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[4–9] 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[8] 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[1,15] (in atomic units)

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

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 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

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

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

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

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

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

and

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

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

n	$\ln[k_0(nl)/R_\infty]$	$\ln[k_0(nl)/R_\infty]$	$\ln[k_0(nl)/R_\infty]$	$\ln[k_0(nl)/R_\infty]$
	$l=0$			
1	2.984 128 555 765 498	$l=1$		
2	2.811 769 893 120 563	−0.030 016 708 630 213	$l=2$	
3	2.767 663 612 491 822	−0.038 190 229 385 312	−0.005 232 148 140 883	$l=3$
4	2.749 811 840 454 057	−0.041 954 894 598 086	−0.006 740 938 876 975	−0.001 733 661 482 126
5	2.740 823 727 854 572	−0.044 034 695 591 878	−0.007 600 751 257 947	−0.002 202 168 381 486
6	2.735 664 206 935 105	−0.045 312 197 688 974	−0.008 147 203 962 354	−0.002 502 179 760 279
7	2.732 429 129 187 092	−0.046 155 177 262 915	−0.008 519 223 293 658	−0.002 709 095 727 000
8	2.730 267 260 690 589	−0.046 741 352 003 557	−0.008 785 042 984 125	−0.002 859 114 559 296
9	2.728 751 166 038 614	−0.047 165 699 952 735	−0.008 982 032 293 858	−0.002 971 901 488 037
10	2.727 646 938 659 466	−0.047 482 893 356 678	−0.009 132 272 249 044	−0.003 059 094 278 891
11	2.726 817 782 527 157	−0.047 726 268 148 058	−0.009 249 570 815 264	−0.003 128 021 134 523
12	2.726 179 340 635 48	−0.047 917 111 573 660	−0.009 342 953 986 099	−0.003 183 519 098 74
13	2.725 677 290 537 02	−0.048 069 543 645 71	−0.009 418 537 646 70	−0.003 228 901 669 23
14	2.725 275 365 172 99	−0.048 193 233 848 14	−0.009 480 591 420 45	−0.003 266 508 236 62
15	2.724 948 600 408 85	−0.048 294 986 397 14	−0.009 532 172 414 71	−0.003 298 032 527 08
16	2.724 679 355 911 28	−0.048 379 702 978 99	−0.009 575 517 770 68	−0.003 324 727 300 68
17	2.724 454 879 738 29	−0.048 450 987 781 85	−0.009 612 295 977 53	−0.003 347 536 419 73
18	2.724 265 768 141 35	−0.048 511 539 184 83	−0.009 643 772 402 77	−0.003 367 182 587 53
19	2.724 104 963 270 95	−0.048 563 410 017 21	−0.009 670 921 054 36	−0.003 384 227 121 23
20	2.723 967 084 293 02	−0.048 608 184 514 61	−0.009 694 501 704 45	−0.003 399 111 574 10
	$l=4$			
5	−0.000 772 098 901 537	$l=5$		
6	−0.000 962 797 424 841	−0.000 407 926 168 297	$l=6$	
7	−0.001 094 472 739 370	−0.000 499 701 854 766	−0.000 240 908 258 717	$l=7$
8	−0.001 190 432 043 318	−0.000 566 532 724 12	−0.000 290 426 172 391	−0.000 153 864 500 961
9	−0.001 263 094 507 064	−0.000 617 234 171 18	−0.000 327 943 900 64	−0.000 182 899 145 591
10	−0.001 319 718 057 354	−0.000 656 886 016 24	−0.000 357 298 649 48	−0.000 205 584 988 395
11	−0.001 364 844 849 466	−0.000 688 630 813 03	−0.000 380 840 963 25	−0.000 223 775 429 151
12	−0.001 401 468 731 72	−0.000 714 523 500 24	−0.000 400 093 505 39	−0.000 238 662 892 56
13	−0.001 431 644 265 75	−0.000 735 967 796 62	−0.000 416 088 536 73	−0.000 251 049 857 96
14	−0.001 456 827 618 98	−0.000 753 956 638 21	−0.000 429 552 243 14	−0.000 261 497 161 38
15	−0.001 478 078 457 94	−0.000 769 212 618 49	−0.000 441 011 226 81	−0.000 270 409 332 42
16	−0.001 496 185 126 95	−0.000 782 274 102 15	−0.000 450 857 082 66	−0.000 278 085 983 83
17	−0.001 511 745 248 80	−0.000 793 550 212 75	−0.000 459 387 218 08	−0.000 284 754 032 72
18	−0.001 525 219 287 83	−0.000 803 357 162 81	−0.000 466 831 590 97	−0.000 290 588 633 45
19	−0.001 536 967 112 49	−0.000 811 942 961 68	−0.000 473 370 767 31	−0.000 295 727 206 73
20	−0.001 547 273 535 58	−0.000 819 504 641 04	−0.000 479 148 442 37	−0.000 300 279 101 37
	$l=8$			
9	−0.000 104 148 092 50	$l=9$		
10	−0.000 122 284 630 82	−0.000 073 724 978 585	$l=10$	
11	−0.000 136 808 195 63	−0.000 085 632 465 91	−0.000 054 079 265 232	$l=11$
12	−0.000 148 688 925 63	−0.000 095 361 612 93	−0.000 062 217 985 59	−0.000 040 833 679 38
13	−0.000 158 576 610 33	−0.000 103 453 844 66	−0.000 068 980 232 23	−0.000 046 584 135 94
14	−0.000 166 922 825 60	−0.000 110 284 190 41	−0.000 074 684 418 41	−0.000 051 430 308 99
15	−0.000 174 051 514 01	−0.000 116 120 527 04	−0.000 079 557 464 81	−0.000 055 567 811 06
16	−0.000 180 201 449 52	−0.000 121 159 422 12	−0.000 083 765 339 93	−0.000 059 139 490 75
17	−0.000 185 552 757 78	−0.000 125 548 542 94	−0.000 087 432 273 14	−0.000 062 252 004 58
18	−0.000 190 244 049 52	−0.000 129 401 107 87	−0.000 090 653 173 76	−0.000 064 986 598 35
19	−0.000 194 383 831 67	−0.000 132 805 476 83	−0.000 093 501 870 64	−0.000 067 406 282 41
20	−0.000 198 058 316 53	−0.000 135 831 685 02	−0.000 096 036 714 01	−0.000 069 560 713 71

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

$$B=B_N+\beta_N\zeta_N(3)+\gamma_N\zeta_N(5)\ , \tag{9}$$

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

$$C=\int_0^\infty u(\nu)d\nu\ , \tag{10}$$

with

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

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

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

C is approximated by

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

where

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

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

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

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 $N\simeq 50$ for $l=0$ and $N\simeq 20$ 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

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

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

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 Maquet[8] to the number of figures they quote. The values for the 1s and 2s states verify the 14 figure results of Haywood and Morgan[11] 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 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.[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,

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

where

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

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 results[3]

$$\sigma(1\,{}^1S)=0.006\,15,\quad \sigma(2\,{}^1S)=-0.020\,40 ,$$
$$\sigma(2\,{}^3S)=-0.013\,88,\quad \sigma(2\,{}^1P)=-0.006\,00 ,$$
$$\sigma(2\,{}^3P)=-0.004\,75 .$$

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 $1s,nL \rightarrow 1s,n''L\pm1$, 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)]

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

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

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

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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