

The Self-Energy of an Electron Bound in a Coulomb Field

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Abstract—Recent progress in calculation of the one-loop self-energy of the electron bound in the Coulomb field is summarized. The relativistic multipole expansion is introduced. This expansion is based on a single assumption: except for the part of the time component of the electron four-momentum corresponding to the electron rest mass, the exchange of four-momentum between the virtual electron and photon can be treated perturbatively. For non S-states and normalized difference $n^3 \Delta E_n - \Delta E_1$ of the S-states this itself yields very accurate results after taking the method to the third order. For the ground state the perturbation treatment of the electron virtual states with very high three-momentum is to be avoided. For these states one can always rearrange the pertinent expression in such a way that free-particle approximation is allowed. Combination of the relativistic multipole expansion and free-particle approximation yields very accurate result after taking the method to the ninth order. These results are in very good agreement with the previous results obtained by the partial wave expansion and definitely exclude the possibility that the uncertainty in determination of the proton radius comes from the uncertainty in the calculation of the one-loop self-energy.

Keywords—Hydrogen-like atoms, self-energy.

I. INTRODUCTION

Recently found disagreement between the radius of proton deduced from a comparison of the theory [1], [2] and experiment [3], [4] of Lamb shifts in the ordinary and muonic hydrogen calls for a verification of correctness of both the theory and experiment [5]. Only when this is done, more interesting possibilities can be examined [5].

Among various contributions to the Lamb shift in ordinary hydrogen, the most important is the self-energy of the bound electron in the one-loop approximation. This effect causes the shift of $2S-1S$ transition of about 7.32 GHz. The difference between the proton radii found in [1] and [4] leads [6] to the difference of about 82.22 kHz for $2S-1S$ transition. Thus the self-energy effect should be known with accuracy significantly better than 1 part in 10^5 .

For years the self-energy for the atoms with low nuclear charges has been calculated via the series in powers of $Z\alpha$

$$\Delta E = \frac{m\alpha(Z\alpha)^4}{\pi n^3 s^3} F(Z\alpha, n, l_j), \quad (1)$$

where [7], [8], [9], [10]

$$\begin{aligned} F(Z\alpha, n, l_j) = & A_{41} \ln s(Z\alpha)^{-2} + A_{40} + A_{50}(Z\alpha) + \\ & +(Z\alpha)^2 [A_{62} \ln^2 s(Z\alpha)^{-2} + A_{61} \ln s(Z\alpha)^{-2} + A_{60}] + \\ & +(Z\alpha)^3 [\ln s(Z\alpha)^{-2} A_{71} + A_{70}] + \dots, \end{aligned} \quad (2)$$

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where $s = 1$ in the non-recoil limit. The dominant part of the recoil effect is taken into account by replacing $s = 1$ in Eqs. (1) and (2) by $s = 1 + m_e/m_n$. Here m_e/m_n is a ratio of the electron and nuclear masses [13]. The coefficients A , $A = A(n, l_j)$, are summarized e.g. in [1], [11]. n , l and j denote the principal, orbital and total momentum quantum numbers of the state under consideration.

Recently, another approach based on the partial wave expansion [12] was developed. For atoms with low nuclear charges this expansion converges very slowly. Nonetheless, the most accurate results obtained so far for the hydrogen atom were obtained in [11] by means of this expansion. In that paper several millions of partial waves were considered. For each partial wave there is a three-dimensional integration to be performed numerically, for details see [11], [12].

It is convenient to write the self-energy effect on general S-state as

$$\Delta E_n = \frac{n^3 \Delta E_n - \Delta E_1}{n^3} + \frac{\Delta E_1}{n^3}, \quad (3)$$

where the first and the second terms on the right member will be referred to as the state-dependent and the state-independent parts, respectively. In comparison with calculation of the state-independent part of the S-states, calculation of the state-dependent part of the S-states and non S-states is substantially simpler: the coefficients A_{41} , A_{50} and A_{62} in Eq. (2) vanish and the estimate obtained by means of series (2) truncated after A_{60} term is quite good, see below. However, the dominant part of the effect is state independent part of the S-states. The relative difference between the series (2) truncated after $\alpha(Z\alpha)^6$ term and the numerical result in [11] for the ground states of the hydrogen is 3 parts in 10^6 . In view of the complexity of the calculation of the A_{60} coefficient [8], there is no hope of achieving significantly better accuracy within purely perturbation approach. Clearly, such an approach is not sufficient any more.

II. THE METHOD

The renormalized expression for the self-energy in the non-recoil limit reads (see [14] for notation used)

$$\Delta E = \langle O - \Delta m \rangle = \langle \psi | \gamma_0 (O - \Delta m) | \psi \rangle, \quad (4)$$

where Δm stands for the electromagnetic mass of the electron and the regularized mass operator O reads

$$O = \frac{\alpha}{\pi} \int_0^{\Lambda^2} d\lambda \int \frac{d^4 k_F}{(k^2 - \lambda)^2} \gamma^\mu \frac{1}{\gamma \cdot (\Pi - k) - m} \gamma^\mu. \quad (5)$$

The wave function ψ is a solution of the stationary Dirac equation with the energy E

$$(\gamma \cdot \Pi - m)\psi = 0. \tag{6}$$

The components of physical momentum Π of the particle in the case of the Coulomb field read

$$\Pi = \left(E + \frac{Z\alpha}{R}, \vec{P} \right) \tag{7}$$

where \vec{P} is the canonical momentum.

Following [7] we multiply $1/(\gamma \cdot (\Pi - k) - m)$ in Eq. (5) by $(\gamma \cdot (\Pi - k) + m)/(\gamma \cdot (\Pi - k) + m)$ from the right. Using Dirac equation and properties of γ matrices [14] we get

$$\langle O \rangle = -\frac{\alpha}{2\pi} \left\langle \gamma_\mu \left(G_4 \Pi_\mu - \frac{m}{2} G \cdot \gamma \gamma_\mu \right) \right\rangle, \tag{8}$$

where

$$G_{4,\nu} = (-4) \int_0^{\Lambda^2} d\lambda \int \frac{d^4 k_F}{(k^2 - \lambda)^2} \frac{(1, k_\nu/m)}{k^2 - 2k \cdot \Pi + H}. \tag{9}$$

Here the second-order Hamilton operator H [7] reads

$$H = (\gamma \cdot \Pi + m)(\gamma \cdot \Pi - m) = \Pi \cdot \Pi - m^2 + \frac{1}{4} [\Pi_\mu, \Pi_\nu] [\gamma_\mu, \gamma_\nu]. \tag{10}$$

Recently an expansion of the electron propagator has been suggested [15], [16], [17], [18]. This expansion is referred to as relativistic generalization of multipole expansion (RME). This expansion is based on a single assumption, namely that the four-momentum Π of the bound electron in the virtual states is dominated by the four-momentum ε of the electron at rest:

$$\frac{1}{k^2 - 2k \cdot \varepsilon + H - 2k \cdot (\Pi - \varepsilon)} = \frac{1}{z - \tilde{H}_0 - \lambda \tilde{H}_1}. \tag{11}$$

Here the propagator is written in a generic form $(z - \tilde{H})^{-1}$, where $\tilde{H} = \tilde{H}_0 + \lambda \tilde{H}_1$ is a generic Hamilton operator. Furthermore, λ is a formal perturbation parameter that is eventually set to one,

$$\varepsilon = (m, 0, 0, 0) \tag{12}$$

and

$$z = k^2 - 2k \cdot \varepsilon, \tilde{H}_0 = -H, \lambda \tilde{H}_1 = 2k \cdot (\Pi - \varepsilon). \tag{13}$$

We form the series

$$\Delta E = m \frac{\alpha}{\pi} (Z\alpha)^4 \sum_{v=1}^{\infty} F_v, \tag{14}$$

where

$$\begin{aligned} -2(Z\alpha)^4 F_v = & \sum_{t=0}^v \left\langle \gamma_0 G_4^{2(v-t),t} + \gamma_\mu G_4^{2(v-t-1),t} \frac{(\Pi - \varepsilon)_\mu}{m} + \right. \\ & \left. + \gamma_0 G_0^{2(v-t),t} - \frac{1}{2} \gamma_\mu [G_0^{2(v-t-3),t}, \gamma_0 \gamma_\mu] + \frac{1}{2} \gamma_\mu G_i^{2(v-t)-1,t} \gamma_i \gamma_\mu \right\rangle. \end{aligned} \tag{15}$$

The superscripts v and t in $G_{4,\nu}^{v,t}$ stand for the number of expanded space and time components of $(\Pi - \varepsilon)$, respectively. The method for generating the individual terms of the expansion is described in [15], [18] for the ground state and in [16] for non S-states and state-dependent part of the S-states.

RME has a number of advantages. Once the renormalization of the electron mass is made all the integrals over either photon or electron variables are finite both at the infrared and ultraviolet. Thus, no separation of any of the integration is necessary. The terms of RME are generated very easily. In fact, by means of computer languages for symbolic calculation like Maple or Mathematica they can be generated automatically. The only integrals to be performed numerically are one-dimensional integrals over the electron wave numbers of the continuous part of the spectrum. These integrals converge very fast. For non S-states and state-dependent part of the S-states it is sufficient to consider the sum in Eq. (14) only up to $v = 3$. Further, for the atoms with low nuclear charges the pertinent expressions can be further simplified and part of the calculation can be carried out analytically, for details see [16].

Question then arises of the relation of the series (14) to (2). As argued in [15], [17], [16] the coefficients A_{41} , A_{40} and A_{62} are contained in $F_1 + F_2$. For non S-states and state-dependent part of the S-states the coefficient A_{61} is contained in $F_1 + F_2$ and the coefficient A_{60} is contained in $F_1 + F_2 + F_3$. For state-independent part of the S-states the coefficient A_{61} and sufficiently great part of the coefficient A_{60} is contained in $F_1 + F_2 + F_3$, see Tables 2 and 3 of [17]. The coefficient A_{50} is contained in complete sum (14). This coefficient is entirely determined by the virtual states with very high wave numbers. For these states one can always rearrange the pertinent expression in such a way that free-particle approximation is appropriate, see [18]. The coefficient A_{50} can then be written as

$$A_{50} = \sum_{v=1}^{\infty} A_{50}^{(v)}, \tag{16}$$

where $A_{50}^{(v)}$ is the part of A_{50} coefficient contained in F_v [17], [18]

$$A_{50}^{(v)} = -2^3 \frac{\Gamma(\frac{1}{2}) \Gamma(v - \frac{5}{2}) (16v^4 - 32v^3 + 296v^2 + 8v - 267)}{\pi \Gamma(v)(2v+5)(2v+3)(2v+1)^2(2v-3)}. \tag{17}$$

For large v this behaves as

$$A_{50}^{(v)} \simeq -\frac{4}{\pi^{1/2}} v^{-7/2}. \tag{18}$$

The complete coefficient A_{50} is [7], [8]

$$A_{50} = 4\pi \left(\frac{139}{128} - \frac{\ln 2}{2} \right). \tag{19}$$

For the self-energy function $F(Z\alpha, 1, 0)$, Eq. (1), we write

$$F(Z\alpha, 1, 0) = (Z\alpha) A_{50} + \sum_{v=1}^{\infty} S_v, \tag{20}$$

where

$$S_v = F_v - (Z\alpha) A_{50}^{(v)}. \tag{21}$$

The point is that if the RME is truncated after finite number of terms, one can exactly determine how much of the free-particle result is contained in it. When considering the self-energy effect of the light hydrogen-like ions this is the greatest advantage of the RME over the method used in [11], [12] based on partial wave expansion.

III. RESULTS

The results obtained for the low lying states of the hydrogen atom are displayed in Tables I and II taken from [16] and [18], respectively.

TABLE I

THE RESULT FOR THE SCALED ENERGY FUNCTION $F(\alpha, n, l_j)$ FOR LOW LYING S- AND P-STATES OF HYDROGEN-LIKE ATOMS OBTAINED BY VARIOUS METHODS. FOR THE S-STATES THE RESULTS FOR THE DIFFERENCE $F(\alpha, n, 0) - F(\alpha, 1, 0)$ ARE GIVEN. THE RESULTS PRESENTED AS 'RME' WERE OBTAINED FROM THE SERIES (14), TRUNCATED AFTER THE THIRD TERM, FOR DETAILS SEE [16]. THE RESULTS OBTAINED BY MEANS OF PARTIAL WAVE EXPANSION ARE TAKEN FROM [11]. THE RESULTS OBTAINED BY MEANS OF EQ. (2) ARE TAKEN FROM [10].

State	RME	Partial waves	Eq. (2)
$2s - 1s$	0.23002947	0.23003154	0.23003040
$2p_{1/2}$	-0.1263965908	-0.12639637	-0.12639773
$2p_{3/2}$	0.1234982498	0.12349856	0.12349766
$3s - 1s$	0.28881828	0.28882057	0.28881946
$4s - 1s$	0.31259262	0.31259475	0.31259391

TABLE II

THE CONVERGENCE OF RME FOR THE GROUND STATE OF THE HYDROGEN. 'LEAD' STANDS FOR THE SUM $S_1 + S_2 + A_{50}$. INSTEAD OF EQ. (15) WE CONSIDERED $-2(Z\alpha)^4 F_v \simeq \left\langle \gamma_0 \sum_{t=0}^T \left(G_4^{2(v-t),t} + G_0^{2(v-t),t} \right) + \sum_{t=0}^{T-1} \left(\gamma_\mu G_4^{2(v-t-1),t} \frac{(\Pi-\varepsilon)_\mu}{m} + \frac{1}{2} \gamma_\mu \sum_{t=0}^{T-1} G_i^{2(v-t-1),t} \gamma_i \gamma_\mu \right) \right\rangle$, WHERE $T = 3$. THE CONTRIBUTION OF THE TERMS $\langle \gamma_0 G_{4,0}^{2v,t} \rangle$ FOR $t > 3$ THE TERMS $\langle \gamma_\mu G_4^{2(v-t-1),t} (\Pi - \varepsilon)_\mu \rangle$ AND $\langle \gamma_\mu G_i^{2(v-t-1),t} \gamma_i \gamma_\mu \rangle$ FOR $t > 2$ AND $\left(-\frac{1}{2}\right) \langle \gamma_\mu [G_0^{2v,t}, \gamma_0 \gamma_\mu] \rangle$ ARE VERY SMALL AND ARE ESTIMATED UNDER HEADING 'SMALL'. WE HAVE FOUND THAT FOR LARGE v THE RATIO S_v/S_{v-1} APPROACHES THE RATIO $A_{50}^{(v)}/A_{50}^{(v-1)}$. THIS ENABLED US TO ESTIMATE THE REMAINDER OF THE SERIES, 'REM'. FOR DETAILS SEE [18]. 'OTHER' IS THE RESULT OF THE PARTIAL WAVE EXPANSION TAKEN FROM [11].

term	$F(\alpha, 1, 0)$
lead	10.315870916
S_3	0.891183 10^{-3}
S_4	0.23509 10^{-4}
S_5	0.4484 10^{-5}
S_6	0.1554 10^{-5}
S_7	0.719 10^{-6}
S_8	0.388 10^{-6}
S_9	0.237 10^{-6}
sum	10.3167929917
small	0.36 10^{-7}
rem	0.648 10^{-6}
total	10.316793675(50)
other	10.316793650(1)

These results agree with the results obtained by partial wave expansion to high degree of accuracy. The difference between the result for the state dependent and state independent part of the S-states obtained by these two completely independent methods amounts to the difference of 210.5 and 18 Hz for $2S - 1S$ transitions in hydrogen, respectively. This definitely excludes the possibility that uncertainty in determination of the proton radius comes from the uncertainty in determination of the one-loop self-energy correction to the energy levels.

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REFERENCES

- [1] P. J. Mohr et al. Rev. Mod. Phys. **80**, 633 (2008); P. J. Mohr in *Springer Handbook of Atomic, Molecular and Optical Physics*, edited by G. W. F. Drake (Springer 2006). See also S. G. Karshenboim, Phys. Rep. **422**, 1 (2005); M. I. Eides et al, Phys. Rep. **342**, 63 (2001).
- [2] E. Borie, Phys. Rev. A **71**, 032508 (2005). See also K. Pachucki, Phys. Rev. A **53**, 2092 (1996); *ibid* **60**, 3593 (1999).
- [3] M. Niering et al, Phys. Rev. Lett. **84**, 5496 (2000); T. Udem et al, *ibid* **79**, 2646 (1997). See also S. Bourzeix et al, *ibid* **76**, 384 (1996).
- [4] R. Pohl et al, Nature **466**, 213 (2010).
- [5] A. Antognini et al, J. Phys.: Conf. Series **312**, 032002 (2011).
- [6] The influence of the non-zero proton radius on the energy levels is given by the formula [1] $\Delta E = \frac{4}{3N^3} \frac{Z^4}{1 + \frac{m_e}{m_p}} (4\pi)^2 \frac{R_\infty^3 c}{\alpha^2} (r_p[m])^2$, where N is the principal quantum number of the state under consideration. The fundamental constants are denoted in the usual way and their values can be found in [1]. The proton radius $r_p = 0.8768 fm$ given in [1] leads to the shift 1.052 MHz between $2S$ and $1S$ states, while the radius $r_p = 0.84184 fm$ found in [4] leads to the shift 0.96977 MHz.
- [7] R. Karplus et al, Phys. Rev. **86**, 288 (1952); G. W. Erickson and D. R. Yennie, Ann. Phys. (NY) **35**, 271 (1965); *ibid* **35**, 447 (1965). See also M. Baranger et al, Phys. Rev. **92**, 482 (1953); A. J. Layzer, J. Math. Phys. **2**, 292 (1961); *ibid* **2**, 308 (1961).
- [8] K. Pachucki, Ann. Phys. (NY) **226**, 1 (1993). See also W. Erickson, Phys. Rev. Lett. **27**, 780 (1971); J. Sapirstein, *ibid* **47**, 1723 (1981).
- [9] S. G. Karshenboim, Z. Phys. D **39**, 109 (1997).
- [10] U. D. Jentschura et al. Phys. Rev. A **72**, 062102 (2005). See also A. Czarnecki et al. Phys. Rev. Lett. **95**, 180404 (2005); U. D. Jentschura et al. Phys. Rev. Lett. **90**, 163001 (2003); E.-O. Le Bigot et al. Phys. Rev. A **68**, 042101 (2003); U. D. Jentschura and K. Pachucki, *ibid* **54**, 1853 (1996); U. D. Jentschura et al. *ibid* **56**, 1739 (1997). B. J. Wundt and U. D. Jentschura, Phys. Lett. B **659**, 571 (2008).
- [11] U. D. Jentschura et al, Phys. Rev. A **63**, 042512 (2001). See also U. D. Jentschura et al, Phys. Rev. Lett. **82**, 53 (1999).
- [12] P. J. Mohr et al., Phys. Rep. **293**, 227 (1998). See also P.J. Mohr, Phys. Rev. A **46**, 4421 (1992); P. J. Mohr and Y. K. Kim, *ibid* **45**, 2727 (1992); P. J. Mohr, *ibid* **26**, 2338 (1982); P. J. Mohr, Ann. Phys. (NY) **88**, 26, (1974); *ibid* **88**, 52 (1974).
- [13] K. Pachucki, Phys. Rev. A **52**, 1079 (1995). See also G. Bhatt and H. Grotch, Ann. Phys. (NY) **178**, 1 (1987).
- [14] The following notation is used: $d^4 k_F$ stands for $i(2\pi)^{-2} d^4 k$ and k stands for the four-momentum of the virtual photon. We use the summation convention $A.B = A_\nu B_\nu = A_0 B_0 - \vec{A} \cdot \vec{B}$. In particular, $k^2 = k_0^2 - \omega^2$, $\omega^2 = \vec{k} \cdot \vec{k}$. The Dirac γ matrices are defined by the anticommutation relation $\{\gamma_\mu, \gamma_\nu\} = 2g_{\mu\nu}$, where $g_{0\mu} = \delta_{0\mu}$ and $g_{ij} = -\delta_{ij}$. Here δ has the usual meaning of the Kronecker symbol. When integrating over k_0 in Eq. (5) we replace the electron mass m by $m - i\eta$ and take the limit $\eta \rightarrow 0$ from above. This is the same notation and the same way of integration as the one used by Feynman in his original papers in Phys. Rev. **76**, 749 (1949); *ibid* **76**, 769 (1949). The natural units ($\hbar = c = 1$) are used throughout the paper. Symbol α stands for the fine structure constant. In actual calculation we took the value $1/137.03599911$ given in [1].
- [15] J. Zamastil, Ann. Phys. (NY) **327**, 297 (2012).
- [16] J. Zamastil and V. Patkóš, Phys. Rev. A **86**, 042514 (2012).
- [17] J. Zamastil, Ann. Phys. (NY) **328**, 139 (2013).
- [18] J. Zamastil and V. Patkóš, to be published.