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Bethe logarithms for hydrogen up to $n = 20$, and approximations for two-electron atoms

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Bethe logarithms accurate to 14 or 15 places to the right of the decimal are tabulated for all states of hydrogen up to $n=20$. Approximation methods for Rydberg states of two-electron atoms are discussed.

I. INTRODUCTION

The Bethe logarithm (BL) represents the essentially nonrelativistic part of the Lamb shift arising from lowest-order quantum electrodynamic (QED) effects in hydrogen and other one-electron ions.¹ The one-electron BL also plays an important role in approximation schemes for many-electron atoms.^{2,3} BL's have been calculated by many authors⁴⁻⁹ in the years since Bethe's¹⁰ original work on the $2s-2p$ Lamb shift in hydrogen, the most extensive tabulation being that of Klarsfeld and Maquet⁸ for all states up to $n=8$. Subsequently, Haywood and Morgan¹¹ obtained higher precision for the $1s$ and $2s$ states by the application of finite basis-set methods. Baker, Hill, and Morgan¹² have recently further improved the $1s$ value to 17 places to the right of the decimal.

Recent high-precision measurements of transition frequencies among the $n=10$ Rydberg states of helium¹³ raise once again the need for a more extensive tabulation of BL's. For example, the one-electron Lamb shift contributes about 13 kHz to the $1s10g-1s10h$ manifold of transitions,¹⁴ which is much larger than the ± 2 -kHz accuracy of the measurements. The purpose of this paper is to tabulate BL's for all one-electron states up to $n=20$, and to discuss screened hydrogenic values for the corresponding Rydberg states of helium. The one-electron values are believed to be accurate to 14 or 15 places to the right of the decimal, which substantially exceeds any previous tabulation.

The lowest-order QED shift for an electron with quantum numbers n, l, j in a point Coulomb field of charge Z and infinite mass is^{1,15} (in atomic units)

$$\Delta E_L(nlj) = \frac{4}{3} Z \alpha^3 (Z^3 / \pi n^3) \left[\delta_{l,0} \left[\ln(Z\alpha)^{-2} + \frac{11}{24} - \frac{1}{5} \right] - \ln[k_0(nl) / Z^2 R_\infty] + \frac{3}{8} \frac{c_{lj}}{(2l+1)} \right], \quad (1)$$

where $c_{lj} = \delta_{j,l+1/2} / (l+1) - \delta_{j,l-1/2} / l$. The terms $\frac{11}{24}$ and $-\frac{1}{5}$ come from electron self-energy and vacuum polarization corrections, respectively, and the last term containing c_{lj} is the anomalous magnetic-moment correction. Bethe's mean excitation energy $k_0(nl)$ is defined by

$$\ln[k_0(nl) / R_\infty] = \sum_{n'} g(nl, n') \ln|\omega(n', n)|, \quad (2)$$

where $\omega(n', n) = (E_{n'} - E_n) / R_\infty$ and the sum includes all discrete states and an integration over the continuous spectrum. The $g(nl, n')$ are related to oscillator strengths for transitions $nl \rightarrow n'l \pm 1$ by

$$g(nl, n') = (3n^3 / 16) f(nl, n') \omega^2(n', n). \quad (3)$$

II. COMPUTATIONAL METHOD

Previous evaluations of $\ln k_0$ have used either an explicit summation of the terms in Eq. (2),^{4,8,10} or implicit summation methods based on the Coulomb Green function.^{5-9,12} In the present work, we have found that results approaching machine accuracy (about 16 figures in double precision) can readily be obtained by direct summation, using Gordon's formula¹ for bound-state transition integrals, and an equivalent formula derived by Karzas and Latter¹⁶ for continuum transition integrals which avoids complex variables. In view of the rather modest accuracy achieved in the past by this method, it seems worthwhile to describe the computational details used here. We first write Eq. (2) in the form

$$\ln[k_0(nl) / R_\infty] = B + C, \quad (4)$$

where B is the bound-state contribution and C the continuum contribution, and define the partial sum

$$B_N = \sum_{n'=l}^N b_{n'}, \quad (5)$$

with $b_{n'} = g(nl, n') \ln|\omega(n', n)|$. The $b_{n'}$ have the asymptotic expansion

$$b_{n'} = \beta / n'^3 + \gamma / n'^5 + \dots \quad (6)$$

Analytic expressions for β and γ could be derived, but it is computationally simpler to estimate them from the last two terms included in (5) according to

$$\gamma_N = \frac{N^2(N-1)^2}{2N-1} [(N-1)^3 b_{N-1} - N^3 b_N] \quad (7)$$

and

$$\beta_N = N^3 b_N - \gamma_N / N^2, \quad (8)$$

obtained by solving two equations in two unknowns. Then $\gamma_N \rightarrow \gamma$ and $\beta_N \rightarrow \beta$ as $N \rightarrow \infty$. The complete sum over bound states is then approximated by

TABLE I. (Continued).

n	$\ln[k_0(nl)/R_\infty]$	$\ln[k_0(nl)/R_\infty]$	$\ln[k_0(nl)/R_\infty]$	$\ln[k_0(nl)/R_\infty]$
$l = 12$				
13	-0.000 031 581 518 92	$l = 13$		
14	-0.000 035 759 246 53	-0.000 024 924 973 82	$l = 14$	
15	-0.000 039 323 101 08	-0.000 028 032 896 20	-0.000 020 014 384 873	$l = 15$
16	-0.000 042 397 776 52	-0.000 030 712 253 25	-0.000 022 374 144 60	-0.000 016 313 053 76
17	-0.000 045 076 278 68	-0.000 033 045 090 67	-0.000 024 427 375 56	-0.000 018 136 888 68
18	-0.000 047 429 319 85	-0.000 035 093 747 13	-0.000 026 229 566 48	-0.000 019 736 795 95
19	-0.000 049 511 611 78	-0.000 036 906 385 55	-0.000 027 823 571 79	-0.000 021 151 218 00
20	-0.000 051 366 162 73	-0.000 038 520 794 22	-0.000 029 242 977 94	-0.000 022 410 278 06
$l = 16$				
17	-0.000 013 470 635 45	$l = 17$		
18	-0.000 014 902 445 73	-0.000 011 251 829 40	$l = 18$	
19	-0.000 016 167 595 63	-0.000 012 391 530 91	-0.000 009 494 620 18	$l = 19$
20	-0.000 017 293 290 47	-0.000 013 405 126 23	-0.000 010 413 063 29	-0.000 008 084 977 84

$$B = B_N + \beta_N \zeta_N(3) + \gamma_N \zeta_N(5), \quad (9)$$

where $\zeta_N(k) = \zeta(k) - \sum_{j=1}^N j^{-k}$ is the N -times-subtracted Riemann ζ function. Loss of precision in making the subtractions can be avoided by starting from

$$\zeta_6(3) = 0.011\,765\,236\,492\,927\,618\,73,$$

$$\zeta_6(5) = 0.000\,137\,365\,482\,876\,099\,17,$$

so that $\zeta_N(k) = \zeta_6(k) - \sum_{j=7}^N j^{-k}$. Complete stability to 16 figures in B is easily obtained for all states studied with N no more than 10 000 for the highest states, and much less for the lower states.

A similar strategy was applied to the continuum part

$$C = \int_0^\infty u(\nu) d\nu, \quad (10)$$

with

$$u(\nu) = (\nu - E_n)^2 \ln(\nu - E_n) \frac{df}{d\nu}. \quad (11)$$

Since $u(\nu)$ has the asymptotic expansion

$$u(\nu) \sim \ln \nu (\tilde{\beta}/\nu^{3/2} + \tilde{\gamma}/\nu^2), \quad (12)$$

C is approximated by

$$C = C_N + \tilde{\beta}_N I_{E(N)}(\frac{3}{2}) + \tilde{\gamma}_N I_{E(N)}(2), \quad (13)$$

where

$$I_E(k) = \int_E^\infty \nu^{-k} \ln \nu d\nu = \frac{\ln E}{(k-1)E^{k-1}} + \frac{1}{(k-1)^2 E^{k-1}} \quad (14)$$

and C_N is evaluated by numerical Romberg integration in a number of subintervals according to

$$C_N = \sum_{i=1}^N \int_{E(i-1)}^{E(i)} u(\nu) d\nu + E(0)u[E(0)], \quad (15)$$

with $E(i) = 2^{i-13} R_\infty$ for $i \geq 1$ and $E(0) = 10^{-13} R_\infty$. The last term in (15) is the small contribution to the integral from the interval $0 \leq \nu \leq E(0)$. The $\tilde{\beta}_N$ and $\tilde{\gamma}_N$ are calculated as in Eqs. (7) and (8) from $u(E)$ evaluated at $E(N)$ and $E(N-1)$, and N increased until C becomes stable to machine precision. This requires $N \approx 50$ for $l=0$ and $N \approx 20$ for $l \neq 0$. The entire calculation takes less than a minute per state on an IBM PC/AT.

The above method was used to calculate simultaneously the check sums

$$\sum_{n'} f(nl, n') = 1, \quad (16)$$

$$\sum_{n'} g(nl, n') = \delta_{i,0}. \quad (17)$$

The largest deviations for $12 \leq n \leq 20$ were 4×10^{-14} for Eq. (16) and 2×10^{-15} for Eq. (17). For $n \leq 11$, the largest deviations were 8×10^{-15} and 1×10^{-15} , respectively. The check sums for each state were used to assess the accuracy of the corresponding BL.

III. RESULTS

The final results for the Bethe logarithms are listed in Table I. All are believed to be accurate to within ± 1 in the final figure quoted. For the lower states, the results agree exactly with the 11 figure (for $n \leq 4$) and 8 figure (for $n \leq 8$) tabulations of Klarsfeld and Maquet⁸ to the number of figures they quote. The values for the $1s$ and $2s$ states verify the 14 figure results of Haywood and Morgan¹¹ to within the $\pm 2 \times 10^{-13}$ uncertainty of their finite basis-set calculation. The one previous calculation which exceeds the accuracy of the present work by two figures is the $1s$ result of Baker, Hill, and Morgan.¹² They obtain (after adding $\ln 2$ to convert from a.u. to rydbergs)

$$\ln[k_0(1s)/R_\infty] = 2.984\,128\,555\,765\,497\,61,$$

in agreement with our value.

The two-electron BL is defined by an expression exactly analogous to Eq. (2) except that the one-electron transition integrals and frequencies are replaced by the corresponding two-electron quantities.¹ Although direct calculations of the two-electron BL are difficult and have only been carried out for the ground state,¹⁷ they can be estimated from the data in Table I as follows. Inserting Z^{-1} expansions for the two-electron wave functions and energies into Eq. (2) yields, for singly excited states,

$$\begin{aligned} & \ln \left[\frac{k_0(1s, nL; {}^{2S+1}L)}{Z^2 R_\infty} \right] \\ &= \ln \left[\frac{k_0^0(1s, nL)}{R_\infty} \right] - \frac{2\sigma}{Z} + O(Z^{-2}) \\ &= \ln \left[\frac{k_0^0(1s, nL)(Z - \sigma)^2}{Z^2 R_\infty} \right] + O(Z^{-2}), \end{aligned} \quad (18)$$

where

$$\begin{aligned} & \ln \left[\frac{k_0^0(1s, nL)}{R_\infty} \right] \\ &= \frac{\ln[k_0(1s)/R_\infty] + n^{-3} \ln[k_0(nL)/R_\infty]}{1 + n^{-3} \delta_{L,0}} \end{aligned} \quad (19)$$

is the leading term, and σ can be expressed in terms of perturbation sums over intermediate states.^{2,3} Values of σ have only been calculated for states up to $n=2$ with the results³

$$\begin{aligned} \sigma(1^1S) &= 0.00615, & \sigma(2^1S) &= -0.02040, \\ \sigma(2^3S) &= -0.01388, & \sigma(2^1P) &= -0.00600, \\ \sigma(2^3P) &= -0.00475. \end{aligned}$$

For the high nL states, a useful approximation to the two-electron BL can be obtained by calculating the mean

excitation energy for the $1s$ electron as if the outer electron were not present, and the nL electron for an effective nuclear charge $Z_{\text{eff}} = Z - 1$. The first corresponds to virtual excitations of the form $1s, nL \rightarrow n'p, nL$ and the second to virtual excitations of the form $1s, nL \rightarrow 1s, n''L \pm 1$, summed over n' with $Z_{\text{eff}} = Z$ and n'' with $Z_{\text{eff}} = Z - 1$. Since the one-electron oscillator strengths are independent of Z while the transition energies scale as Z^2 or $(Z - 1)^2$, respectively, for the two cases, the result is [using Eq. (17)]

$$\begin{aligned} & \ln \left[\frac{k_0(1s, nL)}{Z^2 R_\infty} \right] \\ &= \ln \left[\frac{k_0(1s)}{R_\infty} \right] + \frac{1}{n^3} \left[\frac{Z - 1}{Z} \right]^4 \ln \left[\frac{k_0(nL)}{R_\infty} \right] \end{aligned} \quad (20)$$

for $L > 0$. Comparing with Eq. (18) yields

$$\bar{\sigma}(nL) = (2/n^3) \ln[k_0(nL)]. \quad (21)$$

For the $1s2p$ state, this gives $\bar{\sigma}(2p) = -0.0075$, which is in reasonable accord with the exact values above for the $1s2p^1P$ and 3P states. For the high nL states, one would expect $\bar{\sigma}(nL) \rightarrow \sigma(nL)$.

Since $\ln k_0(1s, nL)$ can easily be calculated from Eq. (20) and the results in Table I, this quantity is not separately tabulated. Values for $n=10$ are given in Ref. 12. The results for the $1s10f-1s10g$ and $1s10g-1s10h$ transition frequencies of helium are in close agreement with experiment.¹²

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