509.3(3)	414 147 508(4)
	(38,34) → (37,33)	505 222 281.1(3)	505 222 296(8)
	(35,33) → (33,31)	1 553 643 102.4(3)	1 553 643 100(7)

photon emission and absorbtion,

$$J(k) = \langle \mathbf{J}_\varphi (E_0 - H_\varphi - k)^{-1} \mathbf{J}_\varphi \rangle. \tag{12}$$

We neglect retardation as is usual for the nonrelativistic Bethe logarithm calculations [19]. It is worth noting that $J(k)$ does not depend on φ for a complete (infinite) basis set, and thus the final value for $\beta(L,v)$ will not depend on the "unphysical" parameter—the rotational angle. Meanwhile, the number itself should be complex with the imaginary part being the radiative correction contribution to the Auger decay rate. The actual calculation of the Bethe logarithm for the metastable states of the antiprotonic helium is performed as a straightforward generalization of the numerical scheme derived in Ref. [21], and all the technical details may be found there.

IV. THE VARIATIONAL WAVE FUNCTION

In our CCR calculations, the initial quasibound state of the antiprotonic helium atom as well as the intermediate states, which appears in the second order perturbation calculations of the Bethe logarithm, are taken in the form [22,23]

$$\begin{aligned}\Psi_L(l_1,l_2) = \sum_{i=1}^{\infty}\{&U_i\,\mathrm{Re}[e^{-\alpha_i R-\beta_i r_1-\gamma_i r_2}]\\ &+ W_i\,\mathrm{Im}[e^{-\alpha_i R-\beta_i r_1-\gamma_i r_2}]\}\mathcal{Y}^{l_1,l_2}_{LM}(\hat{\mathbf{R}},\hat{\mathbf{r}}_1),\end{aligned} \tag{13}$$

where $\mathcal{Y}^{l_1,l_2}_{LM}(\hat{\mathbf{R}},\hat{\mathbf{r}}_1)$ are the solid bipolar harmonics as defined in Ref. [24], and L is the total orbital angular momentum of a state. The initial states have normal spatial parity: $\pi = (-1)^L$. Complex parameters α_i, β_i, and γ_i are generated in a quasirandom manner:

$$\begin{aligned}\mathrm{Re}[\alpha_i] &= \left[\left\lfloor \tfrac{1}{2} i(i+1)\sqrt{p_\alpha}\right\rfloor (A_2 - A_1) + A_1\right],\\ \mathrm{Im}[\alpha_i] &= \left[\left\lfloor \tfrac{1}{2} i(i+1)\sqrt{q_\alpha}\right\rfloor (A_2' - A_1') + A_1'\right],\end{aligned} \tag{14}$$

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

The intermediate states span over $L' = L, L \pm 1$ with the spatial parity $\pi = -(-1)^L$, where L is a total orbital angular momentum of the initial quasibound state. The basis set of intermediate states is composed of a regular part and two extra short-distance trial functions (for $\mathbf{r}_i \to 0$, $i = 1,2$) with exponentially growing parameters (see details in Ref. [21]). To keep the required numerical stability the quadruple and sextuple precision arithmetics have been used.

V. RESULTS

The results of numerical calculations are presented in Tables I and II. The nonrelativistic energies and widths were recalculated with improved precision and using the CODATA10 recommended values for physical constants [1]. The basis sets for these variational CCR calculations were taken up to $N = 7000$ basis functions. In the tables we also present data for the expectation values of the $\mathbf{p}_e^4$, $\delta(\mathbf{r}_{\mathrm{He}})$, and $\delta(\mathbf{r}_{\bar{p}})$ operators. These numbers are of particular importance for evaluating the leading order relativistic corrections ($m\alpha^4$) with precision better than 100 kHz in ro-vibrational transition frequencies. The last column contains data of the CCR calculations of the Bethe logarithm, which are our main result of this work. Only the real part of $\beta(n,l)$ is shown. We estimate that the values presented have a precision of 7–8 significant digits. It allows us to claim that the uncertainty arising in the leading order radiative contribution $m\alpha^5$ is now below 100 kHz.

In Table III a list of transition frequencies of spectroscopic interest both for $^4\mathrm{He}^+\bar{p}$ and $^3\mathrm{He}^+\bar{p}$ atoms are collected. The theoretical data contains a complete set of contributions up to $m\alpha^7$ order and the leading contributions of the $m\alpha^8$ order [13]. The error bars indicate mainly the uncertainty, which is caused by the numerical inaccuracy in the one-loop self-energy calculations. The whole budget of the contributions for the $(36,34) \to (34,32)$ transition of the $^4\mathrm{He}^+\bar{p}$ atom, and a total list of the corrections, which were included, are discussed in detail in Ref. [13]. The last column gives a comparison with the best available experimental measurements for these transitions.

In conclusion, the results of the calculations presented here allows us to infer the electron-to-(anti)proton mass ratio from comparison of theoretical data of Table III and future improved experimental measurements with the ultimate relative precision of about 10^{-10}. That is about an order of magnitude more precise than the CODATA recommended value for the atomic mass of an electron.

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