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Asymptotic Properties of Self-Energy Coefficients

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We investigate the asymptotic properties of higher-order binding corrections to the one-loop self-energy of excited states in atomic hydrogen. We evaluate the historically problematic A_{60} coefficient for all P states with principal quantum numbers $n \leq 7$ and D states with $n \leq 8$ and find that a satisfactory representation of the n dependence of the coefficients requires a three-parameter fit. For the high-energy contribution to A_{60}, we find exact formulas. The results obtained are relevant for the interpretation of high-precision laser spectroscopic measurements.

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Bound-state quantum electrodynamics (QED) occupies a unique position in theoretical physics in that it combines all conceptual intricacies of modern quantum field theories, augmented by the peculiarities of bound states, with the experimental possibilities of ultrahigh resolution laser spectroscopy. Calculations in this area have a long history, and the current status of theoretical predictions is the result of continuous effort. The purpose of this Letter is twofold: first, to present improved evaluations of higher-order binding corrections to the bound-state self-energy for a large number of atomic states, including highly excited states with a principal quantum number as high as $n = 8$, and second, to analyze the asymptotic dependence of the analytic results on the bound-state quantum numbers. Highly excited states (e.g., with $n = 4$ to 12) are of particular importance for high-precision spectroscopy experiments in hydrogen (for a summary, see for instance, [1]).

In the analytic calculations, we focus on a specific higher-order binding correction, known as the A_{60} coefficient or "relativistic Bethe logarithm." We write the (real part of the) one-loop self-energy shift of an electron in the field of a nucleus of charge number Z as

$$\Delta E_{\mathrm{SE}} = \frac{\alpha}{\pi}\frac{(Z\alpha)^4}{n^3} F(nl_j, Z\alpha) mc^2, \tag{1}$$

where $F(nl_j, Z\alpha)$ is a dimensionless quantity. In this Letter, we use natural units with $\hbar = c = m = 1$ and $e^2 = 4\pi\alpha$ (m is the electron mass). The notation nl_j is inspired by the usual spectroscopic nomenclature: n is the level number, j is the total angular momentum, and l is the orbital angular momentum.

The semianalytic expansion of $F(nl_j, Z\alpha)$ about $Z\alpha = 0$ for a general atomic state with quantum numbers n, $l \geq 1$, and j gives rise to the expression,

$$F(nl_j, Z\alpha) = A_{40}(nl_j) + (Z\alpha)^2[A_{61}(nl_j)\ln(Z\alpha)^{-2} + G_{\mathrm{SE}}(nl_j, Z\alpha)] \qquad (l \geq 0), \tag{2}$$

where $G_{\mathrm{SE}}(nl_j, Z\alpha) \to \text{const}$ as $Z\alpha \to 0$. The limit as $Z\alpha \to 0$ of $G_{\mathrm{SE}}(nl_j, Z\alpha)$ is referred to as the A_{60} coefficient, i.e.,

$$A_{60}(nl_j) = \lim_{Z\alpha\to 0} G_{\mathrm{SE}}(nl_j, Z\alpha). \tag{3}$$

It is this coefficient which has proven to be by far the most difficult to evaluate [2–7]. Furthermore, the complexity of the calculation increases sharply with increasing principal quantum number n, both due to the more involved structure of the bound-state wave function (see also Fig. 1), and due to the necessity of subtracting bound-state poles that lie infinitesimally close to the photon integration contour. The atomic states with the highest n for which analytic results are available today are the $4P$ states [9]. In this Letter, we present analytic data for the A_{60} coefficient of P states with $n \leq 7$ and all D states with $n \leq 8$. For a given n, the calculation is more involved for nP than for nD, because there is one more term in the nonrelativistic radial nP wave function than in the corresponding nD wave function (when they are expressed as a function of the electron-nucleus distance). Essentially, the number of terms in the radial wave function determines the complexity of the calculation.

One of the most demanding specific calculations in the evaluation of A_{60} is necessitated by a Bethe-logarithm-type contribution given by the relativistic wave-function correction $F_{\delta\phi}$; this contribution is defined in Eqs. (43) and (53) of [8]. For $7P$ and $8D$ states, we use up to 200 000 terms in intermediate steps in the evaluation of this correction. Because A_{60} involves relativistic corrections to the coefficient A_{40}, which in turn is given mainly by the Bethe logarithm, it is natural to refer to the entire A_{60} coefficient as a relativistic Bethe logarithm.

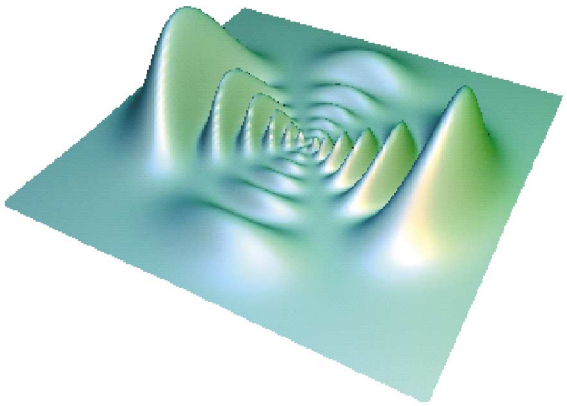

FIG. 1 (color online). Plot of the radial probability density $r^2|\psi(r,\theta,\phi)|^2$ of the nonrelativistic $8D$ wave function (angular momentum projection $m = 0$) in the plane of constant azimuth $\phi = 0$. The calculation of the relativistic Bethe logarithm A_{60} starts from this nonrelativistic wave function, with relativistic corrections being taken into account via generalized Foldy-Wouthuysen transformations [8,9].

The "normal Bethe logarithm" $\ln k_0(nl)$ forms part of the coefficient A_{40} for which a well-known general formula (see, e.g., Ref. [1]) reads

$$A_{40}(nl_j) = -\frac{1}{2\kappa(2l+1)} - \frac{4}{3}\ln k_0(nl), \tag{4}$$

where $\kappa = 2(l-j)(j+1/2)$. Formulas for A_{61} valid for P and D states read as follows (see, e.g., Ref. [1]):

$$A_{61}(nP_{1/2}) = \frac{1}{45}\left(33 - \frac{29}{n^2}\right), \tag{5}$$

$$A_{61}(nP_{3/2}) = \frac{2}{45}\left(9 - \frac{7}{n^2}\right), \tag{6}$$

$$A_{61}(nl_j) = \frac{32\left(3 - \frac{l(l+1)}{n^2}\right)}{3\prod_{m=-1}^{3}(2l+m)} \qquad (l \geq 2). \tag{7}$$

Note that $A_{61}(nl_j) \to \text{const}$ for $n \to \infty$ at constant l and j. It is the purpose of this Letter to present new results for the A_{60} coefficients. Details of our calculations will be presented in a forthcoming article [10]. It has been observed previously by Karshenboim [11] that the n dependence of the $A_{60}(nP)$ coefficients can be fitted to a satisfactory accuracy by an $(n^2-1)/n^2$-type model, and a two-parameter fit has been employed for the n dependence of the S-state coefficients $A_{60}(nS_{1/2})$ [12]. Our data for P states in Table I are roughly consistent with this $(n^2-1)/n^2$ model.

For the atomic states under investigation, the self-energy contribution due to hard virtual photons (high-energy part) obtained by the ϵ method [6,8–10] is

$$F_H(nl_j, Z\alpha) = -\frac{1}{2\kappa(2l+1)} + (Z\alpha)^2 \times \left[\mathcal{K} - \frac{C}{\epsilon} - A_{61}\ln(2\epsilon) + \mathcal{O}(\epsilon)\right] + \cdots. \tag{8}$$

The ellipsis denotes higher-order terms, which are irrelevant for the current investigation. In Eq. (8), $\mathcal{K}$ and C, as well as A_{61}, are state-dependent coefficients. For concrete evaluations of the high-energy part concerning specific atomic states, see Eqs. (18) and (19) of [8] and Eqs. (55)–(58) of [9]. The low-energy part assumes the form

$$F_L(nl_j, Z\alpha) = -\frac{4}{3}\ln k_0(nl) + (Z\alpha)^2 \times \left[\mathcal{L} + \frac{C}{\epsilon} + A_{61}\ln\left(\frac{\epsilon}{(Z\alpha)^2}\right) + \mathcal{O}(\epsilon)\right], \tag{9}$$

TABLE I. A_{60} coefficients for $P_{1/2}$, $P_{3/2}$, $D_{3/2}$, and $D_{5/2}$ states ($n = 2, \ldots, 7$ for P states, and $n = 3, \ldots, 8$ for D). The quantity $\mathcal{L}$ is implicitly defined in Eq. (9) and represents the low-energy contribution to A_{60}.

n	$A_{60}(nP_{1/2})$	$\mathcal{L}(nP_{1/2})$	$A_{60}(nP_{3/2})$	$\mathcal{L}(nP_{3/2})$
2	−0.998 904 402(1)	−0.795 649 812(1)	−0.503 373 464(1)	−0.584 516 780(1)
3	−1.148 189 956(1)[a]	−0.944 288 447(1)	−0.597 569 388(1)	−0.693 566 427(1)
4	−1.195 688 142(1)	−0.997 810 211(1)	−0.630 945 796(1)	−0.730 579 137(1)
5	−1.216 224 512(1)	−1.023 991 781(1)	−0.647 013 509(1)	−0.747 615 653(1)
6	−1.226 702 391(1)	−1.039 079 399(1)	−0.656 154 893(1)	−0.756 897 499(1)
7	−1.232 715 957(1)	−1.048 800 134(1)	−0.662 027 568(1)	−0.762 622 956(1)
n	$A_{60}(nD_{3/2})$	$\mathcal{L}(nD_{3/2})$	$A_{60}(nD_{5/2})$	$\mathcal{L}(nD_{5/2})$
3	0.005 551 575(1)	0.021 250 354(1)	0.027 609 989(1)	0.019 188 397(1)
4	0.005 585 985(1)	0.022 882 528(1)	0.031 411 862(1)	0.020 710 720(1)
5	0.006 152 175(1)	0.023 759 683(1)	0.033 077 571(1)	0.021 511 798(1)
6	0.006 749 745(1)	0.024 294 690(1)	0.033 908 493(1)	0.021 975 925(1)
7	0.007 277 403(1)	0.024 645 479(1)	0.034 355 926(1)	0.022 264 036(1)
8	0.007 723 850(1)	0.024 886 986(1)	0.034 607 492(1)	0.022 452 259(1)

[a]We take the opportunity to correct a computational error for this result as previously reported in Ref. [9], where a value of −1.14768(1) was given.

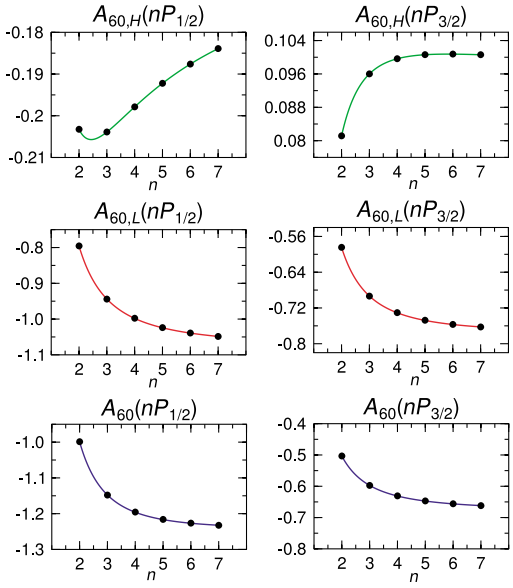

FIG. 2 (color online). The plots show the dependence on the principal quantum number n of the high- and low-energy parts of the A_{60} self-energy coefficient, as well as their sum (A_{60}). The curves for the high-energy contribution $A_{60,H}$ represent the exact results (5)–(7), (11), and (12), with n being generalized to a continuous variable (only integer n values have physical significance). The smooth curves for the low-energy parts $A_{60,L} = \mathcal{L}$ result from a three-parameter fit of the data in Table I to the function in (13); the fit parameters are given in Table II. The curves in the lower row represent the total result for $A_{60} = A_{60,H} + A_{60,L}$.

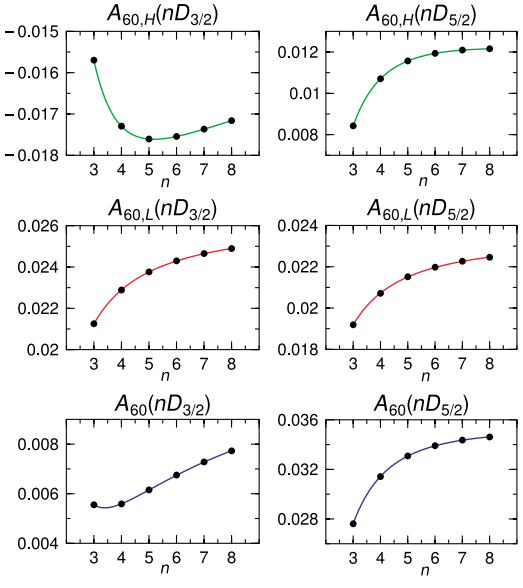

FIG. 3 (color online). The analog of Fig. 2 for $D_{3/2}$ and $D_{5/2}$ states. The minimum in $A_{60,H}(nD_{3/2})$ near $n = 5$ is determined by the exact formulas (7) and (12c).

where we omit terms that are irrelevant at relative order $(Z\alpha)^2$ in the evaluation of $F(nl_j, Z\alpha)$. A detailed explanation of the ϵ method will be given in [10]. The dependence on C cancels when the high- and low-energy parts are added. Specifically, we have

$$A_{60} = \mathcal{K} - A_{61}\ln 2 + \mathcal{L}. \tag{10}$$

Upon inspection of (8) and (9), we identify

$$A_{60,H} = \mathcal{K} - A_{61}\ln 2 \tag{11}$$

as the high-energy contribution to A_{60}, and $A_{60,L} = \mathcal{L}$ as the low-energy contribution (see Figs. 2 and 3).

We obtain the following general formulas for $\mathcal{K}$:

$$\mathcal{K}(nP_{1/2}) = \frac{637}{1800} - \frac{1}{4n} - \frac{767}{5400n^2}, \tag{12a}$$

$$\mathcal{K}(nP_{3/2}) = \frac{2683}{7200} + \frac{1}{16n} - \frac{2147}{5400n^2}, \tag{12b}$$

$$\mathcal{K}(nD_{3/2}) = -\frac{157}{30\,240} - \frac{3}{80n} + \frac{3007}{37\,800n^2}, \tag{12c}$$

$$\mathcal{K}(nD_{5/2}) = \frac{379}{18\,900} + \frac{1}{60n} - \frac{1759}{18\,900n^2}. \tag{12d}$$

All of these formulas are consistent with a limit $\mathcal{K} \to$ const as $n \to \infty$ for constant l and j. The n dependence of the nonrelativistic $\mathcal{L}(nl_j)$ contributions as listed in Table I can be approximated very well using a three-parameter fit inspired by the above structure found for the high-energy $\mathcal{K}$ contributions. We find

$$\mathcal{L}(nl_j) \approx L_1(l_j) + \frac{L_2(l_j)}{n} + \frac{L_3(l_j)}{n^2}, \tag{13}$$

where L_1, L_2, and L_3 assume values as listed in Table II for the series of states under investigation. The n dependence of the low-energy contributions $\mathcal{L}$ is smoother than the corresponding curves for the high-energy part (see Figs. 2 and 3). The excellent agreement of the fits with the numerical values of $A_{60,L}$, together with our exact results for the high-energy part as given by Eqs. (5)–(7), (11), and (12), could suggest a constant limit of $A_{60}(nl_j)$ as $n \to \infty$ for constant l and j.

For Rydberg states with the highest l possible for given n (i.e., $l = \bar{l} = n - 1$), our results are consistent with

$$\lim_{n\to\infty} A_{60}(n\bar{l}_j) = 0 \quad \text{for } \bar{l} = n - 1,\ j = n - 1 \pm 1/2, \tag{14}$$

which is plausible to suggest as a conjecture. The conjecture is indicated by the trend in the numbers ($j = \bar{l} - 1/2$): $A_{60}(3D_{3/2}) = 0.005\,551\,573(1)$, $A_{60}(4F_{5/2}) = 0.002\,326\,988(1)$, $A_{60}(5G_{7/2}) = 0.000\,814\,415(1)$; as well as in the results ($j = \bar{l} + 1/2$): $A_{60}(3D_{5/2}) = 0.027\,609\,989(1)$, $A_{60}(4F_{7/2}) = 0.007\,074\,961(1)$, $A_{60}(5G_{9/2}) = 0.002\,412\,929(1)$. The magnitude of $A_{60}(n\bar{l}_j)$ appears to decrease faster than $1/n$. In general, relativistic corrections acquire at least one more inverse power of n when $n = l + 1$, $j = n - 1 \pm 1/2$, and n large, than S or P states of the same n. This can, for

TABLE II. Coefficients L_1, L_2, and L_3 that result from a least-squares fit of the n dependence of our data for $\mathcal{L}$ in Table I (see also Figs. 2 and 3). The value of L_1 from this global fit should approximate the limit $\lim_{n\to\infty}\mathcal{L}(nl_j)$ in Eq. (13), although it is not necessarily the best estimate.

State	L_1	L_2	L_3
$P_{1/2}$	−1.082	0.0966	0.950
$P_{3/2}$	−0.775	−0.0232	0.811
$D_{3/2}$	0.0264	−0.00952	−0.0175
$D_{5/2}$	0.0235	−0.00568	−0.0220

example, be seen in the relativistic correction of order $(Z\alpha)^4$ to the Schrödinger-Coulomb electron energy [Eqs. (2)–(87) of [13]],

$$E_{nj} = m - \frac{(Z\alpha)^2 m}{2n^2} - \frac{(Z\alpha)^4 m}{n^3}\left[\frac{1}{2j+1} + \frac{3}{8n}\right] + \mathcal{O}[(Z\alpha)^6].$$

For $j = n - 1 \pm 1/2$, this relativistic term acquires an additional inverse power of n. Our results suggest that analogous statements hold for radiative corrections given by relativistic Bethe logarithms.

We have presented results of a calculation of higher-order binding corrections to the one-loop self-energy for highly excited hydrogenic atomic levels (see Table I). Calculational difficulties induced by the more complex analytic structure of the wave functions have been a severe obstacle for evaluations of relativistic Bethe logarithms at high n, and no prior results are available for A_{60} for any state with $n > 4$ (see Ref. [9]). Intermediate expressions contained up to 200 000 terms; without a computer, this work would have been impractical. Our calculation is split into a high- and a low-energy part. We find that the dependence of the low-energy contribution to A_{60} on the principal quantum number of the atomic state under investigation can in many cases be represented accurately using a three-parameter fit [see Eq. (13) and the data in Table II]. As suggested by the exact formulas for the high-energy part given in Eq. (12) and the curves in Figs. 2 and 3, a fit with less than three parameters cannot be assumed to lead to a satisfactory representation of A_{60}. Our final results for A_{60} are given in Table I. We establish that the magnitude of A_{60} decreases rapidly for Rydberg states with the highest possible angular momentum for each principal quantum number. Our calculations improve the knowledge of the self-energy of an electron bound to a nucleus [see Eqs. (1)–(3) and Table I]. They are motivated by the dramatically increasing precision of laser spectroscopy [14–17], which is rapidly approaching the 1 Hz level of accuracy. For the determination of fundamental constants from high-resolution spectroscopy, frequency measurements of at least two different transitions have to be performed. Highly excited, slowly decaying D states are attractive because they can be excited out of S states via two-photon resonance [1,14].

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[1] P. J. Mohr and B. N. Taylor, Rev. Mod. Phys. **72**, 351 (2000).
[2] G. W. Erickson and D. R. Yennie, Ann. Phys. (N.Y.) **35**, 271 (1965).
[3] G. W. Erickson and D. R. Yennie, Ann. Phys. (N.Y.) **35**, 447 (1965).
[4] G. W. Erickson, Phys. Rev. Lett. **27**, 780 (1971).
[5] J. Sapirstein, Phys. Rev. Lett. **47**, 1723 (1981).
[6] K. Pachucki, Ann. Phys. (N.Y.) **226**, 1 (1993).
[7] U. D. Jentschura, P. J. Mohr, and G. Soff, Phys. Rev. Lett. **82**, 53 (1999).
[8] U. Jentschura and K. Pachucki, Phys. Rev. A **54**, 1853 (1996).
[9] U. D. Jentschura, G. Soff, and P. J. Mohr, Phys. Rev. A **56**, 1739 (1997).
[10] E.-O. Le Bigot, U. D. Jentschura, P. J. Mohr, P. Indelicato, and G. Soff (to be published).
[11] S. G. Karshenboim (private communication).
[12] S. G. Karshenboim, Z. Phys. D **39**, 109 (1997).
[13] C. Itzykson and J. B. Zuber, *Quantum Field Theory* (McGraw-Hill, New York, 1980).
[14] B. de Beauvoir, F. Nez, L. Julien, B. Cagnac, F. Biraben, D. Touahri, L. Hilico, O. Acef, A. Clairon, and J. J. Zondy, Phys. Rev. Lett. **78**, 440 (1997).
[15] C. Schwob, L. Jozefowski, B. de Beauvoir, L. Hilico, F. Nez, L. Julien, F. Biraben, O. Acef, J.-J. Zondy, and A. Clairon, Phys. Rev. Lett. **82**, 4960 (1999); **86**, 4193(E) (2001).
[16] J. Reichert, M. Niering, R. Holzwarth, M. Weitz, T. Udem, and T. W. Hänsch, Phys. Rev. Lett. **84**, 3232 (2000).
[17] M. Niering, R. Holzwarth, J. Reichert, P. Pokasov, T. Udem, M. Weitz, T. W. Hänsch, P. Lemonde, G. Santarelli, M. Abgrall, P. Laurent, C. Salomon, and A. Clairon, Phys. Rev. Lett. **84**, 5496 (2000).