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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 authors\(^4\) in the years since Bethe's\(^10\) original work on the 2s-2p Lamb shift in hydrogen, the most extensive tabulation being that of Klarsfeld and Maquet\(^6\) for all states up to \( n = 8 \). Subsequently, Haywood and Morgan\(^11\) obtained higher precision for the 1s and 2s states by the application of finite basis-set methods. Baker, Hill, and Morgan\(^12\) 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 helium\(^13\) 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 \( Ze \) and infinite mass is\(^15\) (in atomic units)

\[
\Delta E_L(nl) = \frac{3}{4} Z \alpha^2 (Z^3/\pi n^3) \left[ \delta_{l0} \left[ \ln(Z \alpha)^2 + \frac{11}{32} - \frac{3}{4} \right] - \ln[k_0(nl)/Z^2 R_\infty^2] \right] + \frac{3}{8} \frac{c_j}{(2l + 1)},
\]

where \( c_j = \delta_{j1/2} (l + 1) - \delta_{j-1/2} l \). The terms \( 1/32 \) and \( -1/2 \) come from electron self-energy and vacuum polarization corrections, respectively, and the last term containing \( c_j \) is the anomalous magnetic-moment correction.

Bethe's mean excitation energy \( k_0(nl) \) is defined by

\[
\ln[k_0(nl)/R_\infty] = \sum \lambda(nl,n') \ln[\omega(n',n)],
\]

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 \( \lambda(nl,n') \) are related to oscillator strengths for transitions \( nl \to n' \pm 1 \) by

\[
\lambda(nl,n') = (3n^3/16) f(nl,n') \omega^2(n',n). \tag{3}
\]

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 formula\(^1\) for bound-state transition integrals, and an equivalent formula derived by Karzas and Latter\(^16\) 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

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

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

\[
B_N = \sum_{n' = l}^{N} b_{n'}, \tag{5}
\]

with \( b_{n'} = \lambda(nl,n') \ln[\omega(n',n)] \). The \( b_{n'} \) have the asymptotic expansion

\[
b_{n'} = \beta / n^{3} + \gamma / n^{12} + \cdots.
\]

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

\[
\gamma_N = N^2[(N - 1)^2 / 2N - 1] \sum_{n' = l - 1}^{N - 1} b_{n'} - N^3 b_N,
\]

and

\[
\beta_N = N^3 b_N - \gamma_N / N^2,
\]

obtained by solving two equations in two unknowns. Then \( \gamma \to \gamma \) and \( \beta \to \beta \) as \( N \to \infty \). The complete sum over bound states is then approximated by

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

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TABLE I. Bethe logarithms for hydrogen. For two-electron atoms, see Eq. (20).

<table>
<thead>
<tr>
<th>$n$</th>
<th>$\ln[k_0(nl)/R_{\infty}]$</th>
<th>$\ln[k_0(nl)/R_{\infty}]$</th>
<th>$\ln[k_0(nl)/R_{\infty}]$</th>
<th>$\ln[k_0(nl)/R_{\infty}]$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$l = 0$</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>1</td>
<td>2.984 128 555 765 498</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>2</td>
<td>2.811 769 893 120 563</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>3</td>
<td>2.767 663 612 491 822</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>4</td>
<td>2.749 811 840 454 057</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>5</td>
<td>2.740 823 728 584 572</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>6</td>
<td>2.735 664 206 935 105</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>7</td>
<td>2.732 429 129 187 092</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>8</td>
<td>2.730 267 260 690 589</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>9</td>
<td>2.728 751 166 038 614</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>10</td>
<td>2.727 646 938 659 466</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>11</td>
<td>2.726 817 782 527 157</td>
<td></td>
<td></td>
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</tr>
<tr>
<td>12</td>
<td>2.726 179 340 635 48</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>13</td>
<td>2.725 677 290 537 02</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>14</td>
<td>2.725 275 397 127 599</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>15</td>
<td>2.724 948 600 408 85</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>16</td>
<td>2.724 679 355 911 28</td>
<td></td>
<td></td>
<td></td>
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<tr>
<td>17</td>
<td>2.724 454 879 738 29</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>18</td>
<td>2.724 265 768 141 35</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>19</td>
<td>2.724 104 963 270 95</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>20</td>
<td>2.723 967 084 293 02</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

| $l = 4$ | | | | |
| 5 | -0.000 772 098 901 537 | | | |
| 6 | -0.000 962 797 424 841 | | | |
| 7 | -0.000 994 792 739 370 | | | |
| 8 | -0.001 190 432 043 318 | | | |
| 9 | -0.001 263 904 507 064 | | | |
| 10 | -0.001 319 718 057 354 | | | |
| 11 | -0.001 364 844 849 466 | | | |
| 12 | -0.001 401 468 731 72 | | | |
| 13 | -0.001 431 644 265 75 | | | |
| 14 | -0.001 456 827 618 98 | | | |
| 15 | -0.001 478 078 457 94 | | | |
| 16 | -0.001 496 185 126 95 | | | |
| 17 | -0.001 511 745 248 80 | | | |
| 18 | -0.001 525 219 287 83 | | | |
| 19 | -0.001 536 967 112 49 | | | |
| 20 | -0.001 547 273 535 58 | | | |

| $l = 8$ | | | | |
| 9 | -0.000 104 148 092 50 | | | |
| 10 | -0.000 136 808 195 63 | | | |
| 11 | -0.000 148 688 925 63 | | | |
| 12 | -0.000 158 576 610 33 | | | |
| 13 | -0.000 166 922 825 60 | | | |
| 14 | -0.000 174 051 514 01 | | | |
| 15 | -0.000 180 201 449 52 | | | |
| 16 | -0.000 185 552 757 78 | | | |
| 17 | -0.000 190 244 049 52 | | | |
| 18 | -0.000 194 383 831 67 | | | |
| 19 | -0.000 198 058 316 53 | | | |
| 20 | -0.000 135 831 685 02 | | | |
TABLE I. (Continued).

<table>
<thead>
<tr>
<th>n</th>
<th>$\ln[k_0(nl)/R_{\infty}]$</th>
<th>$\ln[k_0(nl)/R_{\infty}]$</th>
<th>$\ln[k_0(nl)/R_{\infty}]$</th>
<th>$\ln[k_0(nl)/R_{\infty}]$</th>
</tr>
</thead>
<tbody>
<tr>
<td>13</td>
<td>-0.000 031 581 518 92</td>
<td>-0.000 024 924 973 82</td>
<td>-0.000 020 014 384 873</td>
<td>-0.000 016 313 053 76</td>
</tr>
<tr>
<td>14</td>
<td>-0.000 035 759 246 53</td>
<td>-0.000 028 032 896 20</td>
<td>-0.000 022 374 144 60</td>
<td>-0.000 018 136 888 68</td>
</tr>
<tr>
<td>15</td>
<td>-0.000 039 323 101 08</td>
<td>-0.000 030 712 253 25</td>
<td>-0.000 024 427 375 56</td>
<td>-0.000 019 736 795 95</td>
</tr>
<tr>
<td>16</td>
<td>-0.000 042 397 776 52</td>
<td>-0.000 033 045 090 67</td>
<td>-0.000 026 229 566 48</td>
<td>-0.000 021 151 218 00</td>
</tr>
<tr>
<td>17</td>
<td>-0.000 045 076 278 68</td>
<td>-0.000 035 906 385 55</td>
<td>-0.000 027 823 571 79</td>
<td>-0.000 022 410 278 06</td>
</tr>
<tr>
<td>18</td>
<td>-0.000 047 429 319 95</td>
<td>-0.000 038 520 794 22</td>
<td>-0.000 029 242 977 94</td>
<td></td>
</tr>
<tr>
<td>19</td>
<td>-0.000 049 511 611 78</td>
<td>-0.000 040 013 405 26</td>
<td>-0.000 031 013 405 26</td>
<td></td>
</tr>
<tr>
<td>20</td>
<td>-0.000 051 366 162 73</td>
<td>-0.000 042 470 635 45</td>
<td>-0.000 044 960 472 47</td>
<td></td>
</tr>
</tbody>
</table>

\[ B = B_N + \beta_N \xi_N(3) + \gamma_N \xi_N(5), \]

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

\[ \xi_6(3) = 0.011 765 236 492 927 618 73, \]
\[ \xi_6(5) = 0.000 137 365 482 876 099 17, \]

so that \( \xi_N(k) = \xi_6(k) - \sum_{j=7}^{N} j^{-k} \). 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

\[ C = \int_0^\infty u(v) dv, \]

with

\[ u(v) = (v - E_n)^2 \ln(v - E_n) \frac{df}{dv}. \]

Since \( u(v) \) has the asymptotic expansion

\[ u(v) \sim \ln(\beta/v^{3/2} + \gamma/v^2), \]

\[ C \]

\[ C = C_N + \beta_N I_{E(N)}(\frac{1}{3}) + \gamma_N I_{E(N)}(2), \]

where

\[ I_E(k) = \int_E^\infty v^{-k} \ln v dv = \ln E - (k-1)^{-1} \frac{1}{(k-1)^2 E^{k-1}}, \]

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

\[ C_N = \sum_{i=1}^{N} \int_E^{E(i)} u(v) dv + E(0) u[E(0)], \]

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 \( 0 \leq v \leq E(0) \). The \( \beta_N \) and \( \gamma_N \) 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

\[ \sum_{n'} f(nl, n') = 1, \]
\[ \sum_{n'} g(nl, n') = \delta_{l,0}. \]

The largest deviations for \( 12 \leq n \leq 20 \) were \( 4 \times 10^{-14} \) for Eq. (16) and \( 2 \times 10^{-15} \) for Eq. (17). For \( n \leq 11 \), the largest deviations were \( 8 \times 10^{-15} \) and \( 1 \times 10^{-15} \), 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 \( \pm 1 \) 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 Maquet to the number of figures they quote. The values for the 1s and 2s states verify the 14 figure results of Haywood and Morgan 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. They obtain (after adding ln2 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. Although direct calculations of the two-electron BL are difficult and have only been carried out for the ground state, 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,

$$
\ln \left[ \frac{k_0(1s,nL; 2s+1L)}{Z^2 R_\infty} \right] = \ln \left[ \frac{k_0(1s,nL)}{R_\infty} \right] - \frac{2\sigma}{Z} + O(Z^{-2})
$$

$$
= \ln \left[ \frac{k_0(1s,nL)}{Z} \right] + O(Z^{-2}),
$$

where

$$
\ln \left[ \frac{k_0(1s,nL)}{R_\infty} \right] = \ln \left[ k_0(1s)/R_\infty \right] + n^{-3} \ln \left[ k_0(nL)/R_\infty \right]
$$

is the leading term, and $\sigma$ can be expressed in terms of perturbation sums over intermediate states. Values of $\sigma$ have only been calculated for states up to $n=2$ with the results

$$
\sigma(1S) = 0.00615, \quad \sigma(1P) = -0.02040,
$$

$$
\sigma(2S) = -0.01388, \quad \sigma(2P) = -0.00600,
$$

$$
\sigma(3S) = -0.00475.
$$

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 $Z_{eff} = Z - 1$. The first corresponds to virtual excitations of the form $1s,nL \rightarrow n',nL$ and the second to virtual excitations of the form $1s,nL \rightarrow 1s,n''L \pm 1$, summed over $n'$ with $Z_{eff} = Z$ and $n''$ with $Z_{eff} = Z - 1$. 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)]

$$
\ln \left[ \frac{k_0(1s,nL)}{Z^2 R_\infty} \right] = \ln \left[ \frac{k_0(1s)}{R_\infty} \right] + \frac{1}{n^2} \left( \frac{Z-1}{Z} \right)^4 \ln \left[ \frac{k_0(nL)}{R_\infty} \right]
$$

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

$$
\sigma(nL) = (2/n^3) \ln [k_0(nL)].
$$

For the 1s2p state, this gives $\sigma(2p) = -0.0075$, 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 $\sigma(nL) \rightarrow \sigma(nL)$.

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

ACKNOWLEDGMENTS

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