On the method of precise calculations of energy levels of hydrogen-like atoms

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Abstract

We describe a method for deriving logarithmic corrections in the mass ratio to the S-level of a hydrogen-like atom. With this method, a number of new corrections of this type are calculated analytically for the first time.

The comparison of theoretical and experimental results on non-relativistic bound states in QED is an important source of information about the fundamental physical parameters, such as the fine structure constant, the masses of electron, muon, proton and many others. The promotion of precision of theoretical results requires more and more difficult calculations of higher order corrections. Solution of this problem is impossible without the development of bound state theory, and should use new methods of calculation.

Long debates on the logarithmic contribution $\alpha^6 \ln \alpha$ to the fine shift of S-levels in muonium took place in resent years. It was found eventually that such correction vanishes. However, it is highly probable that there is correction involving the logarithm of parameter $\beta = m_1/m_2$. In the review [1] earlier published recoil corrections are summarized. Among the recoil corrections there is only one logarithmic contribution in the parameter β [2]. The problem of existence of such different corrections is discussed on the basis of the quasipotential approach in [3, 4, 5, 6].

The three-dimensional relativistic approach to the description of bound states of two particles is developed [7, 8, 9] and allows one to find various logarithmic corrections in the parameter β to the magnitude of the fine shift of S-level energies in hydrogen-like atoms in sixth orders in the fine structure constant and to determine the conditions under which the contribution found in [2] is the only one. We consider the methods of quasipotential definition, used for the description of bound states of two particles. The equation for the Green function of two fermions can be written in a Schwinger form:

$$\{(\gamma\pi - M)_1(\gamma\pi - M)_2 - I_{12}\}G = I, \tag{1}$$

where $\pi = p - eA$; p is the 4-momentum of the particle, A is the external field, M is the mass operator of the particle, I_{12} is the interaction kernel of particles 1,2 and I is the unit operator. Equation (1) can also be written in the Bethe-Salpeter form:

$$G = g_0 + g_0 I_{12} G, \qquad g_0 = iG_1G_2 \tag{2}$$

where G_i is the free fermion function. The Coulomb kernel is separated as the main part of interaction:

$$I_{12} = K_C + \tilde{I}, \qquad K_C(\vec{p},\vec{q}) = \frac{e_1e_2\gamma_{10}\gamma_{20}}{(\vec{p}-\vec{q})^2}. \tag{3}$$

Then the Coulomb Green function is determined by the equation

$$\{(\gamma\pi - M)_1(\gamma\pi - M)_2 - K_C\}g_C = I, \qquad g_C = g_0 + g_0 K_C G_C. \tag{4}$$

Using Eq. (1) and (4) the Green's function can be written as

$$G = g_C + g_C \tilde{I} G. \tag{5}$$

To include the mass corrections into the interaction kernel it is convenient to use the expressions

$$G = G_C + G_C \tilde{K} G, \qquad G_C = G_0 + G_0 K_C G_C, \qquad G_0 = iS_1S_2, \qquad S_i^{-1} = (\hat{p} - m)_i. \tag{6}$$

$$\tilde{K} = I_{12} - [M_1 S_2^{-1} + S_1^{-1} M_2 - M_1 M_2] + K_C = K - K_C. \tag{7}$$

The wave function of the two-fermion system with total energy E satisfies the quasipotential equation

$$((\widehat{G^+})^{-1}(\vec{p},\vec{q};E) - \tilde{V}(\vec{p},\vec{q};E)\Psi_E(\vec{q}) = 0, \tag{8}$$

where the quasipotential is determined as

$$\tilde{V} = (\widehat{G_C^+})^{-1}(\widehat{(G_C\tilde{T}G_C)^+})^{-1}(\widehat{G^+})^{-1}, \tilde{T} = \tilde{K} + \tilde{K}G\tilde{K}. \tag{9}$$

This definition is the most general expression for two particles interaction quasipotential. The expansion of quasipotential has the form

$$\tilde{V} = \tilde{\tau}_C - \tilde{\tau}_C\,\widehat{G_C^+}\,\tilde{\tau}_C + \ldots, \qquad \tilde{\tau}_C = (\widehat{G_C^+})^{-1}(\widehat{(G_C\tilde{T}G_C)^+})^{-1}(\widehat{G_C^+})^{-1}. \tag{10}$$

We consider the quasipotential in the lowest approximation

$$\tilde{V}^{(2)} \approx \tilde{\tau}_C. \tag{11}$$

Let us discuss the simplest case, when the amplitude is defined as $\tilde{T}^{(2)} = K_T$,

$$K_T = -\frac{4\pi\alpha}{k_0^2 - \vec{k}^2 + i\varepsilon}(\vec{\gamma}_1\vec{\gamma}_2 - \frac{(\vec{\gamma}_1\vec{k})(\vec{\gamma}_2\vec{k})}{k^2}), \tag{12}$$

where K_T characterizes the exchange with transverse photon. The bound effects can be considered in the approximation

$$G_C \approx G_0 + G_0 K_C G_0. \tag{13}$$

This approximation allows one to describe the exchange by Coulomb and transverse photons. Using the equation for the Green's function of noninteracting particles and the result of projection on positive frequency states the inverse Green's function is represented as

$$(\widehat{G_C^+})^{-1} = F^{-1} - K_C^+, \qquad F = \widehat{G_0^+}\,. \tag{14}$$

Then the amplitude τ_C is defined by

$$\tau_C = (K_T)^+_{0F} + (K_C G_0 K_T)^+_{0F} - K_C^+ F (K_T)^+_{0F}$$
$$+(K_T G_0 K_C)^+_{0F} - (K_T)^+_{0F} F K_C^+ + (K^{(2)})^+_{0F}, \tag{15}$$

where the symbol $(X)^+_{0F}$ means $F^{-1}\,\widehat{X^+}\,F^{-1}$,$K^{(2)} = K_{CT} + K_{TC}$. Excluding the main Coulomb interaction and considering the exchanges by Coulomb and transverse photons, we can write the quasipotential as

$$V(\vec{p}, \vec{q}; E) = F^{-1} - (\widehat{G^+})^{-1} = F^{-1} - \tau_0 + \tau_0 F \tau_0 + \ldots, \tag{16}$$

where

$$\tau_0 = F^{-1}\,\overbrace{(G_0 T G_0)^+}\,F^{-1}, \qquad T = K + KGK. \tag{17}$$

Then using the Coulomb gauge for photon propagator we obtain

$$\tau_0 \cong (K_T)^+_{0F} + (K_C G_0 K_T)^+_{0F} + (K_T G_0 K_C)^+_{0F} + (K_{CT})^+_{0F} + (K_{TC})^+_{0F}. \tag{18}$$

Expression (18) is included in (15). Therefore, the block τ_0 is the part of the expression τ_C and quasipotential $\tilde{V}$. Note that if the quasipotential is determined in terms of τ_C, the reducible graphs and corresponding iterations are considered in the first order of perturbation theory. However, using the quasipotential (16) we obtain iterations only in the second order of the expansion.

$$V^{(2)} = (K_T)^+_{0F}, \tag{19}$$

$$V^{(4)} = (K_C G_0 K_T)^+_{0F} + (K_T G_0 K_C)^+_{0F}$$
$$-K_C^+ F (K_T)^+_{0F} - (K_T)^+_{0F} F K_C^+ + (K_{CT} + K_{TC})_{0F}. \tag{20}$$

The presence of iteration terms for each reducible graph, improving their behavior in the infrared region, is the main feature of the quasipotential. It should be noted that, because of the arising difference of reducible graphs and their iteration contributions, the main corrections to the Coulomb energy level from $V^{(2)}$ and $V^{(4)}$ are in one case of lower order and in the other of higher order in the fine structure constant α. As the number of events of Coulomb photon exchange increases in higher orders of perturbation theory, the conditions for the cancellation of the leading corrections in the differences of reducible diagrams and the corresponding iterations remain unchanged. Since the iterations correspond only to reducible graphs, the non-reducible diagram with single transverse photon is considered taking into account the multiple exchanges with Coulomb photons.

The described methods of constructing the quasipotential (9) and (16) are not isolated and constitute the system, connected by consistent transitions from the general to a particular case. For example, to describe the interactions of particles in hydrogen-like atoms in the low-frequency domain the quasipotential is used in the form

$$\tilde{V} = \frac{\tau_C}{1 + \widehat{G_C^+}\,\tau_C}. \tag{21}$$

The terms of G_C expansion series are of the same order in α, therefore one can use the non-relativistic analog G_C, that is the Green's function of the Schrödinger equation with the Coulomb potential. In the high-frequency domain one can iterate the equation for Coulomb Green's function and obtain the following expression for the quasipotential (21)

$$\tilde{V} = \frac{\tau_0}{1 + F\tau_0}. \tag{22}$$

Performing the contour integration over the zero components of momenta we can simplify the quasipotential (22). Taking the fermion propagator expressions via projection operators and using the residue theory one can obtain the expression for τ_0:

$$\begin{aligned} \tau_0 = T_+(\vec{p},\vec{q};E) + \textstyle\sum_{i=1}^{2}(\varepsilon_{ip} - E_i)\Delta T^{'}_{i+}(\vec{p},\vec{q};E) + \textstyle\sum_{i=1}^{2}(\varepsilon_{iq} - E_i)\Delta T^{''}_{i+}(\vec{p},\vec{q};E) \\ + \textstyle\sum_{i,j=1}^{2}(\varepsilon_{ip} - E_i)\Delta T^{'''}_{ij+}(\vec{p},\vec{q};E)(\varepsilon_{jq} - E_j), \qquad \varepsilon_{ip} = \sqrt{p^2 + m_i^2}. \end{aligned} \tag{23}$$

In many cases of investigation of energy levels of the hydrogen-like atoms up to the accuracy of terms of the order α^5 we can restrict ourselves to the first term of the sum in expression (23) that is we can use

$$\tau_0 \approx T_+(\vec{p},\vec{q};E), \qquad V = \frac{T_+}{1 + FT_+}. \tag{24}$$

Because in the weakly coupled systems the particles are located near the mass shell, one can use the scattering approximation to consider two photon interactions up to accuracy of order α^5 and replace $T_+(\vec{p},\vec{q};E)$ with $T_+(0,0;E)$

$$T_+(\vec{p},\vec{q};E) \Rightarrow T_+(0,0;E) \tag{25}$$

In the high virtual momenta domain, the matrix elements of scattering amplitude can be approximated on the mass shell and calculated at values of the momenta $|\vec{p}| \sim |\vec{q}| \cong 0, E \cong m_1 + m_2$. The on-shell scattering amplitude has poles in the infrared region. The infrared divergences are canceled by introduction of some minimum virtual momentum $k_{min} \cong \varepsilon$. The concrete value of ε is not important, because the infrared divergences are canceled in the sum of the diagrams. Then one can perform the change

$$T_+(0,0;E) \Rightarrow T_+^0(0,0;m_1 + m_2), \tag{26}$$

and the quasipotential is determined as

$$V = \frac{T_+^0(0,0;m_1 + m_2)}{1 + FT_+^0(0,0;m_1 + m_2)}. \tag{27}$$

We note that this quasipotential does not allow one to calculate exactly the corrections up to the accuracy $\alpha^6 \ln\alpha$ to the shift of S-energy levels of hydrogen-like atoms. In papers [8, 10] it is shown that for a more complete calculation of contributions of order $\alpha^6 \ln\alpha$ to the hyperfine shift of muonium it is required to use quasipotential expressed via the amplitude τ_0 (22).

Thus, to consider the concrete problem of bound states different methods of constructing the quasipotential are used. The connection between them is expressed in approximations used for an amplitude and can be describe schematically as:

$$\tau_C \to \tau_0 \to T_+ \to T_+(0,0;E) \to T_+^0(0,0;m_1+m_2). \tag{28}$$

The retardation effects are considered more accurately when the amplitude T_+ is used. The corresponding method of constructing the quasipotential allows one to obtain the correction of order $\alpha^6 \ln \alpha$. However, to calculate the logarithmic contributions completely, it is necessary to use the amplitude τ_0 and the relativistic modification of the Coulomb wave function [11]. So, according to our investigations [10, 12, 13, 14] the result for the hyperfine splitting of the ground energy levels of the positronium atoms was established up to the accuracy of $\alpha^6 \ln \alpha$

$$\Delta E_{hfs} = \frac{\alpha^4 m}{2}[\frac{7}{6} - \frac{\alpha}{\pi}(\frac{16}{9} + \ln 2) + \frac{5\alpha^2}{12}\ln \alpha^{-1}]. \tag{29}$$

The result (29) was obtained also in [15, 16].

Once the theoretical result for the hyperfine splitting of the ground energy levels in the muonium and positronium atoms has been reliably established up to the accuracy of $\alpha^6 \ln \alpha$, an effort to study the effect of recoil of the heavy particles was intensified. According to [11], the relativistic factor can give rise to logarithmic corrections only in the lowest order in α. Taking this into account, first we analyzed the effect of recoil on the fine shift of the S-levels of the muonium atom from the one photon exchange. For the hydrogen-like atom involving a nucleus of charge Ze it is established, that the general expression for the shift of the energy levels due to one photon interaction is given by

$$\delta E_T(n,l) = \frac{(Z\alpha)^6 \mu^5}{m_1^2 m_2^2 n^3}\frac{2\sqrt{2}}{\pi^2}\{\ln(1+\sqrt{2}) - \sqrt{2} - \beta \ln \beta^{-1}\} \ln \beta^{-1}. \tag{30}$$

By estimating the frequencies corresponding to these shifts of the energy levels we arrive at

$$\Delta\mathcal{E}(1S) \simeq 3,8kHz, \qquad \Delta\mathcal{E}(2S) \simeq 0,48kHz, \qquad \Delta\mathcal{E}(2S-1S) = -3,32kHz. \tag{31}$$

Note for comparison that the logarithmic contribution to the hyperfine shift of the ground energy levels in the muonium atom is equal to $11,29\ kHz$.

In analyzing two-photon diagrams, it turns out that one must take into account the multiple exchanges of Coulomb photons. However, the effects of binding manifest themselves only in the low-frequency region at virtual momentum values of $|\vec{k}| < \epsilon, \mu(Z\alpha)^2 \leq \varepsilon \leq \mu$, since the binding energy of a hydrogen-like atoms is small. In view of this it is reasonable to break down the interval of integration into the low- and the high-frequency regions. In the low-frequency domain the non-relativistic approximation can be efficiently applied. The quasipotential is defined via the amplitude τ_C and is given by

$$\tilde{V} = \tau_C - \tau_C(\widehat{G_C})^+ \tau_C + \ldots \ \approx T_+ - T_+ g_C T_+. \tag{32}$$

In the lowest approximation $T = K^{(1)} + K^{(2)}, K^{(1)} = K_T$, $K^{(2)}$ is shown in Figure1.

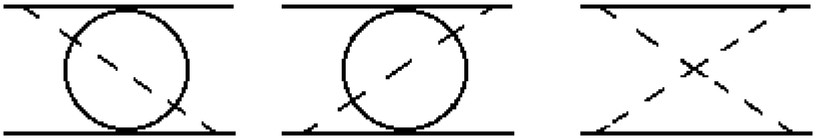

Fig.1. Diagrams of kernel $K^{(2)}$

In the high-frequency domain the Green's function G_C can be expanded in a series and in the investigation of two-photon exchanges, the quasipotential corresponds to the diagrams in Figure2.

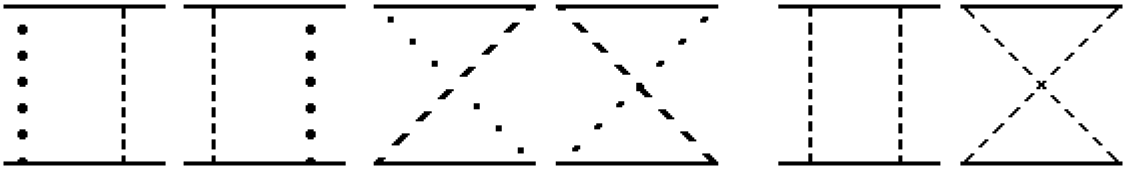

Fig.2. Diagrams of two photon exchange kernel.

The results of calculations of the logarithmic corrections in parameter β from one photon interaction (ΔE_T), two photon exchanges (ΔE_{CT},ΔE_{TT}) and iteration terms (ΔE_{it}) are given in Table 1.

Diagram	ΔE_T	ΔE_{CT}	ΔE_{it}	ΔE_{TT}
$\alpha^6\beta^2\ln\beta^{-1}$	0	0	0	$2\pi^{-1}$
$\alpha^6\ln\beta^{-1}$	$2\sqrt{2}\pi^{-2}[\ln(1+\sqrt{2})-\sqrt{2}]$	0	$-4\sqrt{2}\pi^{-2}[\ln(1+\sqrt{2})-\sqrt{2}]$	0
$\alpha^6\beta\ln^2\beta^{-1}$	$-\pi^{-2}$	$\sqrt{2}\pi^{-2}$	$2\pi^{-2}$	0

Table. 1

Note that the result of calculation of the logarithmic contribution in β of the exchange diagram with two transverse photons obtained in the quasipotential approach coincides with the corresponding quantity in [2]. This is the only such correction that must be found in the δ-approximation of the wave function. Other corrections of this type vanish in this approximation, and can be obtained only with the exact expressions of the Coulomb wave functions and quasipotential taken into account.

So, these new contributions to the $1S-2S$ shift of the energy levels are of order $10,26$ kHz for hydrogen and $66,67$ kHz for muonium. The experimentally determined shift of difference of $1S-2S$ levels is given by

$$\delta\nu^{exp}_{1S-2S} = 2466061413187,34(84)kHz. \tag{33}$$

for hydrogen [17] and

$$\delta\nu^{exp}_{1S-2S} = 2455528941,0(9,8)MHz. \tag{34}$$

for muonium [18]. Therefore, the analytic difference of the contributions to the $1S$ and $2S$ levels that we have found does not exceed the experimental errors. According to [17] new data of the classical Lamb shift of $2S_{1/2}-2P_{1/2}$ levels are

$$\Delta E^{Lth} = 1057833(4)kHz. \tag{35}$$

$$\Delta E^{Lexp} = 1057845(3) kHz. \tag{36}$$

We note that the numerical estimate obtained in our papers for the Lamb shift of $2S$ energy level in the hydrogen atom makes it possible to increase its theoretical value (35) by $1,5$ kHz and to reduce the distinction between the theoretical and experimental values of the classical Lamb shift.

References

[1] M.I. Eides, H. Grotch, V.A. Shelyuto, Phys. Rept. 342 (2001) 63

[2] T. Fulton, P.C. Martin, Phys. Rev. 95 (1954) 811

[3] N.A. Boikova, Yu.N. Tyukhtyaev, R.N. Faustov, Phys. At. Nucl., 61 (1998) 781

[4] N.A. Boikova, Yu.N. Tyukhtyaev, R.N. Faustov, Phys. At. Nucl., 64 (2001) 917

[5] N.A. Boikova, N.E. Nunko, Yu.N. Tyukhtyaev, R.N. Faustov, Teor. Mat. Phys. 132 (2002) 1179

[6] N.A. Boikova, S.V. Kleshchevskaya, Yu.N. Tyukhtyaev, R.N. Faustov, Phys. of At. Nucl., 66 (2003) 893

[7] Yu.N. Tyukhtyaev. Teor. Mat. Phys, 36 (1978) 264

[8] N.A. Boikova, Yu.N. Tyukhtyaev, R.N. Faustov, in: Problems of High Energy Physics and Quantum Field Theory, ed. IHEP, Protvino, 1983, vol. 1, p.116

[9] N.E. Nunko, Yu.N. Tyukhtyaev, R.N. Faustov. Yad. Fiz. 30 (1979) 457

[10] N.A. Boikova, Yu.N. Tyukhtyaev, R.N. Faustov, JINR Communications, Dubna, P2-81-582, 1981

[11] Yu.N. Tyukhtyaev, R.N. Faustov. JINR Communications, Dubna, P2-86-281, 1986

[12] N.E. Nunko, Yu.N. Tyukhtyaev, R.N. Faustov, in: Problems of High Energy Physics and Quantum Field Theory, ed. IHEP, Protvino, 1983, vol. 1, p.104

[13] N.A. Levchenko, Yu.N. Tyukhtyaev, R.N. Faustov, Yad. Fiz. 32 (1980) 1656.

[14] N.A. Levchenko, N.E. Nunko, Yu.N. Tyukhtyaev, JINR Communications, Dubna, P2-12355, 1979

[15] G.P.Lepage, Phys. Rev. A16 (1977) 863

[16] G.T. Bodwin, D.R. Yennie, Phys. Rept. C43 (1978) 267

[17] M.I. Eides, H. Grotch, V.A. Shelyuto, hep-ph/0002158.

[18] V. Meyer, S.N. Bagaev, P.E. Baird et. al., Phys. Rev. A51 (2000) 1854