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Bethe logarithm for the helium atom

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The Bethe logarithm for a large set of states of the helium atom is calculated with a precision of 12–14 significant digits. The numerical data are obtained for the case of infinite mass of a nucleus. Then we study the mass dependence and provide coefficients of the m_e/M expansion, which allows us to calculate accurate values for the Bethe logarithm for any finite mass. An asymptotic expansion for the Rydberg states is analyzed, and a high-quality numerical approximation is found, which ensures 7–8-digit accuracy for the S, P, and D states of the helium atom.

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I. INTRODUCTION

The Bethe logarithm is an important constituent of the leading-order radiative contribution to the energy of light atoms [1]. In the case of the hydrogen atom, the splitting between $2s$ and $2p_{1/2}$ levels of about 1058 MHz detected in the Lamb and Retherford experiment [2], also known as the Lamb shift, was explained by Bethe [3] in a purely nonrelativistic fashion by introducing the mean excitation energy K_0. However, already in the case of a helium atom it was realized that to obtain numerically the mean excitation energy K_0, or more precisely the Bethe logarithm $\ln(K_0/R_\infty)$, is a very nontrivial task [4]. It is astonishing that one of the earliest calculations [5] remained the most accurate for more than 30 years.

The significant breakthrough in numerical studies of the Bethe logarithm was achieved in the 1990s. Almost simultaneously, three independent groups [6–8] using different approaches reached a precision that exceeded the earlier results by three to five orders of magnitude. Since that time, precision calculations of many other atomic and molecular systems have appeared. Among them are calculations of rovibrational states in the hydrogen molecular ions $H_2{}^+$ and HD^+ [9,10], adiabatic two-electron calculation of the Bethe logarithm for molecular hydrogen [11], three electron Li-like [12,13], and four electron Be-like atoms and ions [14,15].

In this work, we present a comprehensive calculation of the Bethe logarithm for the helium atom. This study covers a wide range of orbital angular momentum states up to and including F states. We provide necessary numerical tools, which allow us to calculate a precise value for the Bethe logarithm for a helium atom with a finite nuclear mass M as well as for high n states, where n is the principal quantum number of an excited electron.

Atomic units are used throughout.

II. NUMERICAL APPROACH TO CALCULATE THE BETHE LOGARITHM

In this section, we follow the method described in detail in [16]. We define the Bethe logarithm as the ratio

$$\beta(L,v)=\frac{\mathcal{N}}{\mathcal{D}}, \tag{1}$$

where the numerator $\mathcal{N}(n,L)$ is expressed by the following integral:

$$\begin{aligned}\mathcal{N}(n,L)=&\int_0^{E_h} k\,dk\left\langle \mathbf{J}\left(\frac{1}{E_0-H-k}+\frac{1}{k}\right)\mathbf{J}\right\rangle\\ &+\int_{E_h}^{\infty}\frac{dk}{k}\left\langle \mathbf{J}\frac{(E_0-H)^2}{E_0-H-k}\mathbf{J}\right\rangle,\end{aligned} \tag{2a}$$

while the denominator is

$$\mathcal{D}(n,L)=\langle \mathbf{J}[H,\mathbf{J}]\rangle=\frac{\langle[\mathbf{J}[H,\mathbf{J}]]\rangle}{2}. \tag{2b}$$

Here E_h is the Hartree energy (the atomic unit of energy), $\mathbf{J}$ is the nonrelativistic electric current density operator of the atomic system

$$\mathbf{J}=\sum_i \frac{z_i}{m_i}\mathbf{P}_i, \tag{3}$$

and z_i and m_i are the charges and masses of the particles.

A. First-order perturbation wave function, $\psi_1(\cdot)$, and asymptotic expansion of $J(k)$ at $k\to\infty$

The key quantity for our numerical studies is

$$J(k)=\langle \mathbf{J}(E_0-H-k)^{-1}\mathbf{J}\rangle. \tag{4}$$

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Knowing this function, one immediately gets a value for the nonrelativistic Bethe logarithm using Eq. (2). The relation between $J(k)$ and other forms of the integrand in (2) may be found in [5].

A general procedure to calculate $J(k)$ is to solve the equation

$$(E_0 - H - k)\psi_1 = i\mathbf{J}\psi_0 \tag{5}$$

for different values of k. Since we are interested in the asymptotic behavior of $J(k)$ for $k \to \infty$, it is assumed that k is sufficiently large, and as a first approximation one may take

$$\psi_1^{(0)} = -(i/k)\mathbf{J}\psi_0. \tag{6}$$

Any approximate solution for ψ_1 may be (formally) iteratively improved:

$$\psi_1^{(n)} = -\frac{i}{k}\mathbf{J}\psi_0 + \frac{1}{k}(E_0 - H)\psi_1^{(n-1)} \tag{7}$$

and the next iteration would be

$$\psi_1^{(1)} = -\frac{i}{k}\mathbf{J}\psi_0 + \frac{1}{k^2}[H, i\mathbf{J}]\psi_0, \tag{8}$$

where

$$[H, i\mathbf{J}] = \sum_{i>j} z_i z_j \left(\frac{z_j}{m_j} - \frac{z_i}{m_i}\right)\frac{\mathbf{r}_{ij}}{r_{ij}^3}, \qquad \mathbf{r}_{ij} = \mathbf{r}_j - \mathbf{r}_i. \tag{9}$$

At small r_{ij}, ψ_1 should be smooth. To get a proper solution, one has to consider Eq. (5) for $r_{ij} \to 0$ and keep only important terms [here $m_{ij} = m_i m_j/(m_i + m_j)$ is the reduced mass of a pair; we also use a notation $(\cdot)$ in the list of variables of a function if the particular form of the internal variables is not important],

$$\left(\frac{1}{2m_{ij}}\Delta_{ij} - k\right)\psi_1(r_{ij}, \cdot) = 0,$$

which gives homogeneous solutions of the type

$$\sim \frac{\mathbf{r}_{ij}}{r_{ij}^3}\, e^{-\mu_{ij} r_{ij}}\,(1 + \mu_{ij} r_{ij})$$

with $\mu_{ij} = \sqrt{2m_{ij}k}$. These solutions, taken for different pairs of particles, may be added to $\psi_1^{(1)}$ to make the whole wave function smooth. So, we come to an approximation of ψ_1 for $k \to \infty$, which has the following form:

$$\psi_1^{(1)} = -\frac{i}{k}\mathbf{J}\psi_0(\cdot) + \frac{1}{k^2}\sum_{i>j} z_i z_j \left(\frac{z_j}{m_j} - \frac{z_i}{m_i}\right)\frac{\mathbf{r}_{ij}}{r_{ij}^3}$$
$$\times [1 - e^{-\mu_{ij} r_{ij}}\,(1 + \mu_{ij} r_{ij})]\psi_0(\cdot). \tag{10}$$

As is seen from this equation, there is no singular term in the wave function corresponding to a pair of identical particles.

The integrand $J(k)$ may be evaluated using the variational formalism as a stationary solution of a functional of ψ_1,

$$J(k) = -2\langle\psi_0|i\mathbf{J}|\psi_1\rangle - \langle\psi_1(E_0 - H - k)\psi_1\rangle.$$

To derive the asymptotic expansion, we substitute $\psi_1^{(1)}$ into the functional. That results in [16]

$$J(k) = -\frac{1}{k}\langle\mathbf{J}^2\rangle - \frac{1}{k^2}\frac{\langle\,[i\mathbf{J}, [H, i\mathbf{J}]]\,\rangle}{2} - \frac{1}{k^3}\sum_{\substack{i>j,k>l\\(i,j)\neq(k,l)}} z_i z_j z_k z_l \left(\frac{z_i}{m_i} - \frac{z_j}{m_j}\right)\left(\frac{z_k}{m_k} - \frac{z_l}{m_l}\right)\left\langle\frac{\mathbf{r}_{ij}\mathbf{r}_{kl}}{r_{ij}^2 r_{kl}^2}\right\rangle$$
$$-\frac{1}{k^3}\sum_{i>j} z_i^2 z_j^2 \left(\frac{z_i}{m_i} - \frac{z_j}{m_j}\right)^2 \{4\pi\mathcal{R}_{ij} + [\sqrt{2m_{ij}k} + z_i z_j m_{ij}(\ln(m_{ij}k) - \ln 2 - 1)]4\pi\langle\delta(\mathbf{r}_{ij})\rangle\} + \cdots. \tag{11}$$

Here $\mathcal{R}_{ij}$ is a finite functional, which replaces a divergent $1/r^4$ operator, and it is defined by the following expression:

$$\mathcal{R}_{ij} = \lim_{\rho\to 0}\left\{\left\langle\frac{1}{4\pi r_{ij}^4}\right\rangle_\rho - \left[\frac{1}{\rho}\langle\delta(\mathbf{r}_{ij})\rangle + (\ln\rho + \gamma_E)\langle\delta'(\mathbf{r}_{ij})\rangle\right]\right\}, \tag{12}$$

where

$$\langle\phi_1|\delta'(\mathbf{r})|\phi_2\rangle = \langle\phi_1|\frac{\mathbf{r}}{r}\nabla\delta(\mathbf{r})|\phi_2\rangle$$
$$= -\langle\partial_r\phi_1|\delta(\mathbf{r})|\phi_2\rangle - \langle\phi_1|\delta(\mathbf{r})|\partial_r\phi_2\rangle.$$

The mixed terms $(\mathbf{r}_{ij}\mathbf{r}_{kl})/(r_{ij}r_{kl})^2$ are finite and do not require any regularization.

B. Variational property

If we consider the quantity

$$\mathcal{J}_\Lambda = \int_0^\Lambda k\,dk\,J(k)$$
$$= \sum_n |\langle\psi_0|\mathbf{J}|\psi_n\rangle|^2\left[\Lambda - (E_0 - E_n)\ln\left|\frac{E_0 - E_n}{E_0 - E_n - \Lambda}\right|\right], \tag{13}$$

we would find that for the ground state of a system this quantity possesses the variational property, since for the integrand for all k the following inequality is fulfilled:

$$J_{\text{exact}}(k) \geqslant J_{\text{numerical}}(k).$$

The same property remains satisfied for other states if integration is performed from some $k_0 \sim 1$, which lies above the poles related to the states $E_n < E_0$. It is known from practical calculations that the low-k contribution becomes numerically converged to a high accuracy at a moderate basis length of intermediate states, and thus with good confidence the variational property—the higher the value of $\mathcal{J}_\Lambda$ the more accurate the solution—remains in effect. This allows us to perform optimization of the variational parameters of the basis set.

C. Numerical scheme

Here we consider the numerical scheme for the three-body Coulomb problem, which is then used in calculations of the Bethe logarithm for the helium and $H_2{}^+$ ground states. The wave functions both for the initial bound state and for the first-order perturbation solution (or intermediate state) are taken in the form

$$\Psi_L(l_1,l_2)=\sum_{i=1}^{\infty}\{U_i\,\mathrm{Re}[e^{-\alpha_i r_1-\beta_i r_2-\gamma_i r}] + W_i\,\mathrm{Im}[e^{-\alpha_i r_1-\beta_i r_2-\gamma_i r}]\}\mathcal{Y}^{l_1 l_2}_{LM}(\mathbf{r}_1,\mathbf{r}_2), \quad (14)$$

where $\mathcal{Y}^{l_1 l_2}_{LM}(\mathbf{r}_1,\mathbf{r}_2)$ are the solid bipolar harmonics as defined in [17]; r_1, r_2, and r are the Hylleraas coordinates of the two electrons in the helium atom; $\mathbf{r}=\mathbf{r}_2-\mathbf{r}_1$; and L is the total orbital angular momentum of a state. Complex parameters α_i, β_i, and γ_i are generated in a quasirandom manner [18]:

$$\alpha_i=\left[\left\lfloor\frac{1}{2}i(i+1)\sqrt{p_\alpha}\right\rfloor(A_2-A_1)+A_1\right] + i\left[\left\lfloor\frac{1}{2}i(i+1)\sqrt{q_\alpha}\right\rfloor(A'_2-A'_1)+A'_1\right], \quad (15)$$

where $\lfloor x\rfloor$ designates the fractional part of x; p_α and q_α are some prime numbers, say, 2, 3, 5, etc.; and $[A_1,A_2]$ and $[A'_1,A'_2]$ are real variational intervals that need to be optimized. The parameters β_i and γ_i are obtained in a similar way.

The basis set for intermediate states is constructed as follows:

(i) First we use a regular basis set, which is taken similarly to the initial state with regular values of the parameters (α,β,γ) in the exponentials.

(ii) Then we build a special basis set with exponentially growing parameters for a particular r_{ij},

$$\begin{aligned}A_1^{(0)}&=A_1, \quad A_2^{(0)}=A_2,\\ A_1^{(n)}&=\tau^n A_1, \quad A_2^{(n)}=\tau^n A_2,\end{aligned} \quad (16)$$

where $\tau=A_2/A_1$.

Typically, $[A_1,A_2]=[3,6]$ and $n_{\max}=5\text{–}7$, which corresponds to the photon energy interval $k\in[0,10^4]$.

(iii) For other pairs of (i,j) we take similar basis sets to those in (ii). It is worth noting that for identical particles, this step should be omitted, since, as it follows from Eq. (10), there is no singular behavior of $\psi_1(r_{ij},\cdot)$ for small r_{ij}.

After the complete set of basis functions is constructed, we diagonalize the matrix of the Hamiltonian H_I for intermediate states to get a set of (pseudo)state energies, E_m, and then to calculate $\langle 0|i\mathbf{J}|m\rangle$. These two sets of data are enough to restore $J(k)$:

$$J(k)=-\sum_m\frac{\langle 0|i\mathbf{J}|m\rangle^2}{E_0-E_m-k}, \quad (17)$$

and to integrate the low-energy part of the numerator $\mathcal{N}(L,v)$,

$$\int_0^{E_h}k\,dk\left\langle\mathbf{J}\left(\frac{1}{E_0-H-k}+\frac{1}{k}\right)\mathbf{J}\right\rangle + \int_{E_h}^{\Lambda}\frac{dk}{k}\left\langle\mathbf{J}\frac{(E_0-H)^2}{E_0-H-k}\mathbf{J}\right\rangle. \quad (18)$$

TABLE I. The Bethe logarithm calculations for the ground and excited states of the helium atom with infinite nuclear mass $M_{\mathrm{He}}\to+\infty$ and comparison with most precise previous calculations.

n	$n\,^1S$	$n\,^3S$	$n\,^1P$	$n\,^3P$
1	4.370 160 223 0703(3)			
	4.370 160 218(3)[a]			
	4.370 160 222 9(1)[b]			
	4.370 160 223 06(2)[c]			
2	4.366 412 726 417(1)	4.364 036 820 476(1)	4.370 097 743 554(2)	4.369 985 364 549(3)
	4.366 412 72(7)[a]	4.364 036 82(1)[a]	4.370 097 82(3)[a]	4.369 985 20(2)[a]
	4.366 412 726 2(1)[b]	4.364 036 820 41(2)[b]	4.370 097 743 5(1)[b]	4.369 985 364 4(2)[b]
3	4.369 164 860 824(2)	4.368 666 996 159(2)	4.370 295 862 299(4)	4.370 235 654 775(4)
	4.369 164 871(8)[a]	4.368 666 92(2)[a]	4.370 295 75(9)[a]	4.370 233 9(2)[a]
4	4.369 890 632 356(3)	4.369 723 392 715(4)	4.370 363 160 331(5)	4.370 334 604 477(5)
	4.369 890 66(1)[a]	4.369 723 44(5)[a]	4.370 363 2(2)[a]	4.370 334 16(5)[a]
5	4.370 151 796 310(4)	4.370 078 509 668(4)	4.370 390 514 367(5)	4.370 375 352 464(5)
	4.370 151 7(1)[a]	4.370 078 31(8)[a]	4.370 390 54(4)[a]	4.370 374 6(2)[a]
6	4.370 266 974 319(5)	4.370 229 062 747(5)	4.370 403 502 993(6)	4.370 394 624 37(2)
7	4.370 325 261 772(5)	4.370 303 319 792(5)		
n	$n\,^1D$	$n\,^3D$	$n\,^1F$	$n\,^3F$
3	4.370 413 478 422(3)	4.370 420 247 640(2)		
	4.370 413 470(7)[d]	4.370 420 247(2)[c]		
4	4.370 417 339 045(4)	4.370 421 238 038(4)	4.370 421 511 306(3)	4.370 421 527 144(3)
5	4.370 419 597 74(2)	4.370 421 809 90(2)		

[a] Drake and Goldman [8].
[b] Yerokhin and Pachucki [19].
[c] Korobov [16].
[d] Wienczek *et al.* [20].

From thus obtained $J(k)$ we extrapolate coefficients of asymptotic expansion,

$$f_{\rm fit}(k) = \sum_{m=1}^{M} \frac{C_{1m}\sqrt{k}+C_{2m}\ln k+C_{3m}}{k^{m+3}}, \qquad (19)$$

which is taken in the same form as in analytic expansion for the hydrogen atom. The leading-order terms of $J(k)$ are obtained from Eq. (11). That allows us to calculate the high-energy part of the numerator,

$$\int_{\Lambda}^{\infty} \frac{dk}{k} \left\langle \mathbf{J} \frac{(E_0-H)^2}{E_0-H-k} \mathbf{J} \right\rangle.$$

III. RESULTS

The results of our numerical calculations are presented in Table I, where the infinite mass of the nucleus is assumed. As is seen from the data, our results are in good agreement with previous calculations [8,19], but they exceed them in numerical precision. To calculate the data for a comprehensive analysis of the leading-order radiative corrections, we have to consider the mass dependence of the Bethe logarithm and extrapolation to high-n states. That will be done in the subsections below.

A. Finite mass

For the case of a finite mass M of the nucleus, the results of Table I should be somehow modified. The simplest way is to use an expansion

$$\beta_M = \beta_\infty + \ln(\mu/m_e) + a_1(m_e/M) + a_2(m_e/M)^2 + \cdots . \qquad (20)$$

The major contribution, $\ln(\mu/m_e)$, comes from the scaling of the electron wave function due to the finite mass effect, where $\mu = m_e M/(M+m_e)$ is the reduced mass of an electron. The next linear term may be calculated using the first-order perturbation of the Bethe logarithm by the mass-polarization operator; see [19]. In our case, we utilized a more trivial approach. Since our code was written for a general case of three particles of finite masses, we performed calculations of the Bethe logarithm for two consecutive points of the variable M, namely for $M_1 = M_{^4\mathrm{He}} = 7294.299\,541\,36 m_e$ and $M_2 = M_1/2$. For a mass of the α particle, we take the CODATA14 recommended value [21]. The two coefficients of the linear and quadratic terms in (20) have been obtained from a set of two linear equations. The linear coefficients are in very good agreement with the corresponding coefficients calculated by Yerokhin and Pachucki in [19], as may be expected. We also checked the quality of our approximation for the $1\,^1S$ state using the least-squares approximation for a_1 and a_2 from the three-point data with the third data point $M_3 = M_1/3$. The least-squares result—$a_1 = 0.094\,389\,42$ and $a_2 = -0.164\,903\,2$—agrees well with the simple approximation and demonstrates that the data presented in Table II are sufficient for a precise determination of the Bethe logarithm for real cases of the helium atom for various nuclear isotopes.

TABLE II. Mass dependence of the Bethe logarithm. Coefficients of expansion (20).

State	a_1	a_2
1^1S	0.9438944[−01]	−0.16501[+00]
2^1S	0.1773442[−01]	−0.34889[−01]
2^3S	0.4785558[−02]	−0.95888[−02]
2^1P	−0.3553442[−02]	0.95390[−02]
2^3P	0.8709662[−02]	0.37926[−02]
3^1S	0.5386215[−02]	−0.10813[−01]
3^3S	0.1071013[−02]	−0.29114[−02]
3^1P	−0.1004733[−02]	0.20368[−02]
3^3P	0.2536963[−02]	−0.11556[−02]
3^1D	−0.6358710[−05]	0.36083[−03]
3^3D	0.3792498[−04]	−0.22445[−03]
4^1S	0.2264400[−02]	−0.45874[−02]
4^3S	0.3763586[−03]	−0.12354[−02]
4^1P	−0.4158826[−03]	0.78650[−03]
4^3P	0.1074222[−02]	−0.72991[−03]
4^1D	−0.6179997[−05]	0.17459[−03]
4^3D	0.1964547[−04]	−0.17124[−03]
4^1F	0.3926256[−05]	−0.11805[−03]
4^3F	0.3612599[−05]	−0.11625[−04]
5^1S	0.1151476[−02]	−0.23793[−02]
5^3S	0.1710350[−03]	−0.51711[−03]
5^1P	−0.2113686[−03]	0.38744[−03]
5^3P	0.5516224[−03]	−0.41064[−03]
5^1D	−0.4174068[−05]	0.75987[−03]
5^3D	0.1077559[−04]	−0.64813[−04]
6^1S	0.6621675[−03]	−0.23261[−02]
6^3S	0.9116608[−04]	−0.64837[−04]
6^1P	−0.1225350[−03]	−0.43729[−03]
6^3P	0.3206520[−03]	−0.33082[−03]

B. Asymptotic expansions for Rydberg states

For the Rydberg states, the Bethe logarithm may be calculated using the asymptotic expansion [22,23]

$$\begin{aligned}\beta(1,s;n,l;{}^{1,3}L) = \beta_{1s} + \ln Z^2 + \left(\frac{Z-1}{Z}\right)^4 \frac{\beta_{nl}}{n^3} \\ + \frac{0.316\,205(6)}{Z^6}\langle x^{-4}\rangle \\ + \Delta\beta(1,s;n,l;{}^{1,3}L),\end{aligned} \qquad (21)$$

where x is the distance between the outer Rydberg electron and nucleus. In the approximation of an electron in a field of the effective charge $Z^* = 1$, this quantity given by expression Eq. (21) is valid for states with $L > 0$ [22]. Here $\beta_{1s} = 2.984\,128\,555\,765$ is the Bethe logarithm for the ground state of a hydrogen atom, and $\Delta\beta(1,s;n,l^{1,3}L)$ takes into account contributions from the higher multipole moments [23] [see Eqs. (19) and (20)].

TABLE III. The Bethe logarithm for the Rydberg states. Coefficients of the asymptotic expansion (22).

	n^1S	n^3S	n^1P	n^3P	n^1D	n^3D
c_0	−0.03151	−0.03530	−0.004857	−0.006620	−0.0006212	−0.0003348
c_1	−0.01874	−0.04245	0.003677	0.001407	0.0009306	0.0012734
c_2	0.03409	0.01840	0.001809	0.009856	0.0005059	−0.0014552

In our case, we use a slightly different expansion,

$$\beta(1,s;n,l) = \beta_{1s} + \ln Z^2 + \frac{1}{n^3}\sum_{j=0}^{2}\frac{c_j}{n^j}, \qquad (22)$$

where the coefficients c_i are obtained by the least-squares method [24] and data from Table I. To get a proper extrapolation in the case of S states, we have used data points for states $n = 3$ and up to $n = 7$ in order to eliminate the nonmonotonic behavior of the $\beta(n)$ function for the first two states. Coefficients of the asymptotic expansion (22) are presented in Table III. We estimate that the values obtained using expansion (22) for the Bethe logarithm of the Rydberg states should be accurate up to 7–8 digits.

For the states with $L \geqslant 3$, the asymptotic formula (21) works well. For example, the results for the $4F$ states: $\beta(4^1F) = 4.370\,421\,511(13)$ and $\beta(4^3F) = 4.370\,421\,527(15)$, agree to 10-figure accuracy with our results presented in Table I. For further discussions, we refer the reader to [23].

C. Conclusions

In conclusion, we want to summarize the main results of our work. First, the more accurate values of the Bethe logarithm have been obtained numerically for a wide range of states with a precision that exceeds the published data by at least three orders of magnitude. These data allowed us to make an asymptotic extrapolation to the states with higher n, a principal quantum number of the excited electron. Along with results obtained by Drake in [23], our data cover the whole set of bound states in a helium atom.

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