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 Heρ 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 maρ order and the leading contributions of maρ order, that has allowed us to get theoretical values for ro-vibrational transition frequencies for the Heρ 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 ∼ 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 maρ 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.
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 $\beta$ 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,

$$a_1 = E'(0) = \langle \Psi_0^*(\theta)|W(\theta)|\Psi_0(\theta)\rangle,$$

$$a_2 = \sum_{n\neq 0} \frac{\langle \Psi_0^*(\theta)|W(\theta)|\Psi_n(\theta)\rangle\langle \Psi_n(\theta)|W(\theta)|\Psi_0(\theta)\rangle}{E_n - E_0(\theta)}.$$ (5)

It is assumed that the wave functions are normalized as $\langle \Psi_0^*, \Psi_0 \rangle = 1$. Coefficients $a_1$, $a_2$, etc. do not depend on $\theta$ 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 $m^2\alpha^3/(m/M)$ 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:

$$E^{(3)}_\infty = \alpha^3\frac{4}{3} \left[ \ln \frac{1}{\alpha^2} - \beta(L,\nu) + \frac{5}{6} - \frac{3}{8} \right] \langle Z_{He}\delta(r_{He}) \rangle$$

$$+ Z_p\delta(r_p),$$ (6)

where

$$\beta(L,\nu) = \frac{\langle J|H-E_0\rangle\ln(|H-E_0|/R_\infty|J\rangle)}{\langle J|H,J\rangle/2}$$ (7)

is the nonrelativistic Bethe logarithm [19] for a bound state of the three-body system. Here $J = \sum_{\alpha} Z_{\alpha}\rho_{\alpha}/m_e$ 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]:

$$E^{(3)}_{\text{recoil}} = \sum_{i=1,2} \frac{Z_i\alpha^3}{M_i} \left\{ \frac{2}{3} \left( -\ln \alpha - 4\beta(L,\nu) + \frac{31}{3} \right) \delta(r_i) \right\} - \frac{14}{3} Q(r_i),$$ (8)

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

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

The last term is the one-loop vacuum polarization:

$$E^{(3)}_{\text{vp}} = \frac{4\alpha^3}{3} \left[ -\frac{1}{5} \right] \left( Z_{He}\delta(r_{He}) + Z_p\delta(r_p) \right).$$ (9)

The two quantities, the $Q(r)$ term and the mean value the $\delta$-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 $\Delta l$, nonrelativistic energies $E_{n\nu}$ (in a.u.), Auger widths $\Gamma$ (in a.u.), expectation values of operators: $p_r^2$, $\delta(r_{He})$, and $\delta(r_p)$, and the Bethe logarithm values, $\beta(n,l)$, for the Auger states of $^4$He$^6\tilde{p}$ atom.
TABLE II. Multipolarities of the Auger transition $\Delta l$, nonrelativistic energies $E_{nr}$ (in a.u.), Auger widths $\Gamma$ (in a.u.), expectation values of operators: $p_{x}^{4}$, $\delta(r_{\theta_{m}})$, and $\delta(r_{\phi})$, and the Bethe logarithm values, $\beta(n,l)$, for the Auger states of $^4$He$^+\bar{p}$ atom.

<table>
<thead>
<tr>
<th>$(n,l)$</th>
<th>$\Delta l$</th>
<th>$E_{nr}$</th>
<th>$\Gamma/2$</th>
<th>$p_{x}^{4}$</th>
<th>$\delta(r_{\theta_{m}})$</th>
<th>$\delta(r_{\phi})$</th>
<th>$\beta(n,l)$</th>
</tr>
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<tbody>
<tr>
<td>(31,30)</td>
<td>3</td>
<td>$-3.5073727202819(5)$</td>
<td>$3.3424 \times 10^{-9}$</td>
<td>$28.309519$</td>
<td>$0.99368837$</td>
<td>$0.11287882$</td>
<td>$4.559722(1)$</td>
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<tr>
<td>(32,31)</td>
<td>4</td>
<td>$-3.348832173150003(2)$</td>
<td>$5.169 \times 10^{-10}$</td>
<td>$30.803393$</td>
<td>$1.069407$</td>
<td>$0.10401090$</td>
<td>$4.540686(1)$</td>
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<td>(33,31)</td>
<td>4</td>
<td>$-3.2195072516355(1)$</td>
<td>$8.2761 \times 10^{-9}$</td>
<td>$34.744079$</td>
<td>$1.1871602$</td>
<td>$0.09174227$</td>
<td>$4.511062(1)$</td>
</tr>
<tr>
<td>(34,32)</td>
<td>4</td>
<td>$-3.20767231244689(1)$</td>
<td>$7.8 \times 10^{-13}$</td>
<td>$33.484950$</td>
<td>$1.1497243$</td>
<td>$0.09489883$</td>
<td>$4.522121(1)$</td>
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<tr>
<td>(34,31)</td>
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<td>$-3.1061288628903(2)$</td>
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<td>$38.697601$</td>
<td>$1.3055346$</td>
<td>$0.08005938$</td>
<td>$4.486207(2)$</td>
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<td>$1.709 \times 10^{-11}$</td>
<td>$37.595341$</td>
<td>$1.2729446$</td>
<td>$0.08281128$</td>
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<tr>
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<td>$-$</td>
<td>$36.355772$</td>
<td>$1.2560854$</td>
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<td>$4.501942(5)$</td>
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<td>(35,32)</td>
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<td>$41.676373$</td>
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<td>(35,33)</td>
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<td>$-2.983373123874257(5)$</td>
<td>$1.303 \times 10^{-12}$</td>
<td>$40.593960$</td>
<td>$1.3630401$</td>
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<td>(36,32)</td>
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<td>$45.621175$</td>
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<tr>
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<td>$-2.89719228821683(3)$</td>
<td>$2.915 \times 10^{-10}$</td>
<td>$44.720654$</td>
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<tr>
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<td>$43.723769$</td>
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<td>$4.2678 \times 10^{-9}$</td>
<td>$48.642644$</td>
<td>$1.6040396$</td>
<td>$0.05369086$</td>
<td>$4.441353(3)$</td>
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<tr>
<td>(37,34)</td>
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<td>$7.6 \times 10^{-13}$</td>
<td>$47.831121$</td>
<td>$1.5799277$</td>
<td>$0.05494800$</td>
<td>$4.446893(6)$</td>
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<tr>
<td>(37,32)</td>
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<td>$3.4239 \times 10^{-8}$</td>
<td>$52.279701$</td>
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<td>$0.04549272$</td>
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<td>(38,34)</td>
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<td>$3.90 \times 10^{-12}$</td>
<td>$51.647733$</td>
<td>$1.6942064$</td>
<td>$0.04633993$</td>
<td>$4.431067(4)$</td>
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<tr>
<td>(39,34)</td>
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<td>$1.130 \times 10^{-9}$</td>
<td>$55.114275$</td>
<td>$1.7980611$</td>
<td>$0.03907099$</td>
<td>$4.419510(4)$</td>
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<tr>
<td>(40,35)</td>
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<td>$6.7 \times 10^{-13}$</td>
<td>$57.840699$</td>
<td>$1.8798956$</td>
<td>$0.03318082$</td>
<td>$4.411872(5)$</td>
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</table>
We neglect retardation as is usual for the nonrelativistic Bethe logarithm calculations [19]. It is worth noting that $J(k)$ does not depend on $\varphi$ for a complete (infinite) basis set, and thus the final value for $\beta(L, \nu)$ 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 calculation of the Bethe logarithm for the metastable states.

To keep the required numerical stability the quadrupole 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 re-calculated 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 $p_1^2$, $\delta(r_\alpha)$, and $\delta(r_\beta)$ operators. These numbers are of particular importance for evaluating the leading order relativistic corrections ($ma^0$) 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 $ma^0$ is now below 100 kHz.

In Table III a list of transition frequencies of spectroscopic interest both for $^4\text{He}^+\bar{p}$ and $^4\text{He}^+\bar{\beta}$ atoms are collected. The theoretical data contains a complete set of contributions up to $ma^0$ order and the leading contributions of the $ma^0$ 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) $\rightarrow$ (34, 32) transition of the $^4\text{He}^+\bar{p}$ 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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