Precise theory of levels of hydrogen and deuterium: The one-photon self energy correction

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The one-photon self energy is the dominant quantum electrodynamic correction to the energy levels of hydrogen and deuterium atoms. Calculations of this correction are surveyed, and numerical values, based on extrapolations from higher values of the charge of the nucleus and plausible approximations, are provided for states with $n \leq 200$. The results of an evaluation of the energy levels and transition frequencies in hydrogen and deuterium, based on values of the self energy given here, are available on the NIST Physics Laboratory Web site at physics.nist.gov/hdel.

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I. INTRODUCTION

Energy levels in hydrogen and deuterium are determined primarily by the eigenvalues of the Dirac equation, but to obtain accurate values for the levels, it is necessary to include many additional corrections including those due to quantum electrodynamic (QED) effects. In hydrogen and deuterium, the largest QED effect is the self-energy, due to the emission and reabsorption of a virtual photon by the electron.

II. SELF ENERGY

The level shift due to the one-photon self energy is given by

$$E^{(2)}_{\rm SE} = \frac{\alpha}{\pi}\frac{(Z\alpha)^4}{n^3} F(Z\alpha)\, m_{\rm e}c^2 \,, \tag{1}$$

where

$$\begin{aligned} F(Z\alpha) \;=\; & A_{41}\ln(Z\alpha)^{-2} + A_{40} + A_{50}\,(Z\alpha) \\ & + A_{62}\,(Z\alpha)^2\ln^2(Z\alpha)^{-2} + A_{61}\,(Z\alpha)^2\ln(Z\alpha)^{-2} \\ & + G_{\rm SE}(Z\alpha)\,(Z\alpha)^2 \,, \end{aligned} \tag{2}$$

with [1]

$$\begin{aligned} A_{41} \;=\; & \frac{4}{3}\,\delta_{l0} \\ A_{40} \;=\; & -\frac{4}{3}\ln k_0(n,l) + \frac{10}{9}\,\delta_{l0} - \frac{1}{2\kappa(2l+1)}(1-\delta_{l0}) \\ A_{50} \;=\; & \left(\frac{139}{32} - 2\ln 2\right)\pi\,\delta_{l0} \\ A_{62} \;=\; & -\delta_{l0} \\ A_{61} \;=\; & \left[4\left(1+\frac{1}{2}+\cdots+\frac{1}{n}\right) + \frac{28}{3}\ln 2 - 4\ln n \right. \\ & \left. - \frac{601}{180} - \frac{77}{45n^2}\right]\delta_{l0} + \left(1-\frac{1}{n^2}\right)\left(\frac{2}{15} + \frac{1}{3}\delta_{j\frac{1}{2}}\right)\delta_{l1} \\ & + \frac{96n^2 - 32l(l+1)}{3n^2(2l-1)(2l)(2l+1)(2l+2)(2l+3)}(1-\delta_{l0}) \,. \end{aligned} \tag{3}$$

In Eqs. (1)–(3), n is the principal quantum number of the state, κ is the Dirac angular momentum-parity quantum number, $l = |\kappa + \frac{1}{2}| - \frac{1}{2}$ is the nonrelativistic angular momentum, and $j = |\kappa| + \frac{1}{2}$ is the total angular momentum. Bethe logarithms $\ln k_0(n,l)$ that appear in Eq. (3) needed for this work are given in an accompanying paper.

III. THE COEFFICIENT A_{60}

The next coefficient in the series in Eq. (2) is A_{60}, which is given by

$$\lim_{Z\alpha\to 0} G_{\rm SE}(Z\alpha) = A_{60} \tag{4}$$

There is a long history of calculations of A_{60} [2, 3], leading up to the most accurate values of A_{60} for the 1S and 2S states [4]. These values are given in Tables I and II, along with the results of subsequent calculations for states with higher angular momentum. The references for the data in Tables I and II are listed in Table III.

Asymptotic formulas for A_{60} for the P and D states for values of n higher than those in Table I are given in Ref [9] as

$$\begin{aligned} A_{60}(\mathrm{P}_{1/2}) \;=\; & -1.249(9) + \frac{0.0(2)}{n} + \frac{0.87(45)}{n^2} + \cdots \\ A_{60}(\mathrm{P}_{3/2}) \;=\; & -0.69(2) + \frac{0.15(5)}{n} + \frac{0.25(25)}{n^2} + \cdots \\ A_{60}(\mathrm{D}_{3/2}) \;=\; & 0.011(1) - \frac{0.032(7)}{n} - \frac{0.05(9)}{n^2} + \cdots \\ A_{60}(\mathrm{D}_{5/2}) \;=\; & 0.034(2) + \frac{0.025(5)}{n} - \frac{0.18(4)}{n^2} + \cdots \end{aligned} \tag{5}$$

TABLE I: Calculated values of the constant A_{60} for S, P, and D states.

n	$S_{1/2}$	$P_{1/2}$	$P_{3/2}$	$D_{3/2}$	$D_{5/2}$
1	−30.924 15(1)				
2	−31.840 47(1)	−0.998 904 402(1)	−0.503 373 464(1)		
3		−1.148 189 956(1)	−0.597 569 388(1)	0.005 551 575(1)	0.027 609 989(1)
4		−1.195 688 142(1)	−0.630 945 796(1)	0.005 585 985(1)	0.031 411 862(1)
5		−1.216 224 512(1)	−0.647 013 509(1)	0.006 152 175(1)	0.033 077 571(1)
6		−1.226 702 391(1)	−0.656 154 893(1)	0.006 749 745(1)	0.033 908 493(1)
7		−1.232 715 957(1)	−0.662 027 568(1)	0.007 277 403(1)	0.034 355 926(1)
8				0.007 723 850(1)	0.034 607 492(1)

TABLE II: Calculated values of the constant A_{60} for F and G states.

n	$F_{5/2}$	$F_{7/2}$	$G_{7/2}$	$G_{9/2}$
4	0.002 326 988(1)	0.007 074 961(1)		
5	0.002 403 158(1)	0.008 087 020(1)	0.000 814 415(1)	0.002 412 929(1)

TABLE III: References for calculations of the coefficient A_{60}.

States	Reference
$1S_{1/2}$, $2S_{1/2}$	Pachucki [4, 5]
$2P_{1/2}$, $2P_{3/2}$	Jentschura and Pachucki [6]
$3P_{1/2}$-$4P_{1/2}$, $3P_{3/2}$-$4P_{3/2}$	Jentschura et al. [7]
$2P_{1/2}$-$7P_{1/2}$, $2P_{3/2}$-$7P_{3/2}$	Jentschura et al. [8]
$3D_{3/2}$-$8D_{3/2}$, $3D_{5/2}$-$8D_{5/2}$	Jentschura et al. [8]
$4F_{5/2}$-$5F_{5/2}$, $4F_{7/2}$-$5F_{7/2}$	Le Bigot et al. [9]
$5G_{7/2}$, $5G_{9/2}$	Le Bigot et al. [9]

TABLE IV: Values of the constant A_{60} for P and D states given by Eq. (5).

n	$P_{1/2}$	$P_{3/2}$	$D_{3/2}$	$D_{5/2}$
5	−1.21(5)	−0.65(3)	0.003(9)	0.032(8)
6	−1.22(4)	−0.66(2)	0.004(5)	0.033(5)
7	−1.23(3)	−0.66(2)	0.005(4)	0.034(4)
8	−1.24(3)	−0.67(2)	0.006(3)	0.034(3)
9	−1.24(2)	−0.67(2)	0.007(2)	0.035(3)
10	−1.24(2)	−0.67(2)	0.007(2)	0.035(2)
11	−1.24(2)	−0.67(2)	0.008(2)	0.035(2)
12	−1.24(2)	−0.68(2)	0.008(1)	0.035(2)
13	−1.24(2)	−0.68(2)	0.008(1)	0.035(2)
14	−1.24(2)	−0.68(2)	0.008(1)	0.035(2)
15	−1.25(2)	−0.68(2)	0.009(1)	0.035(2)

These expansions are obtained by making numerical extrapolations of the data in Table I. Numerical results given by the asymptotic formulas are listed in Table IV. The numbers in that table include a component of uncertainty of $1/n^3$ to account for the omitted higher order terms in Eq. (5). The values of A_{60} provide a first approximation to the remainder function $G_{\rm SE}(Z\alpha)$ in the cases where it has not been calculated numerically.

IV. THE REMAINDER FUNCTION $G_{\rm SE}(Z\alpha)$

The function $G_{\rm SE}(Z\alpha)$ in Eq. (2) gives the complete remainder of the self energy. Values for $G_{\rm SE}(\alpha)$ used in the 2002 least-squares adjustment of the fundamental constants are listed in Table V [10]. In that table, the values for states with $n = 1$ and $n = 2$ are based on direct numerical evaluations [11, 12]. More recently an evaluation for the 3S and 4S states has been done with the results [13]

$$G_{\rm SE}(\alpha) = -31.047\,7(9) \qquad \text{3S state} \tag{6}$$

$$G_{\rm SE}(\alpha) = -30.912(4) \qquad \text{4S state} \tag{7}$$

These results are consistent with the values in Table V, however they are not used in the current work in order to maintain consistency of the results with the values of the fundamental constants determined in the 2002 adjustment.

The values of $G_{\rm SE}(\alpha)$ for higher-n states are based on the low-Z limit of this function, $G_{\rm SE}(0) = A_{60}$, in the cases where it is known, together with extrapolations of the results of complete numerical calculations of $F(Z\alpha)$ [see Eq. (2)] at higher Z [9, 14]. Extensive numerical evaluations of $F(Z\alpha)$ at higher Z provide information for the determination of $G_{\rm SE}(Z\alpha)$ [15–18].

For this work, Table V is extended to all states with $n \le 200$. Table VI gives a partial listing of the larger set of values for S, P, and D states, based on updated extrapolations of numerical calculations and calculated and estimated values of the coefficient A_{60}. The values in Table VI are used in the present calculation, unless results are available from Table V, in which case, the latter values are employed in order maintain consistency with the 2002 least-squares adjustment.

For S states with $n \ge 13$, we employ an approximate extrapolation given by

$$G_{\rm SE}(\alpha) = -30.7 - \frac{0.7}{n} \pm 0.2, \tag{8}$$

TABLE V: Values of the function $G_{\rm SE}(\alpha)$ used in the 2002 least-squares adjustment of the fundamental constants.

n	$S_{1/2}$	$P_{1/2}$	$P_{3/2}$	$D_{3/2}$	$D_{5/2}$
1	−30.290 24(2)				
2	−31.185 15(9)	−0.973 5(2)	−0.486 5(2)		
3	−31.01(6)				
4	−30.87(5)	−1.165(2)	−0.611(2)		0.031(1)
6	−30.82(8)				0.034(2)
8	−30.80(9)			0.008(5)	0.034(2)
12				0.009(5)	0.035(2)

TABLE VI: Enlarged table of values of the function $G_{\rm SE}(\alpha)$.

n	$S_{1/2}$	$P_{1/2}$	$P_{3/2}$	$D_{3/2}$	$D_{5/2}$
1	−30.290 24(2)				
2	−31.185 15(9)	−0.973 5(2)	−0.486 5(2)		
3	−31.047 7(9)	−1.118(2)	−0.578(2)	0.005 73(15)	0.027 79(18)
4	−30.912(4)	−1.165(2)	−0.608(2)	0.005 80(9)	0.031 63(22)
5	−30.80(10)	−1.183(3)	−0.625(2)	0.006 37(9)	0.033 32(25)
6	−30.80(10)	−1.193(3)	−0.634(2)	0.006 97(9)	0.034 17(26)
7	−30.79(10)	−1.199(3)	−0.640(2)	0.007 50(9)	0.034 57(22)
8	−30.78(10)	−1.22(5)	−0.65(3)	0.007 94(9)	0.034 84(22)
9	−30.78(15)	−1.22(5)	−0.65(3)	0.008(2)	0.035(3)
10	−30.77(15)	−1.22(5)	−0.65(3)	0.008(2)	0.035(3)
11	−30.77(15)	−1.22(5)	−0.65(3)	0.008(2)	0.035(3)
12	−30.76(15)	−1.22(5)	−0.65(3)	0.008(2)	0.035(3)

and for P and D states with $n \geq 13$, we employ the approximation

$$G_{\rm SE}(\alpha) = A_{60} \pm \Delta, \tag{9}$$

where A_{60} is the value given by Eq. (5), including the uncertainty indicated there, with an additional contribution to the uncertainty Δ given by 0.05, 0.05, 0.005, 0.005 for the $P_{1/2}$, $P_{3/2}$, $D_{3/2}$, and $D_{5/2}$ states, respectively.

For $F_{5/2}$, $F_{7/2}$, $G_{7/2}$, and $G_{9/2}$ states with $n \leq 5$, we use Eq. (9) with values for A_{60} from Table II with uncertainties Δ given by 0.0002, 0.0008, 0.00008, and 0.0002, respectively. For the corresponding states with $n \geq 6$, we use the values for $n = 5$ with uncertainties Δ given by 0.001, 0.005, 0.0005, and 0.001, respectively.

For all states with $l \geq 5$, *i.e.,* H or higher, we use $G_{\rm SE}(\alpha) = 0$, with an uncertainty of 0.01.

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