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Precise theory of levels of hydrogen and deuterium: The two-photon radiative corrections

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The two-photon radiative effects are significant quantum electrodynamic corrections to the energy levels of hydrogen and deuterium atoms. Calculations of higher-order contributions to this correction are reviewed, and the results needed to evaluate energy levels for states with $n \le 200$ are given. The results of such an evaluation 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 two-photon radiative correction is a significant QED effect.

II. TWO-PHOTON CORRECTIONS

Corrections from two virtual photons, of order α^2, have been calculated as a power series in $Z\alpha$:

$$E^{(4)} = \left(\frac{\alpha}{\pi}\right)^2 \frac{(Z\alpha)^4}{n^3} m_e c^2 F^{(4)}(Z\alpha) , \qquad (1)$$

where

$$\begin{aligned} F^{(4)}(Z\alpha) = {} & B_{40} + B_{50}\,(Z\alpha) + B_{63}\,(Z\alpha)^2 \ln^3 (Z\alpha)^{-2} \\ & + B_{62}\,(Z\alpha)^2 \ln^2 (Z\alpha)^{-2} \\ & + B_{61}\,(Z\alpha)^2 \ln (Z\alpha)^{-2} + B_{60}\,(Z\alpha)^2 \\ & + \cdots . \end{aligned} \qquad (2)$$

The leading terms B_{40}, B_{50}, B_{63}, and B_{62} are known for all states and are discussed in Appendix A of Ref. [1]. References to calculations of these terms are also given there. In this note, we are concerned with the information available for the coefficients B_{61} and B_{60}

III. THE COEFFICIENT B_{61}

The single-logarithm coefficient B_{61} for S states has been given as [2]

$$\begin{aligned} B_{61} = {} & \frac{39\,751}{10\,800} + \frac{4N(n)}{3} + \frac{55\pi^2}{27} - \frac{616\,\ln 2}{135} + \frac{3\pi^2 \ln 2}{4} \\ & + \frac{40 \ln^2 2}{9} - \frac{9\,\zeta(3)}{8} + \left(\frac{304}{135} - \frac{32\,\ln 2}{9}\right) \\ & \times \left[\frac{3}{4} + \gamma + \psi(n) - \ln n - \frac{1}{n} + \frac{1}{4n^2}\right] , \end{aligned} \qquad (3)$$

TABLE I: Values of N for S states in this work

n	N
1	17.855 672(1)
2	12.032 209(1)
3	10.449 810(1)
4	9.722 413(1)
5	9.304 114(1)
6	9.031 832(1)
7	8.840 123(1)
8	8.697 639(1)
9	8.2(8)
10	8.2(8)
11	8.1(8)
12	8.1(8)
13	8.1(8)
14	8.0(8)
15	8.0(8)

where $N(n)$ is a term that was numerically evaluated for the 1S state by Pachucki [2]. Jentschura [3] has evaluated $N(n)$ for excited S states with $n = 2$ to $n = 8$, has made an improved evaluation for $n = 1$, and has given an approximate fit to the calculated results in order to extend them to higher n. The fitted function for S states is

$$N(n) = 7.78 + \frac{3.13}{n} + \frac{6.93}{n^2} + \cdots \qquad (4)$$

There are no complete results yet for P, D, or higher-l states for B_{61}, although the term $N(n)$ has been calculated for P states in Ref. [3].

Values of the function $N(n)$ for some S states are given in Table I. The values for $n \ge 9$ are based on Eq. (4), with an assumed uncertainty of type u_n of 10 % of the quoted value. Based on the relative magnitude of A_{61} for the S, P, and D states, we take as uncertainties $u_n(B_{61}) = 5.0$ for P states and $u_n(B_{61}) = 0.5$ for D and higher-l states.

Recent work indicates that there may be an additional contribution to B_{61} and/or B_{60} [4, 5]. The effect of such a contribution would be to change the S-state energy levels by an amount that is likely to be less than half the uncertainty of the nuclear size correction due to uncertainty in the rms radius of the nucleus. However, a change of this size in either coefficient that is independent of n would have a relatively

TABLE II: Values of $b_{\rm L}$ and B_{60} used in the 2002 adjustment

n	$b_{\rm L}$	B_{60}
1	$-81.4(3)$	$-61.6(9.2)$
2	$-66.6(3)$	$-53.2(8.0)$
3	$-61.7(5.0)$	$-50.1(9.0)$
4	$-59.2(5.0)$	$-48.4(8.8)$
5	$-57.7(5.0)$	$-47.4(8.7)$
6	$-56.7(5.0)$	$-46.7(8.6)$
7	$-56.0(5.0)$	$-46.2(8.5)$
8	$-55.5(5.0)$	$-45.8(8.5)$
9	$-55.1(5.0)$	$-46.0(8.6)$
10	$-54.8(5.0)$	$-45.7(8.5)$
11	$-54.5(5.0)$	$-45.5(8.5)$
12	$-54.3(5.0)$	$-45.3(8.5)$
13	$-54.1(5.0)$	$-45.1(8.5)$
14	$-53.9(5.0)$	$-45.0(8.4)$
15	$-53.8(5.0)$	$-44.9(8.4)$

minor effect on the calculated energy levels, based on a least-squares adjustment. The reason is that such a new coefficient, when included in the least-squares adjustment of the constants would lead to a new adjusted value of the nuclear charge radius, since both corrections to the energy level are proportional to $1/n^3$, and the sum of the corrections is determined by the experimental data. Thus, the change in the coefficient and the change in the nuclear size correction would essentially cancel in the net contribution to the energy levels.

IV. THE COEFFICIENT B_{60}

The two-loop Bethe logarithm $b_{\rm L}$, which is expected to be the dominant part of the no-log term B_{60}, has been calculated for the 1S and 2S states by Pachucki and Jentschura [6] who obtained

$$b_{\rm L} = -81.4(3) \quad \text{1S state} \tag{5}$$
$$b_{\rm L} = -66.6(3) \quad \text{2S state .} \tag{6}$$

An additional contribution for S states,

$$b_{\rm M} = \frac{10}{9} N \ , \tag{7}$$

as derived by Pachucki [2], where N is given in Table I as a function of the state n.

These contributions can be combined to obtain an estimate for the coefficient B_{60} for S states:

$$B_{60} = b_{\rm L} + \frac{10}{9} N + \cdots \ , \tag{8}$$

where the dots represent uncalculated contributions to B_{60} which are at the relative level of 15 % [6].

In order to obtain an approximate value for B_{60} for S states with $n \geq 3$, we employ a simple extrapolation formula,

$$b_{\rm L} = a + \frac{b}{n} \ , \tag{9}$$

with a and b fitted to the 1S and 2S values of $b_{\rm L}$, and we include a component of uncertainty $u_0(b_{\rm L}) = 5.0$. The results for $b_{\rm L}$, along with the total estimated values of B_{60} for S states, is given in Table II. For P states, there is a calculation of fine-structure differences [7], but because of the uncertainty in B_{61} for P states, we do not include this result. We assume that for both the P and D states, the uncertainty attributed to B_{61} is sufficiently large to account for the uncertainty in B_{60} and higher-order terms as well.

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