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DOCTORAL THESIS

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Radiation corrections to atomic spectra

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I would like to express my sincerest thanks to my mentor Jaroslav Zamastil for his kind and general help.

I declare that I carried out this doctoral thesis independently, and only with the cited sources, literature and other professional sources.

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Název práce: Radiační korekce k atomovým spektrům.

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Abstrakt: V současné době dosáhla relativní přesnost experimentálních měření atomových spekter fantastické výše 1 díl v 10 na 14-tou. Jsou-li tato měření doprovázena teoretickými výpočty podobné přesnosti lze z porovnání teorie a experimentu testovat kvantovou elektrodynamiku, část standardního modelu zodpovědnou za paritu-narušující slabé interakce a určovat některé základní fyzikální konstanty jako je Rydbergova konstanta, hmotnost a poloměry jader, konstanta jemné struktury a její variace s časem atd. Pro dosažení takové přesnosti výpočtů je potřeba vzít v úvahu tzv. radiační korekce. Tato práce se zaměřuje na zpřesnění výpočtu nejdůležitější z nich, vlastní energie elektronu v jednosmyčkovém přiblížení.

Klíčová slova: Kvantová elektrodynamika, radiační korekce, vlastní energie elektronu.

Title: Radiation corrections to atomic spectra.

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Abstract: In present time accuracy of spectroscopic measurements achieved fantastic accuracy 1 part in 10 to the power 14. If these measures are followed by theoretical calculations of similar accuracy we can test quantum electrodynamics and part of the standard model responsible for parity violating weak forces by comparing theory and experiment and set some of the basic physical constants like Rydberg constant, mass and radius of nucleus, constant of fine structure and it´s variation in time etc. For achieving this kind of accuracy of calculations one must take into account so called radiation corrections. This thesis focus is on accurate calculation of the most important of them, the self-energy of electron in one-loop aproximation.

Keywords: Quantum electrodynamics, radiation corrections, self-energy of electron.

Contents

1. Introduction

1.1 Motivation

Since the early days of quantum mechanics the atomic spectra have been the tool to test our theoretical knowledge with experimental data. The greatest mystery and failure of classical physics, the stability of atom, lies tighly connected with explanation of spectral lines of particular atom. Since the discovery of hydrogen lines series and explanation using Bohr theory we have walked the long path. From the crudest estimate given by Schrödinger equation through relativistic Dirac equation correction to various quantum electrodynamics (QED) effects we have been systematically improving our knowledge and precision of the atomic spectra prediction as the ongoing experiments became more and more precise. At this time the quantum electrodynamics have become one of the most well-tested physical theories in history.

1.1.1 Survey of tests of QED

There are parameters that have to be taken from experiment as electron mass, electron charge, ratios of electron to proton and electron to muon masses $\frac{m_e}{m_p}$, $\frac{m_e}{m_\mu}$, nuclear parameters as nuclear radii, anomalous magnetic moment μ_N etc. Testing QED then means to keep consistency in determination of these parameters from various sources. These tests provide restrictions on the magnitude of the non-renormalizable electromagnetic interactions and give us information about nuclear structure. Brief summary of various experiments and information they provide is in the following table:

Experiment	Information
Lamb shift in hydrogen, deuterium, muonic hydrogen, antiproton helium	Rydberg constant, proton and deuterium charge radii, $\frac{m_e}{m_p}$, $\frac{m_e}{m_D}$
Ground state hyperfine transition in hydrogen, muonium, positronium	In principle α, in practice $\frac{m_e}{m_\mu}$. In hydrogen unknown proton structure. In positronium insufficient accuracy of both theory and experiment
Helium 2^3P fine structure	In principle α but disagreement of theory and experiment
Anomalous magnetic moment of electron and muon	α (the best), tests of hadronic contributions
Electron g-factor of bound electron	$\frac{m_e}{m_N}$, $\frac{\mu_e}{\mu_N}$

More detailed review can be found in [21, 30].

1.1.2 Comparison of theory and experiment in H-like atoms

Deviation of energy levels of hydrogen-like atoms from Dirac equation known as Lamb shift provides up to this day one of the most precise tests of quantum electrodynamics. Among various contributions to energy levels of bound electron the radiation corrections play important role [10]. Magnitude of contribution of the greatest of them, the one-loop self-energy is in the case of hydrogen comparable to that of relativistic correction following from Dirac equation. The greatest terms contributing to the $1s-2s$ energy shift are [30]

$$E^{nr}_{1s-2s} = 2.466038423 \times 10^{15}\text{Hz},$$

$$E^{rel}_{1s-2s} = 3.0117249662 \times 10^{10}\text{Hz},$$
$$E^{se}_{1s-2s} = -7.3120585916 \times 10^{9}\text{Hz},$$
$$E^{vp}_{1s-2s} = 1.879635023 \times 10^{8}\text{Hz},$$
$$E^{rec}_{1s-2s} = -2.0617519462 \times 10^{6}\text{Hz},$$
$$E^{rad-rec}_{1s-2s} = 1.213210227 \times 10^{4}\text{Hz},$$
$$E^{two-loop}_{1s-2s} = -6.3492111653 \times 10^{5}\text{Hz}.$$

The first two terms stand for non-relativistic Schrödinger energy and relativistic correction from effective Dirac equation (Eq. (10) in [30]). The third and fourth terms stand for the one-loop self-energy and one-loop vacuum polarization (Eqs. (19) and (22) in [30]). The term E^{rec}_{1s-2s} stands for the part of the recoil effect that cannot be covered by the shift from electron mass to reduced mass in effective Dirac equation (Eqs. (11) and (13) in [30]). The term $E^{rad-rec}_{1s-2s}$ stands for the radiative recoil. This is correction to the one-loop self-energy and vacuum polarization due to motion of nucleus that cannot be covered by the shift from electron mass to reduced mass (Eq. (56) in [30]). The final term stands for the two-loop correction (Eq. (29) in [30]). The sum of the above contributions is

$$E^{theo}_{1s-2s} = 2.466061414238446 \times 10^{15}\text{Hz}.$$

The most precise experimental data for $1s-2s$ shift are [33]

$$E^{exp}_{1s-2s} = 2.466061413187103(46) \times 10^{15}\text{Hz}.$$

The discrepancy between these two numbers is caused by the finite radius of proton, to which we direct our attention next.

1.1.3 Proton radius puzzle

The greatest uncertainty in theoretical determination of the $1s-2s$ transition comes from uncertainty in determination of the so called proton electric radius. Only when this issue is resolved more stringent tests of QED from Lamb shift can be obtained. The correction from finite structure of proton affects especially S-states whose radial wave function overlaps with proton. Radius of proton is defined as

$$r_p^2 = \int d^3r \rho(\vec{r}) r^2, \tag{1.1}$$

where $\rho(\vec{r})$ is charge density in proton. One possibility of obtaining this radius is from electron-proton scattering experiments. However, as discussed in [45] the value of r_p determined from scattering data depends strongly on the density $\rho(r)$ at large radii r. This density is poorly constrained by the scattering data. From critical analysis of the scattering experiments [4] one obtains root mean square of proton radius

$$r_p = 0.897(18) \times 10^{-15}\text{m}. \tag{1.2}$$

The scattering experiments data are not sufficient since uncertainty of this determination of r_p amounts to uncertainty of 21 kHz for $2s-1s$ transition. Therefore the problem can be reversed. In comparison of theory and experiment in the case of bound electron g-factor the QED holds to accuracy better than 1 part in 10^9 [46]. Thus, assuming that QED holds at least to this accuracy, one can use QED theoretical predictions in hydrogen atom to extract proton radius value. From comparison of theory and experiment in hydrogen (CODATA) [30]

$$r_p = 0.8768(69) \times 10^{-15}\text{m}. \tag{1.3}$$

These two determinations, (1.2) and (1.3) are compatible with each other. One may obtain the value of proton radius also from muonic hydrogen. Muonic hydrogen is more suited for the study of proton structure because mass of muon is about 200 times larger than that of electron. Corresponding Bohr radius for muon is thus smaller and muon feels the effects of finite proton structure more than electron in ordinary ep hydrogen. In contrast with ordinary hydrogen not the self-energy but the vacuum polarization effect is dominant QED effect in muonic hydrogen. From theoretical calculations one gets for the transition energy of $2s_{1/2} - 2p_{3/2}$ states in muonic hydrogen [35, 36, 5, 27, 28]

$$\Delta E = \left[209.9779(49) - 5.2262\langle r_p^2\rangle + 0.00913\langle r_p^3\rangle_{(2)}\right]\text{meV}.$$

The last term corresponds to the so called third Zemach moment,

$$\langle r_p^3\rangle_{(2)} = \int d^3r_1 d^3r_2 \rho(r_1)\rho(r_2)|\vec{r_1} - \vec{r_2}|. \tag{1.4}$$

In the case when the proton form-factor $G_E(-\vec{q}^2)$ is of dipole form,

$$G_E(-\vec{q}^2) = \int d^3\vec{r}\rho_p(\vec{r})e^{-i\vec{q}.\vec{p}} = \frac{m_d^4}{(\vec{q}^2 + m_d^2)^2} \tag{1.5}$$

there is a simple relation between the third Zemach moment and the proton radius [40]:

$$\langle r_p^3\rangle_{(2)} = \sqrt{\frac{3675}{64}}\langle r_p^2\rangle^{\frac{3}{2}}. \tag{1.6}$$

The Lamb shift in muonic hydrogen was measured in [39]. Low-energy muons were stopped at low-density H_2 gas where they formed highly excited μp atoms ($n \approx 14$). Most of these de-excited quickly to the $1s$ ground state but small amount populated the long-lived $2s$ state. Short laser pulse then induced the $2s \to 2p$ transition, immediately followed by the transition into ground state via emission of X-ray. The measured frequency corresponds to energy

$$\Delta E = 206.2949(32)\text{meV},$$

from which and Eq. (1.6) the proton charge radius

$$r_p = 0.84184(67) \times 10^{-15}\text{m} \tag{1.7}$$

can be deduced. Despite good precision of both approaches one arrives at different values for proton radius. Both results (1.3) and (1.7) are within 5σ from each other. This discrepancy is known as proton radius puzzle. In order to start thinking about more exotic explanations, one must first rule out possible error in theoretical calculations. In [40, 41] the possibility of non-dipole proton form factors was discussed. It was shown that the form of charge distribution influences significantly the third Zemach moment and its relation to proton radius and depending on the concrete model one may reduce the discrepancy between results (1.3) and (1.7) to 3σ-4σ. It thus seem highly plausible that the nontrivial charge distribution in proton may play a role in the proton radius puzzle.

1.1.4 Parity-nonconserving interactions

Another example of importance of the self-energy diagrams are the parity-nonconserving (PNC) interactions in atoms [6]. Measurements of the PNC in atoms provide sensitive tests of the Standard model. By comparison of theory and experiment we obtain tests of weak neutral currents and information about neutron distribution in nuclei. Example of these effects is highly forbidden $6s - 7s$ PNC amplitude in Cesium atom. The PNC effects were found to be enhanced by increase of Z (the Z^3 law), see [6] and references therein. Cesium ($Z = 55$) provides perfect compromise between enhancement of PNC effects and complexity of atomic structure. Exchange of Z^0 boson between nucleus and electron results in pseudoscalar term in transition amplitude. This in turn amounts for difference between the transition amplitude for normal and mirrored states. This difference is called left-right asymetry. As summarized in [6] or [8] the asymetry can be expressed as

$$\delta = 2\mathrm{Im}(E_P)/M \tag{1.8}$$

where E_P stands for the parity-violating dipole amplitude and M is the zeroth-order amplitude of magnetic dipole transition. The asymetry can be measured in both atomic measurements and scattering experiments of e^- on protons. In the case of Cesium $6s-7s$ transition the δ is -1.17×10^{-4} and is measured by different absorbtion of left- and right-handed photons. From these measurements one can obtain the weak charge Q_W. In order to establish the agreement with Standard model within 1σ, one has to take into account among other effects also the self-energy corrections to PNC amplitude. In papers [43, 44] the contribution of the self-energy diagrams was established to be $-0.67(3)\%$ of the whole effect. As in the case of proton radius the high-energy scattering experiments and low-energy atomic measurements are complementary to each other as each of them probes different domains of parameter space. This is shown schematicaly in Figure 2.1 (borrowed from the paper [6]).

1.2 Subject of this thesis

The main subject of this thesis is the accurate evaluation of the one-loop self-energy effect. The difference in two determinations of proton radius in (1.3) and (1.7) amounts to 82kHz for the $1s - 2s$ transition. Since the self-energy causes shift of 7.3GHz for the $1s - 2s$ transition one has to calculate the self-energy of bound electron with accuracy significantly better than 1 part in 10^5. The only calculation of such accuracy was performed in [17] using the method of partial wave expansion to be described later. However, in that article several million partial waves had to be calculated with three-dimensional numerical integration at every term and then extrapolated. Thus it is highly desirable to provide independent check of this result.

The self-energy of electron corresponds to interaction of electron with its own electromagnetic field. Electron in the presence of external potential emits and then reabsorbs virtual photon. Calculation of this process leads to divergent expression. One first regularizes the expression to get it well defined by replacing photon propagator $\frac{1}{k^2}$ by $\frac{1}{k^2} - \frac{1}{k^2-\Lambda^2}$, i.e. assumes that aside with "ordinary" massless photons there are very massive photons that couple with electrons in opposite way to massless photons. This procedure was first introduced by Feynman [13] and is rather inaccurately known as Pauli-Villars regularization. The measurable part of the self-energy effect is then the effect of self-interaction of bound electron with its own electromagnetic field from which is subtracted the part of the interaction contributing to the electromagnetic mass. This procedure is called renormalization. By this procedure one obtains convergent result which is at least of the order $\alpha(Z\alpha)^4$.

The expression for the self-energy follows from the formalism of bound state QED (Furry picture) (see [32] for details). The effect of the external potential is included in the wave function and the propagator from the very beginning. The difference from the free-particle case is in replacement of the canonical momentum P_μ by the physical momentum $\Pi_\mu = P_\mu - eA_\mu^{ex}$ where A_μ^{ex} is the four-potential of the external electromagnetic field. The renormalized expression for the self-energy in the non-recoil limit (neglecting motion of nucleus) reads

$$\Delta E = \langle O - \Delta m \rangle =< \psi|\gamma_0(O - \Delta m)|\psi >, \tag{1.9}$$

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

$$O = \frac{\alpha}{\pi} \int_0^{\Lambda^2} d\lambda \int \frac{d^4k_F}{(k^2-\lambda)^2} \gamma_\mu \frac{1}{\gamma.(\Pi - k) - m} \gamma_\mu. \tag{1.10}$$

In this thesis we concentrate on the case that is of greatest interest for determination of fine structure of hydrogen-like atoms, namely the case when the components of physical momentum Π of the particle are taken to be those in the external Coulomb field

$$\Pi = \left(E + \frac{Z\alpha}{R}, \vec{P}\right), \tag{1.11}$$

where $\vec{P}$ is the canonical three-momentum. The wave function ψ of the reference state is a solution of the stationary Dirac equation with the energy E

$$(\gamma.\Pi - m)\psi = 0 \tag{1.12}$$

and m is the electron mass. The notation we use is the following: d^4k_F stands for $i(2\pi)^{-2}d^4k$ and k stands for the four-momentum of the virtual photon. We use the summation convention $A.B = A_\nu B_\nu = A_0B_0 - \vec{A}.\vec{B}$. In particular, $k^2 = k_0^2 - \omega^2$, $\omega^2 = \vec{k}.\vec{k}$. 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. (1.10) we replace the electron mass m by $m - i\eta$ and take the limit $\eta \to 0$ from above. Symbol α stands for the fine structure constant. In actual calculation we took the value 1/137.03599911 given in [30].

It is convenient to write the self-energy in the form

$$\Delta E = \frac{m\alpha(Z\alpha)^4}{\pi n^3 s^3} F(Z\alpha, n, l_j) \tag{1.13}$$

where $F(Z\alpha, n, l_j)$ is dimensionless function. Here n, l, j stand for principal, orbital and total angular momentum quantum numbers, respectively and s is dimensionless factor to be discussed below. Further, it is convenient to write the self-energy effect on general S-state as

$$\Delta E_n = \frac{n^3 \Delta E_n - \Delta E_1}{n^3} + \frac{\Delta E_1}{n^3}, \tag{1.14}$$

where the first and the second terms on the right member will be referred to as the state-dependent and the state-independent parts of the S-states, respectively. The numerator in the first term is called normalized difference. The state-independent part of the S-states is by far the most dominant part of the whole effect.

Using Dirac equation and properties of γ matrices the expression for average of mass operator can be rewritten to more convenient form

$$\langle O \rangle = -\frac{\alpha}{2\pi} \left\langle \gamma_\mu \left(G_4 \Pi_\mu - \frac{m}{2} G.\gamma\gamma_\mu \right) \right\rangle, \tag{1.15}$$

where

$$G_{4,\nu} = (-4) \int_0^{\Lambda^2} d\lambda \int \frac{d^4 k_F}{(k^2 - \lambda)^2} \frac{(1, k_\nu/m)}{k^2 - 2k.\Pi + H}. \tag{1.16}$$

We thus made transition to expression containing the second-order Hamilton operator H

$$H = (\gamma.\Pi + m)(\gamma.\Pi - m) = \Pi.\Pi - m^2 + \frac{1}{4}[\Pi_\mu, \Pi_\nu][\gamma_\mu, \gamma_\nu]. \tag{1.17}$$

As discussed in greater detail in the section 2 we found the second-order form of self-energy (1.15) to be much more advantageous for actual evaluation than the first order form (1.10).

1.3 Difficulties in evaluation of the self-energy

The difficulties in calculation of the self-energy are following. The main problem is the presence of several scales. Integration over soft and hard photon regions are in both semi-analytical and numerical methods discussed in the next section treated separately. The hard photon region is crucial to get renormalization of the electron mass correctly. In this region the momentum imparted on virtual electron is so high that the electron can be in the first approximation treated as free. The electron propagator in (1.10) can then be expanded as

$$\frac{1}{\gamma.(\Pi - k) - m} = \frac{1}{\gamma.(p - k) - m} + \frac{1}{\gamma.(p - k) - m} e\gamma.A \frac{1}{\gamma.(p - k) - m} + \tag{1.18}$$

$$+\frac{1}{\gamma.(p-k)-m}e\gamma.A\frac{1}{\gamma.(p-k)-m}e\gamma.A\frac{1}{\gamma.(p-k)-m}+\dots$$

where the first term corresponds to free electron, second to 1-potential scattering, third to 2-potential scattering etc. The problem can be thus formulated as the multiple scattering of the electron by the external Coulomb field. On the other hand, the soft photon region, that is the region corresponding to emission and absorption of photon with very long wavelengths, is crucial to get rough estimate of the self-energy effect. As shown by Bethe the dominant part of the self-energy comes from this region. In this region the binding potential cannot be treated perturbatively but the motion of electron can be described as non-relativistic and a dipole approximation for the interaction of electron and photon can be used. Moreover, in both regions different gauges for photon propagator are often used in both numerical [32] and analytic [34] calculations. In the high-energy region the Feynman gauge is used while at low-energy region the transition to Coulomb gauge is used. Since the low-energy region itself is not gauge independent the correction term appears.

Another scale involves the integration over momentum of virtual electron. The squared Hamilton operator H, Eq. (1.17), with four-momentum Π given by Eq. (1.11) has for the continuous part of the spectrum eigenvalues

$$-\frac{H}{m^2}=(Z\alpha)^2[1+k_e^2(l_0+1)^2],\ k_e\in(0,\infty),\ l_0=\sqrt{1-(Z\alpha)^2}-1 \qquad (1.19)$$

in the case of ground state and similarly for excited states. The electron low-energy region stands for the discrete part of virtual electron spectra and continuous part for $k_e<\frac{1}{Z\alpha}$ (in atomic units). The high-energy electron region stands for the continuous part of the spectra with $k_e\geq\frac{1}{Z\alpha}$. The low-energy electron region contains dominant part of the effect, high-energy subdominant part.

Calculation of the one-loop self-energy contains integration over 11 variables. Four variables come from integration over photon four-momentum, 3+3 integrations follow from calculation of the matrix elements between reference and virtual electron states and finally one summation over discrete and one integration over continuous virtual electron spectrum. The angular variables can be integrated out analytically and also the radial integrations between reference and virtual states pose no problem as will be shown in section 2. The difficult integrals are those for photon variables k_0 and ω and electron variable k_e. At least the integration over k_e has to be treated numerically. It has long been thought that due to difference between soft and hard photon regions the virtual photon integration over both regions has to be treated separately. As will be shown in next section one actually can perform expansion of virtual electron propagator that covers both photon regions simultanously.

This difficulties in evaluation of the self-energy should be contrasted with evaluation of vacuum polarization, the second largest QED effect in ordinary atoms. There the finite electron mass provides natural cutoff for small momenta of virtual electron and potential expansion of the electron propagator (1.18) can be used without difficulty. The zero-, two- and so on potential scattering vanish because of Furry theorem. The one-potential scattering yields Uehling potential, by far the largest part of the effect. Three-potential term, of the order $(Z\alpha)^2$ smaller than Uehling potential, was calculated long time ago by Wichmann and Kroll

[47] using the exact Green function of the first-order Dirac Hamilton operator $H_D = \vec{\alpha}.\vec{p} + \beta m - \frac{Z\alpha}{R}$.

1.4 History of evaluation of one-loop self-energy

The self-energy of bound electron was first calculated by Bethe [3] in non-relativistic approximation. He used ordinary second order perturbation theory and in somewhat ad hoc manner obtained the energy shift of approximately 1040 MHz in good agreement with 1057 MHz $2s_{\frac{1}{2}} - 2p_{\frac{1}{2}}$ splitting measured for the first time by W. Lamb and R. Retherford [24]. Bethe's approach included non-relativistic and dipole approximations and was valid only for low frequencies ω of the virtual photon. The contribution from the high ω and high p momentum of electron region was calculated in [14, 23] by French and Weisskopf and by Kroll and Lamb. As mentioned above, in this region the bound electron propagator can be expanded in powers of external potential. The problem thus reduces to radiation scattering of free electron on external Coulomb potential. By inclusion of free and one-potential scattering the full contribution of $\alpha(Z\alpha)^4(A_{41}\ln(Z\alpha)^{-2} + A_{40})$ was thus obtained. In the works of Karplus, Klein and Swinger [20] and Baranger, Bethe and Feynman [2, 1] corrections of the order $\alpha(Z\alpha)^5$ were calculated by considering two-potential scattering term in the potential expansion of electron propagator. The corrections of the order $\alpha(Z\alpha)^6\ln(Z\alpha)^{-2}$ and $\alpha(Z\alpha)^6\ln^2(Z\alpha)^{-2}$ were later calculated in works of Layzer, Erickson and Yennie [15, 26, 11, 12]. Both of these corrections come from the region of low ω and the first of them also from the region of small p. After these works there was gap of almost 30 years where no significant progress was made. The advancement of computer power in nineties of last century sparked more progress in the field. In works of Pachucki, Jentschura and others the corrections of the order $\alpha(Z\alpha)^6$ for $1s$, $2s$ [34] and for excited states [16, 18] were added. In work of Karshenboim [22] the correction of order $\alpha(Z\alpha)^7\ln(Z\alpha)^{-2}$ was calculated, however the details of the calculation have not been published.

Thus, the self-energy function $F(Z\alpha, n, l_j)$ has been expressed as semi-analytical $Z\alpha$ expansion

$$
\begin{gathered}
F(Z\alpha, n, l_j) = A_{41}\ln s(Z\alpha)^{-2} + A_{40} + A_{50}(Z\alpha) + \qquad (1.20) \\
+(Z\alpha)^2\left[A_{62}\ln^2 s(Z\alpha)^{-2} + A_{61}\ln s(Z\alpha)^{-2} + A_{60}\right] + \\
+(Z\alpha)^3\left[\ln s(Z\alpha)^{-2}A_{71} + A_{70}\right] + \dots,
\end{gathered}
$$

where $s = 1$ in the non-recoil limit. The dominant part of the nucleus recoil is taken into account by replacing $s = 1$ in Eqs. (1.13) and (1.20) by $s = 1 + m_e/m_n$, see [32] and references therein. Here m_e/m_n is a ratio of the electron and nuclear masses. The coefficients A, $A = A(n, l_j)$, are summarized e.g. in [30, 17]. The first index in coefficients A_{ij} stands for the power of $Z\alpha$ while the second one stands for the power of $\ln s(Z\alpha)^{-2}$. For non-S-states and state-dependent part of the S-states simplification appears: coefficients A_{41}, A_{50} and A_{62} vanish. These are given by contributions of the states with very large electron wave numbers.

With the exception of the coefficients A_{60} and A_{71} the coefficients were calculated more than once. The analytic form of the coefficient A_{70} is unknown and even the form of the series beyond $\alpha(Z\alpha)^7$ term is not known. Considering the difficulty in obtaining the A_{60} coefficient there is no hope in extending this method anymore. Also, the accuracy of this expansion is sufficient for non-S-states and the state-depedent part of the S-states but not for the state-independent part of the S-states. The difference in results for the Lamb shift of the ground state obtained by means of the above mentioned semi-analytical expansion in $Z\alpha$ and non-perturbative result [17, 54] for hydrogen ($Z = 1$) is 24kHz. Such uncertainty is not significantly less than 82kHz coming from the proton radius uncertainity. *It is thus inevitable to leave the $Z\alpha$ expansion and obtain result that does not completely rely on it.*

The more recent approach for calculation of the self-energy that avoids $Z\alpha$ expansion is based on partial wave expansion (PWE). This approach was initiated in early works [7, 9, 31] and considerably improved recently in [17, 48]. For review of the whole approach see [32]. In this method the average of mass operator (1.10) is written as

$$\langle O\rangle = -\frac{\alpha}{\pi}\int_0^{\Lambda^2} d\lambda \int \frac{idk_0}{(2\pi)^2}\int \frac{d^3k}{(k_0^2-\omega^2-\lambda)^2} \tag{1.21}$$

$$\int d^3\vec{r}_1 d^3\vec{r}_2 \psi^+(\vec{r}_1)\gamma_0\gamma_\mu e^{i\vec{k}.\vec{r}_1} G(-k_0+E,\vec{r}_1,\vec{r}_2)e^{-i\vec{k}.\vec{r}_2}\gamma_0\gamma_\mu\psi(\vec{r}_2).$$

The function $G(z,\vec{r_1},\vec{r_2})$ is the Green function of the first-order Dirac Hamilton operator,

$$(z-H_D)G(z,\vec{r}_1,\vec{r}_2) = \delta(\vec{r}_1-\vec{r}_2) \tag{1.22}$$

where

$$H_D = \vec{\alpha}.\vec{p} + \beta m - \frac{Z\alpha}{r}. \tag{1.23}$$

The Green function is expressed in terms of Whittaker functions [32]. Integration contour over k_0 is conveniently deformed. Integrals over $\vec{k}$, $\vec{n}_1$ and $\vec{n}_2$ are performed analytically, however one ends with three-dimensional numerical integration over k_0, r_1 and r_2. This method suffers from problems with renormalization since the manifest Lorentz invariance of mass operator is broken at the very beginning of calculation. The self-energy is expressed as expansion over the angular momentum of virtual photon or, equivalently, the total angular momentum of the virtual electron states $j = |\kappa| - 1/2$ where κ is the relativistic angular-momentum parameter of the Dirac equation. The individual partial-wave expansion contributions to the function $F(Z\alpha)$ go roughly as $F_{|\kappa|} \approx \frac{n^3}{(Z\alpha)^2|\kappa|^3}$. Thus, the convergence of this expansion greatly slows down for light atoms (low Z) and increasing principal quantum number n of the state under consideration. This is the consequence of improper treatment of $\alpha(Z\alpha)^5$ terms that contribute in every order of PWE. This method is thus viable only for high Z and lower lying states. To calculate the self-energy for atoms with $Z < 10$ either the method for acceleration of slowly convergent series was invoked [17] or the terms causing the convergence problem were indentified and evaluated separately [48]. However, the precision of the latter approach is not sufficient, it is lower than the perturbation approach.

2. The Method

2.1 Second-order form of self-energy

Relativistic generalisation of the multipole expansion (RME) is based on the second-order form of self-energy, see Eqs. (1.15), (1.16). The second-order form of self-energy was first introduced in the work of Karplus, Klein and Schwinger [20], later elaborated further in work of Erickson and Yennie [11]. The advantages of using the second-order operator are that with the help of integration over Feynman parameters it enables us to avoid the decomposition into soft and hard photon regions in the integration over photon four-momentum. Moreover, it allows the separation of spinor-angular and radial parts in electron virtual states and the non-relativistic approximation does not spoil renormalizability in contrast to the first-order form [19]. Also, the radial eigenfunctions of the second-order Hamilton operator (1.17) are of similar form as non-relativistic Schrödinger radial functions.

The second-order Hamilton operator H, Eq. (1.17), for the case of the four-momentum of virtual electron given by (1.11) reads

$$H = E^2 - m^2 - \left(P_R^2 + \frac{\Gamma(\Gamma-1)}{R^2} - \frac{2EZ\alpha}{R} \right) \tag{2.1}$$

where the operator Γ is given by

$$\hat{\Gamma} = \gamma_0 \hat{K} + i\alpha Z \vec{\alpha}.\vec{n} \tag{2.2}$$

and

$$\hat{K} = \gamma_0 (\vec{\Sigma} \cdot \hat{\vec{L}} + 1) \tag{2.3}$$

is the relativistic parity operator, $\vec{\Sigma}/2$ is the spin operator and $\vec{L}$ is the angular momentum operator. The corresponding eigenvalues are

$$\Gamma = \pm\sqrt{K^2 - (Z\alpha)^2} \tag{2.4}$$

and

$$K = \pm(j + 1/2). \tag{2.5}$$

Operators $\{\hat{H}, \hat{\Gamma}, \hat{K}, \hat{J}^2, \hat{J}_z\}$, where $\vec{J}$ stands for total momentum, form the complete set of commuting operators. One can thus find their eigenfunctions and decompose Hamilton operator H using them. However, when expressing the solution of the first order Dirac Eq. (1.12) using these eigenfunctions one has to take linear combination of them since the operator Γ does not commute with the first-order Dirac Hamilton operator (1.23). The spectral decomposition of generic function of H reads

$$f(H) = \sum \frac{|\Gamma, K, j, m\rangle\langle\Gamma, K, j, m|\gamma_0}{\langle\Gamma, K, j, m|\gamma_0|\Gamma, K, j, m\rangle} f(H_{l_\Gamma}). \tag{2.6}$$

Here $l_\Gamma = |\Gamma| - 1$ in the case of $\Gamma > 0$ and $l_\Gamma = |\Gamma|$ for $\Gamma < 0$. The presence of the Dirac matrix γ_0 in (2.6) follows from the fact that Γ is not hermitian operator but $\gamma_0\Gamma$ is. The radial Hamiltonian H_{l_Γ} reads

$$H_{l_\Gamma} = E^2 - m^2 - \left(P_R^2 + \frac{l_\Gamma(l_\Gamma+1)}{R^2} - \frac{2EZ\alpha}{R} \right). \tag{2.7}$$

2.2 Expansion of propagator

2.2.1 Operator form of RME

In order to evaluate (1.15) one has to perform expansion of electron propagator. The key idea of our method introduced for the first time in [52] and further elaborated in [53, 54] is that the four-momentum Π of bound electron in the virtual states is dominated by the four-momentum

$$\varepsilon = (m, \vec{0}) \tag{2.8}$$

of the electron at rest and the electron propagator $(k^2 - 2k.\Pi + H)^{-1}$ can thus be expanded in powers of their difference. This expansion has been motivated by the following considerations. First, the dominant contribution to the self-energy of bound electron for low values of nuclear charge Z comes from the integration over low frequencies of the virtual photon and low wave numbers k_e of the virtual electron ($k_e \approx 1$ in atomic units). The greatest overlap between reference state and virtual states of the electron lies in this region. In this region the virtual electron momentum $\vec{p} \approx mZ\alpha k_e \approx mZ\alpha$ is small compared to the rest mass m. The contribution from the soft photon region in the leading order can be expressed in terms of the Bethe logarithm,

$$\langle p_i H_0 \ln(H_0) p_i \rangle, \tag{2.9}$$

which contains explicitly the non-relativistic limit H_0 to the second-order Hamilton operator H. To get this contribution right and to avoid infrared divergencies, H has to be kept at the leading approximation of the propagator. Making transition from natural to atomic-like units

$$R = \frac{r}{EZ\alpha}, \tag{2.10}$$

the difference between physical momentum Π and momentum of the particle at rest ε is

$$\Pi - \varepsilon = \left(E - m + \frac{E(Z\alpha)^2}{r}, EZ\alpha\vec{p} \right). \tag{2.11}$$

Since $E - m = O(Z\alpha)^2$, for small $Z\alpha$ the time component of $\Pi - \varepsilon$ is of the order $(Z\alpha)^2$ while the space component is of the order $Z\alpha$. This will be called naive counting. As will be shown later this naive counting does not entirely work due to contribution from the high-energy electron region. Nonetheless, for the low-energy region this holds and results in fast convergence of the RME.

The operator form of the RME is

$$\frac{1}{k^2 - 2k.\Pi + H} = \frac{1}{k^2 - 2k.\varepsilon + H} + \frac{1}{k^2 - 2k.\varepsilon + H} 2k.(\Pi - \varepsilon) \frac{1}{k^2 - 2k.\varepsilon + H} + \tag{2.12}$$

$$+ \frac{1}{k^2 - 2k.\varepsilon + H} 2k.(\Pi - \varepsilon) \frac{1}{k^2 - 2k.\varepsilon + H} 2k.(\Pi - \varepsilon) \frac{1}{k^2 - 2k.\varepsilon + H} + \dots .$$

This can be brought to more convenient form. The second term on the right member of Eq. (2.12) can be written as

$$\frac{1}{k^2 - 2k.\varepsilon + H} 2k.(\Pi - \varepsilon) \frac{1}{k^2 - 2k.\varepsilon + H} = 2k.(\Pi - \varepsilon)_1 D_1 \left[\frac{1}{k^2 - 2k.\varepsilon + H} \right] \tag{2.13}$$

and the third as

$$\frac{1}{k^2-2k.\varepsilon+H}2k.(\Pi-\varepsilon)\frac{1}{k^2-2k.\varepsilon+H}2k.(\Pi-\varepsilon)\frac{1}{k^2-2k.\varepsilon+H}= \tag{2.14}$$

$$=(2k).(\Pi-\varepsilon)_1(2k).(\Pi-\varepsilon)_2D_2\left[\frac{1}{k^2-2k.\varepsilon+H}\right].$$

The symbols $D_1[f(H)]$ and $D_2[f(H)]$ stand for

$$D_1[f(H)]=\frac{f(H_{01})}{H_{01}-H_{12}}+\frac{f(H_{12})}{H_{12}-H_{01}}, \tag{2.15}$$

$$D_2[f(H)]=\frac{f(H_{01})}{(H_{01}-H_{12})(H_{01}-H_{23})}+ \tag{2.16}$$

$$+\frac{f(H_{12})}{(H_{12}-H_{01})(H_{12}-H_{23})}+\frac{f(H_{23})}{(H_{23}-H_{01})(H_{23}-H_{12})}$$

and so on. Components of Π do not mutually commute and also do not commute with H so the ordering of operators in the latter equations is governed by indices in expressions. For example, $H_{01}(\Pi-\varepsilon)_1H_{12}$ means that the first operator that acts on the bra vector is H_{01}, after that acts the operator $\Pi-\varepsilon$ and finally the operator H_{12}. Using this formalism one can treat the operators involved as numbers.

It seems that with rearrangements (2.13), (2.14) we are going into troubles when integrating over four-momentum k of virtual photon since with increasing order of the expansion more powers of k appears in the numerator while the same power of k is in the denominator. However, since $D_n[f(H)]$ is determined up to the polynomial of the $n-1$ order in H, e.g.

$$D_1[a_0]=0,\ D_2[a_0+a_1H]=0, D_3[a_0+a_1H+a_2H^2]=0 \tag{2.17}$$

and so on, we can rewrite the pertinent expressions by means of parametric differentiation as

$$2k.(\Pi-\varepsilon)_1D_1\left[\int_0^H dw\frac{d}{dw}\frac{1}{k^2-2k.\varepsilon+w}\right]= \tag{2.18}$$

$$=-(\Pi-\varepsilon)_{1\lambda}\frac{\partial}{\partial\varepsilon_\lambda}D_1\left[\int_0^H\frac{dw}{k^2-2k\varepsilon+H}\right]$$

and

$$(2k).(\Pi-\varepsilon)_1(2k).(\Pi-\varepsilon)_2D_2\left[\frac{1}{k^2-2k.\varepsilon+H}\right]= \tag{2.19}$$

$$=(\Pi-\varepsilon)_{1\lambda}(\Pi-\varepsilon)_{2\rho}\frac{\partial^2}{\partial\varepsilon_\lambda\partial\varepsilon_\rho}D_2\left[\int_0^H\frac{d^2w}{k^2-2k.\varepsilon+w}\right].$$

Here $\int_0^H d^2w=\int_0^H dw_2\int_0^{w_2}dw_1$ etc. Now, the crucial observation is that all the terms containing integration over photon four-momentum k are of the same form. The only integral that needs to be evaluated is the integral

$$\int_0^{\Lambda^2}d\lambda\int\frac{d^4k_F}{(k^2-\lambda)^2}\int_0^H d^nw\frac{(1,k_\nu)}{k^2-2k.\varepsilon+w}= \tag{2.20}$$

$$= \int_0^{\Lambda^2} d\lambda \int \frac{d^4k_F H^n}{(k^2-\lambda)^2} \int_0^1 d^n w \frac{(1,k_\nu)}{k^2-2k.\varepsilon+wH} =$$

$$= -\frac{1}{4}H^n \int_0^1 d^n w \int_0^1 dy(1, y\varepsilon_\nu)\Big(\ln(\varepsilon^2 y - wH) - \ln(\Lambda^2(1-y)/y)\Big)\,.$$

In the first equality the transition $w \to wH$ was made. In the last equality we neglected the terms involving inverse powers of cutoff Λ.

The operator form of RME is advantageous when only few terms of RME have to be calculated. This is the case of the non-S-states and normalized difference for the S-states. These cases will be referred to as excited states. In general one can always reduce the number n of spectral decompositions of H in expressions $(\Pi-\varepsilon)_{1\mu}(\Pi-\varepsilon)_{2\nu}\ldots(\Pi-\varepsilon)_{n\rho}D_n[f(H)]$ to one, see [53], but with increasing number of terms it is more advantageous to go to explicit form discussed in next section instead of the operator form.

For the excited states and low Z tremendous simplification appears. Contribution of the high-energy electron region cancels out nearly completely. Then only few terms of RME expansion have to be calculated to get very accurate results. Part of the calculation can be done in good approximation analytically. The other part can be done in non-relativistic approximation. For details see the attached article [53].

2.2.2 Illustrative calculation - leading part of the effect

As illustrative example of the method we evaluate the leading order of the effect using operator form of RME. From expressions (1.9), (1.10) and (1.16) and expansion (2.12) with (2.18) and (2.19) we get the leading order term

$$\begin{aligned}\langle O\rangle \simeq -\frac{\alpha}{2\pi}\langle\gamma_\mu G_4\Pi_\mu\rangle \simeq -\frac{\alpha}{2\pi}(-4)\int_0^{\Lambda^2} d\lambda \int \frac{d^4k_F}{(k^2-\lambda)^2}\Big\langle\gamma_\mu\Big(&\frac{1}{k^2-2k.\varepsilon+H}+ \\ +(\Pi-\varepsilon)_{1\lambda}\frac{\partial}{\partial\varepsilon_\lambda}D_1\left[\int_0^H\frac{dw}{k^2-2k.\varepsilon+w}\right]&+ \\ +(\Pi-\varepsilon)_{1\lambda}(\Pi-\varepsilon)_{2\rho}\frac{\partial^2}{\partial\varepsilon_\lambda\partial\varepsilon_\rho}D_2\left[\int_0^H\frac{d^2w}{k^2-2k.\varepsilon+w}\right]&\Big)\Pi_\mu\Big\rangle\,,\end{aligned} \tag{2.21}$$

where we neglected the terms $\langle\gamma_\mu G_\nu\gamma_\nu\gamma_\mu\rangle(-\frac{m}{2})$ in comparison with $\langle\gamma_\mu G_4\Pi_\mu\rangle$. The term with G_ν contains k_ν in the numerator and contributes mainly to hard photon region. The integral over photon four-momentum can be evaluated using Eq. (2.20). In the second term in (2.21), containing differentiation $\partial/\partial\varepsilon_\lambda$ the following replacement is made

$$\ln\frac{\varepsilon^2 y - w}{m^2 y} \to \frac{2\varepsilon_\lambda y}{m^2 y - w} \tag{2.22}$$

and in the third term with the differentiation $\partial^2/\partial\varepsilon_\lambda\partial\varepsilon_\rho$ the replacement

$$\ln\frac{\varepsilon^2 y - w}{m^2 y} \to \frac{2\eta_{\lambda\rho}y}{m^2 y - w} + \varepsilon_\lambda\varepsilon_\rho\frac{4y^2}{(m^2y-\omega)^2} \tag{2.23}$$

is made. For now we neglect the second term on right member of the last equation. Substituting this into (2.21) we get

$$\begin{aligned}\langle O\rangle \simeq -\frac{\alpha}{2\pi}\Big\langle \gamma_\mu \int_0^1 dy \ln\frac{m^2y-H}{m^2y}\Pi_\mu + \\ +m\Big\{(\Pi-\varepsilon)_{1\lambda}\varepsilon_\lambda D_1\Big[\frac{2}{m^2}\int_0^1 dy\int_0^H dw+\frac{2}{m^4}\int_0^1 dy\int_0^H dw\frac{w}{\left(y-\frac{w}{m^2}\right)}\Big]+ \\ +(\Pi-\varepsilon)_{1\lambda}(\Pi-\varepsilon)_{2\lambda}D_2\Big[\frac{2}{m^2}\int_0^1 dy\int_0^H d^2w+\frac{2}{m^4}\int_0^1 dy\int_0^H d^2w\frac{w}{\left(y-\frac{w}{m^2}\right)}\Big]\Big\}\Big\rangle - \\ -\frac{m\alpha}{2\pi}\langle 1\rangle\int_0^1 dy\ln\frac{m^2y}{\Lambda^2(1-y)}.\end{aligned}\tag{2.24}$$

For the second and third terms on the right member of Eq. (2.21) we used relation

$$\langle\gamma_\mu Q\Pi_\mu\rangle = m\langle Q\rangle + \langle[\gamma_\mu, Q]\Pi_\mu\rangle \tag{2.25}$$

and neglected the second term which is at least by factor $Z\alpha$ smaller. The last term in (2.24) is contributing to the electromagnetic mass and is removed by renormalization. To evaluate the rest of expression (2.24) one must evaluate action of D_1 and D_2. This is however quite simple for polynomial functions of H:

$$D_1[H] = 1,\ D_2[H^2] = 1. \tag{2.26}$$

Furthermore, since $H\psi = 0$ for reference state ψ we have for $f(H) \to H^2$ when $H \to 0$

$$D_1[f(H)]\mid_{H_{01}=H_{12}=0} = 0 \tag{2.27}$$

and similarly for $f(H) \to H^3$ when $H \to 0$ we get

$$D_2[f(H)]\mid_{H_{01}=H_{23}=0} = \frac{f(H_{12})}{H_{12}^2}. \tag{2.28}$$

With help of these equations we may finally write the leading part of the effect as

$$\begin{aligned}\langle O\rangle \simeq -\frac{\alpha}{2\pi}\Big\langle \gamma_\mu \int_0^1 dy \ln\frac{m^2y-H}{m^2y}\Pi_\mu + \\ +m(\Pi-\varepsilon)_\mu\frac{2}{m^4}\int_0^1 dy\frac{1}{H^2}\int_0^H d^2w\frac{w}{\left(y-\frac{w}{m^2}\right)}(\Pi-\varepsilon)_\mu + \frac{1}{m^2}(\Pi.\Pi-m^2)\Big\rangle.\end{aligned}\tag{2.29}$$

In the last term one can recognise part of the anomalous magnetic moment of electron since

$$\langle(\Pi.\Pi-m^2)\rangle = -\frac{1}{4}\langle[\gamma_\mu,\gamma_\nu][\Pi_\mu,\Pi_\nu]\rangle \tag{2.30}$$

where we have again used the fact that the action of H on reference state yields zero and Eq. (1.17). The first two terms in Eq. (2.29) contain the Bethe logarithm in the non-relativistic limit. The equation (2.29) yields 94% of the whole effect for the ground state.

2.2.3 Explicit form of RME

The explicit form of RME is more suited for the cases when the large number of terms in RME has to be calculated. One can eliminate the space component of Π in the electron propagator by formula

$$\frac{1}{k^2 - 2k.\Pi + H} = e^{i\vec{k}.\vec{R}} \frac{1}{k^2 - 2k_0\Pi_0 + H + \omega^2} e^{-i\vec{k}.\vec{R}}. \tag{2.31}$$

The exponentials on the right member of the last equation are then decomposed using partial wave expansion,

$$e^{i\vec{k}.\vec{R}} = 4\pi \sum_{L=0}^{\infty} i^l j_L(\omega R) \sum_{m=-L}^{m=L} Y^*_{L,m}(\vec{n}) Y_{L,m}(\vec{\eta}) \tag{2.32}$$

where $\vec{n}$ and $\vec{\eta}$ are the unit vectors in the direction of $\vec{R}$ and $\vec{k}$, respectivelly. Each of them contains spherical harmonics which contribute to the spinor-angular integration. The spinor-angular integrations can be for all terms contained in (1.16) calculated in the closed form by means of algebraic methods, for details see attachment 4. The expansion in space components of $(\Pi - \varepsilon)$ is then obtained by expanding the whole expression (2.31) in powers of ω. To that end the expansion of spherical Bessel functions $j_L(\omega R)$ in power series in ωR

$$j_L(\omega R) = \sum_{q=0}^{\infty} \left(-\frac{1}{2}\right)^q \frac{(\omega R)^{L+2q}}{q!(2L+2q+1)!!}. \tag{2.33}$$

is usefull.

Furthermore, the explicit appearance of Π_0 in (2.31) can also be eliminated. The term $-2k_0\Pi_0 + H$ can be rewritten by using the form of H, Eq. (2.1), as follows

$$-2k_0\Pi_0 + H = -2k_0E + E^2 - m^2 + \frac{2EZ\alpha}{R}\left(1 - \frac{k_0}{E}\right) - P_R^2 - \frac{\Gamma(\Gamma-1)}{R^2}. \tag{2.34}$$

Performing substitutions

$$R = \frac{r}{EZ\alpha\xi},\ \xi = 1 - \frac{k_0}{E} \tag{2.35}$$

one expresses from Eqs. (2.31)-(2.35) the self-energy as a sum of the terms of the form

$$\left\langle l_0+1, l_0 \left| r^a \frac{1}{k^2 - 2k_0\Pi_0 + H + \omega^2} r^b \right| l_0+1, l_0 \right\rangle = \tag{2.36}$$

$$= \int_0^{\infty} dk_e \frac{\langle l_0+1, l_0|r^a|k_e, l_\Gamma\rangle_\xi\ {}_\xi\langle k_e, l_\Gamma|r^b|l_0+1, l_0\rangle}{(k^2 - 2k_0E - (Z\alpha m)^2(1 + (l_0+1)^2k_e^2\xi^2) + \omega^2)} +$$

$$+ \sum_{n=l_\Gamma+1}^{\infty} \frac{\langle l_0+1, l_0|r^a|n, l_\Gamma\rangle_\xi\ {}_\xi\langle n, l_\Gamma|r^b|l_0+1, l_0\rangle}{(k^2 - 2k_0E - (Z\alpha m)^2(1 - (l_0+1)^2\xi^2/n^2) + \omega^2)}$$

where $\langle r|k_e, l_\Gamma\rangle_\xi = R_{k_e,l_\Gamma}(\xi r)$. The radial overlap integrals between reference and virtual states can be evaluated analytically using formula [25]

$$\langle l_0+1, l_0|r^p|k_e, l_\Gamma\rangle_\xi = \int_0^{\infty} dr r^{2+p} R_{l_0+1,l_0}(r) R_{k_e,l}(\xi r) = \tag{2.37}$$

$$= \frac{2C_{k_e,l}}{(l_0+1)^{l_0+2}} \frac{2^{l_0+l}}{\sqrt{(2l_0+1)!}} \frac{k_e^l}{(2l+1)!} \Gamma(l_0+l+p+3) \left(\frac{1}{l_0+1}+ik_e\xi\right)^{l_0+l+p+3} \times$$

$$\times F\left(i/k_e+l+1, l_0+l+p+3, 2l+2, \frac{2ik_e\xi}{\frac{1}{l_0+1}+ik_e\xi}\right)$$

where

$$C_{k_e,l} = \sqrt{\frac{2}{\pi}} k_e e^{\pi/k_e} |\Gamma(l+1-i/k_e)| \xi^{l+\frac{3}{2}} \tag{2.38}$$

is the normalization constant for the continuous part of the spectrum. The integrals for discrete part of the spectrum are obtained by the substitution $k \to -i/n$ and change of normalization constants $C_{k_e,l}$ to $C_{n,l}$. In the case when the radial function of reference state R_{n_0,l_0} is not nodeless, i.e. $n_0 \neq l_0+1$ one can always bring the integrals $\int_0^\infty drr^{2+p} R_{n_0,l_0} R_{k_e,l}$ to the form of linear combination of integrals (2.37) by recursive relations for radial functions, for details see attached article [53] or [51].

2.2.4 RME and summation of $\alpha(Z\alpha)^5$ terms

For the ground state the contribution of the electron virtual states with very high wave numbers k_e requires separate treatment. These states contribute at the order $\alpha(Z\alpha)^5$ and are contained in RME in the form of slowly convergent series.

The region from which the $\alpha(Z\alpha)^5$ terms come from is characterised by the limit of low $Z\alpha$ and high k_e. The limit of small $Z\alpha$ is obtained by reducing the wave functions into the non-relativistic Schrödinger functions and taken into account relativistic correction due to the term $\vec{\alpha}[\vec{p}, V]$ (spin-orbit interaction) up to the second order. In limit of high k_e and small $Z\alpha$ the matrix elements between the reference and virtual electron states simplify considerably. Contribution of terms $\alpha(Z\alpha)^5$ can then be evaluated analytically. The example how to obtain $\alpha(Z\alpha)^5$ terms is in the next section. The order v of RME is given by collecting all the terms of the order $(Z\alpha)^{2v}$ by naive counting. One can write the expression for $\alpha(Z\alpha)^5$ contribution at order v of RME as [54]

$$A_{50}^{(v)} = -2^3 \frac{\Gamma\left(\frac{1}{2}\right)\Gamma\left(v-\frac{5}{2}\right)(16v^4-32v^3+296v^2+8v-267)}{\pi\Gamma(v)(2v+5)(2v+3)(2v+1)^2(2v-3)}. \tag{2.39}$$

where the full coefficient A_{50} is obtained by summing the terms (2.39) to infinity,

$$A_{50} = \sum_{v=1}^{\infty} A_{50}^{(v)} \tag{2.40}$$

and is equal to

$$A_{50} = 4\pi\left(\frac{139}{128} - \frac{\ln 2}{2}\right) \tag{2.41}$$

in agreement with the results obtained from other methods [1, 2, 11, 12, 15, 20, 26]. With the slowest converging term in RME indentified we can improve the accuracy of the method by subtracting the $\alpha(Z\alpha)^5$ contribution from every order of RME expansion and adding the full A_{50} coefficient. The self-energy function $F(Z\alpha)$ can then be written as

$$F(Z\alpha) = (Z\alpha)A_{50} + \sum_{v=1}^{\infty} S_v, \tag{2.42}$$

where

$$S_v = F_v - (Z\alpha)A_{50}^{(v)}. \tag{2.43}$$

In the function F_v all the terms contributing at the same order of $Z\alpha$ by naive counting are collected. For the explicit form of corresponding terms see the attached article [54]. In [54] RME was calculated up to the ninth order. After this order the results started to be affected by numerical instabilities. However, for the needed accuracy the ninth order was sufficient. Every order of RME contains expansion in both time and space components of $(\Pi - \varepsilon)$. We found the contribution of higher temporal multipoles to be highly suppresed. In fact for low Z one does not have to take the expansion in time component to more than the third order and in some terms even to the second order.

The remainder of terms not accounted for in the expansion up to the ninth order could be estimated. We observed that for increasing v the ratios of S_v/S_{v-1} approach the ratio $A_{50}^{(v)}/A_{50}^{(v-1)}$. One can then make estimate

$$F_{rem} \simeq \frac{S_V}{A_{50}^{(V)}} \sum_{v=V+1}^{\infty} A_{50}^{(v)} = \frac{S_V}{A_{50}^{(V)}} \left(A_{50} - \sum_{v=1}^{V} A_{50}^{(v)} \right), \tag{2.44}$$

where $V = 9$. Even for higher nuclear charges this ratio tends to hold, although the coefficients S_v differ for different Z in the magnitude significantly. Still, this estimate could not be completely justified and remains to be proved. Nonetheless, the estimate of remainder improves agreement with PWE by 1-2 orders for Z up to 20. For stronger fields the significance of the high energy electron virtual states decreases and for $Z > 20$ we did not try to supplement the RME by summation of $\alpha(Z\alpha)^5$ terms.

In [54] the accuracy of numerical integration was up to 12 digits. Since then some terms contributing to RME expansion were recalculated with greater precision. These are displayed in Tables 2.1-2.8.

2.3 Illustrative calculation - subleading part of the effect

In this section the contribution of $\langle \gamma_0 G_4 \rangle$ in the mass operator (1.15) is calculated as illustrative example in non-relativistic approximation. We describe in some detail how the terms of the order $\alpha(Z\alpha)^5$ and higher are calculated.

2.3.1 Non-relativistic approximation

The non-relativistic approximation is obtained by limit of small $Z\alpha$. The quantum number $|\Gamma|$ is then approximately $|\Gamma| \approx (j + 1/2)$. The Hamilton operator (1.17) is then replaced by non-relativistic Hamiltonian

$$H_0 = 2m(\Pi_0 - m) - \vec{P}^2 \tag{2.45}$$

and the wave function of the reference state reduces to the Schrödinger wave function of hydrogen. Non-relativistic approximation avoids expansion into partial waves and is exact in the limit $k_e \to \infty$, $Z\alpha \to 0$. It enables us to get overlap integrals between reference and virtual states in the closed form. Thus, it is suitable for study of the region $k_e \to \infty$, i.e. of the region where RME breaks down.

As an illustration we calculate the part of the self-energy corresponding to

$$-\frac{\alpha}{2\pi}\langle\gamma_0 G_4\rangle \approx -\frac{\alpha m}{2\pi}(-4)\int_0^{\Lambda^2} d\lambda \int \frac{d^4k_F}{(k^2-\lambda)^2}\left\langle\frac{1}{k^2-2k.\Pi+H_0}\right\rangle_0, \tag{2.46}$$

where $\langle O\rangle_0 = \langle\psi_0|O|\psi_0\rangle$ and $\psi_0(\vec{r})$ is Schrödinger wave function.

For the reasons to become clear in the moment we begin by applying formula

$$\frac{1}{A-B} = \frac{1}{A} + \frac{1}{A}B\frac{1}{A-B} \tag{2.47}$$

to the term $1/(k^2 - 2k.\Pi + H_0)$ twice:

$$\frac{1}{k^2-2k.\Pi+H_0} = \frac{1}{k^2-2k.\varepsilon+H_0} + \frac{1}{k^2-2k.\varepsilon+H_0}2k.(\Pi-\varepsilon)\frac{1}{k^2-2k.\varepsilon+H_0} + \tag{2.48}$$
$$+\frac{1}{k^2-2k.\varepsilon+H_0}2k.(\Pi-\varepsilon)\frac{1}{k^2-2k.\Pi+H_0}2k.(\Pi-\varepsilon)\frac{1}{k^2-2k.\varepsilon+H_0}.$$

This expression is taken in the mean value between reference states. In order to obtain terms of the order $\alpha(Z\alpha)^5$ more easily it is advantageous to add and subtract the term $(k^2-2k.\varepsilon)^{-3}\langle 2k.(\Pi-\varepsilon)2k.(\Pi-\varepsilon)\rangle_0$. Because $H_0\psi_0 = 0$ for the reference state the average of the expression (2.48) simplifies to

$$\left\langle\frac{1}{k^2-2k.\Pi+H_0}\right\rangle_0 = \frac{1}{k^2-2k.\varepsilon} + \frac{1}{(k^2-2k.\varepsilon)^2}\langle 2k.(\Pi-\varepsilon)\rangle_0 + \tag{2.49}$$
$$+\frac{1}{(k^2-2k.\varepsilon)^3}\langle 2k.(\Pi-\varepsilon)2k.(\Pi-\varepsilon)\rangle_0 +$$
$$+\frac{1}{(k^2-2k.\varepsilon)^2}\left\langle 2k.(\Pi-\varepsilon)\left(\frac{1}{k^2-2k.\Pi+H_0} - \frac{1}{k^2-2k.\varepsilon}\right)2k.(\Pi-\varepsilon)\right\rangle_0.$$

The first term contributes to the electromagnetic mass and is thus of no interest now. The second and third contribute to the leading term of the order $\alpha(Z\alpha)^4$ and are also of no interest for now. Thus the only term we will be interested in is the last one. The term inside the mean value can be rewritten in similar fashion as (2.19):

$$\left\langle 2k.(\Pi-\varepsilon)\left(\frac{1}{k^2-2k.\Pi+H_0} - \frac{1}{k^2-2k.\varepsilon}\right)2k.(\Pi-\varepsilon)\right\rangle_0 = \int_0^1 du(1-u) \tag{2.50}$$
$$\frac{\partial^2}{\partial\varepsilon_\lambda\partial\varepsilon_\rho}\left(\left\langle(\Pi-\varepsilon)_\lambda\frac{1}{k^2-2k.\varepsilon+u(-2k_0(\Pi_0-m)+2\vec{k}.\vec{P}+H_0)}(\Pi-\varepsilon)_\rho\right\rangle_0 -\right.$$
$$\left.-\left\langle(\Pi-\varepsilon)_\lambda\frac{1}{k^2-2k.\varepsilon}(\Pi-\varepsilon)_\rho\right\rangle_0\right).$$

Using Eq. (2.31)

$$\left\langle (\Pi-\varepsilon)_\lambda \left(\frac{1}{k^2-2k.\varepsilon+u(-2k_0(\Pi_0-m)+2\vec{k}.\vec{P}+H_0)}-\frac{1}{k^2-2k.\varepsilon}\right)(\Pi-\varepsilon)_\rho\right\rangle_0 = \tag{2.51}$$

$$=\left\langle (\Pi-\varepsilon)_\lambda e^{i\vec{k}.\vec{R}}\left(\frac{1}{k^2-2k.\varepsilon+u(-2k_0(\Pi_0-m)+H_0+\omega^2)}-\right.\right.$$

$$\left.\left.-\frac{1}{k^2-2k.\varepsilon}\right)e^{-i\vec{k}.\vec{R}}(\Pi-\varepsilon)_\rho\right\rangle_0 .$$

The part of the denominator proportional to Feynman paramater u can be rewritten with the help of explicit form of non-relativistic Hamiltonian H_0, Eq. (2.45), to

$$-2k_0(\Pi_0-m)+H_0 = 2m\left(1-\frac{k_0}{m}\right)(E-m)+\frac{2Z\alpha}{R}m\left(1-\frac{k_0}{m}\right)-\vec{P}^2 = \tag{2.52}$$

$$= 2m(E-m)\xi-2(Z\alpha m\xi)^2\left(\frac{\vec{p}^2}{2}-\frac{1}{r}\right)$$

where the substitutions

$$R=\frac{r}{mZ\alpha\xi},\ \xi=1-\frac{k_0}{m} \tag{2.53}$$

were made. As shown in [25] using parabolic coordinates one can find eigenfunction $\psi^-_{\vec{p}}$ of the Hamilton operator $(\hat{p}^2/2-1/\hat{r})$ that behaves as plane wave for $r\to\infty$. All the integrals necessary for calculation of the matrix elements of any operator between referrence and virtual states needed in calculation of self-energy can be derived by parametric differentiation with respect to $\vec{q}$ and μ of the equation [25]

$$\int\frac{dV}{r}(\psi^-_{\vec{p}})^* e^{-i\vec{q}\cdot\vec{r}}\psi_0(\mu\vec{r}) = \mu^{3/2}\sqrt{\frac{2}{\pi^2}}e^{\frac{\pi}{2p}}\left(\frac{(\vec{q}+\vec{p})^2+\mu^2}{(\mu-ip)^2+q^2}\right)^{\frac{i}{p}}\frac{\Gamma\left(1-\frac{i}{p}\right)}{\mu^2+(\vec{q}+\vec{p})^2}. \tag{2.54}$$

In this way one can avoid the partial wave expansion.

Since we are making just illustrative calculation we consider further just the term $\lambda=\rho=0$ in Eq. (2.50). Also, for now we neglect in (Π_0-m) the term E_0-m with respect to $\frac{Z\alpha}{R}$. Contribution of the former term is relatively small. Inserting (2.49)-(2.54) into (2.46) and making just described omission the corresponding contribution to the self-energy reads

$$-\frac{\alpha}{2\pi}\langle\gamma_0 G_4^{(R)}\rangle \to -\frac{\alpha m}{2\pi}(-4)\int_0^{\Lambda^2}d\lambda\int\frac{d^4k_F}{(k^2-\lambda)^2}\frac{\partial^2}{\partial\varepsilon_0^2}\int_0^1 du(1-u) \tag{2.55}$$

$$\int d^3\vec{p}\left(\frac{1}{k^2-2k.\varepsilon+u(2m(E-m)\xi-(Z\alpha m\xi)^2\vec{p}^2+\omega^2)}-\frac{1}{k^2-2k.\varepsilon}\right)P(\vec{k},\xi,\vec{p})$$

where $G_4^{(R)}$ stands for the remainder of G_4 since we neglected the leading order. Here using (2.54), (2.53) and

$$\vec{q}=\frac{\vec{k}}{mZ\alpha\xi},\ \mu=\frac{1}{\xi} \tag{2.56}$$

the overlap integrals $P(\vec{k},\xi,\vec{p})$ can be expressed as

$$P(\vec{k},\xi,\vec{p}) = \left\langle \psi_0 \left| \frac{Z\alpha}{R} e^{i\vec{k}.\vec{R}} \right| \psi_{\vec{p}} \right\rangle \left\langle \psi_{\vec{p}} \left| e^{-i\vec{k}.\vec{R}} \frac{Z\alpha}{R} \right| \psi_0 \right\rangle = \tag{2.57}$$

$$= (\xi m Z\alpha)^2 (Z\alpha)^2 \frac{1}{\xi^3} \frac{2}{\pi^2} e^{\pi/p} \left(\frac{\left(\frac{1}{\xi} + ip\right)^2 + \left(\frac{\omega}{mZ\alpha\xi}\right)^2}{\left(\frac{1}{\xi} - ip\right)^2 + \left(\frac{\omega}{mZ\alpha\xi}\right)^2} \right)^{i/p} \frac{|\Gamma(1-i/p)|^2}{\left(\left(\frac{1}{\xi}\right)^2 + \left(\frac{\vec{k}}{mZ\alpha\xi} + \vec{p}\right)^2 \right)^2}.$$

In the next step the substitution

$$\vec{p} = \vec{p'}/\xi Z\alpha \tag{2.58}$$

is used. Dropping the prime in $\vec{p'}$ the Eq. (2.55) can be written as

$$-\frac{\alpha}{2\pi}\langle \gamma_0 G_4^{(R)} \rangle \simeq -\frac{\alpha m}{2\pi} (Z\alpha)^5 (-4) \int_0^{\Lambda^2} d\lambda \int \frac{d^4 k_F}{(k^2-\lambda)^2} m^2 \frac{\partial^2}{\partial \varepsilon_0^2} \int_0^1 du (1-u) \tag{2.59}$$

$$\int d^3\vec{p} \left(\frac{1}{k^2 - 2k.\varepsilon - u m^2 ((Z\alpha)^2 \xi + \vec{p}^2 - \frac{\omega^2}{m^2})} - \frac{1}{2k^2 - 2k.\varepsilon} \right) \bar{P}(\vec{k},\xi,\vec{p}) \Bigg|_{\varepsilon_0 = m}.$$

Here we used $E - m \simeq -m(Z\alpha)^2/2$ and

$$\bar{P}(\vec{k},\xi,\vec{p}) = \frac{2}{\pi^2} e^{\frac{\pi}{p} Z\alpha\xi} \left(\frac{(Z\alpha + ip)^2 + \left(\frac{\omega}{m}\right)^2}{(Z\alpha - ip)^2 + \left(\frac{\omega}{m}\right)^2} \right)^{iZ\alpha\xi/p} \frac{|\Gamma(1 - iZ\alpha\xi/p)|^2}{\left((Z\alpha)^2 + \left(\frac{\vec{k}}{m} + \vec{p}\right)^2 \right)^2}. \tag{2.60}$$

2.3.2 RME

The last expression can now be expanded in the multipole expansion. This is achieved by expanding in powers of $\omega = \sqrt{\vec{k}.\vec{k}}$ and k_0, recall that $\xi = 1 - k_0/m$.

Equation (2.59) then reads

$$-\frac{\alpha}{2\pi}\langle \gamma_0 G_4^{(R)} \rangle = -\frac{\alpha m}{2\pi} (Z\alpha)^5 \sum_{v,t} \int_0^1 du (1-u) \int_0^\infty dp p^2 \int_{-1}^1 dx 2\pi \frac{1}{v! 2^v} \frac{\partial^v}{\partial \sigma^v} \tag{2.61}$$

$$\frac{1}{t! 2^t} \frac{\partial^t}{\partial \xi^t} \bar{P}(\sigma,\xi,p,x) \phi^{2v,t}(m^2[(Z\alpha)^2\xi + \vec{p}^2]u, \sigma) \Bigg|_{\sigma=0} \Bigg|_{\xi=1},$$

where $dx = d\theta \sin\theta$, $x = \cos\theta = \frac{\vec{k}.\vec{p}}{\omega p}$ and

$$\phi^{2v,t}(\Delta,\sigma) = m^2 \frac{\partial^2}{\partial \varepsilon_0^2} (-4) \int_0^{\Lambda^2} d\lambda \int \frac{d^4 k_F}{(k^2-\lambda)^2} \frac{\left(\frac{2\omega}{m}\right)^{2v} \left(-\frac{2k_0}{m}\right)^{2t}}{k^2 - 2k.\varepsilon - \Delta + \sigma m^2 u} = \tag{2.62}$$

$$= (-1)^v (2v+1)!! 2^v (-1)^t \frac{\partial^{t+2}}{\partial \varepsilon_0^{t+2}} \int_0^1 dy y^v \int_0^{\frac{\Delta}{m^2} + \sigma u} d^{v+t} w \left(\ln \frac{\varepsilon_0^2 y + w}{y} - \ln \frac{\Lambda^2 (1-y)}{m^2 y} \right) \Bigg|_{\varepsilon_0 = 1}$$

with

$$\bar{P}(\sigma,\xi,p,x) = \frac{2}{\pi^2} e^{\frac{\pi}{p} Z\alpha\xi} \left(\frac{(Z\alpha + ip)^2 + \sigma}{(Z\alpha - ip)^2 + \sigma} \right)^{iZ\alpha\xi/p} \frac{|\Gamma(1 - iZ\alpha\xi/p)|^2}{\left((Z\alpha)^2 + p^2 + 2p\sigma^{1/2} x + \sigma \right)^2}. \tag{2.63}$$

The integral in (2.62) looks horribly divergent. However, recalling discussion about equations (2.13) and (2.14) what we actually need is $D_{2v+t}[\phi^{2v,t}]$. Therefore the $\phi^{2v,t}$ is determined up to the polynomial of the order $2v+t-1$ in Δ. This is enough to make the integrals over k convergent. Further details on the integration over k_F in (2.62) can be found in [54]. The second term in brackets on right member of Eq. (2.62) does not contribute since it is independent of ε_0.

This form of expansion is suited for symbolic evaluation using computer languages as MATHEMATICA or MAPLE. Differentiations with respect to ε_0, ξ and σ and integrations over x, u, y and w can be done analytically by these programs. After this is done, the numerical integration over p is performed. All the individual terms of RME expansion can be in this way generated automatically. The above calculation illustrates the core of the RME method. In the full relativistic approach the calculation gets more complicated. However, the spirit of the method remains the same as in the case elaborated above.

2.3.3 $\alpha(Z\alpha)^5$ terms

From Eq. (2.63) one can immediately see the problem with RME. In the denominator of the last term in the expression (2.60) the term $\left(\vec{p}+\frac{\vec{k}}{m}\right)$ appears. All the other terms that are about to be expanded contain supressing factor $Z\alpha$ except for this one term. This is the origin of the difficulty with the $\alpha(Z\alpha)^5$ term in the RME expansion. This term will be contributing to all orders of the RME and is not supressed by any power of $Z\alpha$.

In limit of very large p Eq. (2.60) reduces to the simple form

$$\bar{P}(\vec{k},\xi,\vec{p}) = \frac{2}{\pi^2}\frac{1}{\left((Z\alpha)^2+\left(\frac{\vec{k}}{m}+\vec{p}\right)^2\right)^2}. \tag{2.64}$$

In this limit the function $\bar{P}$ depends on $\vec{p}$ only through combination $\vec{p}+\frac{\vec{k}}{m}$. This corresponds to the approximation when $\psi_{\vec{p}}^{-}$ is replaced by plane wave $e^{i\vec{p}.\vec{r}}/(2\pi)^{3/2}$. Then the substitution

$$\vec{p'} = \vec{p}-\vec{k}/m \tag{2.65}$$

is obviously advantageous. In the following the prime in $\vec{p'}$ is again dropped. Substituting (2.64) and (2.65) into (2.55) we get

$$\begin{gathered}
-\frac{\alpha}{2\pi}\langle\gamma_0 G_4^{(R)}\rangle \simeq -\frac{\alpha m}{2\pi}(Z\alpha)^5(-4)\int_0^{\Lambda^2} d\lambda \int \frac{d^4k_F}{(k^2-\lambda)^2}m^2 \qquad (2.66) \\
\frac{\partial^2}{\partial\varepsilon_0^2}\int_0^1 du(1-u)\int d^3\vec{p}\frac{2}{\pi^2}\frac{1}{((Z\alpha)^2+\vec{p}^2)^2} \\
\left(\frac{1}{k^2-2k.\varepsilon-um^2(\xi(Z\alpha)^2+(\vec{p}-\vec{k}/m)^2-\omega^2/m^2)}-\frac{1}{k^2-2k.\varepsilon}\right)\Bigg|_{\varepsilon_0=m}.
\end{gathered}$$

The term $\xi(Z\alpha)^2$ does not contribute to the $\alpha(Z\alpha)^5$ order and can be omitted. Now, writing

$$P_u = (\varepsilon_0, um\vec{p}) \tag{2.67}$$

the denominator in the first term in brackets in (2.66) simplifies to

$$\frac{1}{k^2 - 2k.\varepsilon - um^2((\vec{p} - \vec{k}/m)^2 - \omega^2/m^2)} = \frac{1}{k^2 - 2k.P_u - um^2\vec{p}^2}. \tag{2.68}$$

The integral in (2.66) over k_F reads (see Appendix A in [54] for details)

$$(-4)\int_0^{\Lambda^2} d\lambda \int \frac{d^4k_F}{(k^2-\lambda)^2}\left(\frac{1}{k^2 - 2k.P_u - um^2\vec{p}^2} - \frac{1}{k^2 - 2k.\varepsilon}\right) = \tag{2.69}$$

$$= \int_0^1 dy \int_{\frac{\Lambda^2}{m^2}\frac{1-y}{y}}^0 d\lambda \left(\frac{1}{\frac{P_u^2 y}{m^2} + u\vec{p}^2 + \lambda} - \frac{1}{\frac{\varepsilon_0^2}{m^2}y + \lambda}\right).$$

Now, performing scaling $\frac{\varepsilon_0}{m} \to \varepsilon_0$ and using explicit form of P_u the first term in brackets can be rewritten as $1/(\varepsilon_0^2 y + \vec{p}^2 u(1-uy) + \lambda)$. Substituting this back into (2.66) the integration over $\vec{p}$ can be performed to yield

$$\int d^3\vec{p}\frac{2}{\pi^2}\frac{1}{((Z\alpha)^2 + \vec{p}^2)^2}\left(\frac{1}{\varepsilon_0^2 y + \vec{p}^2 u(1-uy) + \lambda} - \frac{1}{\varepsilon_0^2 y + \lambda}\right) = \tag{2.70}$$

$$= -2^2\frac{(u(1-uy))^{1/2}}{(\varepsilon_0^2 y + \lambda)^{3/2}}\left(1 + O((Z\alpha)^2)\right)$$

where only the terms contributing to $\alpha(Z\alpha)^5$ were taken. After integration over λ and setting $\Lambda \to \infty$ the final contribution of the order $\alpha(Z\alpha)^5$ to self-energy reads

$$-\frac{\alpha}{2\pi}\langle\gamma_0 G_4^{(R)}\rangle \simeq -\frac{\alpha m}{2\pi}(Z\alpha)^5\frac{\partial^2}{\partial\varepsilon_0^2}\int_0^1 du(1-u)\int_0^1 dy 2^3(\varepsilon_0^2 y)^{-1/2}(u(1-uy))^{1/2}\,|_{\varepsilon_0=1} = \tag{2.71}$$

$$= -\frac{\alpha m}{2\pi}(Z\alpha)^5 2^4\int_0^1 du(1-u)\int_0^1 dy\left(\frac{u}{y}\right)^{1/2}(1-uy)^{1/2} =$$

$$= -\frac{\alpha m}{2\pi}(Z\alpha)^5 2^4\int_0^1 du(1-u)\int_0^u dv\frac{(1-\delta v)^{1/2}}{v^{1/2}}$$

where in the last equality the substitution $y = v/u$ was used and the perturbation parameter δ was introduced. This parameter has to be added to keep track of the order of the multipole expansion. The final expression is obtained by performing the remaining integrations,

$$-\frac{\alpha}{2\pi}\langle\gamma_0 G_4^{(R)}\rangle = \frac{\alpha(Z\alpha)^5 m}{\pi}\left(-\frac{1}{2}\right)\frac{5\pi}{2} = \tag{2.72}$$

$$= \sum_v \frac{\alpha(Z\alpha)^5 m}{\pi}\left(-\frac{1}{2}\right)\delta^v\frac{2^3\Gamma(\frac{3}{2})(-1)^v(v-1)}{\Gamma(\frac{7}{2})\Gamma(v)(v-\frac{3}{2})(v-\frac{1}{4})}$$

where the first equality was obtained by setting $\delta = 1$ in (2.71). By calculating all the remaining contributions one can obtain the formula (2.39). Had we started with Eq. (2.46) instead of (2.49) the derivation of $\alpha(Z\alpha)^5$ term would be more complex because the expression (2.46) does not reduce in large $\vec{p}$ to the case when $\psi_{\vec{p}}^-$ is replaced by free particle wave function.

2.4 Technical details

When evaluating expressions contained in RME one has to perform spectral decomposition of the Hamilton operator. This decomposition consists of infinite summation over discrete states and integration over continuous states. The summation is handled by performing summation over finite interval and then using Richardson extrapolation. The integration was evaluated using numerical methods. All the calculations were made using Wolfram MATHEMATICA. However, such an approach is not viable in every situation: once the external potential is not exactly Coulombic the exact eigenfunctions of the entire spectrum are not known in the closed form. Also, when extending the RME method to case where several decompositions of Hamilton operators occur one has to evaluate overlap integrals between two continuous spectra functions. This is not trivial at all since the closed formulas which are used for overlap integrals between discrete-discrete and discrete-continuous functions in this case do not exist.

Therefore we also considered an alternative method to the use of the exact eigenfunction, the method of pseudo-states. The hydrogen pseudo-states are expanded using Sturmian functions. These are obtained by performing energy-dependent scaling $r \to nr$ in radial equation

$$\left[\frac{\vec{p}^2}{2} - \frac{1}{r}\right] |\psi\rangle = -\frac{1}{2n^2}|\psi\rangle. \tag{2.73}$$

One then obtains equation for Sturmian functions

$$\left[r\frac{\vec{p}^2}{2} + \frac{r}{2}\right] |n\rangle = n|n\rangle. \tag{2.74}$$

Resulting functions form complete entirely discrete set and thus may be used in pseudo-state expansion

$$|\psi\rangle = \sum c_n|n\rangle. \tag{2.75}$$

There is no continuous part of the spectra and the whole problem of the spectral decomposition of radial part of the Hamilton operator is then reduced into finding eigenvalues and eigenvectors for sufficiently large matrix to obtain accurate enough results. Similarly as in the discrete spectrum in the case of the exact spectral decomposition of H the extrapolation is used to obtain the most accurate result. This method is elaborated in attached article [55] for P-states and normalized difference of S-states. Some preliminary calculation concerning the low-energy part of the self-energy effect for excited states is described there. We found that for pseudo-state method to work really accurately the contribution of the states with $k_e \to \infty$ has to be suppressed. For the normalized difference of S-states and for P-states this contribution goes like $k_e^{-6} \ln k_e$. Therefore in this case the results obtained by pseudo-state method are very accurate.

Results and Conclusion

Results

Using operator form of RME we calculated the one-loop self-energy of excited states for $n = 2 \dots 10$, $l = 0 \dots 3$ and various Z up to 30 (attached article [53]). The results for normalized difference of S-states for $n \geq 9$, P-states for $n \geq 8$ and F-states for $n \geq 6$ were calculated for the first time. For low Z and non-S-states the accuracy is competing with PWE and $Z\alpha$ expansion. For the normalized diference of S-states there is a small difference between RME and both PWE and $Z\alpha$ expansion. Difference between RME and PWE for normalized difference $8E_{2s} - E_{1s}$, $Z = 1$ is 210.5 Hz. The speed of convergence of RME is fast due to nearly complete suppresion of high-energy part in the case of excited states. Preliminary results using the method of pseudo-states were obtained for the normalized difference of S-states up to $n = 15$ at the leading order (attached article [55]).

In the case of ground state the convergence of method was refined by isolating the slowly converging part of the RME expansion. The accuracy is then again competing with the accuracy of PWE method and is significantly better than $Z\alpha$ expansion. This is crucial for reliability of present calculations of QED effects. The difference between RME and PWE in the case of ground state is 2 parts in 10^9 which corresponds to 18 Hz for the $1s - 2s$ transition. This definitely exludes the possibility that the proton radius puzzle has anything to do with uncertainity in determination of one-loop self-energy. The result for hydrogen and also for case of higher Z up to 90 is in attached article [54].

Conclusion

In this thesis the method for evaluation of one-loop self-energy of bound electron based on generalization of relativistic multipole expansion has been described. In comparison to $Z\alpha$ expansion the RME method is not restricted to low Z and works fairly well for state independent part of the S-states. In comparison to PWE our method is not restricted to high Z and low excited states and is by factor 10^7 simpler (10^6 three-dimensional numerical integrations versus 10 one-dimensional numerical integrations). In the case of excited states the method works so well that only few terms of RME have to be considered. For the ground state it has to be supplemented by free-particle approximation in virtual states. Only one-dimensional integrals are necessary to be performed numerically since closed formulas can be used for all other integrals. For the excited states they converge so fast that even this can be avoided by method of pseudo-states.

Comparing $Z\alpha$ expansion (1.20) and RME in greater detail, the naive counting up to the order $(Z\alpha)^6$ yields for the state-independent part of the S-states complete coefficients A_{41}, A_{40}, A_{62}, A_{61}, almost complete A_{60} coefficient and great part of A_{50} coefficient. For excited states it yields complete A_{40}, A_{61} and A_{60} coefficients. Naive counting to the order $(Z\alpha)^6$ thus yields almost everything. For excited states the error is of the order $\alpha(Z\alpha)^7$ or less. Ground state, when supplemented by $\alpha(Z\alpha)^5$ terms is better than $Z\alpha$ expansion truncated after $(Z\alpha)^6$

term.

Possible directions of further continuation of this work are the following:

1. The method can be pushed further to obtain one-loop self-energy with higher accuracy for both ground and excited states, low and high Z. This is of no immediate concern but can be in the future when the proton radius puzzle is resolved.
2. Self-energy for the case when the external Coulomb potential is accompanied by another small external field. This is the case of hyperfine interaction or external magnetic field. The application of this is the calculation of bound electron g factor and radiation corrections to hyperfine structure in H-like atoms [46, 49].
3. Self-energy for the case when aside from Coulomb potential one considers also potential created by exchange of Z boson between nucleus and electron. The application is thus for radiation corrections to PNC amplitude [42, 44].
4. Inclusion of Uehling potential correction arising from the vacuum polarization. This yields part of two-loop corrections.
5. Self-energy in the case when virtual photon is modified by vacuum polarization. This is also part of two-loop corrections.
6. Radiative recoil effects for light and heavy particle. Applications of this is the fine and hyperfine structure of hydrogen, muonium and positronium [37].
7. Complete two-loops corrections, namely the double self-energy graphs that are the most difficult part and are the most limiting factor of purely QED corrections to the accurate determination of spectra of hydrogen-like atoms at present [38, 50].

Although the effects as two-loop radiation corrections or radiative recoil are by several orders of magnitude smaller than the one-loop self-energy and one thus does not need to evaluate them with such accuracy, the RME method could still be proved to be valuable in their evaluation. Only when confirmed from at least two independent methods we can be sure that our theoretical predictions are not flawed and move forward to more exciting and exotic solutions of the proton radius puzzle.

Finally, we believe that the ideas developed in this thesis are of more general interest and contribute to understanding of non-perturbative aspects of quantum field theory in general.

Bibliography

[1] M. Baranger, H. A. Bethe, R. P. Feynman, Phys. Rev. **92**, 482 (1953).

[2] M. Baranger, Phys. Rev. **84**, 866 (1951).

[3] H. A. Bethe, Phys. Rev. **72**, 339 (1947).

[4] P. G. Blunden, I. Sick, Phys. Rev. C **72**, 057601 (2005).

[5] E. Borie, Phys. Rev. A **71**, 032508 (2005).

[6] M. A. Bouchiat, C. Bouchiat, Rep. Prog. Phys. **60**, 1351 (1997).

[7] G. E. Brown, J. S. Langer, G. W. Schaefer, Proc. R. Soc. London, Ser. A **251**, 92 (1959).

[8] E. D. Commins, P. H. Bucksbaum: Chapter 9 in *Weak interactions of leptons and quarks*, Cambridge University Press (1983).

[9] A. M. Desiderio, W. R. Johnson, Phys. Rev. A **3**, 1267 (1971).

[10] M. I. Eides, H. Grotch, V. A. Shelyuto, Phys. Rep. **342**, 63 (2001).

[11] G. W. Erickson, D. R. Yennie, Ann. Phys. **35**, 271 (1965).

[12] G. W. Erickson, D. R. Yennie, Ann. Phys. **35**, 447 (1965).

[13] R. P. Feynman, Phys. Rev. **76**, 769 (1949).

[14] J. B. French, V. F. Weisskopf, Phys. Rev. **75**, 1240 (1949).

[15] H. M. Fried, D. R. Yennie, Phys. Rev. Lett. **4**, 583 (1960).

[16] U. D. Jentschura, E.-O. Le Bigot, P. J. Mohr, P. Indelicato and G. Soff, Phys. Rev. Lett. **90**, 163001 (2003).

[17] U. D. Jentschura, P. J. Mohr, G. Soff, Phys. Rev. A **63**, 042512 (2001). See also U. D. Jentschura, P. J. Mohr, *ibid* **69**, 064103 (2004).

[18] U. D. Jentschura, A. Czarnecki, K. Pachucki, Phys. Rev. A **72**, 062102 (2005). See also A. Czarnecki, U. D. Jentschura, K. Pachucki, Phys. Rev. Lett. **95**, 180404 (2005).

[19] U. D. Jentschura, K. Pachucki, Phys. Rev. A. **54**, 1853 (1996).

[20] R. Karplus, A. Klein, J. Schwinger, Phys. Rev **86**, 288 (1952).

[21] S. G. Karshenboim, Phys. Rep. **422**, 1 (2005).

[22] S. G. Karshenboim, Z. Phys. D **39**, 109 (1997).

[23] N. M. Kroll, W. E. Lamb, Phys. Rev. **75**, 388 (1949).

[24] W. E. Lamb, R. C. Retherford, Phys. Rev **72**, 241 (1947).

[25] L. D. Landau, E. M. Lifschitz: Appendix f in *Quantum mechanics, non-relativistic theory*, Pergamon press, Oxford, (1968).

[26] A. J. Layzer, J. Math. Phys. **2**, 29 (1961).

[27] A. P. Martynenko, Phys. Rev. A **71**, 0022506 (2005).

[28] A. P. Martynenko, Physics of Atomic Nuclei, **71**, 125 (2008).

[29] V. Meyer et al., Phys. Rev. Lett. 84, 1136 (2000).

[30] P. J. Mohr, B. N. Taylor, D. B. Newell, Rev. Mod. Phys. **80**, 633 (2008).

[31] P.J. Mohr, Phys. Rev. A **46**, 4421 (1992). See also P. J. Mohr, 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).

[32] P. J. Mohr, G. Plunien, G. Soff, Phys. Rep. **293**, 227 (1998).

[33] M. Niering et al., Phys. Rev. Lett. 84, 5496 (2000).

[34] K. Pachucki, Ann. Phys **226**, 1 (1993). See also W. Erickson, Phys. Rev. Lett. **27**, 780 (1971); J. Sapirstein, *ibid* **47**, 1723 (1981).

[35] K. Pachucki, Phys. Rev. A **53**, 2092 (1996).

[36] K. Pachucki, Phys. Rev. A **60**, 3593 (1999).

[37] K. Pachucki, Phys. Rev. A **52**, 1079 (1995). G. Bhatt and H. Grotch, Ann. Phys. (NY) **178**, 1 (1987).

[38] K. Pachucki, Phys. Rev. A **63**, 042503 (2001).

[39] R. Pohl et al., Nature **466**, 213 (2010).

[40] A. De Rújala, Phys. Lett. B **697**, 26 (2011).

[41] A. De Rújala, Phys. Lett. B **693**, 555 (2010).

[42] J. Sapirstein, K. T. Cheng , Phys. Rev. A **71**, 022503 (2005).

[43] V. M. Shabaev, K. Pachucki, I. I. Tupitsyn, G. Plunien V. A. Yerokhin, Phys. Rev. A **72**, 062105 (2005).

[44] V. M. Shabaev, K. Pachucki, I. I. Tupitsyn, V. A. Yerokhin, Phys. Rev. Lett. **94**, 213002 (2005).

[45] I. Sick, Prog. Part. Nucl. Phys. **67**, 473 (2012).

[46] S. Sturm et al., Phys. Rev. Lett. **107**, 023002 (2011).

[47] E. H. Wichmann, N. M. Kroll, Phys. Rev. **101**, 843 (1956).

[48] V. A. Yerokhin, K. Pachucki, V. M. Shabaev, Phys. Rev. A **72**, 042502 (2005).

[49] V. A. Yerokhin, U. D. Jentschura, Phys. Rev. Lett. **100**, 163001 (2008).

[50] V. A. Yerokhin, P. Indelicato, V. M. Shabaev, Phys. Rev. A **77**, 062510 (2008).

[51] J. Zamastil, F. Vinette, M. Šimánek, Phys. Rev. A **75**, 022506 (2007).

[52] J. Zamastil, Ann. Phys. (NY) **327**, 297 (2012).

[53] * J. Zamastil, V. Patkóš, Phys. Rev. A **86**, 042514 (2012).

[54] * J. Zamastil, V. Patkóš, Phys. Rev. A **88**, 032501 (2013).

[55] * V. Patkóš, J. Zamastil, to be published.

Publications with asterisk are attached.

List of Tables

In expressions $G_{4,\mu}^{s,t}$ the numbers s and t stand for number of expanded space and time components of $\Pi - \varepsilon$, respectively.

Table 2.1: The term $\langle \gamma_0 G_0^{2v,t} \rangle$ for $t = 0 \dots 2$ and $Z = 1 \dots 3$.

v, $t = 0$	$Z = 1$	$Z = 2$	$Z = 3$
1	-0.65312870037003	-0.64226142781441	-0.63298254957776
2	0.60548218119228	0.58782415058237	0.57152865838656
3	0.00356619864538	0.00693620747000	0.01012594839375
4	0.00045076692697	0.00091966868721	0.00140469944362
5	0.00012735420606	0.00026169550777	0.00040299468224
6	0.00004949428185	0.00010211012898	0.00015792301593
7	0.00002304507176	0.00004767941643	0.00007396371033
8	0.00001208825027	0.00002506603861	0.00003897517727
9	0.00000690671760	0.00001434798949	0.00002235235323
v, $t = 1$	$Z = 1$	$Z = 2$	$Z = 3$
1	-0.44164157634373	-0.42644465641886	-0.41235500653388
2	-0.00314782874100	-0.00640147626223	-0.00964199591678
3	-0.00036350561651	-0.00077737748896	-0.00123748687124
4	-0.00009786529152	-0.00021019214331	-0.00033715721303
5	-0.00003676768348	-0.00007920506254	-0.00012755769763
6	-0.00001668487240	-0.00003602960047	-0.00005819377382
7	-0.00000857616462	-0.00001855631152	-0.00003004010462
8	-0.00000482005191	-0.00001044649794	-0.00001694301078
v, $t = 2$	$Z = 1$	$Z = 2$	$Z = 3$
0	0.00021410779241	0.00067595787592	0.00129575205992
1	0.00009874151359	0.00026499912463	0.00043884320773
2	0.00000998691598	0.00003954973064	0.00008757744701
3	0.00000235165707	0.00000972115456	0.00002250925626
4	0.00000083051590	0.00000347998217	0.00000817848756
5	0.00000036307304	0.00000153271718	0.00000363126997
6	0.00000018188473	0.00000077164175	0.00000183788000
7	0.00000010029254	0.00000042702473	0.00000102101840

Table 2.2: The term $\langle \gamma_0 G_0^{2v,t} \rangle$ for $t = 0 \ldots 2$ and $Z = 4, 5$.

v, $t = 0$	$Z = 4$	$Z = 5$
1	-0.62487084807674	-0.61768400064748
2	0.55634604895348	0.54211104011501
3	0.01314896881474	0.01601711771550
4	0.00190400248373	0.00241587220565
5	0.00055118712591	0.00070618286092
6	0.00021699679530	0.00027938638226
7	0.00010195482810	0.00013170771985
8	0.00005385611442	0.00006974742070
9	0.00003094859805	0.00004016914513
v, $t = 1$	$Z = 4$	$Z = 5$
1	-0.39917558621829	-0.38677476171789
2	-0.01282296890985	-0.01592057140794
3	-0.00173981175303	-0.00228051836689
4	-0.00047884651695	-0.00063526892289
5	-0.00018205209838	-0.00024289655834
6	-0.00008333411114	-0.00011160512755
7	-0.00004312831129	-0.00005792648218
8	-0.00002437400815	-0.00003279626296
v, $t = 2$	$Z = 4$	$Z = 5$
0	0.00203313025540	0.00286374054276
1	0.00059655555622	0.00072565964746
2	0.00015259106968	0.00023293979831
3	0.00004102601230	0.00006549716676
4	0.00001514502606	0.00002458548911
5	0.00000678245697	0.00001111013090
6	0.00000345175744	0.00000567629845
7	0.00000192643126	0.00000320301521

Table 2.3: The term $\langle \gamma_0 G_4^{2v,t} \rangle$ for $t = 0 \ldots 3$ and $Z = 1 \ldots 3$.

v, $t = 0$	$Z = 1$	$Z = 2$	$Z = 3$
1	-5.18091823206220	-4.30732006647140	-3.81466602281970
2	1.19330939740820	1.14489835841290	1.10174842282170
3	0.00587032439241	0.01134862934959	0.01647416881123
4	0.00062776293009	0.00128132894967	0.00195731014982
5	0.00016308215440	0.00033528121375	0.00051652489785
6	0.00006030828346	0.00012446738969	0.00019256590722
7	0.00002717092845	0.00005623165669	0.00008725345262
8	0.00001392206342	0.00002887492946	0.00004490683739
9	0.00000781589223	0.00001623951236	0.00002530325805
v, $t = 1$	$Z = 1$	$Z = 2$	$Z = 3$
1	-1.76205852131300	-1.70041023994010	-1.64502997304820
2	-0.00786272853371	-0.01595675644351	-0.02399039515965
3	-0.00076152315720	-0.00162522910025	-0.00258266894265
4	-0.00018798424718	-0.00040235616763	-0.00064348225592
5	-0.00006708738731	-0.00014391264064	-0.00023090508764
6	-0.00002942524257	-0.00006324671732	-0.00010172741649
7	-0.00001476319036	-0.00003178642966	-0.00005122805280
8	-0.00000814855455	-0.00001757053218	-0.00002836454308
v, $t = 2$	$Z = 1$	$Z = 2$	$Z = 3$
0	1.22339230444950	1.20133349039060	1.18208667461160
1	0.00294962372572	0.00656708150901	0.01048396852717
2	0.00023044060350	0.00055051251856	0.00095773334156
3	0.00005146691857	0.00012269049995	0.00021509912014
4	0.00001725838757	0.00004115461135	0.00007238645198
5	0.00000724489130	0.00001729794190	0.00003050413708
6	0.00000351733857	0.00000840985997	0.00001486276206
7	0.00000189220221	0.00000453027754	0.00000802120615
v, $t = 3$	$Z = 1$	$Z = 2$	$Z = 3$
0	-0.00014050621275	-0.00039458380462	-0.00068780492226
1	-0.00000739838290	-0.00003158834723	-0.00007425439278
2	-0.00000127661175	-0.00000575526672	-0.00001435648850
3	-0.00000037691071	-0.00000172711446	-0.00000439119969
4	-0.00000014651915	-0.00000067756993	-0.00000174041687
5	-0.00000006753251	-0.00000031425572	-0.00000081267900
6	-0.00000003498720	-0.00000016356393	-0.00000042504642

Table 2.4: The term $\langle \gamma_0 G_4^{2v,t} \rangle$ for $t = 0 \ldots 3$ and $Z = 4, 5$.

v, $t = 0$	$Z = 4$	$Z = 5$
1	-3.47696279726870	-3.22355476138670
2	1.06259252490300	1.02666661344070
3	0.02127909101191	0.02579070551327
4	0.00265263669581	0.00336453878097
5	0.00070669268640	0.00090562971248
6	0.00026467743431	0.00034086388530
7	0.00012030281167	0.00015544239458
8	0.00006206432339	0.00008039097473
9	0.00003503989945	0.00004548694531
v, $t = 1$	$Z = 4$	$Z = 5$
1	-1.59447781729950	-1.54787410411810
2	-0.03185760300055	-0.03950791095266
3	-0.00362572489211	-0.00474676147909
4	-0.00091157038154	-0.00120669609119
5	-0.00032846470469	-0.00043696401257
6	-0.00014512689095	-0.00019370191806
7	-0.00007324907910	-0.00009802491388
8	-0.00004063054928	-0.00005445689918
v, $t = 2$	$Z = 4$	$Z = 5$
0	1.16495998266280	1.14954855897600
1	0.01454780343128	0.01867351157121
2	0.00144850695681	0.00201873074406
3	0.00032991372768	0.00046816564431
4	0.00011163707442	0.00015957172837
5	0.00004721670173	0.00006779552155
6	0.00002307035300	0.00003324097542
7	0.00001248035344	0.00001805647675
v, $t = 3$	$Z = 4$	$Z = 5$
0	-0.00099167599533	-0.00129141315195
1	-0.00013603364089	-0.00021695103238
2	-0.00002792317722	-0.00004721721716
3	-0.00000872105998	-0.00001507559409
4	-0.00000349491978	-0.00000611262783
5	-0.00000164368607	-0.00000289469576
6	-0.00000086204256	-0.00000146899940

Table 2.5: The term $\langle \gamma_\mu G_4^{2v,t} (\Pi - \varepsilon)_\mu \rangle$ for $t = 0 \ldots 2$ and $Z = 1 \ldots 3$.

v, $t = 0$	$Z = 1$	$Z = 2$	$Z = 3$
0	15.79105427089100	13.09627533903000	11.55127280922400
1	-1.18695926223940	-1.13178797043900	-1.08184090728500
2	-0.00397176556312	-0.00757498291679	-0.01084467655070
3	-0.00032538777063	-0.00065111422109	-0.00097469346641
4	-0.00007090694379	-0.00014131395955	-0.00021095383293
5	-0.00002311456316	-0.00004563455844	-0.00006747935682
6	-0.00000944875337	-0.00001842281023	-0.00002688167423
7	-0.00000447256989	-0.00000858876455	-0.00001232322044
8	-0.00000234712423	-0.00000442723075	-0.00000622271614
9	-0.00000132973340	-0.00000245674474	-0.00000336810888
v, $t = 1$	$Z = 1$	$Z = 2$	$Z = 3$
0	0.24506816305461	0.23675334679521	0.22713265341354
1	0.00046378530851	0.00132729028056	0.00234039763190
2	0.00001591146828	0.00006057773809	0.00012934972507
3	0.00000253581436	0.00000990682963	0.00002170484728
4	0.00000071208799	0.00000277883632	0.00000608249190
5	0.00000026649525	0.00000103141516	0.00000223744423
6	0.00000011895071	0.00000045465901	0.00000097249675
7	0.00000005985160	0.00000022513795	0.00000052029941
8	0.00000003284898	0.00000012119745	0.00000031632713
v, $t = 2$	$Z = 1$	$Z = 2$	$Z = 3$
0	-0.00001198671118	-0.00003485048044	-0.00005544193072
1	-0.00000032523553	-0.00000205207743	-0.00000556870493
2	-0.00000003458611	-0.00000025411499	-0.00000078238275
3	-0.00000000810852	-0.00000006153142	-0.00000019579514
4	-0.00000000276059	-0.00000002120699	-0.00000006835365
5	-0.00000000116659	-0.00000000901894	-0.00000002926061
6	-0.00000000056830	-0.00000000441050	-0.00000001436431
7	-0.00000000030631	-0.00000000238324	-0.00000000778189

Table 2.6: The term $\langle \gamma_\mu G_4^{2v,t} (\Pi - \varepsilon)_\mu \rangle$ for $t = 0 \dots 2$ and $Z = 4, 5$.

v, $t = 0$	$Z = 4$	$Z = 5$
0	10.47635496988200	9.65852173434970
1	-1.03596385012300	-0.99344260115805
2	-0.01381000497668	-0.01649600511164
3	-0.00129389970368	-0.00160674545767
4	-0.00027953243625	-0.00034673680596
5	-0.00008855633280	-0.00010876271828
6	-0.00003477874880	-0.00004206200275
7	-0.00001564695675	-0.00001852761610
8	-0.00000771359307	-0.00000887743753
9	-0.00000404926693	-0.00000448445185
v, $t = 1$	$Z = 4$	$Z = 5$
0	0.21687674826935	0.20631747210923
1	0.00339954542678	0.00444746062443
2	0.00021771656532	0.00032140483571
3	0.00003745733026	0.00005663628250
4	0.00001048669839	0.00001583612838
5	0.00000381941497	0.00000570373148
6	0.00000170475140	0.00000246650462
7	0.00000082499317	0.00000115882181
8	0.00000055852727	0.00000093454941
v, $t = 2$	$Z = 4$	$Z = 5$
0	-0.00006545728004	-0.00005936951152
1	-0.00001068177734	-0.00001687301110
2	-0.00000167980837	-0.00000294846406
3	-0.00000043467662	-0.00000078929546
4	-0.00000015379096	-0.00000028315901
5	-0.00000006627637	-0.00000012278103
6	-0.00000003268223	-0.00000006199759
7	-0.00000001785678	-0.00000003707510

Table 2.7: The term $\langle \gamma_0 G_i^{2v-1,t} \gamma_i \gamma_0 \rangle$ for $t = 0, 1$ and $Z = 1 \ldots 3$.

v, $t = 0$	$Z = 1$	$Z = 2$	$Z = 3$
1	0.97215062286048	0.94774163217117	0.92553534783747
2	-1.21851078132680	-1.18963537114490	-1.16274756279690
3	-0.00632635645064	-0.01235104554689	-0.01809823001864
4	-0.00090074301285	-0.00183215100300	-0.00279163386878
5	-0.00028724365230	-0.00058775760582	-0.00090164180824
6	-0.00012486144618	-0.00025635545753	-0.00039468597298
7	-0.00006441453192	-0.00013257059203	-0.00020462449454
8	-0.00003711754843	-0.00007653492611	-0.00011836370444
9	-0.00002312245095	-0.00004775101299	-0.00007396576855
v, $t = 1$	$Z = 1$	$Z = 2$	$Z = 3$
1	0.73497058822949	0.72079834492871	0.70734511885783
2	0.00374965724538	0.00787881921766	0.01216932063700
3	0.00050662318459	0.00109674565596	0.00176555605393
4	0.00016016080938	0.00034620943543	0.00055865667415
5	0.00006922047309	0.00014966094668	0.00024183504240
6	0.00003553100772	0.00007686815491	0.00012435954058
7	0.00002038287843	0.00004412530988	0.00007146023760
8	0.00001264749096	0.00002739619961	0.00004440624932

Table 2.8: The term $\langle \gamma_0 G_i^{2v-1,t} \gamma_i \gamma_0 \rangle$ for $t = 0, 1$ and $Z = 4, 5$.

v, $t = 0$	$Z = 4$	$Z = 5$
1	0.90502410891211	0.88590389325674
2	-1.13752432318430	-1.11374720582780
3	-0.02358865256151	-0.02884060281403
4	-0.00377677765420	-0.00478536461451
5	-0.00122893755084	-0.00156964771113
6	-0.00054003657789	-0.00069257751045
7	-0.00028072538836	-0.00036101870206
8	-0.00016271305929	-0.00020969202718
9	-0.00010184615092	-0.00013147123940
v, $t = 1$	$Z = 4$	$Z = 5$
1	0.69453034920173	0.68229491623553
2	0.01652737103328	0.02089934047688
3	0.00250828485456	0.00332033619946
4	0.00079790340784	0.00106425800671
5	0.00034623750107	0.00046334608927
6	0.00017835428342	0.00023920320412
7	0.00010262574465	0.00013786400615
8	0.00006384340109	0.00008588189433

Figures

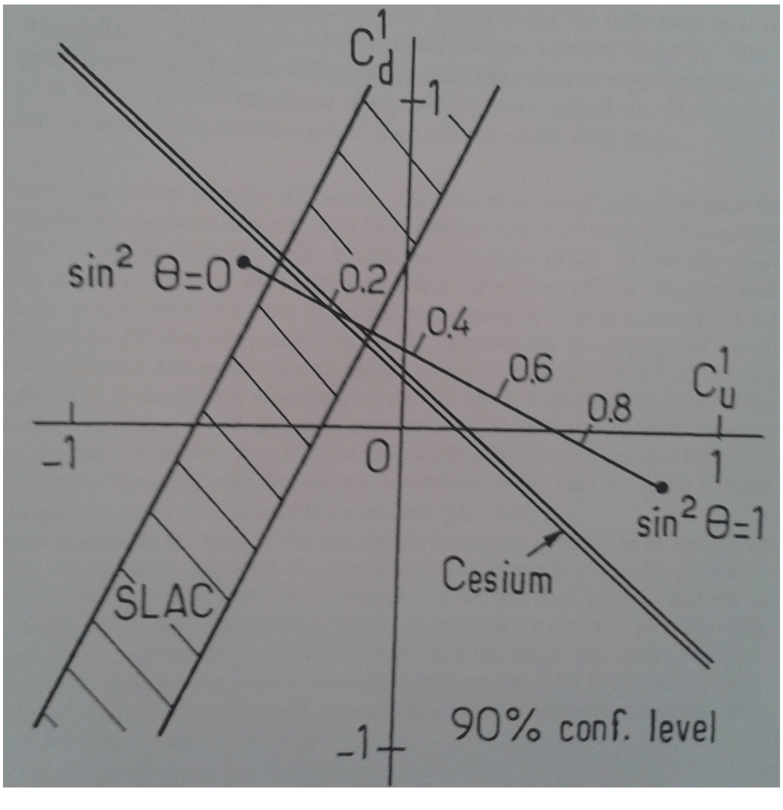

Figure 2.1: Schematic diagram of domains of interests for high-energy scattering experiments and low-energy atomic measurements in determination of weak charge.

Attachments

This thesis includes the following attachments:

1. J. Zamastil, V. Patkóš, Self-energy of bound electron for excited states, Phys. Rev. A **86**, 042514 (2012).
2. J. Zamastil, V. Patkóš, Self-energy of an electron bound in a Coulomb field, Phys. Rev. A **88**, 032501 (2013).
3. V. Patkóš, J. Zamastil, On the application of the pseudo-state method for evaluation of Lamb shift in hydrogen-like atoms, to be published.
4. Analytic evaluation of spinor-angular integrations needed in calculation of the self-energy for the ground state.