Two–Loop Bethe Logarithms

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Abstract

We calculate the two-loop Bethe logarithm correction to atomic energy levels in hydrogen-like systems. The two-loop Bethe logarithm is a low-energy quantum electrodynamic (QED) effect involving multiple summations over virtual excited atomic states. Although much smaller in absolute magnitude than the well-known one-loop Bethe logarithm, the two-loop analog is quite significant when compared to the current experimental accuracy of the $1S$–$2S$ transition: it contributes -8.19 and -0.84 kHz for the $1S$ and the $2S$ state, respectively. The two-loop Bethe logarithm has been the largest unknown correction to the hydrogen Lamb shift to date. Together with the ongoing measurement of the proton charge radius at the Paul Scherrer Institute its calculation will bring theoretical and experimental accuracy for the Lamb shift in atomic hydrogen to the level of 10^{-7}.

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In 1947 Hans Bethe explained the splitting of $2S_{1/2}$ and $2P_{1/2}$ levels in hydrogen by the presence of electron self-interaction [1], and expressed it in terms of the "Bethe" logarithm. For S states this quantity may be represented as a matrix element involving the logarithm of the nonrelativistic Hamiltonian of the hydrogen atom. In natural units with $\hbar = c = \epsilon_0 = 1$ and m denoting the electron mass, it reads

$$\ln k_0(nS) = \frac{\left\langle \vec{p}\,(H-E)\,\ln\left[\dfrac{2(H-E)}{(Z\alpha)^2\,m}\right]\vec{p}\,\right\rangle}{\langle \vec{p}\,(H-E)\vec{p}\,\rangle}\,. \tag{1}$$

This Bethe logarithm is due to the emission and subsequent absorption of a single soft virtual photon (it is independent of the nuclear charge number Z and depends only on the principal quantum number n and the orbital angular momentum which is zero for S states). Over the years, QED theory has been developed and refined [2], and various additional radiative, relativistic, and combined corrections have been obtained to face the increasing precision of the measurements of the hydrogen spectrum [3, 4]. These include higher-order relativistic one–, two–, and three–loop corrections, nuclear recoil, finite size and even the nuclear polarizability. The modern all-order calculation of the leading one-loop self-energy was developed by Mohr in [5] and significantly improved recently using convergence acceleration techniques which led to a highly accurate evaluation of the fully relativistic Green function [6]. One of the conceptually most difficult and as well as interesting corrections involve nuclear recoil effects. The finite nuclear mass, although large as compared to the electron mass, prohibits the use of the one-body Dirac equation, and alternative approaches such as the Bethe-Salpeter equation or nonrelativistic QED [7] have been introduced. Although these methods are quite general, no compact formulas have been derived for relativistic recoil effects. A few years ago, Shabaev tackled the problem of recoil corrections to hydrogenic energy levels of first order in mass ratio, deriving expressions which are nonperturbative in the nuclear charge (see a recent review in [8]), and this has led to the current highly accurate calculations of relativistic recoil corrections.

Another class of effects, namely binding two–loop corrections, are quite difficult from a numerical point of view. A detailed investigation of these effects has been performed only in the last years. The nonperturbative treatment (no $Z\alpha$-expansion) of the two-loop bound-state corrections has been pursued by various groups in Refs. [9–12]. However, these calculations were mostly performed for high-Z hydrogen-like atoms. As yet, complete results

have not been obtained for $Z = 1$ (see for example the most recent work in [12]). In the perturbative treatment of the bound-state two-loop self-energy correction, one calculates terms in a semi-analytic expansion in $Z\alpha$ and $\ln[(Z\alpha)^{-2}]$. For S states, the first nonvanishing terms read

$$\Delta E = \left(\frac{\alpha}{\pi}\right)^2 \frac{(Z\alpha)^4}{n^3} H(Z\alpha)\, m\,, \tag{2}$$

$$\begin{aligned} H(Z\alpha) &= B_{40} + (Z\alpha)\, B_{50} + (Z\alpha)^2 \left\{ B_{63}\, \ln^3(Z\alpha)^{-2} + \right. \\ &\quad \left. B_{62}\, \ln^2(Z\alpha)^{-2} + B_{61}\, \ln(Z\alpha)^{-2} + B_{60} \right\} \\ &\quad + \ldots\,. \end{aligned} \tag{3}$$

It was a perhaps surprising result, found only a few years ago [13], that this expansion has a very slow convergence: because of the large absolute magnitude of higher-order coefficients, many terms have to be included for reliable theoretical predictions which aim to match the current experimental precision. One of the remaining unknown but relevant contributions is the two-loop Bethe logarithm, which forms the dominant part of the problematic nonlogarithmic coefficient B_{60} (note that theoretical effort in evaluating the one-loop analog of this coefficient, A_{60}, has extended over more than three decades [14–17]). The two-loop Bethe logarithm originates from the emission and absorption of two virtual soft photons. Using nonrelativistic QED one derives the following expression for this two-loop correction [18]. For convenience we set $Z = 1$, pull out a common prefactor and express remaining integrand in terms of dimensionless quantities:

$$\Delta E = \left(\frac{2\alpha}{3\pi}\right)^2 \alpha^6\, m \int_0^{\epsilon_1} \mathrm{d}\omega_1 \int_0^{\epsilon_2} \mathrm{d}\omega_2\, f(\omega_1, \omega_2)\,, \tag{4}$$

where

$$
\begin{aligned}
f(\omega_1,\omega_2) \;=\; & \omega_1\omega_2\big\{\big\langle p^i\,G(\omega_1)\,p^j\,G(\omega_1+\omega_2)\,p^i\,G(\omega_2)\,p^j\big\rangle \\
& +\big\langle p^i\,G(\omega_1)\,p^j\,G(\omega_1+\omega_2)\,p^j\,G(\omega_1)\,p^i\big\rangle/2 \\
& +\big\langle p^i\,G(\omega_2)\,p^j\,G(\omega_1+\omega_2)\,p^j\,G(\omega_2)\,p^i\big\rangle/2 \\
& +\big\langle p^i\,G(\omega_1)\,p^i\,G'(0)\,p^j\,G(\omega_2)\,p^i\big\rangle \\
& -\big\langle p^i\,G(\omega_1)\,p^i\big\rangle\,\big\langle p^j\,G^2(\omega_2)\,p^i\big\rangle/2 \\
& -\big\langle p^i\,G(\omega_2)\,p^i\big\rangle\,\big\langle p^j\,G^2(\omega_1)\,p^i\big\rangle/2 \\
& -\big\langle p^i\,G(\omega_1)\,G(\omega_2)\,p^i\big\rangle \\
& -\big\langle p^i\,[G(\omega_1)+G(\omega_2)]\,p^i\big\rangle/(\omega_1+\omega_2)\big\}\,. \qquad (5)
\end{aligned}
$$

Here, $p^k=-i\partial^k$, $G(\omega)=1/[E-(H+\omega)]$ is the nonrelativistic Green function, $E=-1/(2n^2)$ is the Schrödinger energy of the reference state with $H=\vec{p}^{\,2}/2-1/r$, and $G'(0)=1/(E-H)'$ is the reduced Green function with the reference state excluded. The ω-integrals in Eq. (4) depend on ϵ_1 and ϵ_2. We are free to choose the relation between the parameters ϵ_1 and ϵ_2. Following [18], we perform the expansion in large ϵ_2 first, and next in large ϵ_1. All the terms involving $1/\epsilon_1$ or $1/\epsilon_2$ are neglected. The linear and logarithmic terms, using the same relations, have already been considered in [18]. The dependence on the ϵ-parameters cancels when the contributions from the high- and the low-energy photons are added. The constant term, which by definition we call the two-loop Bethe logarithm, is calculated numerically here.

There are two ways to calculate the integrand in Eq. (5). The first one relies on the use of known analytic expressions for the Schrödinger-Coulomb Green function, which involve the product of Whittaker functions. The precise calculation of the ω-integrals requires the use of large ω_1 and ω_2. This leads to a number of problems, including a numerical overflow in the calculation of these functions which persists even in quadruple precision, and this approach has therefore not been pursued here. In the second way, which is chosen here, the Schrödinger Hamiltonian is represented on a numerical grid, as a large symmetric band matrix [19]. Each inversion in Eq. (5) corresponds to a solution of a linear equation with a known right-hand side. This process is quite fast since it scales linearly with the number of grid points and is numerically stable. For the final evaluation we used 10^5 grid points, and

we have checked the numerical accuracy of the results against those obtained with $2 \cdot 10^5$ grid points.

Having calculated the matrix elements, we proceed to the evaluation of the ω_1- and ω_2-integrals. In accordance with the definition of two-loop Bethe logarithm, we first fix ω_1, integrate over ω_2 and expand in large ϵ_2:

$$\begin{aligned} f(\omega_1) &= \int_0^{\epsilon_2} d\omega_2 \, f(\omega_1, \omega_2) \\ &= \epsilon_2 \, a(\omega_1) + \ln(\epsilon_2) \, b(\omega_1) + g(\omega_1) \,. \end{aligned} \tag{6}$$

As in the case of the one-loop Bethe logarithm, the g function finds a representation that is suited for a numerical computation,

$$g(\omega_1) = \mathcal{I}_1 + \mathcal{I}_2 + \mathcal{I}_3 \,, \tag{7}$$

where

$$\mathcal{I}_1 = \int_0^M \mathrm{d}\omega_2 \, f(\omega_1, \omega_2) \,, \tag{8a}$$

$$\mathcal{I}_2 = \int_M^\infty \mathrm{d}\omega_2 \, \left[f(\omega_1, \omega_2) - a(\omega_1) - \frac{b(\omega_1)}{\omega_2} \right] \,, \tag{8b}$$

$$\mathcal{I}_3 = a(\omega_1) \, M + b(\omega_1) \, \ln M \,, \tag{8c}$$

with arbitrary M. The a and b coefficients are the first terms of the expansion of $f(\omega_1, \omega_2)$ for large ω_2 at fixed ω_1,

$$\begin{aligned} f(\omega_1, \omega_2) &= a(\omega_1) + \frac{b(\omega_1)}{\omega_2} + \frac{2\sqrt{2}\, b(\omega_1)}{\omega_2^{3/2}} + \\ & \qquad c(\omega_1) \, \frac{\ln(\omega_2)}{\omega_2^2} + \frac{d(\omega_1)}{\omega_2^2} + \ldots \end{aligned} \tag{9}$$

The first coefficient is

$$a(\omega_1) = \omega_1 \, \left\langle p^i \, \frac{H - E}{(H - E + \omega_1)^2} \, p^i \right\rangle \,, \tag{10}$$

and the second reads

$$b(\omega_1) = \omega_1 \, \delta_{\pi\delta^3(r)} \left\{ \left\langle p^i \, \frac{1}{E - (H + \omega_1)} \, p^i \right\rangle \right\} \,, \tag{11}$$

TABLE I: Sample values of the g function, defined in Eq. (6), for the $1S$ and $2S$ states.

ω	g_{1S}	$8\,g_{2S}$
0	0.000 00	0.000 00
5	-10.281 60	-10.367 94
20	-16.560 34	-16.415 97
80	-22.714 02	-22.439 66
180	-26.232 35	-25.923 09
320	-28.699 64	-28.376 26
500	-30.599 22	-30.268 75
720	-32.142 95	-31.808 43

where by δ_V we denote the first-order correction to the specified matrix elements. Namely, ϕ, E, and H receive corrections according to

$$H \;\to\; H + V\,, \tag{12a}$$

$$|\phi\rangle \;\to\; |\phi\rangle + \frac{1}{(E-H)'}\,V|\phi\rangle\,, \tag{12b}$$

$$E \;\to\; E + \langle V\rangle\,. \tag{12c}$$

The higher-order coefficients $c, d, \ldots$ in Eq. (9) are obtained from the fit to the numerical data and are subsequently used for the analytic integration at large ω_2. The numerical integration over ω_2 is performed with a well adapted set of 400 grid points, and the accuracy is checked by comparison with a calculation involving 200 grid points. Results of this integration for few chosen values of ω_1 is shown in Table I. The next step is the numerical integration over ω_1,

$$\Delta E = \left(\frac{2\alpha}{3\pi}\right)^2 \alpha^6\, m \int_0^{\epsilon_1} \mathrm{d}\omega_1\, g(\omega_1)\,. \tag{13}$$

In order to perform this integration, one needs to know the large-ω_1 asymptotics of g, which

for an nS state reads,

$$
\begin{aligned}
g(\omega_1) \;=\; \Bigg\{ & -4\ln\omega_1 + 2\,[\ln 2 - 1 - \ln k_0(nS)] \\
& + \frac{4\sqrt{2}}{\sqrt{\omega_1}}\,[\ln(\omega_1) + 2\,(\ln 2 - 1) - \pi] + \\
& + \frac{1}{\omega_1}\,\left[\ln^2(\omega_1) + 8 + \frac{3}{2}\,N(nS) + 5\pi^2\right] \\
& + \mathcal{A}\,\frac{\ln^2(\omega_1)}{\omega_1^{3/2}} + \mathcal{B}\,\frac{\ln(\omega_1)}{\omega_1^{3/2}} + \mathcal{C}\,\frac{1}{\omega_1^{3/2}} \\
& + \mathcal{O}\left(\frac{1}{\omega_1^2}\right)\Bigg\}\,\frac{1}{n^3}\,. \qquad (14)
\end{aligned}
$$

Here, N denotes a nonlogarithmic in α correction to the Bethe logarithm induced by a Dirac δ. It has been calculated in [20, Eq. (12)], and the results for the $1S$ and $2S$ states read

$$N(1S) \;=\; 17.855\,672(1)\,, \qquad (15a)$$

$$N(2S) \;=\; 12.032\,209(1)\,. \qquad (15b)$$

The terms proportional to the $\mathcal{A}, \mathcal{B}, \mathcal{C}$-coefficients in Eq. (14), and the omitted higher-order terms are obtained from the fit to the calculated data. The numerical stability of the parameters obtained from the fit, in various ranges of ω_1, indicates consistency of the numerically determined values for $g(\omega_1)$ with the analytically derived logarithmic terms in Eq. (14). This constitutes a check for the large value for the coefficient B_{61} derived in [18] on the basis of the logarithmic asymptotics.

The integral in Eq. (13) is performed in analogy to the algorithm presented in Eq. (6), by choosing an arbitrary value for the parameter M (e.g., $M = 1$), and dropping all linear and logarithmic terms in ϵ_1. For ω_1 larger than 720, the extrapolated values from the fit are employed. However, this part of the integral depends significantly on the unknown analytic behavior of $g(\omega)$ at large ω, and this is the main source of the integration uncertainty. The overall result of the numerical integration leads to the following nonlogarithmic terms of the order of $(\alpha/\pi)^2\,(Z\alpha)^6/n^3$ relative to the electron rest mass, whose numerical coefficients we choose to denote by b_L,

$$b_L(1S) \;=\; -81.4(3)\,, \qquad (16a)$$

$$b_L(2S) \;=\; -66.6(3)\,. \qquad (16b)$$

These terms are much larger than the corresponding one-loop Bethe logarithms for typical hydrogenic states, but suppressed in absolute magnitude by an additional factor $\alpha\,(Z\alpha)^2/\pi$. For hydrogen ($Z = 1$), the above results contribute -8.19 and -0.84 kHz to the $1S$ and $2S$ states, respectively. The other contributions to B_{60} are considered below; the notation is consistent with that of Ref. [18]. The coefficient B_{60} can be represented as the sum

$$B_{60} = b_L + b_M + b_F + b_H + b_{\rm VP}\,. \tag{17}$$

The two-loop Bethe logarithm b_L comes from the region where both photon momenta are small and has been the subject of this work. b_M stems from an integration region where one momentum is large $\sim m$, and the second momentum is small. This contribution is given by a Dirac δ correction to the Bethe logarithm. It has already been derived in [18] but not included in the theoretical predictions for the Lamb shift:

$$b_M = \frac{10}{9}\,N(nS) \tag{18}$$

b_F and b_H originate from a region where both photon momenta are large $\sim m$, and the electron momentum is small and large respectively. Finally, $b_{\rm VP}$ is a contribution from diagrams that involve a closed fermion loop. None of these effects have been calculated as yet. On the basis of our experience with the one- and two-loop calculations [21] we estimate the magnitude of these uncalculated terms to be of the order of 15%. This leads to the following overall result for the B_{60} coefficients:

$$B_{60}(1S) \;=\; -61.6(3) \pm 15\%\,, \tag{19a}$$

$$B_{60}(2S) \;=\; -53.2(3) \pm 15\%\,, \tag{19b}$$

and to the following corrections to transition frequencies

$$\delta\nu(1S) \;=\; -6.20(93)\,\text{kHz}\,, \tag{20a}$$

$$\delta\nu(2S) \;=\; -0.67(10)\,\text{kHz}\,. \tag{20b}$$

In the foreseeable future, we may expect to have results from a direct numerical calculation of the two-loop self-energy at low Z. In addition to improving our knowledge of the Lamb shift at low Z, the obtained result will then serve as a consistency check between two different approaches to bound-state QED.

With the results obtained in Eqs. (19a,19b) we are in a position to present theoretical predictions for the Lamb shifts of $1S$ and $2S$ states. Based on the former result obtained in [18] and the corrections calculated in this work, we obtain:

$$\nu_L(1S) \;=\; 8\,172\,811(32)(2)\,\mathrm{kHz}\,, \tag{21a}$$

$$\nu_L(2S) \;=\; 1\,045\,005(4)\,\mathrm{kHz}\,, \tag{21b}$$

where the first error comes from the current uncertainty in the proton charge radius r_p, and the second one is a rough estimate of uncalculated terms: b_H, b_{VP}, as well as higher-order two-loop corrections denoted by dots in Eq. (3), and the three-loop binding correction C_{50} (for a recent evaluation of C_{40} see Ref. [22]). Theoretical predictions for the $1S$ state agree well with the experimental value of the combined result from the Garching and the Paris groups [3, 4]:

$$\nu_L(1S)_{\mathrm{exp}} = 8\,172\,837(22)\,\mathrm{kHz}\,. \tag{22}$$

Since the uncertainty coming from the proton structure dominates theoretical uncertainties for the Lamb shift in hydrogen, an experiment at the Paul Scherrer Institute (PSI) is currently being pursued with the purpose of a precise measurement of r_p from the Lamb shift in muonic hydrogen [23]. This system is much more sensitive to the proton charge radius. Once it is measured, the combined hydrogen and muonic Lamb shift will test QED at a precision level of 10^{-7}.

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[1] H. A. Bethe, Phys. Rev. A **72**, 339 (1947).

[2] M.I. Eides, H. Grotch, and V.A. Shelyuto, Phys. Rep. **342**, 63 (2001).

[3] Th. Udem *et al.*, Phys. Rev. Lett. **79**, 2646 (1997).

[4] C. Schwob *et al.*, Phys. Rev. Lett. **82**, 4960 (1999).

[5] P. J. Mohr, Ann. Phys. (N.Y) **88**, 26, 52 (1974).

[6] U. D. Jentschura, P. J. Mohr, and G. Soff, Phys. Rev. Lett. **82**, 53 (1999).

[7] W. E. Caswell and G. P. Lepage, Phys. Lett. B **167**, 437 (1986).

[8] V. M. Shabaev, Phys. Rev. A **57**, 59 (1998).

[9] H. Person *et al.*, Phys. Rev. A **54**, 2805 (1996).

[10] S. Mallampalli and J. Sapirstein, Phys. Rev. Lett. **80**, 5297 (1998); Phys. Rev. A **57**, 1548 (1998).

[11] I. Goidenko *et al.*, Phys. Rev. Lett. **83**, 2312 (1999).

[12] V.A. Yerokhin, P. Indelicato, and V.M. Shabaev, e-print hep-ph/0302268 (2003).

[13] K. Pachucki, Phys. Rev. Lett. **72**, 3154 (1994).

[14] G. W. Erickson and D. R. Yennie, Ann. Phys. (N.Y.) **35**, 271, 447 (1965).

[15] G. W. Erickson, Phys. Rev. Lett. **27**, 780 (1971).

[16] J. Sapirstein, Phys. Rev. Lett. **47**, 1723 (1981).

[17] K. Pachucki, Ann. Phys. (N.Y.) **226**, 1 (1993).

[18] K. Pachucki, Phys. Rev. A **63**, 042503 (2001).

[19] S. Salomonson and P. Öster, Phys. Rev. A **40**, 5559 (1989).

[20] U.D. Jentschura, J. Phys. A **36**, L229 (2003).

[21] Concerning logarithmic two-loop vacuum-polarization effects [18]: The contribution of the two-loop self-energy diagrams to B_{61} for the $1S$ state reads 49.7, and the diagrams that involve a closed fermion loop amount to 0.6. Concerning the one-loop higher-order binding correction $A_{60}(1S)$ (analog of B_{60}) as an example: The result for $1S$ is $-30.92415(1)$ (see Refs. [6, 17]). This is the sum of a contribution due to low-energy virtual photons of -27.3 [17, Eq. (5.116)], and a high-energy term of about -3.7 [17, Eq. (6.102)].

[22] K. Melnikov and T. v. Ritbergen, Phys. Rev. Lett. **84**, 1673 (2000).

[23] F. Kottmann *et al.*, Hyp. Int. **138**, 55 (2001).