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LETTER TO THE EDITOR

Radiative energy shifts induced by local potentials**Ulrich D Jentschura**Theoretische Quantendynamik, Fakultät Mathematik und Physik der Universität Freiburg,
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Online at stacks.iop.org/JPhysA/36/L229**Abstract**

We study a specific correction to the Bethe logarithm induced by potentials which are proportional to a Dirac- δ function in coordinate space ('local potentials'). Corrections of this type occur naturally in the calculation of various self-energy corrections to the energy of bound states. Examples include logarithmic higher-order binding corrections to the two-loop self-energy, vacuum-polarization induced corrections to the self-energy and radiative corrections induced by the finite size of the nucleus. We obtain results for excited S and P states and find that the dependence of the corrections on the principal quantum number is remarkable. For the ground state, we find a small modification as compared to previously reported results. Our results are based on mathematical techniques for the treatment of quantum electrodynamic bound states introduced discussed previously by Jentschura and Pachucki (2002 *J. Phys. A: Math. Gen.* **35** 1927).

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(Some figures in this article are in colour only in the electronic version)

1. Introduction

Ever since the quantization of the electromagnetic field was introduced by Dirac in [1], one of the main directions of research in the area of quantum electrodynamics has been the study of bound states and, notably, the corrections to the energy of these states as induced by the virtual quanta. A severe limitation to the accuracy of current theoretical predictions is given by bound-state two-loop self-energy effects whose evaluation has been historically problematic (see [2, 3] and references therein). In this letter, we present complete results for the two-loop (2L) logarithmic self-energy correction of excited S states of order

$$\Delta E_{\log}^{(2L)}(nS) = \left(\frac{\alpha}{\pi}\right)^2 \frac{(Z\alpha)^6 m}{n^3} \ln[(Z\alpha)^{-2}] B_{61}(nS) \quad (1)$$

where $B_{61}(nS)$ is an n -dependent, dimensionless coefficient. Here, n is the principal quantum number, Z is the nuclear charge number, m is the electron mass and α is the fine-structure constant (we work in natural units: $\hbar = c = \epsilon_0 = 1$).

One of the quantities which enter quite universally into higher-order corrections to the one- and two-loop self-energy is that induced by effective potentials which are proportional to a Dirac delta-function in coordinate space. In order to calculate $B_{\delta 1}$ for excited S states, an investigation of such corrections is necessary [3]. Our investigations are based on mathematical techniques which facilitate the treatment of bound states which rely on a separation of the virtual photons into hard (high-energy) and soft (low-energy) quanta; these have recently been generalized to two-loop effects [2, 4].

2. General formulation

Let us consider the Schrödinger Hamiltonian

$$H = \frac{\mathbf{p}^2}{2m} + V \quad (2)$$

where V is the binding Coulomb potential (the energy eigenvalues are $E_n = -(Z\alpha)^2 m / (2n^2)$). We assume a small perturbation of H proportional to a δ -function,

$$\delta V = \frac{\pi(Z\alpha)\delta^{(3)}(\mathbf{r})}{m^2}. \quad (3)$$

For S states, this perturbation leads to an energy shift

$$\delta E = \langle \phi | \delta V | \phi \rangle \quad (4)$$

where $|\phi\rangle$ is the electron wavefunction for which the nonrelativistic approximation may be used in the context of the evaluation of the radiative corrections as discussed in this letter. Correction (4) is nonvanishing only for S states, where the correction to the nS -state energy amounts to $(Z\alpha)^4/n^3$. Perturbation (3) also induces a modification of the wavefunction

$$|\delta\phi\rangle = \left(\frac{1}{E - H} \right)' |\phi\rangle \quad (5)$$

where the prime denotes the reduced Green function (in the spectral decomposition, the reference state $|\phi\rangle$ is excluded).

We calculate the delta-like correction to the one-loop Bethe logarithm,

$$\begin{aligned} \Delta E_{\delta}^{(L)}(nl, \bar{\epsilon}) &= \frac{2\alpha}{3\pi} \delta_{\delta V} \left\{ \int_0^{\bar{\epsilon}} d\omega \omega \left\langle \phi \left| \frac{p^i}{m} \frac{1}{E - (H + \omega)} \frac{p^i}{m} \right| \phi \right\rangle \right\} \\ &= \frac{\alpha}{\pi} (Z\alpha)^6 \frac{m}{n^3} F_6(nl, \bar{\epsilon}) \end{aligned} \quad (6)$$

where nl denotes the bound-state quantum numbers. Notation (6) follows the usual spectroscopic nomenclature, n is the principal quantum number and l is the orbital angular momentum. Correction (6) is independent of the electron spin, and $\bar{\epsilon}$ denotes the quantity

$$\bar{\epsilon} = \frac{\epsilon}{(Z\alpha)^2 m} \quad (7)$$

(the notation has been introduced in [3]). The upper index (L) in equation (6) is assigned because $\Delta E_{\delta}^{(L)}$ represents the low-energy part of the correction (due to soft virtual photons), in the language of the formalism introduced in [2, 5, 6]. In equation (6), the symbol $\delta_{\delta V}$, inspired by the notation of [3], denotes the first-order perturbation received by the quantity in curly brackets through the replacements (see equations (3)–(5))

$$H \rightarrow H + \delta V \quad (8)$$

$$|\phi\rangle \rightarrow |\phi\rangle + |\delta\phi\rangle \quad (9)$$

$$E \rightarrow E + \delta E. \quad (10)$$

The quantity $F_6(nl, \bar{\epsilon})$ in equation (6) is a dimensionless function which parametrizes an effect

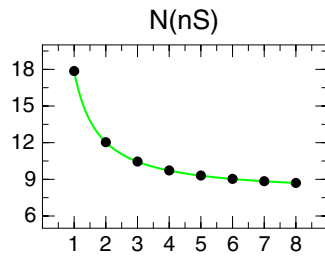


Figure 1. The dependence of the correction $N(nS)$ on the principal quantum number is remarkable. For $n = 8$, the magnitude of the result is less than half $N(1S)$. The smooth curve is a fit based on a model based on a three-parameter fit of the form $a_S + b_S/n + c_S/n^2$ (see equation (14)).

of the order of $(Z\alpha)^6$. Here, we present results for nS states in the range $n = 1, \dots, 8$ and nP states ($n = 2, \dots, 8$).

3. Correction to S states

For S states, F_6 as implicitly defined in equation (6) has the form [3]

$$F_6(nS, \bar{\epsilon}) = -\frac{2}{3} \ln^2(\bar{\epsilon}) + \ln(\bar{\epsilon}) \left[2\{1 - \ln 2\} + \frac{8}{3} \left(\frac{3}{4} + \frac{1}{4n^2} - \frac{1}{n} - \ln(n) + \Psi(n) + C \right) \right] + N(nS). \quad (11)$$

Here, $C = 0.57721\dots$ is Euler's constant, the notation $\bar{\epsilon}$ is explained in equation (7), and $N(nS)$ is a nonlogarithmic term which has been known only for $n = 1$ (see [3]). The dependence on $\bar{\epsilon}$ cancels when the high-energy part is added to the above result [5–7]. The constant term $N(nS)$ has been shown to contribute to the two-loop self-energy coefficient $B_{61}(nS)$ (see [3, equation (50)]). The complexity of the calculation increases with increasing principal quantum number, because of the more complex structure of the bound-state wavefunction and the necessity to subtract poles of the integrand corresponding to the decay into lower-energy states. For states with $n = 8$, we obtain intermediate results with 198 000 terms, and use is made of computer algebra systems [8].

We obtain the following results for $N(nS)$ in the range $n = 1, \dots, 8$:

$$\begin{aligned} N(1S) &= 17.855\,672(1) & N(2S) &= 12.032\,209(1) \\ N(3S) &= 10.449\,810(1) & N(4S) &= 9.722\,413(1) \\ N(5S) &= 9.304\,114(1) & N(6S) &= 9.031\,832(1) \\ N(7S) &= 8.840\,123(1) & N(8S) &= 8.697\,639(1). \end{aligned} \quad (12)$$

The result for $N(1S)$ supersedes the value previously reported in [3] for this correction (see also discussion in section 5 below). A least-squares fit with a functional form

$$N(nS) \approx a_S + b_S/n + c_S/n^2 \quad (13)$$

yields the fit-parameter values

$$a_S = 7.78 \quad b_S = 3.13 \quad c_S = 6.93. \quad (14)$$

The data in equation (12) are well represented by this fit, as is evident from figure 1. The excellent agreement between the fit and the numerical data in equation (12) could suggest a finite limit

$$\lim_{n \rightarrow \infty} N(nS) \approx 7.78. \quad (15)$$

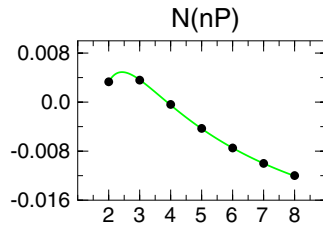


Figure 2. The analogue of figure 1 for P states.

The functional form of the fit is inspired, in particular, by the term proportional to $\ln(\bar{\epsilon})$ in (11). This term can be expanded in a series involving inverse powers of n . Note that the logarithmic term $\ln(n)$, for large n , cancels against a compensating term originating from the expansion of $\Psi(n)$.

4. Correction to P states

For P states, $F_6(nP, \bar{\epsilon})$ assumes the functional form

$$F_6(nP, \bar{\epsilon}) = \frac{2}{9} \left(1 - \frac{1}{n^2} \right) \ln \bar{\epsilon} + N(nP). \quad (16)$$

We obtain the results

$$\begin{aligned} N(2P) &= 0.003\,300\,635(1) & N(3P) &= 0.003\,572\,084(1) \\ N(4P) &= -0.000\,394\,332(1) & N(5P) &= -0.004\,303\,806(1) \\ N(6P) &= -0.007\,496\,998(1) & N(7P) &= -0.010\,014\,614(1) \\ N(8P) &= -0.011\,999\,223(1). \end{aligned} \quad (17)$$

The result for $N(2P)$ was previously obtained in [9, equation (4.159)] . Specifically, the contribution due to this term entered into the result for $F_{\delta H}$ given in [6, table I]. Here, we present the generalization of the result to higher principal quantum numbers. Observe that the correction changes its sign as n is increased. In analogy with the S states, we use a least-squares fit with a functional form

$$N(nP) \approx a_P + b_P/n + c_P/n^2 \quad (18)$$

which results in the fit-parameter values

$$a_P = -0.030 \quad b_P = 0.170 \quad c_P = -0.206. \quad (19)$$

The excellent agreement between the fit and the numerical data is represented in figure 2.

The spin-dependent high-energy part for P states is

$$\Delta E_{\delta}^{(H)}(nP_j, \epsilon) = \frac{\alpha}{\pi} (Z\alpha)^6 \frac{m}{n^3} H_6(nP_j, \bar{\epsilon}). \quad (20)$$

Inspired by the effective treatment of radiative corrections based on form factors [10, ch 7], we take into account the contribution due to hard virtual photons by the replacement

$$\delta V \rightarrow \delta V F_1(-q^2) \quad (21)$$

but this does not give the complete result. We also have to consider the perturbation of the spin-dependent interaction

$$\frac{1}{2m} (i\boldsymbol{\gamma} \cdot \delta \mathbf{E}) \rightarrow \frac{1}{2m} (i\boldsymbol{\gamma} \cdot \delta \mathbf{E}) F_2(-q^2) \quad (22)$$

where δE is the electric field generated by the perturbing potential δV , i.e.

$$\delta E = -i \mathbf{q} \frac{\pi(Z\alpha)}{m^2} \tag{23}$$

in momentum space, and γ is a three-vector whose elements are the spatial Dirac matrices [10]. Both of the above replacement prescriptions (21) and (22) are dictated by the modified Dirac Hamiltonian as given in [2, equation (3)].

We first consider the correction due to the charge form factor F_1 as given in equation (21). Because we consider *a priori* only the one-loop effect, we may take F_1 in the one-loop approximation and expand only up to the order of q^2 . A suitably chosen perturbing potential may be used for an effective treatment of further loops, as discussed in section 5. Formulae relevant to the electron charge form factor F_1 can be found in equations (5), (10) and (31) of [2]. We find

$$\Delta E_\delta^{(H,1)}(nP_j, \epsilon) = \alpha \frac{Z\alpha}{3m^4} \left(\ln\left(\frac{m}{2\epsilon}\right) + \frac{11}{24} \right) \Delta(|\psi_{nP}(\mathbf{r})|^2)|_{r=0} \tag{24}$$

where $\psi_{nP}(\mathbf{r})$ is the nonrelativistic wavefunction of the nP state, and the matrix element reads

$$\Delta(|\psi_{nP}(\mathbf{r})|^2)|_{r=0} = \frac{2}{3} \frac{(Z\alpha)^5 m^5}{\pi n^3} \left(1 - \frac{1}{n^2} \right). \tag{25}$$

Therefore, the result for the scaled high-energy part due to the F_1 form factor reads

$$H_6^{(1)}(nP_j, \epsilon) = \frac{2}{9} \left(1 - \frac{1}{n^2} \right) \left(\ln\left(\frac{m}{2\epsilon}\right) + \frac{11}{24} \right). \tag{26}$$

Now we turn to the spin-dependent correction proportional to the magnetic form factor F_2 as given in equation (22). Again, we may employ the one-loop approximation and take F_2 at zero momentum, where its well-known Schwinger value reads $F_2(0) = \alpha/(2\pi)$. We find

$$\Delta E_\delta^{(H,2)}(nP_j, \epsilon) = F_2(0) \frac{\pi(Z\alpha)}{2m^3} \langle nP_j | \boldsymbol{\gamma} \cdot \mathbf{q} | nP_j \rangle \tag{27}$$

where the expectation value of the momentum space operator $\boldsymbol{\gamma} \cdot \mathbf{q}$ reads

$$\langle nP_j | \boldsymbol{\gamma} \cdot \mathbf{q} | nP_j \rangle = i \left[\frac{\partial}{\partial \mathbf{r}} (\psi_{nP_j}^+(\mathbf{r}) \boldsymbol{\gamma} \psi_{nP_j}(\mathbf{r})) \right]_{r=0} = \frac{n^2 - 1}{\pi n^5} (Z\alpha)^5 m^4 \delta_{j,1/2} \tag{28}$$

i.e. the matrix element vanishes for $P_{3/2}$ states (please observe the missing factor π in the denominator of the right-hand side of equation (29) of [2]). We thus obtain

$$H_6^{(2)}(nP_j, \epsilon) = \frac{1}{4} \left(1 - \frac{1}{n^2} \right) \delta_{j,1/2} \tag{29}$$

in analogy with the result obtained in equation (30) of [2].

Adding the low-energy part (16), and the two high-energy contributions (26) and (29) due to F_1 and F_2 , respectively, we obtain

$$\Delta E_\delta(nP_j) = \Delta E_\delta^{(L)}(nP, \bar{\epsilon}) + \sum_{k=1,2} \Delta E_\delta^{(H,k)}(nP_j, \epsilon) = \frac{\alpha}{\pi} (Z\alpha)^6 \frac{m}{n^3} F_\delta(nP_j) \tag{30}$$

where the function $F_\delta(nP)$ is independent of ϵ and has the form

$$\begin{aligned} F_\delta(nP_j) &= F_6(nP, \bar{\epsilon}) + \sum_{k=1,2} H_6^{(k)}(nP_j, \epsilon) \\ &= \frac{2}{9} \left(1 - \frac{1}{n^2} \right) \left(\ln\left(\frac{1}{(Z\alpha)^2}\right) - \ln(2) + \frac{11}{24} + \frac{9}{8} \delta_{j,1/2} \right) + N(nP). \end{aligned} \tag{31}$$

The numerical values of $N(nP)$ are given in equation (17).

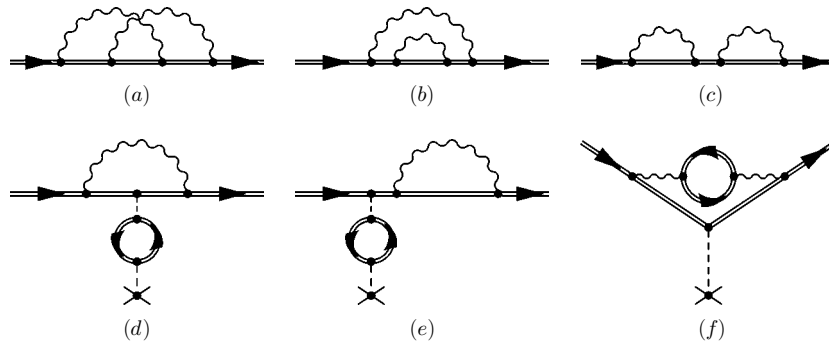


Figure 3. Some of two-loop diagrams involving the bound-state electron self-energy which contribute to the logarithmic coefficient B_{61} . All of these (and others) were taken into account in [3]. The double line in the diagrams denotes the bound electron (Dirac-Coulomb propagator). Figures (a)–(c) contribute also to the triple logarithm of order $\alpha^2(Z\alpha)^6 \ln^3[(Z\alpha)^{-2}]m$, i.e. to the $B_{63}(nS)$ -coefficient. The double logarithm of order $\alpha^2(Z\alpha)^6 \ln^2[(Z\alpha)^{-2}]m$ originates from diagrams (a)–(e). General formulae valid for $B_{62}(nS)$ and $B_{63}(nS)$ of arbitrary n are given in equations (48), (49) and (51) of [3]. The single logarithm $B_{61}(nS)$ involves many more contributions, for example those originating from the diagram (f). This Feynman diagram is considered in equation (40) of [3], together with contributions from other diagrams involving vacuum polarization effects. Complete results for $B_{61}(nS)$ are given in equation (32).

5. Conclusions

We summarize the results of this letter.

- *Dependence of the B_{61} coefficient on the principal quantum number.* Currently, one of the most important limiting factors to a further progress of the theory of the S state Lamb shift is the understanding of higher-order binding corrections to the two-loop bound-state self-energy [11]. The theory of S states is important for the deduction of the Rydberg constant, and it is also necessary to investigate higher excited states because the frequencies of more than one transition have to be theoretically known in order to infer the fundamental constants (see [11] and references therein).

Our result for $N(1S)$ in equation (12) differs slightly from previously published results (see equation (21) of [3]). General formulae, whose structure is valid for $B_{61}(nS)$ of arbitrary n have been given in [3, equations (50) and (52)]; these are relevant to the sum of two-loop self-energy *and* vacuum-polarization effects. Some of the contributing Feynman diagrams are shown in figure 3. However, the quantity $N(nS)$ which enters into the expression for $B_{61}(nS)$ has been known only for $n = 1$. Here, we take into account the slightly shifted value of $N(1S)$ as well as the results presented in equation (12) for $n > 1$. We finally obtain the following results for $B_{61}(nS)$ defined in equation (1),

$$\begin{aligned}
 B_{61}(1S) &= 50.344\,005(1) & B_{61}(2S) &= 42.447\,669(1) \\
 B_{61}(3S) &= 40.289\,637(1) & B_{61}(4S) &= 39.294\,929(1) \\
 B_{61}(5S) &= 38.722\,048(1) & B_{61}(6S) &= 38.348\,805(1) \\
 B_{61}(7S) &= 38.085\,860(1) & B_{61}(8S) &= 37.890\,354(1).
 \end{aligned}
 \tag{32}$$

This completes the calculation of logarithmic two-loop corrections to S states of order $\alpha^2(Z\alpha)^6 \ln^j[(Z\alpha)^{-2}]m$ ($j = 1, 2, 3$).

- *Clarification of a specific intermediate step in the calculation of the muonium hyperfine splitting.* In lowest order, the hyperfine splitting Hamiltonian for an electron bound to an

atomic nucleus with magnetic moment μ_n is given by [10, p 79]:

$$\begin{aligned} V_{\text{hfs}}(\mathbf{r}) &= \frac{e}{2m} \boldsymbol{\sigma}_e \cdot [\nabla \times (\boldsymbol{\mu}_n \times \nabla)] \frac{1}{4\pi r} \\ &= \frac{e}{8\pi m} \boldsymbol{\sigma}_e \cdot [\boldsymbol{\mu}_n \nabla^2 - (\boldsymbol{\mu}_n \cdot \nabla) \nabla] \frac{1}{r} \\ &\rightarrow -\frac{e}{3m} (\boldsymbol{\sigma}_e \cdot \boldsymbol{\mu}_n) \delta^{(3)}(\mathbf{r}) \end{aligned} \quad (33)$$

which is a delta-like potential as in (3). The angular averaging $\nabla_i \nabla_j \rightarrow (1/3) \delta_{ij} \nabla^2$ (see the transition from the second to the third line of equation (33)) is valid when $V_{\text{hfs}}(\mathbf{r})$ is evaluated on S states. Therefore, the quantity $N(nS)$ appears naturally in the evaluation of radiative corrections to the hyperfine splitting of S states, for example in muonium [7, 12].

The results for $N(1S)$ given in equation (12) differ slightly from the corresponding previously published value for the low-energy part of the muonium hyperfine splitting as given in [7]. The difference is

$$\frac{2}{3} \left(\frac{31}{36} - \frac{\pi^2}{12} \right) = 0.025\,7627\dots \quad (34)$$

While the new result reported here does not affect the final result for the hyperfine splitting, it explains the discrepancies between the intermediate results of [7] and those of [12].

- *Vacuum-polarization induced correction to the self-energy.* Our results for $N(nP)$ in equation (17) and the total results in equations (30) and (31) for the energy shift due to the radiative correction to a delta-like potential can be used in order to evaluate the contribution to the energy of a P state due to the diagram in figure 3(d). This is a combined ‘self-energy vacuum-polarization’ correction for P states generated by a vacuum polarization correction to the Coulomb exchange in the bound electron propagator within the one-loop self-energy diagram. The lowest-order one-loop vacuum-polarization potential reads [10, p 327]

$$V_{\text{VP}}(\mathbf{r}) = -\frac{4}{15} \frac{\alpha \pi (Z\alpha) \delta^{(3)}(\mathbf{r})}{\pi m^2} \quad (35)$$

which is proportional to δV defined in equation (3). Our results in equations (17), (30) and (31) contribute to the two-loop coefficients B_{61} and B_{60} for P states as defined in [2].

- *Nuclear finite-size correction to the self-energy.* For an atomic nucleus whose root-mean-square charge radius is small compared to the Bohr radius, the effect of the nuclear finite-size can be incorporated as a form-factor correction to the Coulomb interaction in full analogy with equations (21) and (22). In this case the appropriate form factor reads

$$F(-q^2) = 1 - q^2 \frac{\langle r^2 \rangle}{6} \quad (36)$$

where $\langle r^2 \rangle$ is the mean-square radius of the charge distribution of the atomic nucleus. The Dirac delta-like finite-size ‘potential’ therefore reads

$$V_{\text{fs}} = \frac{2}{3} \langle r^2 \rangle \frac{\pi (Z\alpha) \delta^{(3)}(\mathbf{r})}{m^2} \quad (37)$$

which is again proportional to δV as defined in equation (3). Therefore, the results in this letter can be used for an evaluation of the finite-size correction to the self-energy in atomic systems with a low nuclear charge number. Our result in equation (17) for the case $n = 2$ has been obtained previously in [9]. For the $2P_{1/2}$ and $2P_{3/2}$ states, our calculations are also in agreement with equations (16) and (17) of [13]. Our results in equations (17) and (31) above represent generalizations of this previous work to higher excited states.

Work on the nonlogarithmic term B_{60} for S states is currently in progress and will be presented elsewhere, together with improved theoretical values for the Lamb shift of S states as derived from the results presented in this letter.

Acknowledgement

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