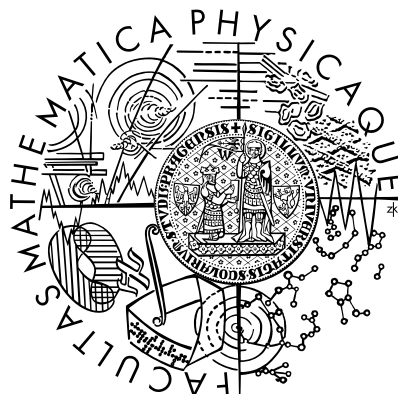


Univerzita Karlova v Praze
Matematicko-fyzikální fakulta

DIPLOMOVÁ PRÁCE



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Polarizace vakua v Coulombickém poli (Vacuum Polarization in Coulomb field)

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I thank to my supervisor doc. Mgr. Jaroslav Zamstil, Ph.D. for an interesting topic, stimulating leadership and his frank and unreserved attitude. I also thank to my parents for their neverending support.

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

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Abstrakt: V předložené práci je studována polarizace vakua a cirkulární dichroismus atomů vodíkového typu. Odvodíme rovnice pro Fourierovu transformaci vakuové hodnoty nábojové hustoty. Ty použijeme k odvození Uehlingova potenciálu a vypočteme jím způsobené posuny energií. Poté diskutujeme efekty ve vyšších řádech α . Ve druhé části definujeme cirkulární dichroismus a vyjádříme jej pomocí redukovaných maticových elementů. Poté odvodíme rovnici pro potenciál narušující paritu, který je vyvolaný slabou interakcí a společně s dalšími výsledky jej použijeme pro vyjádření cirkulárního dichroismu pomocí radálních vodíkových funkcí.

Klíčová slova: Radiační korekce, polarizace vakua, narušení parity, cirkulární dichroismus

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Abstract: In the present work the vacuum polarization and the circular dichroism of hydrogen-like atoms are studied. We derive equations for the Fourier transformation of the vacuum expectation value of the charge density. We use it to derive Uehling potential and calculate energy shifts caused by it. Then we discuss effects of vacuum polarization in higher orders of α . In second part we define circular dichroism and we express it in terms of reduced matrix elements. Then we derive the formula for parity violating potential which is generated by weak interaction and together with other results we use it to find the expression for circular dichroism in terms of hydrogen radial functions.

Keywords: Radiative corrections, vacuum polarization, parity violation, circular dichroism

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Notations and conventions

Throughout this thesis we use natural units, where $\hbar = c = 1$. We also use Einstein summation convention

$$a \cdot b = a^\mu b_\mu = a_\mu b_\mu g^{\mu\nu} = a_0 b_0 - a_j b_j \quad (1)$$

where $g_{00} = g^{00} = 1$, $g_{jj} = g^{jj} = -1$ for $j = 1, 2, 3$ and other $g_{\mu\nu}$ are zero. Other notation we use is the so called Feynman slash notation

$$\not{x} = a_\mu \gamma^\mu \quad (2)$$

where γ^μ are gamma matrices. In calculations we use Pauli-Dirac representation of them (see [6], Appendix A).

At last we use for description of the Dirac field and solutions of the Dirac equation following designation

- $\Psi(x)$... Dirac field
- $\psi(x)$... solution of the time-dependent Dirac equation
- $\Phi(\mathbf{x}) = \langle \mathbf{x} | n, p, j, m \rangle$... solution of the time-independent Dirac equation, where n is the principal quantum number, p is parity, j is the total angular momentum quantum number and m is the magnetic quantum number.

Introduction

Nowadays, high-precision spectroscopic measurements have achieved astonishing accuracy in determining transition frequencies. For example, the frequency for transition between $1S_{1/2} - 2S_{1/2}$ in hydrogen atom has been measured with the relative standard uncertainty only 1.4×10^{-14} [11]. With such accuracy even the tiny effects of quantum electrodynamics (QED) or weak interactions can be seen. Such experiments are very effective in testing standard model (SM) of elementary particles and they provide complementary information to the high energy experiments.

If we want to theoretically explain the measured frequencies, we have to take into account the so called radiative corrections. One of them is caused by virtual production and annihilation of the single e^+e^- pair which is called vacuum polarization. In this work we study the effect of vacuum polarization on atomic levels of electronic or muonic hydrogen-like atom. Especially in muonic atoms the vacuum polarization is the most important QED effect [4].

Other effects now accessible by experiment are those caused by weak interaction. One of the fundamental property of weak interaction is its non-conservation of parity. High-precision measurements of parity violation in atoms can be combined with measurements of the scattering of high-energy polarized electrons on nucleons. It gives constraints on fundamental constants - weak charges of u and d quarks. In Figure 1 taken from [5] we can see that the band obtained by the high-energy SLAC experiment [13, 14] is nearly orthogonal to that obtained by measurements of parity violation in cesium [22]. In this work we aim to calculate circular dichroism in stable atoms caused by weak interaction.

The thesis is organized as follows. At the beginning of chapter 1, we firstly summarize some bases of QED and then we derive the expression for the energy shift caused by Vacuum Polarization. Then we write the solution for hydrogen-like atom in relativistic treatment and discuss the use of the reduced mass in calculations. At the second part of chapter 1 we derive the expression for vacuum expectancy value (VEV) of the charge density which we approximate and solve using free particle and hydrogen function approach. At the end of chapter 1 we discuss the effects of the Uehling potential on hydrogen-like atoms.

In chapter 2 we show how a weak interaction violates the parity conservation in atomic processes. We describe a semiempirical theory that allows us to calculate form factors for neutral weak current. Finally, we derive the formula for circular dichroism in terms of reduced matrix elements which are then expressed by using just radial operators.

In Mathematical supplement we calculate several nontrivial integrals that are

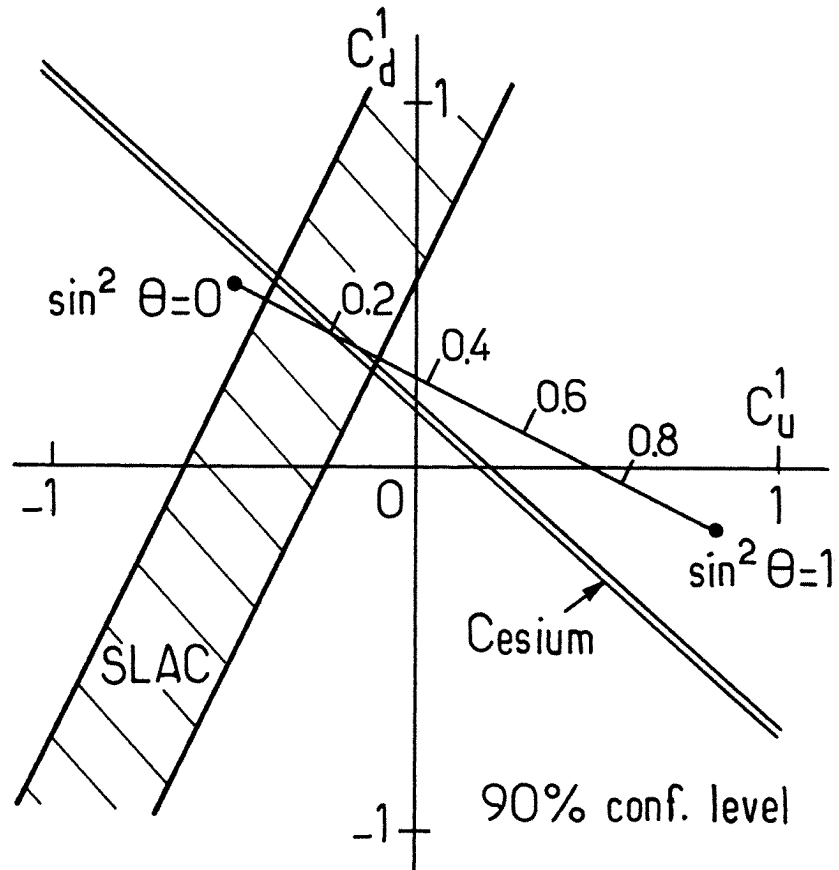


Figure 1: Experimental, model-independent determination of the weak charges of the u and d quarks. The two bands represent the domains allowed by the high-energy SLAC and by the cesium experiments. The graduated segment represents the prediction of the standard model for values of the parameter $\sin^2 \theta$ from 0 to 1.

needed in chapter 1. We also derive expansions to the second or third order for several types of hypergeometric functions.

Chapter 1

Vacuum Polarization in Coulomb Field

1.1 Current situation

In general sense, the Quantum Electrodynamics (QED) is a relativistic quantum field theory that describes interaction between light and matter. To quote Richard Feynmann, QED is the “jewel of physics” because of its extraordinary agreement with experimental results.

The unique system, on which QED can be tested, is a hydrogen atom. The Dirac equation can be solved exactly; therefore, the fundamental theory can be compared with high accuracy experiments.

Recently, the paper [2] was published and a possible discrepancy between the theory and experiment was reported therein.

The authors of [2] measured the $2S_{1/2} - 2P_{3/2}$ transition frequency in muonium ($\mu^- p^+$) by means of the pulse laser spectroscopy. They compared the experimental result with the theoretical prediction and the difference is believed to be caused by finite size nucleus effect. From this difference the proton radius was determined to be $r_p = (0.84184 \pm 0.00067)$ fm. It differs from previously determined values $r_p = (0.8768 \pm 0.0069)$ fm by 5σ extracted from comparison of theory and experiment for “ordinary” hydrogen [11].

What lies behind these discrepancies? The authors of [2] offer some possible explanations:

1. Some fundamental problem with bound-state QED.
2. Unknown effect related to proton or muon.
3. Supposed relation between measured energy shift and proton radius is wrong.
4. Computational error in calculation of radiative corrections.
5. Experimental error.

In this chapter we aim to check the values of radiative correction caused by vacuum polarization.

1.2 Bases of QED with respect to Vacuum Polarization

In this section we define some essential concepts and we describe the derivation of some equations that are necessary for the understanding of the Vacuum Polarization effect.

1.2.1 Time-independent derivation of the Vacuum Polarization

Let us derive energy shift caused by Vacuum Polarization using only time-independent perturbation theory. Dirac field has the form

$$\Psi(x) = \sum_k \psi_k(x) \hat{b}_k, \quad (1.1)$$

where \hat{b}_{k+} is the annihilation operator and \hat{b}_{k+}^\dagger is the creation operator of the electron (similarly \hat{b}_{k-} is the creation operator and \hat{b}_{k-}^\dagger is the annihilation operator of the positron) and $\psi_k(x)$ is the wave function of the electron (or positron) in state k . In this work we use stationary states $\Phi_k(\mathbf{x})$, which are defined as

$$\psi_k(x) = \Phi_k(\mathbf{x}) e^{-iE_k t}. \quad (1.2)$$

The summation in equation (1.1) is formal – it is summation over discrete part and integration over continuous part of the spectrum. For electrons (as for all fermions with spin 1/2) there is an anticommutation relation

$$\{\hat{b}_k^\dagger, \hat{b}_l\} = \delta_{k,l}. \quad (1.3)$$

Next we define charge-symmetric (see [23]) density operator of the Dirac field

$$\rho(x) = -\frac{e}{2} [\Psi^\dagger, \Psi]. \quad (1.4)$$

The vacuum expectation value (shortly VEV) of the charge density in vacuum is therefore defined as

$$\langle \rho(x) \rangle = \langle 0 | \rho(x) | 0 \rangle, \quad (1.5)$$

where $|0\rangle$ stands for vacuum state. Later we will show, that VEV of the charge density is time-independent, i. e.

$$\langle \rho(x) \rangle = \langle \rho(\mathbf{x}) \rangle. \quad (1.6)$$

If the $\langle \rho(\mathbf{x}) \rangle$ is nonzero, it interacts with the Dirac field. The Hamiltonian describing the interaction between the external potential and the Dirac field has the form

$$\hat{H}_{int} = -e \int d^3\mathbf{x}_2 \frac{1}{2} [\bar{\Psi}(x_2), \gamma^\mu \Psi(x_2)] A_\mu(\mathbf{x}_2), \quad (1.7)$$

where γ^μ are gamma matrices. Time-independent VEV of the charge density generates electrostatic potential

$$A_0(\mathbf{x}_2) = e \int d^3\mathbf{x}_1 \frac{\langle \rho(\mathbf{x}_1) \rangle}{4\pi|\mathbf{x}_1 - \mathbf{x}_2|} \quad \text{and} \quad A_i = 0. \quad (1.8)$$

In the first order of the time-independent perturbation theory is the energy shift of the electron in state n caused by vacuum polarization

$$\begin{aligned} \Delta E_n^{VP} &= \langle 0 | \hat{b}_n \hat{H}_{int} \hat{b}_n^\dagger | 0 \rangle = e \langle 0 | \hat{b}_n \int d^3\mathbf{x}_2 \Psi^\dagger(x_2) \Psi(x_2) \int d^3\mathbf{x}_1 \frac{\langle \rho(\mathbf{x}_1) \rangle}{4\pi|\mathbf{x}_1 - \mathbf{x}_2|} \hat{b}_n^\dagger | 0 \rangle = \\ &= e \int \int d^3\mathbf{x}_1 d^3\mathbf{x}_2 \frac{\langle \rho(\mathbf{x}_1) \rangle}{4\pi|\mathbf{x}_1 - \mathbf{x}_2|} \sum_{k,l} \langle 0 | \hat{b}_n \hat{b}_k^\dagger \hat{b}_l \hat{b}_n^\dagger | 0 \rangle \Phi_k^\dagger(\mathbf{x}_2) \Phi_l(\mathbf{x}_2) e^{-i(E_l - E_k)t_2}. \end{aligned}$$

We use relation (1.3) and for the part containing creation and annihilations operators we get

$$\langle 0 | \hat{b}_n \hat{b}_k^\dagger \hat{b}_l \hat{b}_n^\dagger | 0 \rangle = \langle 0 | (\delta_{k,n} - \hat{b}_k^\dagger \hat{b}_n) (\delta_{l,n} - \hat{b}_n^\dagger \hat{b}_l) | 0 \rangle = \delta_{k,n} \delta_{l,n}. \quad (1.9)$$

We also use a Fourier transformation

$$\frac{1}{4\pi|\mathbf{x}_1 - \mathbf{x}_2|} = \int \frac{d^3\mathbf{k}}{(2\pi)^3} \frac{e^{-i\mathbf{k}\cdot(\mathbf{x}_1 - \mathbf{x}_2)}}{\omega^2} \quad (1.10)$$

and then the final equation for the energy shift reads

$$\Delta E_n^{VP} = e \int d^3\mathbf{x}_2 \Phi_n(\mathbf{x}_2)^\dagger \Phi_n(\mathbf{x}_2) \int \frac{d^3\mathbf{k}}{(2\pi)^3} \frac{e^{i\mathbf{k}\cdot\mathbf{x}_2}}{\omega^2} \underbrace{\int d^3\mathbf{x}_1 \langle \rho(\mathbf{x}_1) \rangle e^{-i\mathbf{k}\cdot\mathbf{x}_1}}_{\langle \tilde{\rho}(\mathbf{k}) \rangle}. \quad (1.11)$$

We have used the symbol ω for the magnitude of the vector \mathbf{k} , i. e. $|\mathbf{k}| = \omega$ and $\langle \tilde{\rho}(\mathbf{k}) \rangle$ is the Fourier transformation of the current operator in vacuum.

1.2.2 Green's function of the Dirac field

In this subsection we are going to find an expression for the Green's function of the Dirac field which we will find useful in the next subsection.

By definition of Green's function it holds (from the operator point of view)

$$(\not{\mathbb{I}} - m) G = 1. \quad (1.12)$$

We want to calculate how the Green's function is evolving in time $G(t_1, t_2) = \langle t_1 | G | t_2 \rangle$. From (1.12) we get the equation for $G(t_1, t_2)$

$$\gamma_0 \left(i \frac{\partial}{\partial t_1} - H_0 \right) G(t_1, t_2) = \langle t_1 | t_2 \rangle = \delta(t_1 - t_2), \quad (1.13)$$

where

$$H_0 = eA_0 + \gamma_0 \gamma_j (-i\partial_j - eA_j) + \gamma_0 m \quad (1.14)$$

is the time-independent Hamiltonian (we restrict ourselves to static potentials). From the properties of Greens' functions we know that they depend on the difference of the time $(t_1 - t_2)$, for further information see [8], chapter 1. We use this knowledge and we write the Fourier transformations

$$G(t_1, t_2) = \int \frac{dE}{2\pi} e^{-iE(t_1-t_2)} R(E), \quad (1.15)$$

$$\delta(t_1 - t_2) = \int \frac{dE}{2\pi} e^{-iE(t_1-t_2)}, \quad (1.16)$$

where $R(E)$ is called resolvent. Substituting Fourier transforms (1.15) and (1.16) into equation (1.13) we can calculate the resolvent

$$\begin{aligned} \gamma_0 \left(i \frac{\partial}{\partial t_1} - H_0 \right) \int \frac{dE}{2\pi} e^{-iE(t_1-t_2)} R(E) &= \int \frac{dE}{2\pi} e^{-iE(t_1-t_2)} \\ \gamma_0 (E - H_0) R(E) &= 1 \\ R(E) &= \frac{\gamma_0}{E - H_0}, \end{aligned} \quad (1.17)$$

where we have used the fact that $\gamma_0^2 = 1$. We can use a resolution of identity

$$1 = \sum_n |\Phi_n\rangle \langle \Phi_n|, \quad (1.18)$$

where $|\Phi_n\rangle$ are eigenvectors of the time-independent Hamiltonian. It is obvious from (1.2) that it holds

$$H_0 |\Phi_n\rangle = E_n |\Phi_n\rangle. \quad (1.19)$$

The Green's function can be then written using (1.17) and (1.18)

$$\begin{aligned} G(t_1, t_2) &= \int \frac{dE}{2\pi} \frac{\gamma_0 e^{-iE(t_1-t_2)}}{E - H_0} = \lim_{\epsilon \rightarrow 0} \sum_{n+} \int_{\Gamma} \frac{dE}{2\pi} \frac{\gamma_0 e^{-iE(t_1-t_2)}}{E - E_n + i\epsilon} |\Phi_{n+}\rangle \langle \Phi_{n+}| + \\ &+ \sum_{n-} \int_{\Gamma} \frac{dE}{2\pi} \frac{\gamma_0 e^{-iE(t_1-t_2)}}{E - E_n - i\epsilon} |\Phi_{n-}\rangle \langle \Phi_{n-}|, \end{aligned} \quad (1.20)$$

We have added the parameter ϵ according to Feynmans prescription to know how to round singularities in the complex E-plane. The integration path Γ is shown on the Figure 1.1. After the integration we get the Green's function in the form

$$\begin{aligned} G(t_1, t_2) &= -i\theta(t_1 - t_2) \sum_{n+} e^{-E_{n+}(t_1-t_2)} |\Phi_{n+}\rangle \langle \Phi_{n+}| + \\ &+ i\theta(t_2 - t_1) \sum_{n-} e^{-E_{n-}(t_1-t_2)} |\Phi_{n-}\rangle \langle \Phi_{n-}|. \end{aligned} \quad (1.21)$$

To simplify the discussion we will use symbol \mathbb{H} where the zeroth component is now (after the Fourier transform) equal to $\Pi_0 = E - eA_0^e$, where A_0^e is the static potential in which the electron is bound.

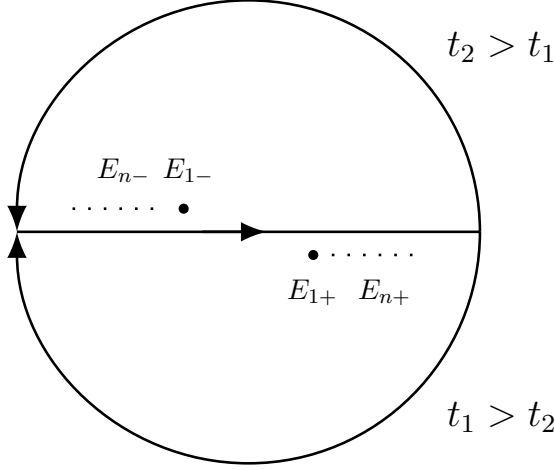


Figure 1.1: Integration path Γ in the complex E -plane

For further calculations we need to know the diagonal matrix element of the Green's function $G(x, x)$. We can write it in the following form

$$\begin{aligned}
 G(x, x) &= \langle \mathbf{r} | G(t, t) | \mathbf{r} \rangle = \langle \mathbf{r} | \int \frac{dE}{2\pi} \frac{1}{\mathbb{I} - m} | \mathbf{r} \rangle = \\
 &= \int \frac{dE}{2\pi} \langle \mathbf{r} | (\mathbb{I} + m) \frac{1}{\mathbb{I}^2 - m^2} | \mathbf{r} \rangle = \int \frac{dE}{2\pi} \langle \mathbf{r} | \frac{1}{\mathbb{I}^2 - m^2} (\mathbb{I} + m) | \mathbf{r} \rangle \quad (1.22)
 \end{aligned}$$

From the equation (1.22) it is also obvious that the "diagonal matrix element" of the Green's function does not depend on the timelike component, i. e.

$$G(x, x) = G(\mathbf{x}, \mathbf{x}). \quad (1.23)$$

1.2.3 Charge density operator in vacuum expressed in terms of Green's function

In the equation (1.5) we have defined the VEV of the charge density. In this section we will show how to calculate $\langle \rho(\mathbf{x}) \rangle$ with the use of the Green's function. We have

$$\begin{aligned}
 \langle \rho(x) \rangle &= -\frac{e}{2} \langle 0 | \Psi^\dagger(x) \Psi(x) - \Psi(x) \Psi^\dagger(x) | 0 \rangle = \frac{e}{2} \sum_{n,k} \langle 0 | \hat{b}_n^\dagger \hat{b}_k \psi_n^\dagger(x) \psi_k(x) - \\
 &\quad - \hat{b}_k \hat{b}_n^\dagger | 0 \rangle \psi_k(x) \psi_n^\dagger(x) = -\frac{e}{2} \sum_{n,k} \langle 0 | \hat{b}_{n+}^\dagger \hat{b}_{k+} \psi_{n+}^\dagger(x) \psi_{k+}(x) + \\
 &\quad + (\delta_{n-,k-} - \hat{b}_{n-} \hat{b}_{k-}^\dagger) \psi_{n-}^\dagger(x) \psi_{k-}(x) - (\delta_{n+,k+} - \hat{b}_{n+}^\dagger \hat{b}_{k+}) \times \\
 &\quad \times \psi_{k+}(x) \psi_{n+}^\dagger(x) - \hat{b}_{n-} \hat{b}_{k-}^\dagger \psi_{k-}(x) \psi_{n-}^\dagger(x) | 0 \rangle = \\
 &= -\frac{e}{2} \sum_n \Phi_{n-}^\dagger(\mathbf{x}) \Phi_{n-}(\mathbf{x}) - \Phi_{n+}(\mathbf{x}) \Phi_{n+}^\dagger(\mathbf{x}), \quad (1.24)
 \end{aligned}$$

because $\hat{b}_{n+}|0\rangle = \hat{b}_{n-}^\dagger|0\rangle = 0$. From the last equation it is also obvious that VEV of the charge density does not depend on the timelike component, as was presumed in section 1.2.1, equation (1.6).

In the next step we rewrite wave function into the form $\Phi_{n+}(\mathbf{x}) = \langle \mathbf{x} | \Phi_{n+} \rangle$ and use tr to emphasize that we have to trace over spinor components (trace over 4x4 matrices)

$$\langle \rho(\mathbf{x}) \rangle = -\frac{e}{2} \text{tr} \langle \mathbf{x} | \left(\sum_n |\Phi_{n-}\rangle \langle \Phi_{n-}| - |\Phi_{n+}\rangle \langle \Phi_{n+}| \right) | \mathbf{x} \rangle. \quad (1.25)$$

Now we use equation (1.21) from the last section and we get

$$\sum_{n-} |\Phi_{n-}\rangle \langle \Phi_{n-}| = \lim_{t_2 \rightarrow t_1^-} -iG(t_1, t_2), \quad (1.26)$$

$$\sum_{n+} -|\Phi_{n+}\rangle \langle \Phi_{n+}| = \lim_{t_2 \rightarrow t_1^+} -iG(t_1, t_2). \quad (1.27)$$

Finally we insert (1.26) and (1.27) into (1.25) and we get the final expression

$$\langle \rho(\mathbf{x}) \rangle = ie \text{tr} \langle \mathbf{x} | \left(\frac{1}{2} \lim_{t_2 \rightarrow t_1^+} + \frac{1}{2} \lim_{t_2 \rightarrow t_1^-} \right) G(t_1, t_2) | \mathbf{x} \rangle = ie \text{tr} G(\mathbf{x}, \mathbf{x}). \quad (1.28)$$

We have used the fact, that neither VEV of the charge density, nor diagonal matrix element of the Green's function depend on the time-like component.

1.2.4 Bound State QED and Vacuum Polarization

In this section we will briefly outline a different approach to equations such as (1.11) and (1.28).

We want to solve problems, where electron is bound; therefore, the common free particle approach is not valid. The way to do so is to use the so called Furry picture. After some technical problems it is possible to extend the Feynman-Dyson formalism for this class of problems. Details can be found in the book [16], chapter 15g.

The radiative correction of the vacuum polarization can be represented by the Feynman diagram on the Figure 1.2. The energy level of the bound electron in state $\Phi_n(x)$ is changed by vacuum polarization

$$\Delta E_n^{VP} = e \int d^3 \mathbf{x}_1 \int d^3 \mathbf{x}_2 \int d(t_2 - t_1) \bar{\psi}_n(x_2) \gamma^\mu \psi_n(x_2) D_F(x_2 - x_1) \times \underbrace{ie \text{tr} [\gamma_\mu G(x_1, x_1)]}_{\langle j_\mu(x_1) \rangle} \quad (1.29)$$

where $G(x, x)$ is the Green's function of the Dirac field, to be discussed below, D_F is the photon propagator of the form

$$D_F(x_2 - x_1) = \int \frac{d^4 k}{(2\pi)^4} \frac{e^{-ik_0(t_2-t_1)+i\mathbf{k}\cdot(\mathbf{x}_2-\mathbf{x}_1)}}{k_0^2 - \omega^2}. \quad (1.30)$$

and $\langle j_\mu(x) \rangle$ is the vacuum expectation value (VEV) of the current operator defined as

$$j_\mu(x) = -\frac{e}{2} [\bar{\Psi}(x), \gamma_\mu \Psi(x)]. \quad (1.31)$$

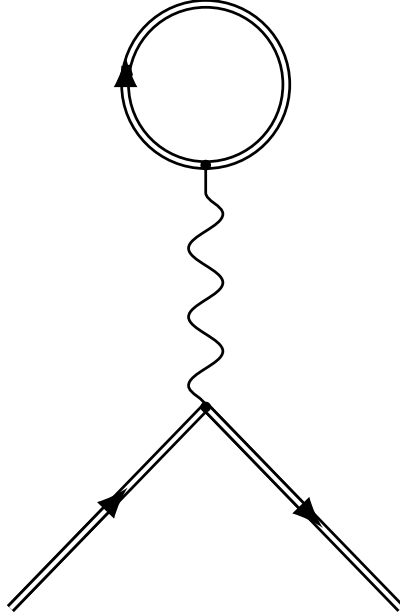


Figure 1.2: Feynman Diagram representing the Vacuum Polarization

We can see the definitions (1.4) and (1.31) are consistent, because $j_0(x) = \rho(x)$.

The diagonal matrix element of the Green's function $G(x_1, x_1)$ does not depend on the timelike component t_1 as was mentioned in the last subsection. Timelike component t_2 cancels, after the substitution from equation (1.2). As a consequence, we can integrate over $(t_2 - t_1)$ and then k_0 , which gives for the energy shift (1.29) following formula

$$\Delta E_n^{VP} = e \int d^3 \mathbf{x}_2 \bar{\Phi}_n(\mathbf{x}_2) \gamma^\mu \Phi_n(\mathbf{x}_2) \underbrace{\int \frac{d^3 \mathbf{k}}{(2\pi)^3} \frac{e^{i\mathbf{k} \cdot \mathbf{x}_2}}{\omega^2}}_{A_\mu(\mathbf{x}_2)} \overbrace{\int d^3 \mathbf{x}_1 \langle \tilde{j}_\mu(\mathbf{x}_1) \rangle e^{-i\mathbf{k} \cdot \mathbf{x}_1}}^{\langle \tilde{j}_\mu(\mathbf{k}) \rangle}, \quad (1.32)$$

where $\langle \tilde{j}_\mu(\mathbf{k}) \rangle$ is the Fourier transformation of the current operator in vacuum and $A_\mu(\mathbf{x})$ is the potential created by $\langle j_\mu(\mathbf{x}) \rangle$.

For $\mu = 0$ we can see that (1.32) is equal to (1.11). In this work we are interested in an electron in a Coloumb potential and as is mentioned in [17] the integrals with $\mu \neq 0$ vanish. In that case we get the same results for the just described approach and the one from the subsection 1.2.1.

1.3 Hydrogen-like atom in relativistic treatment

In this work we use solutions of the Dirac equation for hydrogen-like atoms (with infinitely massive and point nucleus) written as the linear combination of functions which are similar to the solutions of the non-relativistic hydrogen-like atom. This approach was firstly published in [3], the summarization of that approach can be found in [12] or [24].

The time-independent Dirac equation for hydrogen-like atom is

$$H_0\Phi = E\Phi, \quad (1.33)$$

where H_0 is defined in (1.14). We multiply equation (1.33) by γ_0 and write it in the form

$$(\mathbb{I} - m)\Phi = 0. \quad (1.34)$$

It is convenient to find the solutions Φ of the (1.34) using ansatz

$$\Phi = (\mathbb{I} + m)\phi, \quad (1.35)$$

The function ϕ is the solution of the equation

$$\mathcal{H}\phi = 0, \quad (1.36)$$

where the so called iterated Hamiltonian is defined as

$$\mathcal{H} = \mathbb{I}^2 - m^2. \quad (1.37)$$

1.3.1 Solutions of the iterated Hamiltonian

The set of mutually commuting operators is $\{\mathcal{H}, J^2, J_3, K, \Gamma\}$. Here \mathbf{J} is the operator of the total angular momentum,

$$\mathbf{J} = \mathbf{L} + \frac{1}{2}\boldsymbol{\Sigma}, \quad (1.38)$$

where \mathbf{L} is the orbital angular momentum operator and $\boldsymbol{\Sigma}/2$ is the spin operator. The operator Γ is defined as

$$\Gamma = \gamma_0 (K + i(Z\alpha)\boldsymbol{\gamma} \cdot \mathbf{n}), \quad (1.39)$$

where \mathbf{n} denotes the arbitrary unit vector and K stands for the relativistic parity operator

$$K = \gamma_0 (\boldsymbol{\Sigma} \cdot \mathbf{L} + 1). \quad (1.40)$$

We also use the so called effective orbital quantum number l_Γ , which (in relativistic treatment) is not an integer, but has a value

$$\begin{aligned} l_\Gamma &= |\Gamma| - 1 && \text{for } \Gamma > 0, \\ l_\Gamma &= |\Gamma| && \text{for } \Gamma < 0. \end{aligned}$$

The eigenvalues of the set of the mutually commuting operators are

$$\hat{J}^2\phi = j(j+1)\phi, \quad \text{where } j = \frac{1}{2}, \frac{3}{2}, \frac{5}{2}, \dots \quad (1.41)$$

$$\hat{J}_3\phi = m\phi, \quad \text{where } m = -j, -j+1, \dots, j-1, j \quad (1.42)$$

$$\hat{\Gamma}\phi = \Gamma\phi, \quad \text{where } \Gamma = \pm \sqrt{\left(j + \frac{1}{2}\right)^2 - (Z\alpha)^2}, \quad (1.43)$$

$$\hat{\mathcal{H}}\phi = \left(E^2 - m^2 + \frac{(EZ\alpha)^2}{n^2}\right)\phi, \quad \text{where } n = l_\Gamma + 1 + n_r, \quad (1.44)$$

with $n_r = 0, 1, \dots$

$$\hat{K}\phi = K\phi, \quad \text{where } K = p \left(j + \frac{1}{2}\right), \quad \text{with } p = \pm 1. \quad (1.45)$$

It is obvious from the equation (1.45) that quantum number p can be used instead of K . From equations (1.36) and (1.44) we get for the energy E in state n the relation

$$E_n = \frac{m}{\sqrt{1 + \frac{(Z\alpha)^2}{n^2}}}. \quad (1.46)$$

The iterated Hamiltonian \mathcal{H} has the same structure as the Hamiltonian operator for the non-relativistic hydrogen-like atom. As a consequence, the functions ϕ are

$$\phi = \langle \mathbf{r} | n, \Gamma, K, j, m \rangle = \langle r | n, \Gamma \rangle \langle \mathbf{n} | \Gamma, p, j, m \rangle = R_{n,l_\Gamma}(r) \left(\frac{c_{1,p}^\Gamma \langle \mathbf{n} | j, m \rangle^p}{c_{2,p}^\Gamma \langle \mathbf{n} | j, m \rangle^{-p}} \right). \quad (1.47)$$

Here $R_{n,l_\Gamma}(r)$ is the radial function of the non-relativistic hydrogen-like atom. The explicit form of the radial functions can be found in [10], §37. The symbol $\langle \mathbf{n} | j, m \rangle^p$ denotes the spherical spinors, where we have for $p = +1$

$$\langle \mathbf{n} | j, m \rangle^+ = \begin{pmatrix} \sqrt{\frac{j+m}{2j}} Y_{j-\frac{1}{2}, m-\frac{1}{2}}(\mathbf{n}) \\ \sqrt{\frac{j-m}{2j}} Y_{j-\frac{1}{2}, m+\frac{1}{2}}(\mathbf{n}) \end{pmatrix} \quad (1.48)$$

$$(1.49)$$

and for $p = -1$

$$\langle \mathbf{n} | j, m \rangle^- = \begin{pmatrix} -\sqrt{\frac{j-m+1}{2j+2}} Y_{j+\frac{1}{2}, m-\frac{1}{2}}(\mathbf{n}) \\ \sqrt{\frac{j+m+1}{2j+2}} Y_{j+\frac{1}{2}, m+\frac{1}{2}}(\mathbf{n}) \end{pmatrix}, \quad (1.50)$$

where functions of the form $Y_{j-\frac{p}{2}, m\pm\frac{1}{2}}(\mathbf{n})$ are spherical harmonics. Using the equations defined in [12] the constants $c_{1,p}^\Gamma$ and $c_{2,p}^\Gamma$ has the form (up to an arbitrary phase factor $e^{i\varphi}$)

$$c_{1,p}^\Gamma = p^{\theta(-\Gamma)} \frac{Z\alpha}{\sqrt{(Z\alpha)^2 + (\Gamma - p|K|)^2}}, \quad (1.51)$$

$$c_{2,p}^\Gamma = ip^{\theta(-\Gamma)} \frac{\Gamma - p|K|}{\sqrt{(Z\alpha)^2 + (\Gamma - p|K|)^2}}, \quad (1.52)$$

where $\theta(x)$ is Heaviside function, therefore $p^{\theta(-\Gamma)} = 1$ for $\Gamma > 0$ and $p^{\theta(-\Gamma)} = p$ for $\Gamma < 0$. We have thus found a spectrum of the iterated Hamiltonian operator \mathcal{H} .

1.3.2 Solution of the Dirac equation for the hydrogen-like atom

In the last section, we have found the solution ϕ of the iterated equation (1.36). According to (1.35), after the action of the operator $(\not{V} + m)$ we get the solution Φ of the Dirac equation (1.34). But there is a complication. The operator Γ (unlike operators J^2 , J_3 and K) does not commute with operator $(\not{V} + m)$. As

a consequence, the operator Γ is no longer an integral of the motion; thus, the solution Φ is in general a linear combination of both possible values of Γ . After a series of algebraic modifications we get (for particulars see [12])

$$\begin{aligned} \Phi(\mathbf{r}) = \langle \mathbf{r} | n, p, j, m \rangle = \frac{1}{N} & \left[AR_{n,|\Gamma|-1}(r) \begin{pmatrix} c_{1,p}^{|\Gamma|} \langle \mathbf{n} | j, m \rangle^p \\ c_{2,p}^{|\Gamma|} \langle \mathbf{n} | j, m \rangle^{-p} \end{pmatrix} + \right. \\ & \left. + BR_{n,|\Gamma|}(r) \begin{pmatrix} c_{1,p}^{-|\Gamma|} \langle \mathbf{n} | j, m \rangle^p \\ c_{2,p}^{-|\Gamma|} \langle \mathbf{n} | j, m \rangle^{-p} \end{pmatrix} \right], \end{aligned} \quad (1.53)$$

where constants A and B are

$$A = 1 + \frac{p|K|n}{|\Gamma|\sqrt{n^2 + (Z\alpha)^2}}, \quad (1.54)$$

$$B = \frac{Z\alpha}{|\Gamma|} \frac{\sqrt{n^2 - \Gamma^2}}{\sqrt{n^2 + (Z\alpha)^2}}, \quad (1.55)$$

and N is the normalization constant. We determine its value from the normalization condition $\langle \Phi | \Phi \rangle = 1$, which gives

$$N = \left[A^2 + B^2 + 2p \frac{Z\alpha}{(j + \frac{1}{2})} AB \int dr r^2 R_{n,|\Gamma|}(r) R_{n,|\Gamma|-1}(r) \right]^{\frac{1}{2}}. \quad (1.56)$$

1.3.3 Reduced mass in relativistic wave-functions

We can always (in the absence of external fields) write the nonrelativistic two-body problem in the terms of relative and centre-of-mass motion. From the approximation of an atom with the infinitely massive nucleus we move to the real problem with finite masses just by changing the mass of the electron (or muon) m to a reduced mass $m_r = mM_N/(m + M_N)$. When we treat the two-body problem relativistically the center-of-mass motion cannot be factored out rigorously because the Dirac Hamiltonian

$$H = \boldsymbol{\alpha} \cdot \mathbf{p} + \beta m + \boldsymbol{\alpha}_N \cdot \mathbf{p}_N + \beta_N M_N + V(|\mathbf{r} - \mathbf{r}_N|), \quad (1.57)$$

is incorrect. Here $\alpha_j = \gamma\gamma_j$ and $\beta = \gamma_0$ are Dirac matrices and quantities with subscript N stands for the quantities of nucleus.

The correct equation that describes two-interacting-fermion problem is Bethe-Salpeter equation [15], which is too complicated to be solved in practice.

Simpler approach is described in the articles [9] and [4]. It is based on extraction of the effective potential V_{eff} from the $e^- - p^+$ scattering amplitude. It is shown there that V_{eff} is the sum of Coulomb and Breit potential and for the point-like nucleus it has a form

$$V_{\text{eff}} = -\frac{Z\alpha}{r} + \frac{1}{M_N} \left[\frac{-Z\alpha(E_0 - \beta m)}{r} - \frac{(Z\alpha)^2}{2r^2} \right], \quad (1.58)$$

where the symbol E_0 is the eigenvalue of the Dirac Hamiltonian

$$H_0\Phi = \left[\boldsymbol{\alpha} \cdot \mathbf{p} + \beta m - \frac{Z\alpha}{r} \right] \Phi = E_0\Phi. \quad (1.59)$$

The effective Dirac equation for the electron (or muon) in potential generated by nucleus with mass M_N can be then written in the form

$$H_{\text{eff}} = \boldsymbol{\alpha} \cdot \mathbf{p} + \beta m + \frac{\mathbf{p}^2}{2M_N} + V_{\text{eff}}. \quad (1.60)$$

From (1.58) and (1.60) it is also obvious that in limit $M_N \rightarrow \infty$ we get $V_{\text{eff}} = -Z\alpha/r$ and $H_{\text{eff}} = H_0$. The terms proportional to $1/M_N$ will be treated as the first-order perturbation. In [4] it is shown that using the reduced mass m_r instead of m cancels most of the perturbation. We define

$$H_r\Phi_r = \left[\boldsymbol{\alpha} \cdot \mathbf{p} + \beta m_r - \frac{Z\alpha}{r} \right] \Phi_r = E_r\Phi_r \quad (1.61)$$

and the energy $E = \langle \Phi | H_{\text{eff}} | \Phi \rangle$ evaluated in the first order of m/M_N then yields

$$E = E_0 - \frac{E_0 m}{2M_N} - \frac{(E_0 - m)^2}{2M_N} \approx E_r - \frac{(E_0 - m)^2}{2M_N}. \quad (1.62)$$

For values in (1.62) it holds $E_0 \approx m \gg (E_0 - m)$ and thus the greater part of the perturbation is canceled when the reduced mass is used.

In the calculations in this work we use the reduced masses, but all corrections beyond that are neglected. For the sake of brevity we drop the subscript r .

1.4 Derivation of equations for $\langle \tilde{j}_0 \rangle$

In section 1.2 we have shown that the energy shift caused by vacuum polarization depend on the VEV of charge density (the zeroth component of the current operator). In this section we show how a Fourier transform of VEV of charge density could be expressed in terms of integrals I and J .

Using (1.22) we can write the VEV of the current operator in the form

$$\begin{aligned} \langle j_\mu(\mathbf{r}) \rangle &= ie \int \frac{dE}{2\pi} \text{tr} \gamma_\mu G(\mathbf{r}, \mathbf{r}) = ie \int \frac{dE}{2\pi} \text{tr} \gamma_\mu \langle \mathbf{r} | \frac{1}{2} \left\{ \gamma_\nu \Pi^\nu, \frac{1}{\mathcal{H}} \right\} | \mathbf{r} \rangle + \\ &+ ie \int \frac{dE}{2\pi} \langle \mathbf{r} | \underbrace{\text{tr} \gamma_\mu \frac{1}{2} \left\{ m, \frac{1}{\mathcal{H}} \right\}}_{=\dots \text{ odd } \gamma \dots = 0} | \mathbf{r} \rangle = \frac{ie}{2} \int \frac{dE}{2\pi} \langle \mathbf{r} | \text{tr} \gamma_\mu \left\{ \gamma_\nu \Pi^\nu, \frac{1}{\mathcal{H}} \right\} | \mathbf{r} \rangle \end{aligned} \quad (1.63)$$

where \mathcal{H} is defined in (1.37). It is convenient to use the following relation

$$\gamma_\mu \gamma_\nu = \frac{1}{2} \{ \gamma_\mu, \gamma_\nu \} + \frac{1}{2} [\gamma_\mu, \gamma_\nu]. \quad (1.64)$$

Using (1.64) we can simplify trace from equation (1.63)

$$\begin{aligned}
\text{tr } \gamma_\mu \left\{ \gamma_\nu \Pi^\nu, \frac{1}{\mathcal{H}} \right\} &= \text{tr } \gamma_\mu \gamma_\nu \Pi^\nu \frac{1}{\mathcal{H}} + \underbrace{\text{tr } \gamma_\mu \frac{1}{\mathcal{H}} \Pi^\nu \gamma_\nu}_{=\text{tr } \frac{1}{\mathcal{H}} \Pi^\nu \gamma_\nu \gamma_\mu} = \\
&= \left(\frac{1}{2} \text{tr } \{ \gamma_\mu, \gamma_\nu \} \Pi^\nu \frac{1}{\mathcal{H}} + \frac{1}{2} \text{tr} [\gamma_\mu, \gamma_\nu] \Pi^\nu \frac{1}{\mathcal{H}} + \right. \\
&\quad \left. + \frac{1}{2} \text{tr } \frac{1}{\mathcal{H}} \Pi^\nu \underbrace{\{ \gamma_\nu, \gamma_\mu \}}_{=\{ \gamma_\mu, \gamma_\nu \}} + \frac{1}{2} \text{tr } \underbrace{[\gamma_\nu, \gamma_\mu]}_{=-[\gamma_\mu, \gamma_\nu]} \frac{1}{\mathcal{H}} \Pi^\nu \right) = \\
&= \frac{1}{2} \left(\underbrace{\text{tr } \{ \gamma_\mu, \gamma_\nu \}}_{=2g_{\mu\nu}} \Pi^\nu \frac{1}{\mathcal{H}} + \text{tr } \underbrace{\{ \gamma_\mu, \gamma_\nu \}}_{=2g_{\mu\nu}} \frac{1}{\mathcal{H}} \Pi^\nu + \right. \\
&\quad \left. + \text{tr} [\gamma_\mu, \gamma_\nu] \Pi^\nu \frac{1}{\mathcal{H}} - \text{tr} [\gamma_\mu, \gamma_\nu] \frac{1}{\mathcal{H}} \Pi^\nu \right) = \\
&= \text{tr } \left\{ \Pi_\mu, \frac{1}{\mathcal{H}} \right\} + \frac{1}{2} \text{tr} [\gamma_\mu, \gamma_\nu] \left[\Pi^\nu, \frac{1}{\mathcal{H}} \right].
\end{aligned}$$

In order to calculate energy shift we need to know the value of the Fourier transformation of the current operator in vacuum (see (1.32))

$$\begin{aligned}
\langle \tilde{j}_\mu(\mathbf{k}) \rangle &= \int d^3\mathbf{r} \langle j_\mu(\mathbf{r}) \rangle e^{-i\mathbf{k}\cdot\mathbf{r}} = \\
&= \frac{ie}{4\pi} \int dE \int d^3\mathbf{r} \langle \mathbf{r} | \left(\text{tr } \left\{ \Pi_\mu, \frac{1}{\mathcal{H}} \right\} + \frac{1}{2} \text{tr} [\gamma_\mu, \gamma_\nu] \left[\Pi^\nu, \frac{1}{\mathcal{H}} \right] \right) | \mathbf{r} \rangle e^{-i\mathbf{k}\cdot\mathbf{r}}.
\end{aligned} \tag{1.65}$$

Let us focus our attention to the vacuum polarization in the hydrogen atom. As discussed at the end of the previous chapter 1.2.4 only terms with $\mu = 0$ are nonzero [17]. Therefore we have for the energy shift

$$\Delta E_n^{VP} = e \int d^3\mathbf{x}_2 \bar{\Phi}_n^*(x_2) \Phi_n(x_2) \int \frac{d^3\mathbf{k}}{(2\pi)^3} \frac{e^{i\mathbf{k}\cdot\mathbf{x}_2}}{\omega^2} \langle \tilde{j}_0(\mathbf{k}) \rangle. \tag{1.66}$$

That means the Fourier transform of the current operator in vacuum is equal to the sum of two integrals

$$\langle \tilde{j}_0(\mathbf{k}) \rangle = \frac{ie}{4\pi} (I + J) \tag{1.67}$$

where

$$\begin{aligned}
I &= \int dE \int d^3\mathbf{r} \text{tr} \left\{ \Pi_0(\mathbf{r}), \langle \mathbf{r} | \frac{1}{\mathcal{H}} | \mathbf{r} \rangle \right\} e^{-i\mathbf{k}\cdot\mathbf{r}} = \\
&= \int dE \int d^3\mathbf{r} \text{tr} \left\{ E + \frac{Z\alpha}{r}, \langle \mathbf{r} | \frac{1}{\mathcal{H}} | \mathbf{r} \rangle \right\} e^{-i\mathbf{k}\cdot\mathbf{r}}
\end{aligned} \tag{1.68}$$

and

$$\begin{aligned}
J &= \int dE \int d^3\mathbf{r} \frac{1}{2} \underbrace{\text{tr} [\gamma_0, \gamma_i]}_{=2\gamma_0\gamma_i} \langle \mathbf{r} | \left[\Pi^i, \frac{1}{\mathcal{H}} \right] | \mathbf{r} \rangle e^{-i\mathbf{k}\cdot\mathbf{r}} = \\
&= \int dE \int d^3\mathbf{r} \text{tr } \gamma_0 \gamma_i \langle \mathbf{r} | \left[p^i, \frac{1}{\mathcal{H}} \right] | \mathbf{r} \rangle e^{-i\mathbf{k}\cdot\mathbf{r}}.
\end{aligned} \tag{1.69}$$

From (1.37) we have

$$\begin{aligned} \mathcal{H} &= \cancel{\mathbb{V}}^2 - m^2 = \Pi^2 - m^2 + \gamma_0 \gamma_j [p_j, \Pi_0] = \\ &= \underbrace{E^2 - m^2 - \mathbf{p}^2}_{\mathcal{H}_0} + \underbrace{\frac{2EZ\alpha}{r}}_{\mathcal{V}} + \underbrace{\gamma_0 \gamma_j \left[p_j, \frac{Z\alpha}{r} \right]}_{\mathcal{V}'} + \underbrace{\frac{(Z\alpha)^2}{r^2}}_{\mathcal{V}''}. \end{aligned} \quad (1.70)$$

The perturbations \mathcal{V} and \mathcal{V}' are of the first order and \mathcal{V}'' is of the second order in $Z\alpha$.

There are two ways to write the $1/\mathcal{H}$ operator as a useful series in $Z\alpha$

$$\begin{aligned} \frac{1}{\mathcal{H}} &= \frac{1}{\mathcal{H}_0} - \frac{1}{\mathcal{H}_0} (\mathcal{V} + \mathcal{V}' + \mathcal{V}'') \frac{1}{\mathcal{H}_0} + \\ &+ \frac{1}{\mathcal{H}_0} (\mathcal{V} + \mathcal{V}' + \mathcal{V}'') \frac{1}{\mathcal{H}_0} (\mathcal{V} + \mathcal{V}' + \mathcal{V}'') \frac{1}{\mathcal{H}_0} + \dots, \end{aligned} \quad (1.71)$$

called free particle approach or

$$\frac{1}{\mathcal{H}} = \frac{1}{\mathcal{H}'_0} - \frac{1}{\mathcal{H}'_0} (\mathcal{V}' + \mathcal{V}'') \frac{1}{\mathcal{H}'_0} + \frac{1}{\mathcal{H}'_0} (\mathcal{V}' + \mathcal{V}'') \frac{1}{\mathcal{H}'_0} (\mathcal{V}' + \mathcal{V}'') \frac{1}{\mathcal{H}'_0} + \dots, \quad (1.72)$$

called hydrogen functions approach. We can proceed to calculate I and J integrals using both (1.71) and (1.72) approaches.

Let us introduce labeling $I_n^{(k)}$, resp. $J_j^{(i)}$. The lower index j is equal to number of first terms of expansion (1.71) that are used to calculate the integrals I , resp. J . The upper index (i) stands for the order of α to which the integral is proportional.

1.5 Calculation of the 1. order in α

1.5.1 Hydrogen function approach

In order to calculate the first order in α we need to use only first two terms of expansion (1.72); consequently, we calculate integrals I_2 and J_2

$$\begin{aligned} I_2 &= \int dE \int d^3\mathbf{r} \operatorname{tr} 2 \left(E + \frac{Z\alpha}{r} \right) \langle \mathbf{r} | \frac{1}{\mathcal{H}'_0} | \mathbf{r} \rangle e^{-i\mathbf{k}\cdot\mathbf{r}} - \\ &- \int dE \int d^3\mathbf{r} \underbrace{\operatorname{tr} \gamma_0 \gamma_j}_{=0} 2 \left(E + \frac{Z\alpha}{r} \right) \langle \mathbf{r} | \frac{1}{\mathcal{H}'_0} \left[p_j, \frac{Z\alpha}{r} \right] \frac{1}{\mathcal{H}'_0} | \mathbf{r} \rangle e^{-i\mathbf{k}\cdot\mathbf{r}} \end{aligned} \quad (1.73)$$

The integral I_2 is equal to the sum of two nonzero integrals $I_2 = I_{2a} + I_{2b}$, where

$$I_{2a} = 8 \int dE \int d^3\mathbf{r} E \langle \mathbf{r} | \frac{1}{\mathcal{H}'_0} | \mathbf{r} \rangle e^{-i\mathbf{k}\cdot\mathbf{r}} \quad (1.74)$$

and

$$I_{2b} = 8Z\alpha \int dE \int d^3\mathbf{r} \frac{1}{r} \langle \mathbf{r} | \frac{1}{\mathcal{H}'_0} | \mathbf{r} \rangle e^{-i\mathbf{k}\cdot\mathbf{r}}. \quad (1.75)$$

Let us start with calculation of the integral I_{2a} .

The resolution of identity using eigenfunctions of \mathcal{H}'_0 has the form

$$1 = \sum_{n_1, n_2, m} |n_1, n_2, m\rangle \langle n_1, n_2, m| + \int d^3\mathbf{K}_e |\mathbf{K}_e\rangle \langle \mathbf{K}_e| \quad (1.76)$$

where $\mathcal{H}'_0|\mathbf{K}_e\rangle = (E^2 - m^2 - (EZ\alpha)^2\mathbf{K}_e^2)|\mathbf{K}_e\rangle$. Integers n_1, n_2 are called parabolic quantum numbers and m is the magnetic quantum number. For more information about motion in a Coloumb field in parabolic coordinates see [10], §37. For reasons which will be clarified later, we use only the continuous part of the (1.76)

$$\begin{aligned} I_{2a} &= 8 \int dE E \int d^3\mathbf{r} \langle \mathbf{r} | \int d^3\mathbf{K}_e |\mathbf{K}_e\rangle \langle \mathbf{K}_e| \frac{1}{\mathcal{H}'_0} | \mathbf{r} \rangle e^{-i\mathbf{k}\cdot\mathbf{r}} = \\ &= 8 \int dE E \int d^3\mathbf{K}_e \int d^3\mathbf{r} \frac{\langle \mathbf{r} | \mathbf{K}_e \rangle \langle \mathbf{K}_e | \mathbf{r} \rangle}{E^2 - m^2 - (EZ\alpha)^2\mathbf{K}_e^2} e^{-i\mathbf{k}\cdot\mathbf{r}}, \end{aligned} \quad (1.77)$$

with hydrogen wave functions (see [10], §135).

$$\begin{aligned} \langle \mathbf{r} | \mathbf{K}_e \rangle &= (EZ\alpha)^{\frac{3}{2}} \frac{e^{\frac{\pi}{2}|\mathbf{K}_e|}}{(2\pi)^{\frac{3}{2}}} \Gamma\left(1 + \frac{i}{|\mathbf{K}_e|}\right) e^{iEZ\alpha\mathbf{K}_e\cdot\mathbf{r}} \times \\ &\quad \times F\left(-\frac{i}{|\mathbf{K}_e|}, 1, iEZ\alpha(|\mathbf{K}_e|r - \mathbf{K}_e\cdot\mathbf{r})\right), \end{aligned} \quad (1.78)$$

where $F(a, b, z)$ is a confluent hypergeometric function.

Because we integrate over $d^3\mathbf{K}_e$ it is convenient to make substitution

$$\mathbf{K}_e \rightarrow \mathbf{k}_e / (EZ\alpha), \quad (1.79)$$

which gives

$$\begin{aligned} \langle \mathbf{r} | \mathbf{k}_e \rangle \langle \mathbf{k}_e | \mathbf{r} \rangle &= (EZ\alpha)^3 \frac{e^{\frac{EZ\alpha\pi}{|\mathbf{k}_e|}}}{(2\pi)^3} \Gamma\left(1 + \frac{iEZ\alpha}{|\mathbf{k}_e|}\right) \Gamma\left(1 - \frac{iEZ\alpha}{|\mathbf{k}_e|}\right) \times \\ &\quad \times F\left(-\frac{iEZ\alpha}{|\mathbf{k}_e|}, 1, i(|\mathbf{k}_e|r - \mathbf{k}_e\cdot\mathbf{r})\right) F\left(\frac{iEZ\alpha}{|\mathbf{k}_e|}, 1, -i(|\mathbf{k}_e|r - \mathbf{k}_e\cdot\mathbf{r})\right). \end{aligned} \quad (1.80)$$

For the sake of transparency let us denote

$$a = \frac{iEZ\alpha}{|\mathbf{k}_e|}. \quad (1.81)$$

Henceforth (1.77) has the form

$$\begin{aligned} I_{2a} &= 8 \int dE E \int \int d^3\mathbf{r} \frac{d^3\mathbf{k}_e}{(EZ\alpha)^3} \frac{e^{-i\pi a}}{E^2 - m^2 - \mathbf{k}_e^2} \frac{(EZ\alpha)^3}{(2\pi)^3} \Gamma(1+a) \Gamma(1-a) \times \\ &\quad \times F(-a, 1, i(|\mathbf{k}_e|r - \mathbf{k}_e\cdot\mathbf{r})) F(a, 1, -i(|\mathbf{k}_e|r - \mathbf{k}_e\cdot\mathbf{r})) e^{-i\mathbf{k}\cdot\mathbf{r}} = \\ &= \int dE \frac{E}{\pi^3} \int d^3\mathbf{k}_e \frac{e^{-i\pi a}}{E^2 - m^2 - \mathbf{k}_e^2} \Gamma(1+a) \Gamma(1-a) \times K, \end{aligned}$$

where

$$K = \int d^3\mathbf{r} e^{-i\mathbf{k}\cdot\mathbf{r}} F\left(-a, 1, i(|\mathbf{k}_e|r - \mathbf{k}_e \cdot \mathbf{r})\right) F\left(a, 1, -i(|\mathbf{k}_e|r - \mathbf{k}_e \cdot \mathbf{r})\right). \quad (1.82)$$

The detailed calculation of the nontrivial integral K can be found in the appendix A.1.1. The final result is

$$\begin{aligned} I_{2a} = & \frac{16i}{\pi^2\omega^2} \int dE \int d^3\mathbf{k}_e \frac{aEe^{-i\pi a}}{E^2 - m^2 - \mathbf{k}_e^2} \frac{\Gamma(1+a)\Gamma(1-a)|\mathbf{k}_e|}{4\mathbf{k}_e^2 \cos^2\theta - \omega^2} \times \\ & \times \left(\frac{\omega + 2|\mathbf{k}_e| \cos\theta}{\omega - 2|\mathbf{k}_e| \cos\theta} \right)^a \left[F\left(-a, a, 1, \frac{4\mathbf{k}_e^2 \cos^2\theta}{4\mathbf{k}_e^2 \cos^2\theta - \omega^2}\right) - \right. \\ & \left. - a \frac{2\omega|\mathbf{k}_e| \cos\theta}{4\mathbf{k}_e^2 \cos^2\theta - \omega^2} F\left(-a+1, a+1, 2, \frac{4\mathbf{k}_e^2 \cos^2\theta}{4\mathbf{k}_e^2 \cos^2\theta - \omega^2}\right) \right]. \quad (1.83) \end{aligned}$$

The first order in α is the same as the first order in a , so we can neglect some parts of the integral I_{2a} . We can also use some useful expansions

$$\begin{aligned} \left(\frac{\omega + 2|\mathbf{k}_e| \cos\theta}{\omega - 2|\mathbf{k}_e| \cos\theta} \right)^a = & 1 + a \ln \left(\frac{\omega + 2|\mathbf{k}_e| \cos\theta}{\omega - 2|\mathbf{k}_e| \cos\theta} \right) + \\ & + \frac{a^2}{2} \ln^2 \left(\frac{\omega + 2|\mathbf{k}_e| \cos\theta}{\omega - 2|\mathbf{k}_e| \cos\theta} \right) + O(a^3), \quad (1.84) \end{aligned}$$

$$\Gamma(1+a)\Gamma(1-a) = 1 - \frac{\pi^2 a^2}{6} + O(a^4), \quad (1.85)$$

$$e^{-i\pi a} = 1 - i\pi a - \frac{\pi^2 a^2}{2} + O(a^3). \quad (1.86)$$

$$F\left(-a, a, 1, \frac{4\mathbf{k}_e^2 \cos^2\theta}{4\mathbf{k}_e^2 \cos^2\theta - \omega^2}\right) = 1 + O(a^2), \quad (1.87)$$

In the first order of α we use only the ones from the expansions (1.84) – (1.87) and after the substitution for a defined in (1.81) we get

$$\boxed{I_{2a}^{(1)} = \frac{-16Z\alpha}{\pi^2\omega^2} \int dE \int d^3\mathbf{k}_e \frac{E^2}{E^2 - m^2 - \mathbf{k}_e^2} \cdot \frac{1}{4\mathbf{k}_e^2 \cos^2\theta - \omega^2}} \quad (1.88)$$

Let us turn our attention to the integral I_{2b} . We use the same steps as when modifying the expression of the integral I_{2a}

$$I_{2b} = \frac{Z\alpha}{\pi^3} \int dE \int d^3\mathbf{k}_e \frac{e^{-i\pi a}}{E^2 - m^2 - \mathbf{k}_e^2} \Gamma(1+a)\Gamma(1-a) \times K',$$

where

$$K' = \int d^3\mathbf{r} e^{-i\mathbf{k}\cdot\mathbf{r}} \frac{1}{r} F\left(-a, 1, i(|\mathbf{k}_e|r - \mathbf{k}_e \cdot \mathbf{r})\right) F\left(a, 1, -i(|\mathbf{k}_e|r - \mathbf{k}_e \cdot \mathbf{r})\right). \quad (1.89)$$

Calculation of the integral K' can be found in the appendix A.1.2. For the integral I_{2b} we then have formula

$$I_{2b} = \frac{4Z\alpha}{\pi^2\omega^2} \int dE \int d^3\mathbf{k}_e \frac{e^{-i\pi a}}{E^2 - m^2 - \mathbf{k}_e^2} \Gamma(1+a) \Gamma(1-a) \times \\ \times \left(\frac{\omega + 2|\mathbf{k}_e| \cos \theta}{\omega - 2|\mathbf{k}_e| \cos \theta} \right)^a F \left(-a, a, 1, \frac{4\mathbf{k}_e^2 \cos^2 \theta}{4\mathbf{k}_e^2 \cos^2 \theta - \omega^2} \right). \quad (1.90)$$

In this section we only want the first order in α , so we again use the expansions (1.84) – (1.87) and we get

$$I_{2b}^{(1)} = \frac{4Z\alpha}{\pi^2\omega^2} \int dE \int d^3\mathbf{k}_e \frac{1}{E^2 - m^2 - \mathbf{k}_e^2} \quad (1.91)$$

Our next goal is to calculate the integral J_2 . We can use a fact that p_j commute with \mathcal{H}_0 but not with $1/r$. It means we can write

$$\frac{1}{\mathcal{H}'_0} [p^j, \Pi_0] \frac{1}{\mathcal{H}'_0} = \frac{1}{\mathcal{H}'_0} \left[p^j, \frac{\mathcal{H}'_0}{2E} \right] \frac{1}{\mathcal{H}'_0} = -\frac{1}{2E} \left[p^j, \frac{1}{\mathcal{H}'_0} \right], \quad (1.92)$$

where we have used an operator relation

$$\frac{1}{A} [A, B] \frac{1}{A} = \left[B, \frac{1}{A} \right]. \quad (1.93)$$

After this we can do similar procedure for integral J_2 as we did for integral I_2

$$J_2 = \int dE \int d^3\mathbf{r} \underbrace{\text{tr} \gamma_0 \gamma_i}_{=0} \langle \mathbf{r} | \left[p^i, \frac{1}{\mathcal{H}'_0} \right] | \mathbf{r} \rangle e^{-i\mathbf{k}\cdot\mathbf{r}} - \int dE \int d^3\mathbf{r} \frac{1}{2E} \times \\ \times \underbrace{\text{tr} \gamma_0 \gamma_i \gamma_0 \gamma_j}_{-4g_{ij}} \langle \mathbf{r} | \left[p^i, \left[p_j, \frac{1}{\mathcal{H}'_0} \right] \right] | \mathbf{r} \rangle e^{-i\mathbf{k}\cdot\mathbf{r}} = \\ = \int dE \int d^3\mathbf{r} \frac{2}{E} \langle \mathbf{r} | \left[\mathbf{p}^2 \frac{1}{\mathcal{H}'_0} - 2p_j \frac{1}{\mathcal{H}'_0} p_j + \frac{1}{\mathcal{H}'_0} \mathbf{p}^2 \right] | \mathbf{r} \rangle e^{-i\mathbf{k}\cdot\mathbf{r}}.$$

At this time we again use the continuous part of hydrogen functions system (1.76)

$$J_2 = \int dE \int d^3\mathbf{r} \int d^3\mathbf{K}_e \frac{2}{E} \langle \mathbf{r} | \left(\mathbf{p}^2 | \mathbf{K}_e \rangle \langle \mathbf{K}_e | \frac{1}{\mathcal{H}'_0} - \right. \\ \left. - 2p_j | \mathbf{K}_e \rangle \langle \mathbf{K}_e | \frac{1}{\mathcal{H}'_0} p_j + \frac{1}{\mathcal{H}'_0} | \mathbf{K}_e \rangle \langle \mathbf{K}_e | \mathbf{p}^2 \right) | \mathbf{r} \rangle e^{-i\mathbf{k}\cdot\mathbf{r}}, \quad (1.94)$$

where we can use a relation

$$\langle \mathbf{r} | p_j | \mathbf{K}_e \rangle = -i \frac{\partial}{\partial x_j} \langle \mathbf{r} | \mathbf{K}_e \rangle, \quad (1.95)$$

which gives

$$J_2 = \int dE \int d^3\mathbf{K}_e \frac{-2}{E} \frac{1}{E^2 - m^2 - (EZ\alpha)^2 \mathbf{K}_e^2} \int d^3\mathbf{r} e^{-i\mathbf{k}\cdot\mathbf{r}} \nabla^2 (\langle \mathbf{r} | \mathbf{K}_e \rangle \langle \mathbf{K}_e | \mathbf{r} \rangle).$$

At this time we again make substitution for \mathbf{K}_e defined in (1.79) and then we use a from equation (1.81)

$$\begin{aligned} J_2 &= \int dE \int \frac{d^3 \mathbf{k}_e}{(EZ\alpha)^3} \frac{-2}{E} \frac{1}{E^2 - m^2 - \mathbf{k}_e^2} \int d^3 \mathbf{r} e^{-i\mathbf{k} \cdot \mathbf{r}} (EZ\alpha)^3 \frac{e^{-i\pi a}}{(2\pi)^3} \Gamma(1+a) \times \\ &\quad \times \Gamma(1-a) \nabla^2 F\left(-a, 1, i(|\mathbf{k}_e|r - \mathbf{k}_e \cdot \mathbf{r})\right) F\left(a, 1, -i(|\mathbf{k}_e|r - \mathbf{k}_e \cdot \mathbf{r})\right) = \\ &= \frac{1}{4\pi^3} \int dE \int d^3 \mathbf{k}_e \frac{1}{E} \frac{e^{-i\pi a}}{E^2 - m^2 - \mathbf{k}_e^2} \Gamma(1+a) \Gamma(1-a) \times L, \end{aligned}$$

where

$$L = \int d^3 \mathbf{r} e^{-i\mathbf{k} \cdot \mathbf{r}} \nabla^2 F\left(-a, 1, i(|\mathbf{k}_e|r - \mathbf{k}_e \cdot \mathbf{r})\right) F\left(a, 1, -i(|\mathbf{k}_e|r - \mathbf{k}_e \cdot \mathbf{r})\right). \quad (1.96)$$

After calculation of the integral L (for detailed calculation see appendix A.1.3) we get

$$\begin{aligned} J_2 &= \frac{-1}{2\pi^2} \int dE \int d^3 \mathbf{k}_e \frac{a}{E} \frac{e^{-i\pi a}}{E^2 - m^2 - \mathbf{k}_e^2} \Gamma(1+a) \Gamma(1-a) \times \\ &\quad \times \frac{1}{\cos^2 \theta} \left(\frac{\omega + 2|\mathbf{k}_e| \cos \theta}{\omega - 2|\mathbf{k}_e| \cos \theta} \right)^a \left[\frac{2i \cos \theta}{\omega + 2|\mathbf{k}_e| \cos \theta} \times \right. \\ &\quad \times F\left(-a+1, a, 1, \frac{4\mathbf{k}_e^2 \cos^2 \theta}{4\mathbf{k}_e^2 \cos^2 \theta - \omega^2}\right) - \\ &\quad \left. - \frac{2i \cos \theta}{\omega - 2|\mathbf{k}_e| \cos \theta} F\left(-a, a+1, 1, \frac{4\mathbf{k}_e^2 \cos^2 \theta}{4\mathbf{k}_e^2 \cos^2 \theta - \omega^2}\right) \right]. \quad (1.97) \end{aligned}$$

In the first order of a we can simplify the square bracket from the expression (1.97)

$$\begin{aligned} \frac{1}{\cos^2 \theta} \left[\frac{2i \cos \theta}{\omega + 2|\mathbf{k}_e| \cos \theta} - \frac{2i \cos \theta}{\omega - 2|\mathbf{k}_e| \cos \theta} \right] &= \\ &= \frac{2i}{\cos \theta} \left[\frac{\omega - 2|\mathbf{k}_e| \cos \theta - \omega - 2|\mathbf{k}_e| \cos \theta}{\omega^2 - 4\mathbf{k}_e^2 \cos^2 \theta} \right] = -\frac{8i|\mathbf{k}_e|}{\omega^2 - 4\mathbf{k}_e^2 \cos^2 \theta}. \end{aligned}$$

In the first order in a we again use the expansions (1.84) – (1.87) and then we substitute $a = iEZ\alpha/|\mathbf{k}_e|$

$$\boxed{J_2^{(1)} = \frac{4Z\alpha}{\pi^2} \int dE \int d^3 \mathbf{k}_e \frac{1}{E^2 - m^2 - \mathbf{k}_e^2} \frac{1}{4\mathbf{k}_e^2 \cos^2 \theta - \omega^2}}. \quad (1.98)$$

1.5.2 Free particle approach

The free particle approach means to use the series (1.72). So for integrals I and J in the first order of α we get (we use subscript F to emphasize the use of the free particle approach)

$$\begin{aligned}
I_F^{(1)} = & \underbrace{\int dE \int d^3\mathbf{r} \operatorname{tr} \left\{ E, \langle \mathbf{r} | \frac{1}{\mathcal{H}_0} | \mathbf{r} \rangle \right\}}_{=0 \text{ (odd in E)}} e^{-i\mathbf{k}\cdot\mathbf{r}} + \int dE \int d^3\mathbf{r} \operatorname{tr} \left\{ \frac{Z\alpha}{r}, \langle \mathbf{r} | \frac{1}{\mathcal{H}_0} | \mathbf{r} \rangle \right\} \times \\
& \times e^{-i\mathbf{k}\cdot\mathbf{r}} - \int dE \int d^3\mathbf{r} \operatorname{tr} \left\{ E + \underbrace{\frac{Z\alpha}{r}}_{2. \text{ order}}, \langle \mathbf{r} | \frac{1}{\mathcal{H}_0} \mathcal{V} \frac{1}{\mathcal{H}_0} | \mathbf{r} \rangle \right\} e^{-i\mathbf{k}\cdot\mathbf{r}} - \\
& - \int dE \int d^3\mathbf{r} \underbrace{\operatorname{tr} \gamma_0 \gamma_j}_{=0} \left\{ E - \frac{Z\alpha}{r}, \langle \mathbf{r} | \frac{1}{\mathcal{H}_0} [p^j, \Pi_0] \frac{1}{\mathcal{H}_0} | \mathbf{r} \rangle \right\} e^{-i\mathbf{k}\cdot\mathbf{r}}.
\end{aligned}$$

We then have two integrals

$$I_{Fa}^{(1)} = 8 \int dE \int d^3\mathbf{r} E \langle \mathbf{r} | \frac{1}{\mathcal{H}_0} \mathcal{V} \frac{1}{\mathcal{H}_0} | \mathbf{r} \rangle e^{-i\mathbf{k}\cdot\mathbf{r}} \quad (1.99)$$

and

$$I_{Fb}^{(1)} = 8 \int dE \int d^3\mathbf{r} \frac{Z\alpha}{r} \langle \mathbf{r} | \frac{1}{\mathcal{H}_0} | \mathbf{r} \rangle e^{-i\mathbf{k}\cdot\mathbf{r}} \quad (1.100)$$

In order to deal with operators we again use the resolution of identity. Now we use eigenfunctions of the free particle problem (i. e. plain waves)

$$1 = \int d^3\mathbf{p} |\mathbf{p}\rangle \langle \mathbf{p}| \quad \text{where} \quad \langle \mathbf{r} | \mathbf{p} \rangle = \frac{1}{(2\pi)^{\frac{3}{2}}} e^{i\mathbf{p}\cdot\mathbf{r}} \quad (1.101)$$

and it also holds $\mathcal{H}_0 |\mathbf{p}\rangle = E^2 - m^2 - \mathbf{p}^2 |\mathbf{p}\rangle$. So we insert two resolutions of the form (1.101) into calculation of integral $I_a^{(1)}$ and we get

$$\begin{aligned}
I_{Fa}^{(1)} = & -8 \int dE \int d^3\mathbf{r} \int d^3\mathbf{p}_1 \int d^3\mathbf{p}_2 E \langle \mathbf{r} | \frac{1}{\mathcal{H}_0} | \mathbf{p}_1 \rangle \langle \mathbf{p}_1 | \mathcal{V} | \mathbf{p}_2 \rangle \langle \mathbf{p}_2 | \frac{1}{\mathcal{H}_0} | \mathbf{r} \rangle e^{-i\mathbf{k}\cdot\mathbf{r}} \\
= & -8 \int dE \int d^3\mathbf{p}_1 \int d^3\mathbf{p}_2 E \frac{1}{E^2 - m^2 - \mathbf{p}_1^2} \frac{1}{E^2 - m^2 - \mathbf{p}_2^2} \langle \mathbf{p}_1 | \mathcal{V} | \mathbf{p}_2 \rangle \times \\
& \times \int d^3\mathbf{r} \underbrace{\langle \mathbf{r} | \mathbf{p}_1 \rangle}_{=\frac{e^{i\mathbf{p}_1\cdot\mathbf{r}}}{(2\pi)^{\frac{3}{2}}}} \underbrace{\langle \mathbf{p}_2 | \mathbf{r} \rangle}_{=\frac{e^{-i\mathbf{p}_2\cdot\mathbf{r}}}{(2\pi)^{\frac{3}{2}}}} e^{-i\mathbf{k}\cdot\mathbf{r}}.
\end{aligned} \quad (1.102)$$

We calculate the expression $\langle \mathbf{p}_1 | \mathcal{V} | \mathbf{p}_2 \rangle$ using spectral decomposition of the potential operator

$$\mathcal{V} = \int d^3\mathbf{r} \frac{2EZ\alpha}{r} |\mathbf{r}\rangle \langle \mathbf{r}| \quad (1.103)$$

and it gives

$$\langle \mathbf{p}_1 | \mathcal{V} | \mathbf{p}_2 \rangle = 2EZ\alpha \int d^3\mathbf{r} \frac{1}{(2\pi)^3} \frac{e^{-i(\mathbf{p}_2 - \mathbf{p}_1)\cdot\mathbf{r}}}{r} = \frac{EZ\alpha}{\pi^2 (\mathbf{p}_2 - \mathbf{p}_1)^2}. \quad (1.104)$$

Using (1.104) we can calculate the integral $I_{Fa}^{(1)}$

$$\begin{aligned}
I_{Fa}^{(1)} &= \frac{-8Z\alpha}{\pi^2} \int dE \int d^3\mathbf{p}_1 \int d^3\mathbf{p}_2 \frac{E^2}{E^2 - m^2 - \mathbf{p}_1^2} \frac{1}{E^2 - m^2 - \mathbf{p}_2^2} \frac{1}{(\mathbf{p}_2 - \mathbf{p}_1)^2} \times \\
&\quad \times \underbrace{\int d^3\mathbf{r} \frac{1}{(2\pi)^3} e^{-i(\mathbf{p}_1 + \mathbf{k} - \mathbf{p}_2) \cdot \mathbf{r}}}_{=\delta^3(\mathbf{p}_1 + \mathbf{k} - \mathbf{p}_2)} = \\
&= \frac{-8Z\alpha}{\pi^2\omega^2} \int dE \int d^3\mathbf{p}_1 \frac{E^2}{E^2 - m^2 - \mathbf{p}_1^2} \frac{1}{E^2 - m^2 - (\mathbf{p}_1 - \mathbf{k})^2} \quad (1.105)
\end{aligned}$$

Calculation of the $I_{Fb}^{(1)}$ is similar to the calculation of the $I_{Fa}^{(1)}$ as in the hydrogen function approach

$$\begin{aligned}
I_{Fb}^{(1)} &= 8 \int dE \int d^3\mathbf{r} \int d^3\mathbf{p}_1 \int d^3\mathbf{p}_2 \langle \mathbf{r} | \frac{1}{\mathcal{H}_0} | \mathbf{p}_1 \rangle \langle \mathbf{p}_1 | \frac{\mathcal{V}}{2E} | \mathbf{p}_2 \rangle \langle \mathbf{p}_2 | \mathbf{r} \rangle e^{-i\mathbf{k} \cdot \mathbf{r}} = \\
&= 4 \int dE \int d^3\mathbf{p}_1 \int d^3\mathbf{p}_2 \frac{1}{E} \frac{1}{E^2 - m^2 - \mathbf{p}_1^2} \langle \mathbf{p}_1 | \mathcal{V} | \mathbf{p}_2 \rangle \delta^3(\mathbf{p}_1 + \mathbf{k} - \mathbf{p}_2) = \\
&= \frac{4Z\alpha}{\pi^2\omega^2} \int dE \int d^3\mathbf{p}_1 \frac{1}{E^2 - m^2 - \mathbf{p}_1^2}. \quad (1.106)
\end{aligned}$$

Finally, let us calculate integral $J_F^{(1)}$ and show that it is equal to integral $J_2^{(1)}$.

$$\begin{aligned}
J_F^{(1)} &= \int dE \int d^3\mathbf{r} \underbrace{\text{tr} \gamma_0 \gamma_i}_{=0} \langle \mathbf{r} | \left[p^i, \frac{1}{\mathcal{H}_0} \right] | \mathbf{r} \rangle e^{-i\mathbf{k} \cdot \mathbf{r}} + \\
&\quad + \int dE \int d^3\mathbf{r} \underbrace{\text{tr} \gamma_0 \gamma_i}_{=0} \langle \mathbf{r} | \left[p^i, \frac{1}{\mathcal{H}_0} \mathcal{V} \frac{1}{\mathcal{H}_0} \right] | \mathbf{r} \rangle e^{-i\mathbf{k} \cdot \mathbf{r}} - \\
&\quad - \int dE \int d^3\mathbf{r} \text{tr} \gamma_0 \gamma_i \langle \mathbf{r} | \left[p^i, \frac{1}{\mathcal{H}_0} \mathcal{V}' \frac{1}{\mathcal{H}_0} \right] | \mathbf{r} \rangle e^{-i\mathbf{k} \cdot \mathbf{r}} = \\
&= - \int dE \int d^3\mathbf{r} \underbrace{\text{tr} \gamma_0 \gamma_i \gamma_0 \gamma_j}_{=-4g_{ij}} \langle \mathbf{r} | \left[p^i, \frac{1}{\mathcal{H}_0} [p_j, \Pi_0] \frac{1}{\mathcal{H}_0} \right] | \mathbf{r} \rangle e^{-i\mathbf{k} \cdot \mathbf{r}} = \\
&= 4 \int dE \int d^3\mathbf{r} \langle \mathbf{r} | \left[p_j, \frac{1}{\mathcal{H}_0} \underbrace{[p_j, E]}_{=0} \frac{1}{\mathcal{H}_0} \right] | \mathbf{r} \rangle e^{-i\mathbf{k} \cdot \mathbf{r}} - \\
&= 4 \int dE \int d^3\mathbf{r} \langle \mathbf{r} | \frac{1}{\mathcal{H}_0} \left[p_j, \left[p_j, \frac{1}{2E} \mathcal{V} \right] \right] \frac{1}{\mathcal{H}_0} | \mathbf{r} \rangle e^{-i\mathbf{k} \cdot \mathbf{r}} = \\
&= 2 \int dE \int d^3\mathbf{r} \frac{1}{E} \langle \mathbf{r} | \frac{1}{\mathcal{H}_0} \left[\mathbf{p}^2 \mathcal{V} - 2p_j \mathcal{V} p_j + \mathcal{V} \mathbf{p}^2 \right] \frac{1}{\mathcal{H}_0} | \mathbf{r} \rangle e^{-i\mathbf{k} \cdot \mathbf{r}}. \quad (1.107)
\end{aligned}$$

The following calculation is similar to the calculation of the integral $I_F^{(1)}$. We

again insert the resolution of identity (1.101) and use formula (1.104)

$$\begin{aligned}
J_F^{(1)} &= 2 \int dE \int d^3\mathbf{p}_1 \int d^3\mathbf{p}_2 \int d^3\mathbf{r} \frac{1}{E} \langle \mathbf{r} | \mathbf{p}_1 \rangle \langle \mathbf{p}_1 | \frac{1}{\mathcal{H}_0} \times \\
&\quad \times [\mathbf{p}_1^2 \mathcal{V} - 2p_{1j} \mathcal{V} p_{2j} + \mathcal{V} \mathbf{p}_2^2] \frac{1}{\mathcal{H}_0} |\mathbf{p}_2\rangle \langle \mathbf{p}_2 | \mathbf{r} \rangle e^{-i\mathbf{k}\cdot\mathbf{r}} = \\
&= 2 \int dE \int d^3\mathbf{p}_1 \int d^3\mathbf{p}_2 \frac{1}{E} \frac{1}{E^2 - m^2 - \mathbf{p}_1^2} \frac{1}{E^2 - m^2 - \mathbf{p}_2^2} \times \\
&\quad \times [\mathbf{p}_1^2 - 2p_{1j} p_{2j} + \mathbf{p}_2^2] \langle \mathbf{p}_1 | \mathcal{V} | \mathbf{p}_2 \rangle \int d^3\mathbf{r} \frac{e^{-i(\mathbf{p}_1 + \mathbf{k} - \mathbf{p}_2)\cdot\mathbf{r}}}{(2\pi)^3} = \\
&= \frac{2Z\alpha}{\pi^2 \omega^2} \int dE \int d^3\mathbf{p}_1 \frac{1}{E^2 - m^2 - \mathbf{p}_1^2} \frac{1}{E^2 - m^2 - (\mathbf{p}_1 - \mathbf{k})^2} \times \\
&\quad \times \underbrace{[\mathbf{p}_1^2 - 2\mathbf{p}_1 \cdot (\mathbf{p}_1 - \mathbf{k}) + (\mathbf{p}_1 - \mathbf{k})^2]}_{=\omega^2} \\
&= \frac{2Z\alpha}{\pi^2} \int dE \int d^3\mathbf{p}_1 \frac{1}{E^2 - m^2 - \mathbf{p}_1^2} \frac{1}{E^2 - m^2 - (\mathbf{p}_1 - \mathbf{k})^2}. \tag{1.108}
\end{aligned}$$

1.5.3 Comparison of both approaches

We want to show that the approaches from the last two subsections give the same results. The easiest way to do so is to show that $I_{Fa}^{(1)} = I_{2a}^{(1)}$, $I_{Fb}^{(1)} = I_{2b}^{(1)}$ and $J_F^{(1)} = J_2^{(1)}$. Firstly, let us modify the expression (1.105) (we set $\mathbf{p}_1 = \mathbf{p}$)

$$\begin{aligned}
I_{Fa}^{(1)} &= \frac{-8Z\alpha}{\pi^2} \int dE \int d^3\mathbf{p} \frac{-E^2}{\omega^2 - 2\mathbf{p}\cdot\mathbf{k}} \left[\frac{1}{E^2 - m^2 - \mathbf{p}^2} - \right. \\
&\quad \left. - \frac{1}{E^2 - m^2 - (\mathbf{p} - \mathbf{k})^2} \right] = \frac{8\pi Z\alpha}{\pi^2 \omega^2} \int dE \int d^3\mathbf{p} E^2 \times \\
&\quad \underbrace{\left[\frac{1}{\omega^2 - 2\mathbf{p}\cdot\mathbf{k}} \frac{1}{E^2 - m^2 - \mathbf{p}^2} - \frac{1}{\omega^2 - 2\mathbf{p}\cdot\mathbf{k} - 2\omega^2} \frac{1}{E^2 - m^2 - \mathbf{p}^2} \right]}_{\text{substitution } \mathbf{p} \rightarrow \mathbf{p} + \mathbf{k}} = \\
&= \frac{8Z\alpha}{\pi^2 \omega^2} \int dE \int d^3\mathbf{p} \frac{E^2}{E^2 - m^2 - \mathbf{p}^2} \left[\frac{1}{\omega^2 - 2\mathbf{p}\cdot\mathbf{k}} + \frac{1}{\omega^2 + 2\mathbf{p}\cdot\mathbf{k}} \right] = \\
&= \frac{8Z\alpha}{\pi^2 \omega^2} \int dE \int d^3\mathbf{p} \frac{E^2}{E^2 - m^2 - \mathbf{p}^2} \frac{2\omega^2}{\omega^4 - 4(|\mathbf{p}|\omega \cos \theta)^2} = \\
&= \frac{-16Z\alpha}{\pi^2 \omega^2} \int dE \int d^3\mathbf{p} \frac{E^2}{E^2 - m^2 - \mathbf{p}^2} \frac{1}{4\mathbf{p}^2 \cos^2 \theta - \omega^2}. \tag{1.109}
\end{aligned}$$

which is equal to $I_{2a}^{(1)}$ (1.88).

Secondly the expression for $I_{Fb}^{(1)}$ (1.106) is exactly the same as $I_{2b}^{(1)}$ (1.91).

Eventually, if we use the same procedure as in equation (1.109), we get the final expression in the form (we set $\mathbf{p}_1 = \mathbf{p}$)

$$J_F^{(1)} = \frac{4Z\alpha}{\pi^2} \int dE \int d^3\mathbf{p} \frac{1}{E^2 - m^2 - \mathbf{p}^2} \frac{1}{4\mathbf{p}^2 \cos^2 \theta - \omega^2}. \tag{1.110}$$

Again we have obtained the same relation using free particle (1.110) and hydrogen functions (1.98) approach.

1.5.4 Uehling potential

In the last section we have calculated integrals which give the Fourier transformation of the VEV of the current operator in the first order in α

$$\begin{aligned}\langle \tilde{j}_0^{(1)}(\mathbf{k}) \rangle &= \frac{ie}{4\pi} \left(I_{2a}^{(1)} + I_{2b}^{(1)} + J_2^{(1)} \right) = \frac{ie}{4\pi} \left(I_{Fa}^{(1)} + I_{Fb}^{(1)} + J_{2F}^{(1)} \right) = \\ &= \frac{ieZ\alpha}{2\pi^3\omega^2} \int dE \int d^3\mathbf{p} \frac{-4E^2 + 2[E^2 - m^2 - (\mathbf{p} - \mathbf{k})^2] + \omega^2}{(E^2 - m^2 - \mathbf{p}^2)(E^2 - m^2 - (\mathbf{p} - \mathbf{k})^2)} = \\ &= \frac{ieZ\alpha}{2\pi^3\omega^2} \int dE \int d^3\mathbf{p} \frac{-2E^2 - 2\mathbf{p}^2 + 4\mathbf{p} \cdot \mathbf{k} - \omega^2 - 2m^2}{(E^2 - m^2 - \mathbf{p}^2)(E^2 - m^2 - (\mathbf{p} - \mathbf{k})^2)}.\end{aligned}\quad (1.111)$$

For simplicity we rewrite the equations using fourvectors $k = (0, \mathbf{k})$ and $p = (E, \mathbf{p})$ which gives $k^2 = -\omega^2$ and $p^2 = E^2 - \mathbf{p}^2$.

$$\langle \tilde{j}_0^{(1)}(\mathbf{k}) \rangle = \frac{ieZ\alpha}{2\pi^3\omega^2} \int d^4p \frac{-4E^2 + 2p^2 - 4p \cdot k + k^2 - 2m^2}{(p^2 - m^2)((p - k)^2 - m^2)}.\quad (1.112)$$

Further we use Feynmann parametrization

$$\begin{aligned}\langle \tilde{j}_0^{(1)}(\mathbf{k}) \rangle &= \frac{ieZ\alpha}{2\pi^3\omega^2} \int_0^1 dy \int d^4p \frac{-4E^2 + 2p^2 - 4p \cdot k + k^2 - 2m^2}{[(p^2 - m^2)(1 - y) + ((p - k)^2 - m^2)y]^2} = \\ &= \frac{ieZ\alpha}{2\pi^3\omega^2} \int_0^1 dy \int d^4p \frac{-4E^2 + 2p^2 - 4p \cdot k + k^2 - 2m^2}{(p^2 - 2p \cdot ky - m^2 + k^2y)^2},\end{aligned}\quad (1.113)$$

and we substitute $p' = p - ky$ and drop the prime

$$\begin{aligned}\langle \tilde{j}_0^{(1)}(\mathbf{k}) \rangle &= \frac{ieZ\alpha}{2\pi^3\omega^2} \int_0^1 dy \int d^4p \times \\ &\times \frac{-4E^2 + 2p^2 + 4p \cdot ky + 2k^2y^2 - 4p \cdot k - 4k^2y + k^2 - 2m^2}{(p^2 - m^2 + k^2y - k^2y^2)^2} = \\ &= \frac{ieZ\alpha}{2\pi^3\omega^2} \int_0^1 dy \int d^4p \frac{-p^2 + 2p^2 + 2k^2y^2 - 4k^2y + k^2 - 2m^2}{(p^2 - m^2 + k^2y - k^2y^2)^2}\end{aligned}\quad (1.114)$$

In the last step we have used symmetric integration

$$\int d^4p \frac{p_\mu p_\nu}{(p^2 - L)^n} = \int d^4p \frac{1}{4} \frac{p^2 g_{\mu\nu}}{(p^2 - L)^n}.\quad (1.115)$$

which holds for $n > 3$. We have used the relation for the sake of simplicity, even though the integrals are divergent ($n = 2$). After the regularization all integrals will be convergent and the above manipulation will formally take place. We have also used a fact, that integration of the odd function is zero

$$\int d^4p \frac{p_\mu}{(p^2 - L)^n} = 0\quad (1.116)$$

The integral we have (1.114) is quadratically divergent, so we have to use a procedure called Pauli-Villars regularization. We subtract the same expression, but we change mass m to auxiliary mass M . At the end of the calculation we must perform the limit $M \rightarrow \infty$. It can be expressed in the following way

$$f(m^2) \rightarrow f(m^2) - f(M^2) = \int_{M^2}^{m^2} d\lambda \left(\frac{\partial}{\partial \lambda} f(\lambda) \right) \quad (1.117)$$

it gives the regularized expression

$$\begin{aligned} \langle \tilde{j}_0^{(1)}(\mathbf{k}) \rangle &= \frac{ieZ\alpha}{2\pi^3\omega^2} \int_{M^2}^{m^2} d\lambda \int_0^1 dy \int d^4p \left(2 \frac{p^2 + 2k^2y^2 - 4k^2y + k^2 - 2\lambda}{(p^2 - \lambda + k^2y - k^2y^2)^3} - \right. \\ &\quad \left. - \frac{2}{(p^2 - \lambda + k^2y - k^2y^2)^2} \right) = \\ &= \frac{ieZ\alpha}{2\pi^3\omega^2} \int_{M^2}^{m^2} d\lambda \int_0^1 dy \int d^4p \left(\frac{4p^2 - 4\lambda + 4k^2y - 4k^2y^2}{(p^2 - \lambda + k^2y - k^2y^2)^3} + \right. \\ &\quad \left. + \frac{-2p^2 + 8k^2y^2 - 12k^2y + 2k^2}{(p^2 - \lambda + k^2y - k^2y^2)^3} - \frac{2}{(p^2 - \lambda + k^2y - k^2y^2)^2} \right) = \\ &= \frac{ieZ\alpha}{2\pi^3\omega^2} \int_{M^2}^{m^2} d\lambda \int_0^1 dy \int d^4p \left(\frac{8k^2y^2 - 12k^2y + 2k^2}{(p^2 - \lambda + k^2y - k^2y^2)^3} + \right. \\ &\quad \left. + \underbrace{\frac{-2p^2}{(p^2 - \lambda + k^2y - k^2y^2)^3} + \frac{2}{(p^2 - \lambda + k^2y - k^2y^2)^2}}_{=D} \right) \quad (1.118) \end{aligned}$$

We want to show that expression D is zero. To do so we use another formula

$$\int d^4p \frac{1}{(p^2 - L)^3} = \frac{-i\pi^2}{2L}. \quad (1.119)$$

Now let us derive useful relation using formulas (1.116) and (1.119)

$$\int d^4p \frac{p_\mu}{((p-l)^2 - L)^3} = \int d^4p \frac{p_\mu + l_\mu}{(p^2 - L)^3} = \frac{-i\pi^2 l_\mu}{8L}. \quad (1.120)$$

Next we differentiate both sides of equation (1.120) with respect to parameter l_μ and then set $l_\mu = 0$

$$\begin{aligned} -3 \int d^4p \frac{p_\mu 2(p-l)^\mu \cdot (-1)}{((p-l)^2 - L)^4} &= \frac{-i\pi^2 g_\mu^\mu}{8L}, \\ \int d^4p \frac{6p^2}{(p^2 - L)^4} &= \int d^4p \frac{4}{(p^2 - L)^3}. \quad (1.121) \end{aligned}$$

The integral D is still divergent therefore we differentiate D with respect to λ (this can be viewed as an another step in regularization)

$$\frac{\partial D}{\partial \lambda} = \int d^4p \left(\frac{-6p^2}{(p^2 - \lambda + k^2y - k^2y^2)^4} + \frac{4}{(p^2 - \lambda + k^2y - k^2y^2)^3} \right) = 0 \quad (1.122)$$

where we have used just derived formula (1.121).

We can now integrate over d^4p in equation (1.118) using formula (1.119) which gives the final expression of the Fourier transformation of the VEV of the current operator

$$\begin{aligned} \langle \tilde{j}_0^{(1)}(\mathbf{k}) \rangle &= \frac{eZ\alpha}{2\pi\omega^2} \int_0^1 dy \int_{M^2}^{m^2} d\lambda \frac{8k^2y^2 - 12k^2y + 2k^2}{2(\lambda - k^2y + k^2y^2)} = \\ &= \frac{eZ\alpha}{2\pi\omega^2} \int_0^1 dy \omega^2 (1 - 6y + 4y^2) \ln \left(\frac{M^2 - k^2y + k^2y^2}{m^2 - k^2y + k^2y^2} \right) = \\ &= \underbrace{\frac{eZ\alpha}{3\pi} \ln \frac{M^2}{m^2}}_{\text{renorm. term}} + \frac{eZ\alpha}{2\pi} \int_0^1 dy (1 - 6y + 4y^2) \ln \left(1 - \frac{k^2}{m^2} (y - y^2) \right) \end{aligned} \quad (1.123)$$

In the last step we have modified the expression using $M \rightarrow \infty$. The renormalized Fourier transform of the VEV of the current operator is defined as

$$\langle \tilde{j}_0^{(1)}(\mathbf{k}) \rangle^R = \langle \tilde{j}_0^{(1)}(\mathbf{k}) \rangle - \langle \tilde{j}_0^{(1)}(0) \rangle. \quad (1.124)$$

This modification can be seen as replacing the "bare" charge e for a "renormalized" charge e_R . For more about this topic see [8] or any introduction to QED. In the following text we drop the subscript R and we continue to use symbol e although it stands for renormalized charge.

The renormalized Fourier transform of the VEV of the current operator has the form

$$\langle \tilde{j}_0^{(1)}(\mathbf{k}) \rangle^R = \frac{eZ\alpha}{2\pi} \int_0^1 dy (1 - 6y + 4y^2) \ln \left(1 - \frac{k^2}{m^2} (y - y^2) \right) \quad (1.125)$$

In order to eliminate the logarithm we integrate (1.125) by parts and then we transform the integration variable to $v = 2y - 1$

$$\begin{aligned} \langle \tilde{j}_0^{(1)}(\mathbf{k}) \rangle^R &= -\frac{eZ\alpha}{2\pi} \int_0^1 dy (y - 3y^2 + \frac{4}{3}y^3) \frac{1}{1 - \frac{k^2}{m^2}(y - y^2)} \left[-\frac{k^2}{m^2}(1 - 2y) \right] = \\ &= \frac{eZ\alpha k^2}{2\pi m^2} \int_{-1}^1 \frac{1}{2} dv \left(\frac{1}{2} + \frac{v}{2} - \frac{3}{4}(1+v)^2 + \frac{1}{6}(1+v)^3 \right) \frac{-v}{1 - \frac{k^2}{4m^2}(1-v^2)} = \\ &= -\frac{eZ\alpha}{4\pi} \frac{\omega^2}{m^2} \int_0^1 dv (v^2 - \frac{1}{3}v^4) \frac{1}{1 + \frac{\omega^2}{4m^2}(1-v^2)}. \end{aligned}$$

In the last step we have used the symmetry of the integrand. Now we want to calculate the Uehling potential. We use a formula

$$\int \frac{d^3\mathbf{k}}{(2\pi)^3} \frac{e^{i\mathbf{k}\cdot\mathbf{x}_2}}{\omega^2 + a^2} = \frac{1}{4\pi r_2} e^{-ar_2}, \quad (1.126)$$

which allows us to calculate the Fourier integral. The potential then is

$$\begin{aligned} A_0(\mathbf{x}_2) &= \int \frac{d^3\mathbf{k}}{(2\pi)^3} \frac{e^{i\mathbf{k}\cdot\mathbf{x}_2}}{\omega^2} \langle \tilde{j}_0(\mathbf{k}) \rangle^R = \\ &= -\frac{eZ\alpha}{4\pi m^2} \int_0^1 dv \left(v^2 - \frac{1}{3}v^4 \right) \int \frac{d^3\mathbf{k}}{(2\pi)^3} \frac{e^{i\mathbf{k}\cdot\mathbf{x}_2}}{1 + \frac{\omega^2}{4m^2}(1-v^2)} = \\ &= -\frac{eZ\alpha}{\pi} \int_0^1 dv \frac{v^2 - \frac{1}{3}v^4}{1-v^2} \int \frac{d^3\mathbf{k}}{(2\pi)^3} \frac{e^{i\mathbf{k}\cdot\mathbf{x}_2}}{\omega^2 + \frac{4m^2}{1-v^2}}. \end{aligned} \quad (1.127)$$

The final expression of the Uehling potential (firstly derived by Uehling in [19]) is

$$\boxed{A_0(\mathbf{x}_2) = -\frac{eZ\alpha}{4\pi^2 r_2} \int_0^1 dv \frac{v^2 - \frac{1}{3}v^4}{1-v^2} e^{-\frac{2m}{\sqrt{1-v^2}}r_2}} \quad (1.128)$$

A further transformation $\zeta = 1/\sqrt{1-v^2}$ with $v dv = \zeta^{-3} d\zeta$ gives the commonly used form of the Uehling potential (see [8])

$$A_0(\mathbf{x}_2) = -\frac{eZ\alpha}{6\pi^2 r_2} \int_1^\infty d\zeta \left(1 + \frac{1}{2\zeta^2} \right) \frac{\sqrt{\zeta^2 - 1}}{\zeta^2} e^{-2m\zeta r_2}. \quad (1.129)$$

It is very common to use an approximation of the Uehling potential. If we consider the limit $k^2/m^2 \ll 1$, we can calculate only with the first term of the Taylor expansion of the logarithm from the expression (1.125).

$$\langle \tilde{j}_0^{(1)}(\mathbf{k}) \rangle_{app}^R = \frac{eZ\alpha}{2\pi} \int_0^1 dy (1 - 6y + 4y^2) \left(-\frac{k^2}{m^2} (y - y^2) \right) = -\frac{eZ\alpha}{15\pi} \frac{\omega^2}{m^2} \quad (1.130)$$

Therefore, the approximate potential has the form

$$\begin{aligned} A_0(\mathbf{x}_2)_{app} &= \int \frac{d^3\mathbf{k}}{(2\pi)^3} \frac{e^{i\mathbf{k}\cdot\mathbf{x}_2}}{\omega^2} \langle \tilde{j}_0(\mathbf{k}) \rangle_{app}^R = \\ &= -\frac{eZ\alpha}{15\pi m^2} \int \frac{d^3\mathbf{k}}{(2\pi)^3} e^{i\mathbf{k}\cdot\mathbf{x}_2} = -\frac{eZ\alpha}{15\pi m^2} \delta^3(\mathbf{x}_2). \end{aligned} \quad (1.131)$$

1.5.5 Calculations with Uehling potential

The energy shift caused by Uehling potential can be easily calculated using equation (1.11) which gives the formula

$$\Delta E_{VP}^{(1)} = e \int d^3\mathbf{x} |\Phi_n(E_n Z\alpha\mathbf{x})|^2 A_0(\mathbf{x}). \quad (1.132)$$

We use a dimensionless function F_{VP} to express the $\Delta E_{VP}^{(1)}$ in a form

$$E_{VP}^{(1)} = \frac{\alpha}{\pi} \frac{(Z\alpha)^4}{n^3} F_{VP}^{(1)} \frac{m_r^3}{m_e^2}, \quad (1.133)$$

where m_e is the mass of the electron and $m_r = m_{e,\mu}m_p/(m_{e,\mu} + m_p)$ is the reduced mass. We calculate function $F_{VP}^{(1)}$ on three levels of approximation.

1. We use the approximative form of the Uehling potential (1.131) and non-relativistic wave functions

$$F_{VP}(app.) = -\frac{4}{15}\delta_{l,0} \quad (1.134)$$

2. We use the exact form of the Uehling potential (1.128) and nonrelativistic wave functions

$$F_{VP}(nonrel.) = -n^3 \int_0^1 dv \frac{v^2 - \frac{1}{3}v^4}{1 - v^2} \int dr r e^{-\frac{2m_e}{\sqrt{1-v^2}}r} R_{n,l}^2(m_r Z\alpha r). \quad (1.135)$$

3. We use the exact form of the Uehling potential (1.128) and relativistic wave functions (1.53)

$$F_{VP}(rel.) = -\frac{n^4}{N^2 \sqrt{n^2 + (Z\alpha)^2}} \int_0^1 dv \frac{v^2 - \frac{1}{3}v^4}{1 - v^2} \int dr r e^{-\frac{2m_e}{\sqrt{1-v^2}}r} \times \\ \times \left[A^2 R_{n,|\Gamma|-1}^2(E_n Z\alpha r) + B^2 R_{n,|\Gamma|}^2(E_n Z\alpha r) + \right. \\ \left. + \frac{2pZ\alpha}{(j + \frac{1}{2})} AB R_{n,|\Gamma|}(E_n Z\alpha r) R_{n,|\Gamma|-1}(E_n Z\alpha r) \right]. \quad (1.136)$$

The calculated energy shifts are written in Tables 1.1 and 1.2 using just mentioned three levels of approximation and numerical values taken from [11]

$$\alpha^{-1} = 137.035999074(44) \quad (1.137)$$

$$m_e = 0.510998928(11) \text{ MeV} \quad (1.138)$$

$$\frac{m_e}{m_\mu} = 4.83633166(12) \times 10^{-3} \quad (1.139)$$

$$\frac{m_e}{m_p} = 5.4461702178(22) \times 10^{-4} \quad (1.140)$$

$$R_\infty c = 3.289841960364(17) \times 10^{15} \text{ Hz} \quad (1.141)$$

In Table 1.1 we have results for an electron which is bound by point-like proton with hypothetical charge Z . In Table 1.2 we have the same situation, but the electron is replaced by a muon. The values in Tables 1.1 and 1.2 are given in [MHz] which we get from [eV] by multiplication by $R_\infty c/\alpha^2 m_e$.

State	Z	E_{Dir}	$\Delta E_{VP}^{(1)}(app.)$	$\Delta E_{VP}^{(1)}(nonrel.)$	$\Delta E_{VP}^{(1)}(rel.)$
$1s_{\frac{1}{2}}$	1	$-3.288 \cdot 10^9$	-216.7	-214.8	-214.8
$2s_{\frac{1}{2}}$	1	$-8.219 \cdot 10^8$	-27.08	-26.84	-26.85
$2p_{\frac{1}{2}}$	1	$-8.219 \cdot 10^8$	0	$-7.634 \cdot 10^{-5}$	$-3.461 \cdot 10^{-4}$
$2p_{\frac{3}{2}}$	1	$-8.219 \cdot 10^8$	0	$-7.634 \cdot 10^{-5}$	$-7.635 \cdot 10^{-5}$
$1s_{\frac{1}{2}}$	10	$-3.329 \cdot 10^{11}$	$-2.167 \cdot 10^6$	$-1.987 \cdot 10^6$	$-2.027 \cdot 10^6$
$2s_{\frac{1}{2}}$	10	$-8.234 \cdot 10^{10}$	$-2.708 \cdot 10^5$	$-2.481 \cdot 10^5$	$-2.543 \cdot 10^5$
$2p_{\frac{1}{2}}$	10	$-8.234 \cdot 10^{10}$	0	-69.29	-340.7
$2p_{\frac{3}{2}}$	10	$-8.223 \cdot 10^{10}$	0	-69.29	-70.02
$1s_{\frac{1}{2}}$	20	$-1.322 \cdot 10^{12}$	$-3.467 \cdot 10^7$	$-2.929 \cdot 10^7$	$-3.132 \cdot 10^7$
$2s_{\frac{1}{2}}$	20	$-3.310 \cdot 10^{11}$	$-4.334 \cdot 10^6$	$-3.651 \cdot 10^6$	$-3.975 \cdot 10^6$
$2p_{\frac{1}{2}}$	20	$-3.983 \cdot 10^{11}$	0	-3995	$-2.226 \cdot 10^4$
$2p_{\frac{3}{2}}$	20	$-3.292 \cdot 10^{11}$	0	-3995	-4136

Table 1.1: Dirac binding energies and energy shifts caused by Uehling term in [MHz] for system e^-p^{+Z}

Let us comment the results in Table 1.1:

- The approximative form of the Uehling potential gives a good estimation in the leading order for the s -states.
- The calculations with nonrelativistic wave-functions give good results for all calculated states except for $2p_{\frac{1}{2}}$ where relativistic wave functions give approximately 5 times bigger energy shift. It is caused by the relativistic $2p_{\frac{1}{2}}$ state contains a small mixture of the $2s_{\frac{1}{2}}$ state, which has few orders of magnitude higher interaction with the Uehling potential.
- When we compare the last two columns we can see that relativistic wave-functions generally give greater energy shift than the nonrelativistic. This is due to the fact that relativistic wave functions are localized closer to the nucleus where the Uehling potential is more intense.

State	Z	E_{Dir}	$\Delta E_{VP}^{(1)}(app.)$	$\Delta E_{VP}^{(1)}(nonrel.)$	$\Delta E_{VP}^{(1)}(rel.)$
$1s_{\frac{1}{2}}$	1	$-6.114 \cdot 10^{11}$	$-1.393 \cdot 10^9$	$-4.591 \cdot 10^8$	$-4.592 \cdot 10^8$
$2s_{\frac{1}{2}}$	1	$-1.528 \cdot 10^{11}$	$-1.741 \cdot 10^8$	$-5.310 \cdot 10^7$	$-5.310 \cdot 10^7$
$2p_{\frac{1}{2}}$	1	$-1.528 \cdot 10^{11}$	0	$-3.525 \cdot 10^6$	$-3.526 \cdot 10^6$
$2p_{\frac{3}{2}}$	1	$-1.528 \cdot 10^{11}$	0	$-3.525 \cdot 10^6$	$-3.525 \cdot 10^6$
$1s_{\frac{1}{2}}$	10	$-6.122 \cdot 10^{13}$	$-1.393 \cdot 10^{13}$	$-3.086 \cdot 10^{11}$	$-3.100 \cdot 10^{11}$
$2s_{\frac{1}{2}}$	10	$-1.531 \cdot 10^{13}$	$-1.741 \cdot 10^{12}$	$-3.888 \cdot 10^{10}$	$-3.918 \cdot 10^{10}$
$2p_{\frac{1}{2}}$	10	$-1.531 \cdot 10^{13}$	0	$-2.405 \cdot 10^{10}$	$-2.425 \cdot 10^{10}$
$2p_{\frac{3}{2}}$	10	$-1.529 \cdot 10^{13}$	0	$-2.405 \cdot 10^{10}$	$-2.408 \cdot 10^{10}$
$1s_{\frac{1}{2}}$	20	$-2.459 \cdot 10^{14}$	$-2.229 \cdot 10^{14}$	$-1.700 \cdot 10^{12}$	$-1.728 \cdot 10^{12}$
$2s_{\frac{1}{2}}$	20	$-6.155 \cdot 10^{13}$	$-2.786 \cdot 10^{13}$	$-2.410 \cdot 10^{11}$	$-2.475 \cdot 10^{11}$
$2p_{\frac{1}{2}}$	20	$-6.155 \cdot 10^{13}$	0	$-1.790 \cdot 10^{11}$	$-1.840 \cdot 10^{11}$
$2p_{\frac{3}{2}}$	20	$-6.122 \cdot 10^{13}$	0	$-1.790 \cdot 10^{11}$	$-1.799 \cdot 10^{11}$

Table 1.2: Binding energies and energy shifts caused by Uehling term in [MHz] for system μ^-p^+Z

Let us comment the results in Table 1.2 again and compare them with those in Table 1.1:

- The approximative form of the Uehling potential gives energy shift bigger by several orders because the assumption $k^2/m_e^2 \ll 1$ is not valid for muon.
- The results for nonrelativistic and relativistic wave-functions have the same trends as in Table 1.1, but the differences between energy shifts of $2p_{\frac{1}{2}}$ and $2p_{\frac{3}{2}}$ states are much smaller. The reason is that the mass of the muon is approximately 207 times bigger than mass of the electron; therefore, all relativistic effects are smaller.
- In both Tables we can read that the Vacuum Polarization effect is greater for more massive particles in stronger Coulomb fields both absolutely and relatively to binding energies.

1.6 Calculation of the 2. order in α

In this section we want to show that the Fourier transformation of the VEV of the current operator in the second order in α is zero. We can see that the integration over E in the n -th order in α has the form

$$\int dE \frac{E^{n\pm 1}}{E^2 - m^2 - \mathbf{k}_e^2}, \quad (1.142)$$

where the plus sign in exponent is for integral I_{2a} (1.83) and the minus sign is for integrals I_{2b} (1.90) and J_2 (1.97). If we calculate contribution from the odd order in α we integrate odd function in E in integral (1.142). Therefore, we do not have any contributions in the second (and every odd) order in α .

This result is also a cosequence of the more general Furry theorem (see [8], Excercise 4.1).

1.7 Calculation of the 3. order in α

In order to calculate the third order in α we need to extend the expansion of hypergeometric function from (1.87). The expansions are written in the Mathematical Supplement A.2 with a hint how to obtain them. When we use expansions (1.84) – (1.86) and (A.37) – (A.40) we get the formula for the integrals $I_{2a}^{(3)}$, $I_{2b}^{(3)}$ and $J_2^{(3)}$ in the form

$$\begin{aligned}
I_{2a}^{(3)} = & \frac{16i}{\omega^2 \pi^2} \int dE \int d^3 \mathbf{k}_e \frac{a^3 E}{E^2 - m^2 - \mathbf{k}_e^2} \frac{|\mathbf{k}_e|}{4\mathbf{k}_e^2 \cos^2 \theta - \omega^2} \left[-\frac{2\pi^2}{3} + \right. \\
& + \frac{1}{2} \ln^2 \left(\frac{\omega + 2|\mathbf{k}_e| \cos \theta}{\omega - 2|\mathbf{k}_e| \cos \theta} \right) - \text{dilog} \left(\frac{-\omega^2}{4\mathbf{k}_e^2 \cos^2 \theta - \omega^2} \right) + \\
& \left. + \frac{\omega}{2|\mathbf{k}_e| \cos \theta} \ln \left(\frac{\omega + 2|\mathbf{k}_e| \cos \theta}{\omega - 2|\mathbf{k}_e| \cos \theta} \right) \ln \left(\frac{-\omega^2}{4\mathbf{k}_e^2 \cos^2 \theta - \omega^2} \right) \right]. \quad (1.143)
\end{aligned}$$

$$\begin{aligned}
I_{2b}^{(3)} = & \frac{4Z\alpha}{\pi^2 \omega^2} \int dE \int d^3 \mathbf{k}_e \frac{a^2}{E^2 - m^2 - \mathbf{k}_e^2} \left[-\frac{2\pi^2}{3} + \right. \\
& \left. + \frac{1}{2} \ln^2 \left(\frac{\omega + 2|\mathbf{k}_e| \cos \theta}{\omega - 2|\mathbf{k}_e| \cos \theta} \right) - \text{dilog} \left(\frac{-\omega^2}{4\mathbf{k}_e^2 \cos^2 \theta - \omega^2} \right) \right] \quad (1.144)
\end{aligned}$$

$$\begin{aligned}
J_2^{(3)} = & -\frac{4i}{\pi^2} \int dE \int d^3 \mathbf{k}_e \frac{a^3}{E} \frac{1}{E^2 - m^2 - \mathbf{k}_e^2} \frac{|\mathbf{k}_e|}{4\mathbf{k}_e^2 \cos^2 \theta - \omega^2} \times \\
& \times \left[-\frac{2\pi^2}{3} + \frac{1}{2} \ln^2 \left(\frac{\omega + 2|\mathbf{k}_e| \cos \theta}{\omega - 2|\mathbf{k}_e| \cos \theta} \right) + \right. \\
& + \frac{\omega}{2|\mathbf{k}_e| \cos \theta} \ln \left(\frac{\omega + 2|\mathbf{k}_e| \cos \theta}{\omega - 2|\mathbf{k}_e| \cos \theta} \right) \ln \left(\frac{-\omega^2}{4\mathbf{k}_e^2 \cos^2 \theta - \omega^2} \right) + \\
& \left. + 2 \ln \left(\frac{-\omega^2}{4\mathbf{k}_e^2 \cos^2 \theta - \omega^2} \right) - \text{dilog} \left(\frac{-\omega^2}{4\mathbf{k}_e^2 \cos^2 \theta - \omega^2} \right) \right]. \quad (1.145)
\end{aligned}$$

The Fourier transformation of the VEV of the current operator in the third order in α has the form

$$\begin{aligned}
\langle \tilde{j}_0^{(3)}(\mathbf{k}) \rangle &= \frac{ie}{4\pi} \left(I_{2a}^{(3)} + I_{2b}^{(3)} + J_2^{(3)} \right) = \frac{ie(Z\alpha)^3}{\pi^3\omega^2} \times \\
&\times \int dE \int d^3\mathbf{k}_e \frac{E^2}{\mathbf{k}_e^2} \frac{1}{E^2 - m^2 - \mathbf{k}_e^2} \frac{1}{4\mathbf{k}_e^2 \cos^2 \theta - \omega^2} \times \\
&\times \left\{ (4E^2 - 4\mathbf{k}_e^2 \cos^2 \theta) \left[-\frac{2\pi^2}{3} + \right. \right. \\
&+ \left. \frac{1}{2} \ln^2 \left(\frac{\omega + 2|\mathbf{k}_e| \cos \theta}{\omega - 2|\mathbf{k}_e| \cos \theta} \right) - \text{dilog} \left(\frac{-\omega^2}{4\mathbf{k}_e^2 \cos^2 \theta - \omega^2} \right) \right] + \\
&+ 2\omega^2 \ln \left(\frac{-\omega^2}{4\mathbf{k}_e^2 \cos^2 \theta - \omega^2} \right) + \frac{(4E^2 - \omega^2)\omega}{2|\mathbf{k}_e| \cos \theta} \times \\
&\times \left. \ln \left(\frac{\omega + 2|\mathbf{k}_e| \cos \theta}{\omega - 2|\mathbf{k}_e| \cos \theta} \right) \ln \left(\frac{-\omega^2}{4\mathbf{k}_e^2 \cos^2 \theta - \omega^2} \right) \right\} \quad (1.146)
\end{aligned}$$

This result does not contain all relativistic corrections because we have used only first two terms in expansion (1.72) to calculate $\langle \tilde{j}_0^{(3)}(\mathbf{k}) \rangle$. However, it can be used as a partial check when using the partial wave expansion of $\langle j_0 \rangle$.

Chapter 2

Parity violation in Atoms

2.1 Current situation

The interaction between electron and nucleus is predominantly electromagnetic, but there are many orders of magnitude lesser effects of weak interaction. As a result, the manifestation of the weak force can only be detected with very high accuracy experiments. Very important attribute of the weak interaction is that it does not conserve parity. Therefore, we can observe the effects of the weak interaction in atoms by the measurement of the atomic parity violation. The parity violation effects were measured by optical rotation or Stark-PNC on the following atoms: ^{209}Bi , ^{208}Pb , ^{203}Tl and ^{205}Tl , ^{133}Cs [7]. Lately the largest weak interaction effect were measured on ^{174}Yb [18].

The mirror symmetry in stable atoms is broken during absorptions and emissions of polarized photon which is caused by exchange of Z^0 massive boson. The Lagrangian describing weak interaction possesses part which has an opposite sign for left (L) and right (R) handed coordinate system.

In this chapter, we give a full derivation of the formula for circular dichroism δ_{LR} , which is usually written without detailed explanation (see e. g. [6], chapter 9 or [5]). We will express circular dichroism for the M_1 highly forbidden transitions, where the parity violation effect could be seen.

2.2 Circular dichroism and transition rates

In the case of atomic processes, we measure the so called circular dichroism δ_{LR} , which is defined as

$$\delta_{LR} = \frac{w_L - w_R}{w_L + w_R}, \quad (2.1)$$

where w_L and w_R stands for the transition rate from initial (i) to final (f) state.

The transition rate of the photon is given by a Fermi golden rule

$$w_{i \rightarrow f} = 2\pi\delta(E_f - E_i)|\langle f|H_{int}|i\rangle|^2, \quad (2.2)$$

where $\langle f|H_{int}|i\rangle$ is the matrix element of the perturbation between the and final f and initial i state with energies E_f and E_i . In the case of the absorption of the

photon the matrix element is

$$\langle f | \hat{H}_{int} | i \rangle = \langle f | e \int d^3 \mathbf{x} \hat{A}^\mu \hat{j}_\mu | i \rangle = e \langle f | \int d^3 \mathbf{x} A_0 j_0 - \mathbf{A} \cdot \mathbf{j} | i \rangle. \quad (2.3)$$

At the beginning, let us assume just that the \hat{j}_μ has the form

$$\hat{j}_\mu = \Psi^\dagger j_\mu \Psi \quad (2.4)$$

where \mathbf{j} is a vector. Later, we will use a concrete form of j_μ and we will prove assumed behaviour.

Because we want to describe the interaction with a photon, the vector potential has the form

$$\hat{\mathbf{A}}(\mathbf{x}) = \frac{1}{\sqrt{(2\pi)^3}} \int \frac{d^3 \mathbf{k}'}{\sqrt{2|\mathbf{k}'|}} \sum_{\lambda=L,R} \epsilon^\lambda (\hat{a}(\mathbf{k}', \epsilon^\lambda) e^{i\mathbf{k}' \cdot \mathbf{x}} + \hat{a}^\dagger(\mathbf{k}', \epsilon^\lambda) e^{-i\mathbf{k}' \cdot \mathbf{x}}) \quad (2.5)$$

and

$$A_0 = 0. \quad (2.6)$$

For the initial and final state we have

$$|i\rangle = \hat{a}^\dagger(\mathbf{k}, \epsilon^{(L)}) \hat{b}_i^\dagger |0\rangle \quad (2.7)$$

$$|f\rangle = \hat{b}_f^\dagger |0\rangle, \quad (2.8)$$

where we use a coordinate system in which the wave vector is

$$\mathbf{k} = (0, 0, \omega), \quad (2.9)$$

and the circular polarization vector is

$$\epsilon^{(L)} = \frac{1}{\sqrt{2}} (1, \pm i, 0). \quad (2.10)$$

We put just defined relations together and we get for the matrix element

$$\begin{aligned} \langle f | \hat{H}_{int} | i \rangle &= \int d^3 \mathbf{x} \langle 0 | \hat{b}_f \sum_m \Phi_m^\dagger(\mathbf{x}) \hat{b}_m^\dagger \frac{-e}{\sqrt{(2\pi)^3}} \int \frac{d^3 \mathbf{k}'}{\sqrt{2|\mathbf{k}'|}} \sum_{\lambda=L,R} \epsilon^\lambda \cdot \mathbf{j} (\hat{a}(\mathbf{k}', \epsilon^\lambda) \times \\ &\quad \times e^{i\mathbf{k}' \cdot \mathbf{x}} + \hat{a}^\dagger(\mathbf{k}', \epsilon^\lambda) e^{-i\mathbf{k}' \cdot \mathbf{x}}) \sum_n \Phi_n(\mathbf{x}) \hat{b}_n a^\dagger(\mathbf{k}, \epsilon^{(L)}) \hat{b}_i^\dagger |0\rangle = \\ &= \frac{-e}{\sqrt{(2\pi)^3}} \sum_{m,n,\lambda} \int d^3 \mathbf{x} \int \frac{d^3 \mathbf{k}'}{\sqrt{2|\mathbf{k}'|}} \Phi_m^\dagger(\mathbf{x}) \epsilon^\lambda \cdot \mathbf{j} \Phi_n(\mathbf{x}) \times \\ &\quad \times \langle 0 | \hat{b}_f \hat{b}_m^\dagger (\hat{a}(\mathbf{k}', \epsilon^\lambda) e^{i\mathbf{k}' \cdot \mathbf{x}} + \hat{a}^\dagger(\mathbf{k}', \epsilon^\lambda) e^{-i\mathbf{k}' \cdot \mathbf{x}}) \hat{b}_n a^\dagger(\mathbf{k}, \epsilon^{(L)}) \hat{b}_i^\dagger |0\rangle. \end{aligned} \quad (2.11)$$

Only when we have equal number of the annihilation and creation operators we get the nonzero result, therefore the part in (2.11) containing creation and annihilation operators is

$$\langle 0 | \hat{b}_f \hat{b}_m^\dagger \hat{a}(\mathbf{k}', \epsilon^\lambda) \hat{b}_n a^\dagger(\mathbf{k}, \epsilon^{(L)}) \hat{b}_i^\dagger |0\rangle = \delta_{f,m} \delta_{n,i} \delta_{\lambda, (L)} \delta(\mathbf{k} - \mathbf{k}'). \quad (2.12)$$

As a result, after trivial summations and integration over \mathbf{k}' we get for (2.11) a result

$$\begin{aligned}\langle f|\hat{H}_{int}|i\rangle &= \frac{-e}{\sqrt{16\omega\pi^3}} \int d^3\mathbf{x} \Phi_f^\dagger(\mathbf{x})(\mathbf{x}) e^{i\mathbf{k}\cdot\mathbf{x}} \epsilon^{(L)} \cdot \mathbf{J} \Phi_i(\mathbf{x}) = \\ &= \frac{-e}{\sqrt{16\omega\pi^3}} \langle \Phi_f | e^{i\mathbf{k}\cdot\mathbf{x}} \epsilon^{(L)} \cdot \mathbf{J} | \Phi_i \rangle\end{aligned}\quad (2.13)$$

Our goal is to calculate the second power of the matrix element (2.13). We use a substitution $\mathbf{x} \rightarrow Z\alpha\mathbf{x}$ and then we expand the exponential to the first order in $(Z\alpha)$. Consequently, we get

$$\begin{aligned}|\langle \Phi_f | e^{iZ\alpha\mathbf{k}\cdot\mathbf{x}} \epsilon^{(L)} \cdot \mathbf{J} | \Phi_i \rangle|^2 &\approx |\langle \Phi_f | (1 + iZ\alpha\mathbf{k}\cdot\mathbf{x}) \epsilon^{(L)} \cdot \mathbf{J} | \Phi_i \rangle|^2 = \\ &= |\langle \Phi_f | \epsilon^{(L)} \cdot \mathbf{J} | \Phi_i \rangle|^2 + (Z\alpha)^2 |\langle \Phi_f | \mathbf{k}\cdot\mathbf{x} \epsilon^{(L)} \cdot \mathbf{J} | \Phi_i \rangle|^2 + \\ &\quad + 2Z\alpha \text{Im} \langle \Phi_f | \epsilon^{(L)} \cdot \mathbf{J} | \Phi_i \rangle \langle \Phi_i | \mathbf{k}\cdot\mathbf{x} \epsilon^{*(L)} \cdot \mathbf{J} | \Phi_f \rangle\end{aligned}\quad (2.14)$$

We use a relation

$$r_{iJk} = \underbrace{\frac{1}{2}(r_{iJk} + r_{iJk})}_{=S[r_{iJk}]} + \underbrace{\frac{1}{2}(r_{iJk} - r_{iJk})}_{=A[r_{iJk}]}. \quad (2.15)$$

From (2.15) we take only the antisymetrized part which is responsible for M_1 transitions and, unlike the symetrized part (responsible for E_2 transitions), enables us to see the parity violation. We define

$$\mu_p = \varepsilon_{pst} x_s J_t \quad (2.16)$$

and we get

$$A[r_{iJk}] = \frac{1}{2} \varepsilon_{pik} \varepsilon_{pst} x_s J_t = \frac{1}{2} \varepsilon_{pik} \mu_p. \quad (2.17)$$

Therefore, for the operators in (2.14) we have

$$A[k_i r_i \epsilon_k^{*(L)} J_k] = \frac{1}{2} k_i \epsilon_k^{*(L)} \varepsilon_{pik} \mu_p = \pm \frac{i}{2} \frac{\omega}{\sqrt{2}} \mu_{\mp}, \quad (2.18)$$

$$\epsilon_i^{(L)} J_i = \frac{1}{\sqrt{2}} J_{\pm}, \quad (2.19)$$

where we have used the concrete form of k (2.9) and ϵ (2.10).

With the described approximations we have for the transition rates of the left and right handed photons

$$\begin{aligned}w_L &= \frac{e^2}{8\pi^2\omega} \delta(E_f - E_i) \left(\frac{1}{2} |\langle \Phi_f | \mathbf{J}_+ | \Phi_i \rangle|^2 + \frac{(Z\alpha)^2 \omega^2}{8} |\langle \Phi_f | \mu_- | \Phi_i \rangle|^2 + \right. \\ &\quad \left. + \frac{Z\alpha\omega}{2} \text{Re} \langle \Phi_f | \mathbf{J}_+ | \Phi_i \rangle \langle \Phi_i | \mu_- | \Phi_f \rangle \right)\end{aligned}\quad (2.20)$$

$$\begin{aligned}w_R &= \frac{e^2}{8\pi^2\omega} \delta(E_f - E_i) \left(\frac{1}{2} |\langle \Phi_f | \mathbf{J}_- | \Phi_i \rangle|^2 + \frac{(Z\alpha)^2 \omega^2}{8} |\langle \Phi_f | \mu_+ | \Phi_i \rangle|^2 - \right. \\ &\quad \left. - \frac{Z\alpha\omega}{2} \text{Re} \langle \Phi_f | \mathbf{J}_- | \Phi_i \rangle \langle \Phi_i | \mu_+ | \Phi_f \rangle \right)\end{aligned}\quad (2.21)$$

The states $|\Phi_i\rangle$ and $|\Phi_f\rangle$ are bound states of the relativistic hydrogen-like atom (see subsection 1.3.2). Therefore, they are eigenstates of the total angular momentum operator, i. e.

$$|\Phi_i\rangle = |n_i, p_i, j_i, m_i\rangle, \quad (2.22)$$

$$|\Phi_f\rangle = |n_f, p_f, j_f, m_f\rangle, \quad (2.23)$$

where n is the principal quantum number, p is parity, j is total angular momentum quantum number and m is the magnetic quantum number.

As was mentioned earlier, we assume that J (and consequently μ) is a vector operator. Arbitrary vector operator \mathbf{V} has to meet the condition

$$[J_i, V_j] = i\varepsilon_{ijk}V_k \quad (2.24)$$

and then it holds (see [1])

$$\begin{aligned} \langle n_f, p_f, j_i - 1, m_i + 1 | V_+ | n_i, p_i, j_i, m_i \rangle &= \\ &= \langle n_f, p_f, j_i - 1 | | \mathbf{V} | | n_i, p_i, j_i \rangle \sqrt{(j_i - m_i - 1)(j_i - m_i)}, \end{aligned} \quad (2.25)$$

$$\begin{aligned} \langle n_f, p_f, j_i, m_i + 1 | V_+ | n_i, p_i, j_i, m_i \rangle &= \\ &= \langle n_f, p_f, j_i | | \mathbf{V} | | n_i, p_i, j_i \rangle \sqrt{(j_i + m_i + 1)(j_i - m_i)}, \end{aligned} \quad (2.26)$$

$$\begin{aligned} \langle n_f, p_f, j_i + 1, m_i + 1 | V_+ | n_i, p_i, j_i, m_i \rangle &= \\ &= \langle n_f, p_f, j_i + 1 | | \mathbf{V} | | n_i, p_i, j_i \rangle \sqrt{(j_i + m_i + 2)(j_i + m_i + 1)}, \end{aligned} \quad (2.27)$$

$$\begin{aligned} \langle n_f, p_f, j_i - 1, m_i - 1 | V_- | n_i, p_i, j_i, m_i \rangle &= \\ &= \langle n_f, p_f, j_i - 1 | | \mathbf{V} | | n_i, p_i, j_i \rangle \sqrt{(j_i + m_i - 1)(j_i + m_i)}, \end{aligned} \quad (2.28)$$

$$\begin{aligned} \langle n_f, p_f, j_i, m_i - 1 | V_- | n_i, p_i, j_i, m_i \rangle &= \\ &= \langle n_f, p_f, j_i | | \mathbf{V} | | n_i, p_i, j_i \rangle \sqrt{(j_i - m_i + 1)(j_i + m_i)}, \end{aligned} \quad (2.29)$$

$$\begin{aligned} \langle n_f, p_f, j_i + 1, m_i - 1 | V_- | n_i, p_i, j_i, m_i \rangle &= \\ &= \langle n_f, p_f, j_i + 1 | | \mathbf{V} | | n_i, p_i, j_i \rangle \sqrt{(j_i - m_i + 2)(j_i - m_i + 1)}, \end{aligned} \quad (2.30)$$

where the reduced matrix element $\langle n_f, p_f, j_f | | \mathbf{V} | | n_i, p_i, j_i \rangle$ has a value, which is independent of m . Therefore, the w_L and w_R from (2.20) and (2.21) are nonzero only for $j_f = j_i$ or $j_f = j_i \pm 1$ and $m_f = m_i \pm 1$.

We want to get the transition rate independent of m_i ; thus, we have to sum over all possible values of this quantum number. We use a fact that

$$\sum_{m=-j}^j 1 = 2j + 1, \quad (2.31)$$

$$\sum_{m=-j}^j m = 0, \quad (2.32)$$

$$\sum_{m=-j}^j m^2 = \frac{j}{3} (j + 1) (2j + 1). \quad (2.33)$$

After summation, we denote transition as \bar{w} and after substituing (2.25) – (2.30) into (2.20) and (2.21) we get

$$\begin{aligned} \bar{w}_{(R)}^{(L)} &= \sum_{m_i=-j_i}^{j_i} w_{(R)}^{(L)} = \frac{e^2 C_{j_i j_f}}{64\pi^2 \omega} \delta(E_f - E_i) \times \\ &\times \left(4 |\langle n_f, p_f, j_f || \mathbf{J} || n_i, p_i, j_i \rangle|^2 + (Z\alpha)^2 \omega^2 |\langle n_f, p_f, j_f || \boldsymbol{\mu} || n_i, p_i, j_i \rangle|^2 \pm \right. \\ &\quad \left. \pm 4Z\alpha\omega \operatorname{Re} \langle n_f, p_f, j_f || \mathbf{J} || n_i, p_i, j_i \rangle \langle n_f, p_f, j_f || \boldsymbol{\mu} || n_i, p_i, j_i \rangle^* \right), \end{aligned} \quad (2.34)$$

where

$$C_{j_i j_f} = \begin{cases} \frac{2j_i}{3} (4j_i^2 - 1), & \text{for } j_f = j_i - 1 \\ \frac{2j_i}{3} (j_i + 1) (2j_i + 1), & \text{for } j_f = j_i \\ \frac{2}{3} (4j_i^3 + 12j_i^2 + 11j_i + 3), & \text{for } j_f = j_i + 1 \\ 0, & \text{otherwise.} \end{cases} \quad (2.35)$$

For the circular dichroism defined in (2.1) we get

$$\bar{\delta}_{LR} = \frac{4Z\alpha\omega \operatorname{Re} \langle n_f, p_f, j_f || \mathbf{J} || n_i, p_i, j_i \rangle \langle n_f, p_f, j_f || \boldsymbol{\mu} || n_i, p_i, j_i \rangle^*}{4 |\langle n_f, p_f, j_f || \mathbf{J} || n_i, p_i, j_i \rangle|^2 + (Z\alpha)^2 \omega^2 |\langle n_f, p_f, j_f || \boldsymbol{\mu} || n_i, p_i, j_i \rangle|^2}, \quad (2.36)$$

2.2.1 Concrete forms of j

In the last section, we have derived the expression (2.1) for calculating circular dichroism in a case of a general \mathbf{j} . Now we focus on the hydrogen-like atoms and take $\mathbf{j} = e\boldsymbol{\alpha}$. As a result, we have to prove that $\boldsymbol{\alpha}$ and also $\boldsymbol{\mu} = \boldsymbol{\alpha} \times \mathbf{x}$ are a vector operators, i. e. we verify that they meet the condition (2.24)

$$\begin{aligned} [J_i, \alpha_j] &= \underbrace{[L_i, \alpha_j]}_{=0} + \frac{1}{2} [\Sigma_i, \alpha_j] = \\ &= \frac{1}{2} \begin{pmatrix} \sigma_i & 0 \\ 0 & \sigma_i \end{pmatrix} \begin{pmatrix} 0 & \sigma_j \\ \sigma_j & 0 \end{pmatrix} - \frac{1}{2} \begin{pmatrix} 0 & \sigma_j \\ \sigma_j & 0 \end{pmatrix} \begin{pmatrix} \sigma_i & 0 \\ 0 & \sigma_i \end{pmatrix} = \\ &= \frac{1}{2} \begin{pmatrix} 0 & [\sigma_i, \sigma_j] \\ [\sigma_i, \sigma_j] & 0 \end{pmatrix} = i\varepsilon_{ijk} \alpha_k \end{aligned} \quad (2.37)$$

where we have used a known property of Pauli matrices $[\sigma_i, \sigma_j] = 2i\varepsilon_{ijk} \sigma_k$. For the second commutator we use just calculated result and a known commutation relation between L_i and x_p

$$\begin{aligned} [J_i, \mu_j] &= \varepsilon_{jpk} \left(\underbrace{[L_i, x_p]}_{=i\varepsilon_{ipk} x_k} \alpha_q + \frac{1}{2} x_p \underbrace{[\Sigma_i, \alpha_q]}_{2i\varepsilon_{iqk} \alpha_l} \right) = i(\varepsilon_{jpl} \varepsilon_{ipk} x_k \alpha_l + \varepsilon_{jkq} \varepsilon_{iqk} x_k \alpha_l) = \\ &= i(\delta_{i,j} \delta_{k,l} - \delta_{i,l} \delta_{j,k} + \delta_{i,k} \delta_{j,l} - \delta_{i,j} \delta_{k,l}) x_k \alpha_l = i(\delta_{i,k} \delta_{j,l} - \delta_{i,l} \delta_{j,k}) x_k \alpha_l = \\ &= i\varepsilon_{ijm} \varepsilon_{klm} x_k \alpha_l = i\varepsilon_{ijm} \mu_m \end{aligned} \quad (2.38)$$

We can see that both operators $\boldsymbol{\alpha}$ and $\boldsymbol{\mu}$ are vector operators and all results from the last subsection are valid for them.

2.2.2 Analysis of the matrix elements

Let us analyse when the matrix elements are nonzero. All matrix elements are linear combination of the

$$Q_i = \langle n_f, p_f, j_f, m_f | \begin{pmatrix} 0 & q_i \\ q_i & 0 \end{pmatrix} | n_i, p_i, j_i, m_i \rangle \propto \\ \propto c_{1f}^* c_{2i} \langle j_f, m_f |^{p_f} q_i | j_i, m_i \rangle^{-p_i} + c_{2f}^* c_{1i} \langle j_f, m_f |^{-p_f} q_i | j_i, m_i \rangle^{p_i}, \quad (2.39)$$

where q_i is either $q_i = \sigma_i$, or $q_i = \varepsilon_{ijk} x_j \sigma_k$. The form of spherical spinors $|j_f, m_f\rangle^\pm$ (1.48) and (1.50) contains spherical harmonics. As a result, we have in (2.39) the integrals of the form

$$\int d\mathbf{n} Y_{j_f - \frac{p_f}{2}, m_f}^* Y_{j_i - \frac{p_i}{2}, m_i} = \delta_{j_f - \frac{p_f}{2}, j_i - \frac{p_i}{2}} \delta_{m_f, m_i}, \quad (2.40)$$

$$\int d\mathbf{n} Y_{j_f - \frac{p_f}{2}, m_f}^* n_i Y_{j_i - \frac{p_i}{2}, m_i} = k_{i-} \delta_{j_f - \frac{p_f}{2} - 1, j_i - \frac{p_i}{2}} \delta_{m_f, m'} + \\ + k_{i+} \delta_{j_f - \frac{p_f}{2} + 1, j_i - \frac{p_i}{2}} \delta_{m_f, m'}, \quad (2.41)$$

where $d\mathbf{n} = \sin^2 \theta d\theta d\phi$ and $\mathbf{x} = r\mathbf{n}$. We have also used a known property of the spherical harmonics (see [23])

$$n_i Y_{l, m} = k_{i-} Y_{l-1, m'} + k_{i+} Y_{l+1, m'}. \quad (2.42)$$

Using integration over the angular part and equations (2.40) and (2.41) we get nonzero matrix element (2.39) only when

1. For $q_i = \sigma_i$ (E_1 transitions) we have nonzero first term of (2.39) when

$$j_f - \frac{p_f}{2} = j_i + \frac{p_i}{2} \quad (2.43)$$

and the second term when

$$j_f + \frac{p_f}{2} = j_i - \frac{p_i}{2} \quad (2.44)$$

2. For $q_i = \varepsilon_{ijk} x_j \sigma_k$ (M_1 transitions) we have nonzero first term when

$$j_f - \frac{p_f}{2} \pm 1 = j_i + \frac{p_i}{2} \quad (2.45)$$

and the second term when

$$j_f + \frac{p_f}{2} \pm 1 = j_i - \frac{p_i}{2} \quad (2.46)$$

Consequently, when $j_f = j_i \pm 1$ we have nonzero matrix element for E_1 transitions between states of the same parity ($p_f = p_i$) and for M_1 transitions between states of the different parity ($p_f \neq p_i$).

For $j_f = j_i$, the situation is exactly the opposite. We have nonzero matrix element for E_1 transitions between states of the different parity and for M_1 transitions between states of the same parity.

It would seem that the circular dichroism is always zero, because in the numerator of (2.36) we have matrix elements for both E_1 and M_1 transition and either of them should be zero. But in the next subsection we will show that thanks to the weak interaction every state of even parity contains admixture of states with the odd parity and vice versa.

2.3 Parity non-conserving weak interaction between electron and nucleus

As was mentioned in the subsection 1.3.2, the parity operator K commutes with the hydrogen-like Dirac Hamiltonian H_0 . Therefore, the wave functions Φ has exact parity $p = \pm 1$. But if we consider the exchange of the Z^0 boson between electron and nucleus, we get additional term in the effective Hamiltonian

$$H = H_0 + H' = H_0 + H_S + H_P \quad (2.47)$$

which possesses both scalar H_S and pseudoscalar H_P parts. Because the pseudoscalar part H_P does not commute with parity operator K , the eigenstate $|\Phi^{(0)}\rangle$ of the hydrogen-like Dirac Hamiltonian defined in (1.53) changes as

$$|\Phi^{(0)}\rangle \rightarrow |\Phi\rangle = |\Phi^{(0)}\rangle + |\Phi^{(1)}\rangle + \dots \quad (2.48)$$

Using the standard perturbation theory we get

$$|\Phi^{(1)}\rangle = \sum_l \frac{|\chi_l^{(0)}\rangle \langle \chi_l^{(0)} | H_P | \Phi^{(0)}\rangle}{E(\Phi^{(0)}) - E(\chi_l^{(0)})}, \quad (2.49)$$

where sum over l is formal – it is summation over discrete part of the spectrum and integration over continuous part of the spectrum. States $|\chi_l^{(0)}\rangle$ has opposite parity than $|\Phi^{(0)}\rangle$ and energies E are defined in (1.46).

2.3.1 Neutral weak current interaction

In this subsection we show how to get form factors that describe the coupling between Z^0 boson and nucleus.

The standard model (SM) of elementary particles describes the interaction between the electron and Z^0 boson. The Z_μ field (which describes the Z^0 boson) is coupled to the electron field Ψ_e through the interaction

$$\mathcal{L}_e = \frac{-g}{4 \cos \theta_W} \bar{\Psi}_e \gamma^\mu (1 - 4 \sin^2 \theta_W - \gamma_5) \Psi_e Z_\mu, \quad (2.50)$$

where g is a weak coupling constant and θ_W is the Weinberg mixing angle and Ψ 's are the Dirac fields defined in (1.1). Our goal is to find a Lagrangian similar

to 2.50 which would couple the nucleons (protons p and neutrons n) to the Z_μ . We expect the Lagrangian in a form

$$\mathcal{L}_{pn} = \frac{g}{2 \cos \theta_W} J_Z^\mu Z_\mu, \quad (2.51)$$

where J_Z^μ is the neutral nucleonic weak current.

A proper understanding of this subject could be achieved only from equations of quantum chromodynamics (QCD) and from detailed knowledge of the structure of nucleons. However, the methods of QCD are not applicable in the processes we want to study. Thus we will use a semiempirical theory proposed in [20] which allows us to calculate form factors for any neutral current process from several experimentally determined values.

A theory from [20] is based on an assumed gauge-invariance group of total Lagrangian consisting of SU(2) and U(1) groups. We also assume that proton and neutron have same masses ($m_p = m_n$) and they are $\frac{1}{2}$ and $-\frac{1}{2}$ components of an nucleon isospin doublet (isodoublet)

$$\Psi_N = \begin{pmatrix} \Psi_p \\ \Psi_n \end{pmatrix}. \quad (2.52)$$

Then the nucleonic currents are

$$\mathbf{J}^\mu = \bar{\Psi}_N \gamma^\mu (1 - \gamma_5) \mathbf{t} \Psi_N, \quad (2.53)$$

$$J_{EM}^\mu = \bar{\Psi}_N \gamma^\mu \left(\frac{1}{2} + t_3 \right) \Psi_N, \quad (2.54)$$

where t_i are the usual isospin matrices (half the Pauli matrices) and the electromagnetic current J_{EM} contains isovector part (proportional to t_3) and isoscalar part (proportional to $\frac{1}{2}$).

The spontaneous symmetry breaking allows us to write the Lagrangian using fields with definite masses A_μ , W_μ , W_μ^\dagger and Z_μ

$$\mathcal{L}_{nuc} = \frac{g}{2\sqrt{2}} J_W^{\mu\dagger} W_\mu + \frac{g}{2\sqrt{2}} J_W^\mu W_\mu^\dagger + \frac{g}{2 \cos \theta_W} J_Z^\mu Z_\mu + e J_{EM}^\mu A_\mu, \quad (2.55)$$

with charged weak nucleonic current

$$J_W^\mu = J_1^\mu - i J_2^\mu, \quad (2.56)$$

containing isovector V^μ and axial isovector A^μ parts which are put together according to $V - A$ law ($J_W^\mu = V^\mu - A^\mu$). In (2.55) we also have neutral weak nucleonic current defined as

$$J_Z^\mu = J_3^\mu - 2 \sin^2 \theta_W J_{EM}^\mu. \quad (2.57)$$

The matrix element of J_{EM}^μ between two proton states $|p(l)\rangle$, resp. $|p(l')\rangle$ with four-momentum l , resp. l' is given by the general expression

$$\begin{aligned} M_p &= \langle p(l') | J_{EM}^\mu | p(l) \rangle = \\ &= e^{iq \cdot x} \bar{u}_p(l') [C_p(q^2) \gamma^\mu + i G_p(q^2) \sigma^{\mu\nu} q_\nu + F_p(q^2) q^\mu] u_p(l), \end{aligned} \quad (2.58)$$

where $q = l' - l$ is the momentum transfer, C_p , G_p and F_p are form factors and u_p are momentum-space wave functions (Dirac spinors). Condition $\partial_\mu J_{EM}^\mu = 0$ implies very useful restriction $F_p(q^2) = 0$.

Furthermore, in the limit $q^2 \rightarrow 0$ we get $C_p(0) = 1$ because the proton charge is $+|e|$. The anomalous part of the magnetic moment of the proton is accounted for by the ‘‘Pauli moment term’’ which gives $G_p(0) = 1.79/2m_p$. We can construct the matrix element of J_{EM}^μ between two neutron states in the same fashion

$$M_n = e^{iq \cdot x} \bar{u}_n(l') [C_n(q^2)\gamma^\mu + iG_n(q^2)\sigma^{\mu\nu}q_\nu] u_n(l). \quad (2.59)$$

Since the neutron does not interact with the electric field we have $C_n(0) = 0$. Its magnetic momentum is entirely anomalous which gives $G_p(0) = -1.91/2m_p$. We unite the matrix elements M_p and M_n using the nucleon isodoublet u , where spinors u_p and u_n are recovered with the aid of projection operators

$$\left(\frac{1}{2} + t_3\right) u = u_p \quad \text{and} \quad \left(\frac{1}{2} - t_3\right) u = u_n. \quad (2.60)$$

In place of (2.58) and (2.59) we then get

$$M = e^{iq \cdot x} \bar{u} \left\{ \frac{1}{2} [C_{is}(q^2)\gamma^\mu + iG_{is}(q^2)\sigma^{\mu\nu}q_\nu] + [C_{iv}(q^2)\gamma^\mu + iG_{iv}(q^2)\sigma^{\mu\nu}q_\nu] t_3 \right\} u, \quad (2.61)$$

where we have isoscalar (is) and isovector (iv) formfactors defined as

$$C_{is}(q^2) = C_p(q^2) + C_n(q^2), \quad (2.62)$$

$$C_{iv}(q^2) = C_p(q^2) - C_n(q^2), \quad (2.63)$$

$$G_{is}(q^2) = G_p(q^2) + G_n(q^2), \quad (2.64)$$

$$G_{iv}(q^2) = G_p(q^2) - G_n(q^2). \quad (2.65)$$

We now write the corresponding nucleonic weak current between neutron and proton states

$$\begin{aligned} \langle p(l') | J_W^\mu | n(l) \rangle &= \langle p(l') | V^\mu | n(l) \rangle - \langle p(l') | A^\mu | n(l) \rangle = \\ &= e^{iq \cdot x} \bar{u} [f_1(q^2)\gamma^\mu + if_2(q^2)\sigma^{\mu\nu}q_\nu + f_3(q^2)q^\mu] t_+ u - \\ &- e^{iq \cdot x} \bar{u} [g_1(q^2)\gamma^\mu\gamma_5 + ig_2(q^2)\sigma^{\mu\nu}q_\nu\gamma_5 + g_3(q^2)q^\mu\gamma_5] t_+ u. \end{aligned} \quad (2.66)$$

The isovector part of the current (2.53) is conserved because of the global SU(2) gauge invariance. As a result, we have the conserved vector current (CVC) hypothesis which states that the vector charged weak nucleonic current V^μ , its conjugate V^μ and the isovector portion of the electromagnetic current J_{EM}^μ form a single isospin triplet of conserved currents. In other words, for form factors from (2.66) and (2.61) we thus have

$$f_1(q^2) = C_{iv}(q^2), \quad (2.67)$$

$$f_2(q^2) = G_{iv}(q^2), \quad (2.68)$$

$$f_3(q^2) = 0. \quad (2.69)$$

and for limit $q^2 \rightarrow 0$ we get

$$f_1(0) = C_p(0) - C_n(0) = 1 \quad (2.70)$$

$$f_2(0) = M_p(0) - M_n(0) = \frac{3.70}{2m_p} \quad (2.71)$$

Similarly we can use the hypothesis archaically called partially conserved axial current (PCAC) hypothesis which together with experimental data on β -decay give

$$g_1(0) = 1.25, \quad (2.72)$$

$$g_2(0) = 0. \quad (2.73)$$

For more information see [6], section 4.11.

From the derived expressions we can finally write the matrix element of the neutral weak nucleonic current between proton and neutron states

$$\begin{aligned} \langle p(l') | J_Z^\mu | p(l) \rangle &= e^{iq \cdot x} \times \\ &\times \bar{u}_p(l') \left[f_{1p}(q^2) \gamma^\mu + \overbrace{if_{2p}(q^2) \sigma^{\mu\nu} q_\nu}^{=0 \text{ for } q^2 \rightarrow 0} + g_{1p}(q^2) \gamma^\mu \gamma_5 + \overbrace{g_{3p} q^\mu \gamma_5}^{=0 \text{ for } q^2 \rightarrow 0} \right] u_p(l) \end{aligned} \quad (2.74)$$

and

$$\begin{aligned} \langle n(l') | J_Z^\mu | n(l) \rangle &= e^{iq \cdot x} \times \\ &\times \bar{u}_n(l') \left[f_{1n}(q^2) \gamma^\mu + \overbrace{if_{2n}(q^2) \sigma^{\mu\nu} q_\nu}^{=0 \text{ for } q^2 \rightarrow 0} + g_{1n}(q^2) \gamma^\mu \gamma_5 + \overbrace{g_{3n} q^\mu \gamma_5}^{=0 \text{ for } q^2 \rightarrow 0} \right] u_n(l). \end{aligned} \quad (2.75)$$

We have discarded terms with zero formfactors (f_3 and g_2). From definition (2.57) we can write for the formfactors from (2.74) and (2.75) following relations

$$f_{1p}(q^2) = \frac{1}{2} f_1(q^2) - 2 \sin^2 \theta_W C_p(q^2), \quad (2.76)$$

$$f_{1n}(q^2) = -\frac{1}{2} f_1(q^2) - 2 \sin^2 \theta_W C_n(q^2), \quad (2.77)$$

$$f_{2p}(q^2) = \frac{1}{2} f_2(q^2) - 2 \sin^2 \theta_W G_p(q^2), \quad (2.78)$$

$$f_{2n}(q^2) = -\frac{1}{2} f_2(q^2) - 2 \sin^2 \theta_W G_n(q^2), \quad (2.79)$$

$$g_{1p}(q^2) = \frac{1}{2} g_1(q^2) = -g_{1n}(q^2), \quad (2.80)$$

$$g_{3p}(q^2) = \frac{1}{2} g_3(q^2) = -g_{3n}(q^2). \quad (2.81)$$

At low q^2 we may ignore the terms with f_{2p} , f_{2n} , g_{3p} and g_{3n} and after performing the limit $q^2 \rightarrow 0$ we get

$$f_{1p}(0) = \frac{1}{2} (1 - 4 \sin^2 \theta_W) \approx 0.04, \quad (2.82)$$

$$f_{1n}(0) = -\frac{1}{2}, \quad (2.83)$$

$$g_{1p}(0) = -g_{1n}(0) = 0.625. \quad (2.84)$$

These results will be used in the following subsection.

2.3.2 Derivation of expression for effective Hamiltonian H_P

Let us now turn our attention to the pseudoscalar Hamiltonian H_P , which arises from the Z^0 exchange between electron and the atomic nucleus. We want to write H_P as the effective potential caused by nucleus and acting on the electron.

We will use a several approximations

1. As was said earlier we assume limit $q \rightarrow 0$ (momentum transfer between electron and nucleus is negligible).
2. We assume that the nucleus is static so the nucleonic three-current is zero

$$\bar{\Phi}_{n,p}(\mathbf{x})\gamma_i\Phi_{n,p}(\mathbf{x}) = 0. \quad (2.85)$$

3. We also assume a point-like nucleus

$$\Phi_{n,p}^\dagger(\mathbf{x})\Phi_{n,p}(\mathbf{x}) = \delta(\mathbf{x}_N). \quad (2.86)$$

The functions $\Phi_{n,p}(\mathbf{x})$ is related to the momentum wave function $u_{p,n}$ via the Fourier transformation

$$\Phi_{n,p}(\mathbf{x}) = \int \frac{d^3\mathbf{l}}{(2\pi)^{\frac{3}{2}}} e^{i\mathbf{l}\cdot\mathbf{x}} u_{p,n}(\mathbf{l}). \quad (2.87)$$

In electrostatics we can write the interaction between charge density ρ and the test charge e as $H_{elec} = e\varphi$, where φ is determined by the Poisson equation $-\nabla^2\varphi = \rho$. We use approximation 2) and in analogy with electrostatics we write the effective Hamiltonian H' describing the exchange of Z^0 boson between electron and nucleus as

$$H' = q_e^{weak}\varphi_N^{weak}(\mathbf{x}), \quad (2.88)$$

where the weak charge of the electron q_e^{weak} is according to (2.50) equal to

$$q_e^{weak} = \frac{-g}{4\cos\theta_W}(1 - 4\sin^2\theta_W - \gamma_5). \quad (2.89)$$

The nucleonic weak potential $\varphi_N^{weak}(\mathbf{x})$ can be calculated from the equation for static massive field

$$(-\nabla^2 + M_Z^2)\varphi_N^{weak}(\mathbf{x}) = \varrho_N^{weak}(\mathbf{x}), \quad (2.90)$$

where M_Z is mass of the Z^0 boson and the nucleonic weak charge density $\varrho_N^{weak}(\mathbf{x})$ is according to (2.74), (2.75) and (2.82) – (2.84) with approximation 1) in the form

$$\begin{aligned} \varrho_N^{weak}(\mathbf{x}) = \frac{g}{4\cos\theta_W} \left[\sum_p \Phi_p^\dagger(\mathbf{x}) (1 - 4\sin^2\theta_W - 1.25\gamma_5) \Phi_p(\mathbf{x}) - \right. \\ \left. - \sum_n \Phi_n^\dagger(\mathbf{x}) (1 - 1.25\gamma_5) \Phi_n(\mathbf{x}) \right]. \quad (2.91) \end{aligned}$$

We neglect the part of (2.91) which is proportional to γ_5 , because it gives at least one order of magnitude lesser contribution (see [6], section 9.3). Together with approximation 3) we can write (2.91) as

$$\varrho_N^{weak}(\mathbf{x}) = \frac{g}{4 \cos \theta_W} Q_W \delta(\mathbf{x}). \quad (2.92)$$

The so called weak charge Q_W has the form

$$Q_W = \left[\sum_p (1 - 4 \sin^2 \theta_W) + \sum_n (-1) \right] = (1 - 4 \sin^2 \theta_W) Z - N, \quad (2.93)$$

where Z is the proton number and N is the neutron number. For point charge (2.92) the solution of equation (2.90) is Yukawa potential

$$\varphi_N^{weak}(\mathbf{x}) = \frac{g}{4 \cos \theta_W} \frac{Q_W}{4\pi} \frac{e^{-M_Z r}}{r} \quad (2.94)$$

We insert expression (2.94) into (2.88) and we get

$$H' = \frac{-g^2}{16 \cos^2 \theta_W} \frac{Q_W}{4\pi} (1 - 4 \sin^2 \theta_W - \gamma_5) \frac{e^{-M_Z r}}{r} \quad (2.95)$$

We separate the pseudoscalar Hamiltonian H_P from (2.95) (it is the part proportional to γ_5) and we get

$$H_p(\mathbf{x}) = \rho_N(r_e) \gamma_5, \quad (2.96)$$

where $\rho_N(r)$ is defined as

$$\rho_N(r) = \frac{g^2 Q_W}{64\pi \cos^2 \theta_W} \frac{e^{-M_Z r}}{r}. \quad (2.97)$$

2.3.3 Matrix element of H_P

Now we know the form of H_P and we can study the matrix element $\langle \chi_l^{(0)} | H_P | \Phi^{(0)} \rangle$ from equation (2.49), where we take for the zeroth order functions $|\Phi^{(0)}\rangle =$

$|n, p, j, m\rangle$ defined in (1.53)

$$\begin{aligned}
\langle \chi_l^{(0)} | H_P | \Phi^{(0)} \rangle &= \langle n_l, -p, j_l, m_l | \rho_N \gamma_5 | n, p, j, m \rangle = \frac{1}{NN_l} \left[A_l^{-p} \langle n_l, |\Gamma_m| \rangle \times \right. \\
&\times \left(\begin{array}{c} c_{1,-p}^{*|\Gamma_l|} \langle j_l, m_l |^{-p} \\ c_{2,-p}^{*|\Gamma_l|} \langle j_l, m_l |^p \end{array} \right)^T + B_l \langle n_l, |\Gamma_m| - 1 \rangle \left(\begin{array}{c} c_{1,-p}^{*|\Gamma_l|} \langle j_l, m_l |^{-p} \\ c_{2,-p}^{*|\Gamma_l|} \langle j_l, m_l |^p \end{array} \right)^T \left. \right] \\
&\left(\begin{array}{cc} 0 & \rho_N \\ \rho_N & 0 \end{array} \right) \left[A^p |n, |\Gamma\rangle \left(\begin{array}{c} c_{1,p}^{|\Gamma|} |j, m\rangle^p \\ c_{2,p}^{|\Gamma|} |j, m\rangle^{-p} \end{array} \right) + B |n, |\Gamma| - 1 \rangle \left(\begin{array}{c} c_{1,p}^{-|\Gamma|} |j, m\rangle^p \\ c_{2,p}^{-|\Gamma|} |j, m\rangle^{-p} \end{array} \right) \right] = \\
&= \frac{1}{NN_l} \int \rho_N(r) dr r^2 \left\{ A_l^{-p} A^p R_{n_l, |\Gamma_l| - 1} R_{n, |\Gamma| - 1} \times \right. \\
&\times \left[c_{1,-p}^{*|\Gamma_l|} c_{2,p}^{|\Gamma|} \langle j_l, m_l |^{-p} |j, m\rangle^{-p} + c_{2,-p}^{*|\Gamma_l|} c_{1,p}^{|\Gamma|} \langle j_l, m_l |^p |j, m\rangle^p \right] + \\
&+ A_l^{-p} B R_{n_l, |\Gamma_l| - 1} R_{n, |\Gamma|} \times \\
&\times \left[c_{1,-p}^{*|\Gamma_l|} c_{2,p}^{-|\Gamma|} \langle j_l, m_l |^{-p} |j, m\rangle^{-p} + c_{2,-p}^{*|\Gamma_l|} c_{1,p}^{-|\Gamma|} \langle j_l, m_l |^p |j, m\rangle^p \right] + \\
&+ B_l A^p R_{n_l, |\Gamma_l|} R_{n, |\Gamma| - 1} \times \\
&\times \left[c_{1,-p}^{*|\Gamma_l|} c_{2,p}^{|\Gamma|} \langle j_l, m_l |^{-p} |j, m\rangle^{-p} + c_{2,-p}^{*|\Gamma_l|} c_{1,p}^{|\Gamma|} \langle j_l, m_l |^p |j, m\rangle^p \right] + \\
&+ B_l B R_{n_l, |\Gamma_l|} R_{n, |\Gamma|} \times \\
&\times \left. \left[c_{1,-p}^{*|\Gamma_l|} c_{2,p}^{-|\Gamma|} \langle j_l, m_l |^{-p} |j, m\rangle^{-p} + c_{2,-p}^{*|\Gamma_l|} c_{1,p}^{-|\Gamma|} \langle j_l, m_l |^p |j, m\rangle^p \right] \right\}, \quad (2.98)
\end{aligned}$$

where constants A, B, Γ, N and so on are defined in subsections 1.3.1 and 1.3.2. We use subscript l , resp. nothing to emphasize the use of n_l, j_l, \dots , resp. n, j, \dots .

For the scalar product of two spherical spinors (1.48) and (1.50) we get

$$\langle j_l, m_l |^{\pm p} |j, m\rangle^{\pm p} = \delta_{j_l, j} \delta_{m_l, m}, \quad (2.99)$$

and after substitution of c_1 and c_2 from (1.51) and (1.52) we get the matrix element (2.98) in the form

$$\begin{aligned}
\langle n_l, -p, j, m | \rho_N \gamma_5 | n, p, j, m \rangle &= \frac{-ip}{(2j+1) NN_l} \int dr r^2 \rho_N(r) \times \\
&\times \left[(2j+1) A_l^{-p} A^p R_{n_l, |\Gamma_l| - 1} R_{n, |\Gamma| - 1} + 2pZ\alpha A_l^{-p} B R_{n_l, |\Gamma_l| - 1} R_{n, |\Gamma|} - \right. \\
&\left. - 2pZ\alpha B_l A^p R_{n_l, |\Gamma_l|} R_{n, |\Gamma| - 1} - (2j+1) B_l B R_{n_l, |\Gamma_l|} R_{n, |\Gamma|} \right]. \quad (2.100)
\end{aligned}$$

2.4 Calculation of $\bar{\delta}_{LR}$

In this section we can finally derive the theoretical expression for circular dichroism. The parity nonconservation is most easily seen by measurements of circular dichroism in the M_1 transitions, where $j_f = j_i = j$ and $p_f = p_i = p$. From

the expression (2.36) we get formula for the circular dichroism $\bar{\delta}_{LR}$ in the lowest nonzero order of the perturbation theory

$$\bar{\delta}_{LR} \approx \frac{4Z\alpha\omega \text{Re}\langle n_f, p_i, j_i | \boldsymbol{\alpha} | n_i, p_i, j_i \rangle^{(1)} \langle n_f, p_i, j_i | \boldsymbol{\mu} | n_i, p_i, j_i \rangle^{*(0)}}{4|\langle n_f, p_i, j_i | \boldsymbol{\alpha} | n_i, p_i, j_i \rangle^{(1)}|^2 + (Z\alpha)^2\omega^2 |\langle n_f, p_i, j_i | \boldsymbol{\mu} | n_i, p_i, j_i \rangle^{(0)}|^2} \quad (2.101)$$

We also assume that

$$|\langle n_f, p_i, j_i | \boldsymbol{\alpha} | n_i, p_i, j_i \rangle^{(1)}| \ll Z\alpha\omega |\langle n_f, p_i, j_i | \boldsymbol{\mu} | n_i, p_i, j_i \rangle^{(0)}| \quad (2.102)$$

and with the just mentioned assumption (2.102) we have for the expression (2.101)

$$\boxed{\bar{\delta}_{LR} \approx \text{Re} \frac{4\langle n_f, p_i, j_i | \boldsymbol{\alpha} | n_i, p_i, j_i \rangle^{(1)}}{Z\alpha\omega \langle n_f, p_i, j_i | \boldsymbol{\mu} | n_i, p_i, j_i \rangle^{(0)}}} \quad (2.103)$$

The assumption (2.102) could be verified after the calculation from the obtained value of $\bar{\delta}_{LR}$.

2.4.1 Reduced matrix element of the M_1 transition

At first, let us focus our attention on the denominator. We use equation (2.26) to calculate the reduced matrix element. The value of m_i is arbitrary (we choose $m_i = -j$) and we get

$$\langle n_f, p, j | \boldsymbol{\mu} | n_i, p, j \rangle^{(0)} = \frac{1}{\sqrt{2j}} \langle n_f, p, j, -j + 1 | \mu_+ | n_i, p, j, -j \rangle. \quad (2.104)$$

Operator μ_+ has the form

$$\begin{aligned} \mu_+ &= \mu_1 + i\mu_2 = x_2\alpha_3 - x_3\alpha_2 + i(x_3\alpha_1 - x_1\alpha_3) = \\ &= -i(x_1 + ix_2)\alpha_3 + ix_3(\alpha_1 + i\alpha_2) = i(x_3\alpha_+ - x_+\alpha_3) = \begin{pmatrix} 0 & q_+ \\ q_+ & 0 \end{pmatrix} \end{aligned} \quad (2.105)$$

where $\mathbf{x} = r\mathbf{n}$ and q_+ is then

$$q_+ = ir(n_3\sigma_+ - n_+\sigma_3) = ir \begin{pmatrix} -n_+ & n_3 \\ 0 & n_+ \end{pmatrix}. \quad (2.106)$$

Let us write the matrix element using relativistic wave functions (1.53). Because we have $j_f = j_i = j$ and $p_f = p_i = p$, the constants $c_{1,p}^\Gamma$ and $c_{2,p}^\Gamma$ are the same for both wave functions with values defined in (1.51) and (1.52). We also use

subscript i or f to emphasize the use of n_i or n_f in constants A , B and N .

$$\begin{aligned}
\langle n_f, p, j | | \boldsymbol{\mu} | | n_i, p, j \rangle^{(0)} &= \frac{1}{N_i N_f \sqrt{2j}} \times \\
&\times \left[A_f^p \langle n_f, |\Gamma| - 1 | \begin{pmatrix} c_{1,p}^{*|\Gamma|} \langle j, -j + 1 |^p \\ c_{2,p}^{*|\Gamma|} \langle j, -j + 1 |^{-p} \end{pmatrix}^T + B_f \langle n_f, |\Gamma| | \begin{pmatrix} c_{1,p}^{*-|\Gamma|} \langle j, -j + 1 |^p \\ c_{2,p}^{*-|\Gamma|} \langle j, -j + 1 |^{-p} \end{pmatrix}^T \right] \\
&\begin{pmatrix} 0 & q_+ \\ q_+ & 0 \end{pmatrix} \left[A_i^p | n_i, |\Gamma| - 1 \rangle \begin{pmatrix} c_{1,p}^{|\Gamma|} | j, -j \rangle^p \\ c_{2,p}^{|\Gamma|} | j, -j \rangle^{-p} \end{pmatrix} + B_i | n_f, |\Gamma| \rangle \begin{pmatrix} c_{1,p}^{-|\Gamma|} | j, -j \rangle^p \\ c_{2,p}^{-|\Gamma|} | j, -j \rangle^{-p} \end{pmatrix} \right] = \\
&= \frac{1}{N_i N_f \sqrt{2j}} \int dr r^2 \left\{ A_f^p A_i^p R_{n_f, |\Gamma| - 1} R_{n_i, |\Gamma| - 1} \frac{-ipZ\alpha}{2(j + \frac{1}{2})} S_{\pm}^q + \right. \\
&\quad + A_f^p B_i R_{n_f, |\Gamma| - 1} R_{n_i, |\Gamma|} \frac{-ip}{2(j + \frac{1}{2})} \left[|\Gamma| S_+^q + p(j + \frac{1}{2}) S_-^q \right] + \\
&\quad + B_f A_i^p R_{n_f, |\Gamma|} R_{n_i, |\Gamma| - 1} \frac{ip}{2(j + \frac{1}{2})} \left[|\Gamma| S_+^q - p(j + \frac{1}{2}) S_-^q \right] + \\
&\quad \left. + B_f B_i R_{n_f, |\Gamma|} R_{n_i, |\Gamma|} \frac{-ipZ\alpha}{2(j + \frac{1}{2})} S_{\pm}^q \right\}, \tag{2.107}
\end{aligned}$$

where the spin-angular part is

$$\begin{aligned}
S_{\pm}^q &= (\langle j, -j + 1 |^p q_+ | j, -j \rangle^{-p} \pm \langle j, -j + 1 |^{-p} q_+ | j, -j \rangle^p) = \\
&= \begin{cases} 1 \\ p \end{cases} \times (\langle j, -j + 1 |^+ q_+ | j, -j \rangle^- \pm \langle j, -j + 1 |^- q_+ | j, -j \rangle^+). \tag{2.108}
\end{aligned}$$

In order to calculate S_{\pm}^q from the last equation, we use the explicit values of spherical spinors (1.48) and (1.50). We can solve the problem for general j

$$\begin{aligned}
\langle j, -j + 1 |^+ q_+ | j, -j \rangle^- &= ir \int d\mathbf{n} \begin{pmatrix} \frac{1}{\sqrt{2j}} Y_{j-\frac{1}{2}, -j+\frac{1}{2}}^*(\mathbf{n}) \\ \sqrt{\frac{2j-1}{2j}} Y_{j-\frac{1}{2}, -j+\frac{3}{2}}^*(\mathbf{n}) \end{pmatrix}^T \begin{pmatrix} -n_+ & n_3 \\ 0 & n_+ \end{pmatrix} \\
&\begin{pmatrix} -\sqrt{\frac{2j+1}{2j+2}} Y_{j+\frac{1}{2}, -j-\frac{1}{2}}(\mathbf{n}) \\ \sqrt{\frac{1}{2j+2}} Y_{j+\frac{1}{2}, -j+\frac{1}{2}}(\mathbf{n}) \end{pmatrix} = ir \int d\mathbf{n} \left(\sqrt{\frac{2j+1}{2j(2j+2)}} Y_{j-\frac{1}{2}, -j+\frac{1}{2}}^*(\mathbf{n}) \times \right. \\
&\quad \times n_+ Y_{j+\frac{1}{2}, -j-\frac{1}{2}}(\mathbf{n}) + \sqrt{\frac{1}{2j(2j+2)}} Y_{j-\frac{1}{2}, -j+\frac{1}{2}}^*(\mathbf{n}) n_3 Y_{j+\frac{1}{2}, -j+\frac{1}{2}}(\mathbf{n}) + \\
&\quad \left. + \sqrt{\frac{2j-1}{2j(2j+2)}} Y_{j-\frac{1}{2}, -j+\frac{3}{2}}^*(\mathbf{n}) n_+ Y_{j+\frac{1}{2}, -j+\frac{1}{2}}(\mathbf{n}) \right) = \\
&= \frac{ir}{\sqrt{2j}} \frac{2j+1}{2j+2} + \frac{ir}{\sqrt{2j}} \frac{1}{2j+2} + \frac{ir}{\sqrt{2j}} \frac{2j-1}{2j+2} = \frac{ir}{\sqrt{2j}} \frac{4j+1}{2j+2}, \tag{2.109}
\end{aligned}$$

where the integration over $d\mathbf{n}$ was done using formula (2.41). For the second term we get

$$\begin{aligned}
\langle j, -j+1 |^{-q_+} | j, -j \rangle^+ &= ir \int d\mathbf{n} \left(-\sqrt{\frac{2j}{2j+2}} Y_{j+\frac{1}{2}, -j+\frac{1}{2}}^*(\mathbf{n}) \right)^T \begin{pmatrix} -n_+ & n_3 \\ 0 & n_+ \end{pmatrix} \\
&\begin{pmatrix} 0 \\ Y_{j-\frac{1}{2}, -j+\frac{1}{2}}(\mathbf{n}) \end{pmatrix} = ir \int d\mathbf{n} \left(-\sqrt{\frac{2j}{2j+2}} Y_{j+\frac{1}{2}, -j+\frac{1}{2}}^*(\mathbf{n}) \times \right. \\
&\quad \left. \times n_3 Y_{j-\frac{1}{2}, -j+\frac{1}{2}}(\mathbf{n}) + \sqrt{\frac{2}{2j+2}} Y_{j+\frac{1}{2}, -j+\frac{3}{2}}^*(\mathbf{n}) n_+ Y_{j-\frac{1}{2}, -j+\frac{1}{2}}(\mathbf{n}) \right) = \\
&= -\frac{ir}{\sqrt{2j}} \frac{2j}{2j+2} - \frac{ir}{\sqrt{2j}} \frac{2}{2j+2} = -\frac{ir}{\sqrt{2j}} \tag{2.110}
\end{aligned}$$

Altogether we have for the reduced matrix element a relation

$$\begin{aligned}
\langle n_f, p, j | |\boldsymbol{\mu}| | n_i, p, j \rangle^{(0)} &= \frac{1}{2j(2j+2)(2j+1)N_i N_f} \times \\
&\times \int dr r^3 \left\{ 3Z\alpha(2j+1) A_f^p A_i^p R_{n_f, |\Gamma|-1} R_{n_i, |\Gamma|-1} + \right. \\
&\quad + p \left[(2j-1)|\Gamma| + \frac{3}{2}(2j+1)^2 \right] A_f^p B_i R_{n_f, |\Gamma|-1} R_{n_i, |\Gamma|-} \\
&\quad - p \left[(2j-1)|\Gamma| - \frac{3}{2}(2j+1)^2 \right] B_f A_i^p R_{n_f, |\Gamma|} R_{n_i, |\Gamma|-1} + \\
&\quad \left. + 3Z\alpha(2j+1) B_f B_i R_{n_f, |\Gamma|} R_{n_i, |\Gamma|} \right\} \tag{2.111}
\end{aligned}$$

2.4.2 Reduced matrix element of the E_1 transition

At last, we need to calculate the numerator of the fraction (2.103)

$$\begin{aligned}
\langle n_f, p, j | |\boldsymbol{\alpha}| | n_i, p, j \rangle^{(1)} &= \frac{1}{\sqrt{2j}} \left(\langle n_f, p, j, -j+1 | \alpha_+ | n_i, p, j, -j \rangle^{(1)} + \right. \\
&\quad \left. + \langle n_f, p_i, j_i, -j_i+1 |^{(1)} \alpha_+ | n_i, p_i, j_i, -j_i \rangle \right) = \frac{1}{\sqrt{2j}} \times \\
&\times \sum_l \left(\frac{\langle n_f, p, j, -j+1 | \alpha_+ | n_l, -p, j, -j \rangle \langle n_l, -p, j, -j+1 | \rho_N \gamma_5 | n_i, p, j, -j \rangle}{E_i - E_l} + \right. \\
&\quad \left. + \frac{\langle n_f, p, j, -j+1 | \rho_N \gamma_5 | n_l, -p, j, -j+1 \rangle \langle n_l, -p, j, -j+1 | \alpha_+ | n_i, p, j, -j \rangle}{E_f - E_l} \right), \tag{2.112}
\end{aligned}$$

The procedure of calculating matrix elements in (2.112) is very similar to the one we have just done. The only difference is we have operator α_+ instead of μ_+ and

the parity of both functions is different.

$$\begin{aligned}
\langle n_f, p, j, -j+1 | \alpha_+ | n_l, -p, j, -j \rangle &= \frac{1}{N_l N_f} \int dr r^2 \times \\
&\left\{ A_f^p A_l^{-p} R_{n_f, |\Gamma|-1} R_{n_l, |\Gamma|-1} \frac{i}{2(j+\frac{1}{2})} \left[|\Gamma| S_-^\sigma + p(j+\frac{1}{2}) S_+^\sigma \right] + \right. \\
&\quad + \left[-A_f^p B_l R_{n_f, |\Gamma|-1} R_{n_l, |\Gamma|} + B_f A_l^p R_{n_f, |\Gamma|} R_{n_l, |\Gamma|-1} \right] \frac{iZ\alpha}{2(j+\frac{1}{2})} S_+^\sigma + \\
&\quad \left. - B_f B_l R_{n_f, |\Gamma|} R_{n_l, |\Gamma|} \frac{i}{2(j+\frac{1}{2})} \left[-|\Gamma| S_-^\sigma + p(j+\frac{1}{2}) S_+^\sigma \right] \right\}, \quad (2.113)
\end{aligned}$$

where S_\pm^σ is defined just as (2.108) as

$$S_\pm^\sigma = \begin{cases} 1 \\ p \end{cases} \times (\langle j, -j+1 |^+ \sigma_+ | j, -j \rangle^+ \pm \langle j, -j+1 |^- \sigma_+ | j, -j \rangle^-). \quad (2.114)$$

Again, we have to calculate only the spin-angular parts to get the S_\pm^σ and, consequently, the matrix element (2.113)

$$\begin{aligned}
\langle j, -j+1 |^+ \sigma_+ | j, -j \rangle^+ &= \int d\mathbf{n} \begin{pmatrix} \frac{1}{\sqrt{2j}} Y_{j-\frac{1}{2}, -j+\frac{1}{2}}^*(\mathbf{n}) \\ \sqrt{\frac{2j-1}{2j}} Y_{j-\frac{1}{2}, -j+\frac{3}{2}}^*(\mathbf{n}) \end{pmatrix}^T \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} \\
\begin{pmatrix} 0 \\ Y_{j-\frac{1}{2}, -j+\frac{1}{2}}(\mathbf{n}) \end{pmatrix} &= \frac{1}{\sqrt{2j}}, \quad (2.115)
\end{aligned}$$

and

$$\begin{aligned}
\langle j, -j+1 |^- \sigma_+ | j, -j \rangle^+ &= ir \int d\mathbf{n} \begin{pmatrix} -\sqrt{\frac{2j}{2j+2}} Y_{j+\frac{1}{2}, -j+\frac{1}{2}}^*(\mathbf{n}) \\ \sqrt{\frac{2}{2j+2}} Y_{j+\frac{1}{2}, -j+\frac{3}{2}}^*(\mathbf{n}) \end{pmatrix}^T \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} \\
\begin{pmatrix} -\sqrt{\frac{2j+1}{2j+2}} Y_{j+\frac{1}{2}, -j-\frac{1}{2}}(\mathbf{n}) \\ \sqrt{\frac{1}{2j+2}} Y_{j+\frac{1}{2}, -j+\frac{1}{2}}(\mathbf{n}) \end{pmatrix} &= -\frac{\sqrt{2j}}{2j+2}. \quad (2.116)
\end{aligned}$$

We use results from (2.113), (2.115) and (2.116) and from the formula (2.113) we get

$$\begin{aligned}
\langle n_f, p, j, -j+1 | \alpha_+ | n_l, -p, j, -j \rangle &= \frac{2ip}{\sqrt{2j}(2j+1)(2j+2)N_l N_f} \int dr r^2 \times \\
&\left\{ (2j+1) \left[|\Gamma| + \frac{1}{2} \right] A_f^p A_l^{-p} R_{n_f, |\Gamma|-1} R_{n_l, |\Gamma|-1} + \right. \\
&\quad + pZ\alpha \left[-A_f^p B_l R_{n_f, |\Gamma|-1} R_{n_l, |\Gamma|} + B_f A_l^p R_{n_f, |\Gamma|} R_{n_l, |\Gamma|-1} \right] + \\
&\quad \left. + (2j+1) \left[|\Gamma| - \frac{1}{2} \right] B_f B_l R_{n_f, |\Gamma|} R_{n_l, |\Gamma|} \right\}, \quad (2.117)
\end{aligned}$$

We put the results from (2.117) and (2.100) to (2.112) and we get for the reduced matrix element for the E_1 transition in the first order the final relation

$$\begin{aligned}
\langle n_f, p, j || \boldsymbol{\alpha} || n_i, p, j \rangle^{(1)} &= \frac{2}{2j(2j+1)^2(2j+2)N_i N_f} \sum_l \frac{1}{N_l^2} \times \\
&\left(\frac{1}{E_i - E_l} \int dr r^2 \times \left\{ (2j+1) \left[|\Gamma| + \frac{1}{2} \right] A_f^p A_l^{-p} R_{n_f, |\Gamma|-1} R_{n_i, |\Gamma|-1} + \right. \right. \\
&\quad + pZ\alpha \left[-A_f^p B_l R_{n_f, |\Gamma|-1} R_{n_i, |\Gamma|} + B_f A_l^p R_{n_f, |\Gamma|} R_{n_i, |\Gamma|-1} \right] + \\
&\quad \left. \left. + (2j+1) \left[|\Gamma| - \frac{1}{2} \right] B_f B_l R_{n_f, |\Gamma|} R_{n_i, |\Gamma|} \right\} \times \right. \\
&\quad \times \int dr' r'^2 \rho_N(r') \left\{ (2j+1) A_l^{-p} A_i^p R_{n_i, |\Gamma|-1} R_{n_i, |\Gamma|-1} + \right. \\
&\quad \left. + 2pZ\alpha A_l^{-p} B_i R_{n_i, |\Gamma|-1} R_{n_i, |\Gamma|} - 2pZ\alpha B_l A_i^p \times \right. \\
&\quad \left. \left. \times R_{n_i, |\Gamma|} R_{n_i, |\Gamma|-1} - (2j+1) B_l B_i R_{n_i, |\Gamma|} R_{n_i, |\Gamma|} \right\} + \right. \\
&\quad + \frac{1}{E_f - E_l} \int dr r^2 \rho_N(r) \left\{ (2j+1) A_l^{-p} A_f^p R_{n_i, |\Gamma|-1} R_{n_f, |\Gamma|-1} + \right. \\
&\quad \left. + 2pZ\alpha A_l^{-p} B_f R_{n_i, |\Gamma|-1} R_{n_f, |\Gamma|} - 2pZ\alpha B_l A_f^p \times \right. \\
&\quad \left. \left. \times R_{n_i, |\Gamma|} R_{n_f, |\Gamma|-1} - (2j+1) B_l B_f R_{n_i, |\Gamma|} R_{n_f, |\Gamma|} \right\} \times \right. \\
&\quad \times \int dr' r'^2 \times \left\{ (2j+1) \left[|\Gamma| + \frac{1}{2} \right] A_i^p A_l^{-p} R_{n_i, |\Gamma|-1} R_{n_i, |\Gamma|-1} + \right. \\
&\quad \left. + pZ\alpha \left[-A_i^p B_l R_{n_i, |\Gamma|-1} R_{n_i, |\Gamma|} + B_i A_l^p R_{n_i, |\Gamma|} R_{n_i, |\Gamma|-1} \right] + \right. \\
&\quad \left. \left. + (2j+1) \left[|\Gamma| - \frac{1}{2} \right] B_i B_l R_{n_i, |\Gamma|} R_{n_i, |\Gamma|} \right\} \right) \tag{2.118}
\end{aligned}$$

Together with (2.111) we have derived the expression for circular dichroism (2.103). Let us revise the meaning of constants used in (2.111) and (2.118). The constants A , B and N are constants defined by relations (1.54), (1.55) and (1.56). The radial hydrogen function $R_{n, l\Gamma}(r)$ has the form defined in [10], §37. The energy E can be calculated from the expression (1.46).

Conclusion

The aim of this thesis was to calculate the radiative corrections caused by vacuum polarization and to find the expression for the circular dichroism. Firstly, we have derived the formula for energy shift caused by vacuum polarization. Then we have found the equations for Fourier transformation of the vacuum expectation value of charge density and we have suggested two approximative schemes – free particle and hydrogen function expansions. We have used them to derive the Fourier transformation of the vacuum expectation value of charge density in the first order in α and we compared both approximative schemes. Those relations were used to derive Uehling potential and some numerical values of energy shift caused by it were calculated. Then the higher orders contribution were discussed.

In the second chapter we have defined circular dichroism and we have found an expression for it in terms of reduced matrix elements of an arbitrary vector operator. We have analyzed the matrix elements for the case of hydrogen-like atom. Then we have studied the effect of weak interaction that can be seen in atomic spectrum. We have derived the expression for neutral weak nucleonic current and we have shown how it generates the parity violating potential that acts on electrons. Finally, we have used all the results from this section to find the expression for circular dichroism in terms of hydrogen radial functions.

The results achieved in this thesis are thus following:

- We have shown an alternative derivation of the Uehling potential and also how it is contained in the exact result. We have also calculated the energy shift caused by Uehling potential in different levels of approximation, see Tables 1.1 and 1.2.
- The formula (1.146) is important as the check for the calculations which use the partial wave expansion.
- We have derived the formula for circular dichroism in terms of the reduced matrix elements. The angular-spinor degrees of freedom were integrated out, see (2.111) and (2.118).

In the future we are going to continue to work on the topics described in this work. Our plan is following:

- To derive equations for energy shift caused by vacuum polarization effect by means of partial wave expansion and check the results in [21].
- To complete the derivation of circular dichroism for appropriate transitions.

- To calculate numerical values of circular dichroism including self-energy and vacuum polarization radiative corrections.

Appendix A

Mathematical supplement

A.1 Calculation of some integrals using parabolic coordinates

In order to calculate some integrals, it is convenient to use parabolic coordinates defined by relations

$$\xi = r + z, \quad \eta = r - z \quad \text{and} \quad \phi = \arctan \frac{y}{x} \quad (\text{A.1})$$

or inversely

$$x = \sqrt{\xi\eta} \cos \phi, \quad y = \sqrt{\xi\eta} \sin \phi, \quad z = \frac{1}{2}(\xi - \eta)$$
$$\text{and} \quad r = \sqrt{x^2 + y^2 + z^2} = \frac{1}{2}(\xi + \eta) \quad (\text{A.2})$$

with element of volume $dV = d^3\mathbf{r} = \frac{1}{4}(\xi + \eta) d\xi d\eta d\phi$.

In the integrals K , K' and L defined in equations (1.82), (1.89) and (1.96) we integrate over $d^3\mathbf{r}$, so vectors \mathbf{k} and \mathbf{k}_e are parameters. We can choose an arbitrary direction of coordinate axes. In order to keep formulas as easy as possible we set the z -axis in the same direction as vector \mathbf{k}_e and the x -axis in the plane defined by vectors \mathbf{k} and \mathbf{k}_e :

$$\mathbf{r} = (x, y, z), \quad (\text{A.3})$$

$$\mathbf{k}_e = (0, 0, |\mathbf{k}_e|), \quad (\text{A.4})$$

$$\mathbf{k} = (\omega \sin \theta, 0, \omega \cos \theta), \quad (\text{A.5})$$

where θ is angle between vectors \mathbf{k} and \mathbf{k}_e . Expressions (A.3) – (A.5) give

$$\mathbf{k}_e \cdot \mathbf{k} = |\mathbf{k}_e| \omega \cos \theta, \quad (\text{A.6})$$

$$\mathbf{k} \cdot \mathbf{r} = \omega x \sin \theta + \omega z \cos \theta. \quad (\text{A.7})$$

A.1.1 Integral K

After substitution to parabolic coordinates we get for the integral (1.82)

$$\begin{aligned}
K &= \int_0^\infty d\xi \int_0^\infty d\eta \int_0^{2\pi} d\phi \frac{1}{4} (\xi + \eta) e^{-i(\omega \cos \theta \frac{\xi - \eta}{2} + \omega \sin \theta \sqrt{\xi \eta} \cos \phi)} \times \\
&\quad \times F(-a, 1, i|\mathbf{k}_e|\eta) F(a, 1, -i|\mathbf{k}_e|\eta) = \\
&= -\frac{\partial}{\partial \lambda} \int_0^\infty d\xi \int_0^\infty d\eta \int_0^{2\pi} d\phi \frac{1}{4} e^{-\lambda(\xi + \eta)} e^{-i(\omega \cos \theta \frac{\xi - \eta}{2} + \omega \sin \theta \sqrt{\xi \eta} \cos \phi)} \times \\
&\quad \times F(-a, 1, i|\mathbf{k}_e|\eta) F(a, 1, -i|\mathbf{k}_e|\eta) \Big|_{\lambda=0}
\end{aligned}$$

Now we make another substitution defined by formulas

$$u = \sqrt{\xi} \cos \phi, \quad v = \sqrt{\xi} \sin \phi, \quad \text{which gives} \quad du dv = \frac{1}{2} d\phi d\xi \quad (\text{A.8})$$

and then we get

$$\begin{aligned}
K &= -\frac{\partial}{\partial \lambda} \int_{-\infty}^\infty du \int_{-\infty}^\infty dv \int_0^\infty d\eta \frac{1}{2} e^{-\lambda(u^2 + v^2 + \eta)} e^{-i(\omega \cos \theta \frac{u^2 + v^2 - \eta}{2} + \omega \sin \theta \sqrt{\eta} u)} \times \\
&\quad \times F(-a, 1, i|\mathbf{k}_e|\eta) F(a, 1, -i|\mathbf{k}_e|\eta) \Big|_{\lambda=0} = \\
&= -\frac{1}{2} \frac{\partial}{\partial \lambda} \int_0^\infty d\eta e^{-(\lambda - \frac{1}{2}i\omega \cos \theta)\eta} F(-a, 1, i|\mathbf{k}_e|\eta) F(a, 1, -i|\mathbf{k}_e|\eta) \times \\
&\quad \times \underbrace{\int_{-\infty}^\infty dv e^{-\overbrace{(\lambda + \frac{1}{2}i\omega \cos \theta)}^{\alpha} v^2}}_{= \int_{-\infty}^\infty dv e^{-\alpha v^2} = \sqrt{\frac{\pi}{\alpha}}} \int_{-\infty}^\infty du e^{-\overbrace{(\lambda + \frac{1}{2}i\omega \cos \theta)}^{\alpha} u^2 - \overbrace{i\omega \sin \theta \sqrt{\eta}}^{\beta} u}}_{= \int_{-\infty}^\infty du e^{-\alpha(u + \frac{\beta}{2\alpha})^2} e^{\frac{\beta^2}{4\alpha}} = \sqrt{\frac{\pi}{\alpha}} e^{\frac{\beta^2}{4\alpha}}} \Big|_{\lambda=0} = \\
&= -\frac{1}{2} \frac{\partial}{\partial \lambda} \int_0^\infty d\eta \frac{\pi}{\lambda + \frac{1}{2}i\omega \cos \theta} e^{-\left(\lambda - \frac{1}{2}i\omega \cos \theta + \frac{\omega^2 \sin^2 \theta}{4\lambda + 2i\omega \cos \theta}\right)\eta} \times \\
&\quad \times F(-a, 1, i|\mathbf{k}_e|\eta) F(a, 1, -i|\mathbf{k}_e|\eta) \Big|_{\lambda=0}.
\end{aligned}$$

Let us simplify the argument of the exponential and denote it as Λ , so

$$\begin{aligned}
\Lambda &= \lambda - \frac{1}{2}i\omega \cos \theta + \frac{\omega^2 \sin^2 \theta}{4\lambda + 2i\omega \cos \theta} = \\
&= \frac{-i\omega \cos \theta(2\lambda + i\omega \cos \theta) + \lambda(4\lambda + 2i\omega \cos \theta) + \omega^2 \sin^2 \theta}{4\lambda + 2i\omega \cos \theta} = \\
&= \frac{4\lambda^2 + \omega^2 \cos^2 \theta + \omega^2 \sin^2 \theta}{4\lambda + 2i\omega \cos \theta} = \frac{4\lambda^2 + \omega^2}{4\lambda + 2i\omega \cos \theta}. \quad (\text{A.9})
\end{aligned}$$

This gives us the final expression for the integral K

$$K = -\frac{\partial}{\partial \lambda} \int_0^\infty d\eta \frac{\pi}{2\lambda + i\omega \cos \theta} e^{-\Lambda \eta} F(a, 1, i|\mathbf{k}_e|\eta) F(-a, 1, -i|\mathbf{k}_e|\eta) \Big|_{\lambda=0}. \quad (\text{A.10})$$

The integrals of the form (A.10) can be integrated as follows (see [10], Mathematica Appendix §f)

$$\begin{aligned} \int_0^\infty dz e^{-\Lambda z} F(\alpha, \gamma, cz) F(\alpha', \gamma, c'z) &= \\ &= \Gamma(\gamma) \Lambda^{\alpha+\alpha'-\gamma} (\Lambda - c)^{-\alpha} (\Lambda - c')^{-\alpha'} F\left(\alpha, \alpha', \gamma, \frac{cc'}{(\Lambda - c)(\Lambda - c')}\right), \end{aligned} \quad (\text{A.11})$$

where $F(a, b, c, z)$ is the hypergeometric function. Using this formula we get

$$\begin{aligned} K &= -\frac{\partial}{\partial \lambda} \frac{\pi}{2\lambda + i\omega \cos \theta} \Gamma(1) \Lambda^{-1} (\Lambda - i|\mathbf{k}_e|)^a (\Lambda + i|\mathbf{k}_e|)^{-a} \times \\ &\quad \times F\left(-a, a, 1, \frac{\mathbf{k}_e^2}{(\Lambda - i|\mathbf{k}_e|)(\Lambda + i|\mathbf{k}_e|)}\right) \Big|_{\lambda=0} = \\ &= -\frac{\partial}{\partial \lambda} \frac{\pi}{2\lambda + i\omega \cos \theta} \Lambda^{-1} \left(\frac{\Lambda - i|\mathbf{k}_e|}{\Lambda + i|\mathbf{k}_e|}\right)^a F\left(-a, a, 1, \frac{\mathbf{k}_e^2}{\Lambda^2 + \mathbf{k}_e^2}\right) \Big|_{\lambda=0} \end{aligned} \quad (\text{A.12})$$

Using equations

$$-\frac{\partial}{\partial \lambda} \frac{\pi}{2\lambda + i\omega \cos \theta} \Big|_{\lambda=0} = -\frac{2\pi}{\omega^2 \cos^2 \theta}, \quad (\text{A.13})$$

$$-\frac{\partial}{\partial \lambda} \Lambda^{-1} \Big|_{\lambda=0} = -\frac{4}{\omega^2}, \quad (\text{A.14})$$

$$-\frac{\partial}{\partial \lambda} \left(\frac{\Lambda - i|\mathbf{k}_e|}{\Lambda + i|\mathbf{k}_e|}\right)^a \Big|_{\lambda=0} = \frac{8ai|\mathbf{k}_e|}{4\mathbf{k}_e^2 \cos^2 \theta - \omega^2} \left(\frac{\omega + 2|\mathbf{k}_e| \cos \theta}{\omega - 2|\mathbf{k}_e| \cos \theta}\right)^a, \quad (\text{A.15})$$

$$\begin{aligned} -\frac{\partial}{\partial \lambda} F\left(-a, a, 1, \frac{\mathbf{k}_e^2}{\Lambda^2 + \mathbf{k}_e^2}\right) \Big|_{\lambda=0} &= -a^2 F\left(-a + 1, a + 1, 2, \frac{4\mathbf{k}_e^2 \cos^2 \theta}{4\mathbf{k}_e^2 \cos^2 \theta - \omega^2}\right) \times \\ &\quad \times \frac{16i\omega \mathbf{k}_e^2 \cos \theta}{(4\mathbf{k}_e^2 \cos^2 \theta - \omega^2)^2}, \end{aligned} \quad (\text{A.16})$$

we get from equation (A.12) the final expression

$$\begin{aligned}
K &= -\frac{4\pi i}{\omega^3 \cos \theta} \left(\frac{\omega + 2|\mathbf{k}_e| \cos \theta}{\omega - 2|\mathbf{k}_e| \cos \theta} \right)^a F \left(-a, a, 1, \frac{4\mathbf{k}_e^2 \cos^2 \theta}{4\mathbf{k}_e^2 \cos^2 \theta - \omega^2} \right) + \\
&\quad + \frac{4\pi i}{\omega^3 \cos \theta} \left(\frac{\omega + 2|\mathbf{k}_e| \cos \theta}{\omega - 2|\mathbf{k}_e| \cos \theta} \right)^a F \left(-a, a, 1, \frac{4\mathbf{k}_e^2 \cos^2 \theta}{4\mathbf{k}_e^2 \cos^2 \theta - \omega^2} \right) - \\
&\quad - \frac{\pi}{i\omega \cos \theta} \frac{2i \cos \theta}{\omega} \frac{8ai|\mathbf{k}_e|}{4\mathbf{k}_e^2 \cos^2 \theta - \omega^2} \left(\frac{\omega + 2|\mathbf{k}_e| \cos \theta}{\omega - 2|\mathbf{k}_e| \cos \theta} \right)^a \times \\
&\quad \times F \left(-a, a, 1, \frac{4\mathbf{k}_e^2 \cos^2 \theta}{4\mathbf{k}_e^2 \cos^2 \theta - \omega^2} \right) - \\
&\quad - \frac{\pi}{i\omega \cos \theta} \frac{2i \cos \theta}{\omega} \left(\frac{\omega + 2|\mathbf{k}_e| \cos \theta}{\omega - 2|\mathbf{k}_e| \cos \theta} \right)^a \frac{16i\omega \mathbf{k}_e^2 \cos \theta}{(4\mathbf{k}_e^2 \cos^2 \theta - \omega^2)^2} \times \\
&\quad \times a^2 F \left(-a + 1, a + 1, 2, \frac{4\mathbf{k}_e^2 \cos^2 \theta}{4\mathbf{k}_e^2 \cos^2 \theta - \omega^2} \right) = \\
&= a \frac{16i\pi |\mathbf{k}_e|}{\omega^2 (4\mathbf{k}_e^2 \cos^2 \theta - \omega^2)} \left(\frac{\omega + 2|\mathbf{k}_e| \cos \theta}{\omega - 2|\mathbf{k}_e| \cos \theta} \right)^a F \left(-a, a, 1, \frac{4\mathbf{k}_e^2 \cos^2 \theta}{4\mathbf{k}_e^2 \cos^2 \theta - \omega^2} \right) - \\
&\quad - a^2 \frac{32i\pi \mathbf{k}_e^2 \cos \theta}{k (4\mathbf{k}_e^2 \cos^2 \theta - \omega^2)^2} \left(\frac{\omega + 2|\mathbf{k}_e| \cos \theta}{\omega - 2|\mathbf{k}_e| \cos \theta} \right)^a \times \\
&\quad \times F \left(-a + 1, a + 1, 2, \frac{4\mathbf{k}_e^2 \cos^2 \theta}{4\mathbf{k}_e^2 \cos^2 \theta - \omega^2} \right).
\end{aligned}$$

A.1.2 Integral K'

Calculation of the integral K' (1.89) is practically identical to calculation of the integral K , except we do not have to differentiate

$$\begin{aligned}
K &= \frac{1}{2} \int_0^\infty d\xi \int_0^\infty d\eta \int_0^{2\pi} d\phi e^{-i(\omega \cos \theta \frac{\xi - \theta}{2} + \omega \sin \theta \sqrt{\xi \eta} \cos \phi)} \times \\
&\quad \times F(-a, 1, i|\mathbf{k}_e|\eta) F(a, 1, -i|\mathbf{k}_e|\eta) = \\
&= \frac{4\pi}{\omega^2} \left(\frac{\omega + 2|\mathbf{k}_e| \cos \theta}{\omega - 2|\mathbf{k}_e| \cos \theta} \right)^a F \left(-a, a, 1, \frac{4\mathbf{k}_e^2 \cos^2 \theta}{4\mathbf{k}_e^2 \cos^2 \theta - \omega^2} \right).
\end{aligned}$$

A.1.3 Integral L

When calculating the integral L (1.96) it is again useful to use parabolic coordinates. It is clear from (A.1) that the Laplacian operator has the form

$$\nabla^2 = \frac{4}{\xi + \eta} \left[\frac{\partial}{\partial \xi} \left(\xi \frac{\partial}{\partial \xi} \right) + \frac{\partial}{\partial \eta} \left(\eta \frac{\partial}{\partial \eta} \right) \right] + \frac{1}{\eta \xi} \frac{\partial^2}{\partial \phi^2}. \quad (\text{A.17})$$

Only differentiation with respect to η does not give zero, because the Laplacian operator acts on the function depending only on the coordinate η . After substi-

tution to parabolic coordinates we get

$$\begin{aligned}
L &= \int_0^\infty d\xi \int_0^\infty d\eta \int_0^{2\pi} d\phi \frac{1}{4} (\xi + \theta) e^{-i(\omega \cos \theta \frac{\xi - \theta}{2} + \omega \sin \theta \sqrt{\xi \eta} \cos \phi)} \times \\
&\quad \times \frac{4}{\xi + \eta} \frac{\partial}{\partial \eta} \left(\eta \frac{\partial}{\partial \eta} [F(-a, 1, i|\mathbf{k}_e|\eta) F(a, 1, -i|\mathbf{k}_e|\eta)] \right) = \\
&= \int_0^\infty d\xi \int_0^\infty d\eta \int_0^{2\pi} d\phi e^{-i(\omega \cos \theta \frac{\xi - \theta}{2} + \omega \sin \theta \sqrt{\xi \eta} \cos \phi)} \times \\
&\quad \times \frac{\partial}{\partial \eta} \left(\eta \frac{\partial}{\partial \eta} [F(-a, 1, i|\mathbf{k}_e|\eta) F(a, 1, -i|\mathbf{k}_e|\eta)] \right)
\end{aligned}$$

Next we use substitution (A.8)

$$\begin{aligned}
L &= \int_{-\infty}^\infty du \int_{-\infty}^\infty dv \int_0^\infty d\eta 2e^{-i(\omega \cos \theta \frac{u^2 + v^2 - \theta}{2} + \omega \sin \theta \sqrt{\eta} u)} \times \\
&\quad \times \frac{\partial}{\partial \eta} \left(\eta \frac{\partial}{\partial \eta} [F(-a, 1, i|\mathbf{k}_e|\eta) F(a, 1, -i|\mathbf{k}_e|\eta)] \right) = \\
&= \int_0^\infty d\eta \frac{4\pi}{i\omega \cos \theta} e^{-\frac{\omega}{2i \cos \theta} \eta} \frac{\partial}{\partial \eta} \left(\eta \frac{\partial}{\partial \eta} [F(-a, 1, i|\mathbf{k}_e|\eta) F(a, 1, -i|\mathbf{k}_e|\eta)] \right) \quad (\text{A.18})
\end{aligned}$$

Before we continue let us simplify the expression from the equation (A.18) using formula for confluent hypergeometric functions

$$zF(a+1, b+1, z) = b[F(a+1, b, z) - F(a, b, z)], \quad (\text{A.19})$$

so we can write

$$\begin{aligned}
&\eta \frac{\partial}{\partial \eta} [F(-a, 1, i|\mathbf{k}_e|\eta) F(a, 1, -i|\mathbf{k}_e|\eta)] = \\
&= \eta [-aF(-a+1, 2, i|\mathbf{k}_e|\eta) i|\mathbf{k}_e| F(a, 1, -i|\mathbf{k}_e|\eta) + \\
&\quad + aF(-a, 1, i|\mathbf{k}_e|\eta) F(a+1, 2, -i|\mathbf{k}_e|\eta) (-i|\mathbf{k}_e|)] = \\
&= a[-i|\mathbf{k}_e|\eta F(-a+1, 2, i|\mathbf{k}_e|\eta) F(a, 1, -i|\mathbf{k}_e|\eta) + \\
&\quad + F(-a, 1, i|\mathbf{k}_e|\eta) (-i|\mathbf{k}_e|\eta) F(a+1, 2, -i|\mathbf{k}_e|\eta)] = \\
&= a\{-F(-a+1, 1, i|\mathbf{k}_e|\eta) + F(-a, 1, i|\mathbf{k}_e|\eta)\} F(a, 1, -i|\mathbf{k}_e|\eta) + \\
&\quad + F(-a, 1, i|\mathbf{k}_e|\eta) [F(a+1, 1, -i|\mathbf{k}_e|\eta) - F(a, 1, -i|\mathbf{k}_e|\eta)] = \\
&= -a[F(-a+1, 1, i|\mathbf{k}_e|\eta) F(a, 1, -i|\mathbf{k}_e|\eta) - \\
&\quad - F(-a, 1, i|\mathbf{k}_e|\eta) F(a+1, 1, -i|\mathbf{k}_e|\eta)].
\end{aligned}$$

To eliminate the other derivative we use integration by parts

$$\begin{aligned}
L &= \frac{-4\pi a}{i\omega \cos \theta} \int_0^\infty d\eta e^{\frac{\omega i}{2 \cos \theta} \eta} \frac{\partial}{\partial \eta} [F(a+1, 1, i|\mathbf{k}_e|\eta) F(-a, 1, -i|\mathbf{k}_e|\eta) - \\
&\quad - F(a, 1, i|\mathbf{k}_e|\eta) F(-a+1, 1, -i|\mathbf{k}_e|\eta)] = \\
&= \underbrace{\left[\frac{-4\pi a}{i\omega \cos \theta} e^{\frac{\omega i}{2 \cos \theta} \eta} [F(a+1, 1, i|\mathbf{k}_e|\eta) F(-a, 1, -i|\mathbf{k}_e|\eta) - \right.}_{=A} \\
&\quad \left. - F(a, 1, i|\mathbf{k}_e|\eta) F(-a+1, 1, -i|\mathbf{k}_e|\eta)] \right]_0^\infty} + \\
&+ \frac{4\pi a}{i\omega \cos \theta} \frac{\omega i}{2 \cos \theta} \int_0^\infty d\eta e^{-\frac{\omega i}{2 \cos \theta} \eta} [F(a+1, 1, i|\mathbf{k}_e|\eta) F(-a, 1, -i|\mathbf{k}_e|\eta) - \\
&\quad - F(a, 1, i|\mathbf{k}_e|\eta) F(-a+1, 1, -i|\mathbf{k}_e|\eta)] = \\
&= A + \frac{2\pi a}{\cos^2 \theta} \int_0^\infty d\eta e^{-\frac{\omega}{2i \cos \theta} \eta} [F(a+1, 1, i|\mathbf{k}_e|\eta) F(-a, 1, -i|\mathbf{k}_e|\eta) - \\
&\quad - F(a, 1, i|\mathbf{k}_e|\eta) F(-a+1, 1, -i|\mathbf{k}_e|\eta)]. \tag{A.20}
\end{aligned}$$

To calculate the integral over η we again use the formula (A.11)

$$\begin{aligned}
L &= A - \frac{2\pi a}{\cos^2 \theta} \Gamma(1) \left(\frac{\omega}{2i \cos \theta} \right)^0 \left[\left(\frac{\omega}{2i \cos \theta} - i|\mathbf{k}_e| \right)^{a-1} \left(\frac{\omega}{2i \cos \theta} + i|\mathbf{k}_e| \right)^{-a} \times \right. \\
&\quad \times F \left(-a+1, a, 1, \frac{\mathbf{k}_e^2}{\left(\frac{\omega}{2i \cos \theta} - i|\mathbf{k}_e| \right) \left(\frac{\omega}{2i \cos \theta} + i|\mathbf{k}_e| \right)} \right) - \\
&\quad - \left(\frac{\omega}{2i \cos \theta} - i|\mathbf{k}_e| \right)^a \left(\frac{\omega}{2i \cos \theta} + i|\mathbf{k}_e| \right)^{-a-1} \times \\
&\quad \left. \times F \left(-a, a+1, 1, \frac{\mathbf{k}_e^2}{\left(\frac{\omega}{2i \cos \theta} - i|\mathbf{k}_e| \right) \left(\frac{\omega}{2i \cos \theta} + i|\mathbf{k}_e| \right)} \right) \right] = \\
&= A - \frac{2\pi a}{\cos^2 \theta} \left(\frac{\omega + 2|\mathbf{k}_e| \cos \theta}{\omega - 2|\mathbf{k}_e| \cos \theta} \right)^a \left[\left(\frac{\omega + 2|\mathbf{k}_e| \cos \theta}{2i \cos \theta} \right)^{-1} \times \right. \\
&\quad \times F \left(-a+1, a, 1, \frac{4\mathbf{k}_e^2 \cos^2 \theta}{4\mathbf{k}_e^2 \cos^2 \theta - \omega^2} \right) - \\
&\quad \left. - \left(\frac{\omega - 2|\mathbf{k}_e| \cos \theta}{2i \cos \theta} \right)^{-1} F \left(-a, a+1, 1, \frac{4\mathbf{k}_e^2 \cos^2 \theta}{4\mathbf{k}_e^2 \cos^2 \theta - \omega^2} \right) \right].
\end{aligned}$$

We want to show, that limit A from equation (A.20) does not play any role in the following calculations.

$$\begin{aligned}
A &= \lim_{\eta \rightarrow \infty} \left[\frac{-4\pi a}{i\omega \cos \theta} e^{\frac{\omega i}{2 \cos \theta} \eta} [F(a+1, 1, i|\mathbf{k}_e|\eta) F(-a, 1, -i|\mathbf{k}_e|\eta) - \right. \\
&\quad \left. - F(a, 1, i|\mathbf{k}_e|\eta) F(-a+1, 1, -i|\mathbf{k}_e|\eta)] - \frac{-4\pi a}{i\omega \cos \theta} e^{\frac{\omega i}{2 \cos \theta} \eta} \cdot (1-1) \right]. \tag{A.21}
\end{aligned}$$

In the next part we will use the substitution

$$z = i|\mathbf{k}_e|\eta. \quad (\text{A.22})$$

According to [10], Mathematical Appendix §d the behaviour of the confluent hypergeometric functions $F(\alpha, \gamma, z)$ for $z \rightarrow \infty$ is as follows

$$\begin{aligned} F(\alpha, \gamma, z) &= \frac{\Gamma(\gamma)}{\Gamma(\gamma - \alpha)}(-z)^{-\alpha}G(\alpha, \alpha - \gamma + 1, -z) + \\ &+ \frac{\Gamma(\gamma)}{\Gamma(\alpha)}e^z z^{\alpha - \gamma}G(\gamma - \alpha, 1 - \alpha, z), \end{aligned} \quad (\text{A.23})$$

where the asymptotic series of the $G(\alpha, \beta, z)$ has the form

$$G(\alpha, \beta, z) = 1 + \frac{\alpha\beta}{1!z} + \frac{\alpha(\alpha + 1)\beta(\beta + 1)}{2!z^2} + \dots \quad (\text{A.24})$$

Using (A.23) we get for the limit A from (A.21) an expression

$$\begin{aligned} A &= \frac{-4\pi a}{i\omega \cos \theta} \lim_{\eta \rightarrow \infty} e^{\frac{\omega i}{2 \cos \theta} \eta} \times \\ &\times \left[\left(\frac{(-z)^{-a-1}}{\Gamma(-a)} G(1+a, 1+a, -z) + \frac{e^z z^a}{\Gamma(1+a)} G(-a, -a, z) \right) \times \right. \\ &\times \left(\frac{z^a}{\Gamma(1+a)} G(-a, -a, z) + \frac{e^{-z} (-z)^{-a-1}}{\Gamma(-a)} G(1+a, 1+a, -z) \right) - \\ &- \left(\frac{(-z)^{-a}}{\Gamma(1-a)} G(a, a, -z) + \frac{e^z z^{a-1}}{\Gamma(a)} G(1-a, 1-a, z) \right) \times \\ &\left. \times \left(\frac{z^{a-1}}{\Gamma(a)} G(1-a, 1-a, z) + \frac{e^{-z} (-z)^{-a}}{\Gamma(1-a)} G(a, a, -z) \right) \right] \end{aligned} \quad (\text{A.25})$$

In the equation (A.25) all the terms containing z^{-n} for $n \geq 1$ are zero, because $\lim_{\eta \rightarrow \infty} \eta^{-n} = 0$ for $n \geq 1$. Therefore, after using asymptotic series (A.24) and performing limit to zero terms, we get

$$A = \frac{-4\pi a}{i\omega \cos \theta} \lim_{\eta \rightarrow \infty} e^{\frac{\omega i}{2 \cos \theta} \eta} \left(\frac{e^z z^{2a}}{\Gamma^2(1+a)} - \frac{e^{-z} z^{-2a}}{\Gamma^2(1-a)} \right) \quad (\text{A.26})$$

The limit A from equation (A.26) is not zero. But it has the physical meaning as a part extracted from J_2 (1.97) integrated over vector \mathbf{k}_e . The integration over angle θ will make the expression easier

$$\begin{aligned} \int d^3\mathbf{k}_e \frac{A}{E^2 - m^2 - \mathbf{k}_e^2} &= \int_0^\infty d|\mathbf{k}_e| \int_0^\pi d\theta \int_0^{2\pi} d\varphi \frac{\mathbf{k}_e^2 \sin \theta}{E^2 - m^2 - \mathbf{k}_e^2} \frac{-4\pi a}{i\omega \cos \theta} \lim_{\eta \rightarrow \infty} e^{\frac{\omega i}{2 \cos \theta} \eta} \times \\ &\times \left(\frac{e^z z^{2a}}{\Gamma^2(1+a)} - \frac{e^{-z} z^{-2a}}{\Gamma^2(1-a)} \right) = \int_0^\infty d|\mathbf{k}_e| \frac{-8\pi^2 \mathbf{k}_e^2 a}{\omega(E^2 - m^2 - \mathbf{k}_e^2)} \times \\ &\times \lim_{\eta \rightarrow \infty} \left[\pi - 2\text{Si}\left(\frac{\omega\eta}{2}\right) \right] \left(\frac{e^z z^{2a}}{\Gamma^2(1+a)} - \frac{e^{-z} z^{-2a}}{\Gamma^2(1-a)} \right), \end{aligned} \quad (\text{A.27})$$

where $\text{Si}(x)$ is defined as follows

$$\text{Si}(x) = \int_0^x dt \frac{\sin(t)}{t}. \quad (\text{A.28})$$

We can turn our attention from the general point of view to expansion for $a \rightarrow 0$. We thus get

$$\Gamma^{-2}(1+a) = 1 + 2\gamma a + \left(2\gamma^2 - \frac{\pi^2}{6}\right)a^2 + O(a^3), \quad (\text{A.29})$$

$$z^{2a} = 1 + 2a \ln z + 2a^2 \ln^2 z + O(a^3), \quad (\text{A.30})$$

where $\gamma \doteq 0,5772$ is the Euler-Mascheroni constant. Using (A.29) and (A.30) we can write the limit A as a series in a

$$\begin{aligned} \int d^3\mathbf{k}_e \frac{A}{E^2 - m^2 - \mathbf{k}_e^2} &= \int_0^\infty d|\mathbf{k}_e| \frac{\mathbf{k}_e^2}{E^2 - m^2 - \mathbf{k}_e^2} \sum_{n=1}^\infty a^n \lim_{\eta \rightarrow \infty} \left[\pi - 2\text{SI}\left(\frac{\omega\eta}{2}\right) \right] \times \\ &\quad \times \sum_{k=0}^{n-1} (B_l \sin |z| + C_l \cos |z|) \ln^k z, \quad (\text{A.31}) \end{aligned}$$

where B_l and C_l are constants. For any finite n it holds

$$\lim_{\eta \rightarrow \infty} \left[\pi - 2\text{SI}\left(\frac{\omega\eta}{2}\right) \right] (B_l \sin |\mathbf{k}_e|\eta + C_l \cos |\mathbf{k}_e|\eta) \ln^l i|\mathbf{k}_e|\eta = 0. \quad (\text{A.32})$$

We have therefore showed that the calculation of energy shift in any finite order of a (and therefore $Z\alpha$) is not changed by the limit A and we can omit it in the following calculations.

A.2 Expansion of hypergeometric function in a

For functions $F(-a, a, 1, z)$, $F(-a+1, a, 1, z)$, $F(-a, a+1, 1, z)$ we need the expansion to the second order of a and for $F(-a+1, a+1, 2, z)$ to the first order of a .

We write the hypergeometric function $F(-a, a, 1, z)$ in the form

$$F(-a, a, 1, z) = 1 + au_1(z) + a^2u_2(z) + \dots \quad (\text{A.33})$$

The hypergeometric function $F(-a, a, 1, z)$ satisfy the differential equation

$$z(z-1)F''(-a, a, 1, z) + (1-z)F'(-a, a, 1, z) - a^2F(-a, a, 1, z) = 0 \quad (\text{A.34})$$

We also have boundary conditions of the form

$$F(-a, a, 1, 0) = 1 \quad \text{and} \quad F'(-a, a, 1, 0) = -a^2, \quad (\text{A.35})$$

which for functions u_1 and u_2 implies

$$u_1(0) = 0, \quad u_1'(0) = 0 \quad u_2(0) = 0, \quad u_2'(0) = -1. \quad (\text{A.36})$$

If we insert (A.33) into (A.34) we get differential equations for functions $u_1(z)$, $u_2(z)$, etc. We solve them using boundary conditions (A.36) and hereby we get the expansion of the hypergeometric function $F(-a, a, 1, z)$ to the second order in a

$$F(-a, a, 1, z) = 1 - a^2 \operatorname{dilog}(1 - z) + O(a^3). \quad (\text{A.37})$$

Using the same procedure as above we get the expansions of others hypergeometric functions

$$F(1 - a, a, 1, z) = 1 - a \ln(1 - z) + a^2 [2 \ln(1 - z) - \operatorname{dilog}(1 - z)] + O(a^3), \quad (\text{A.38})$$

$$F(-a, 1 + a, 1, z) = 1 + a \ln(1 - z) + a^2 [2 \ln(1 - z) - \operatorname{dilog}(1 - z)] + O(a^3), \quad (\text{A.39})$$

$$F(1 - a, 1 + a, 1, z) = -\frac{1}{z} \ln(1 - z) + O(a^2), \quad (\text{A.40})$$

where the function dilogarithm (or Spence's function) is defined as

$$\operatorname{dilog}(x) = -\int_0^x d\xi \frac{\ln(1 - \xi)}{\xi} = \sum_{k=1}^{\infty} \frac{x^k}{k^2}. \quad (\text{A.41})$$

Bibliography

- [1] Adams B. G., Čížek J. and Paldus J., *Adv. Quant. Chem.*, **19** (1988), 1
- [2] Antognini A., Amaro F. D., Biraben F., Cardoso J. M. R., Covita D. S., Dax A., Dhawan S., Fernandez L. M. P., Giesen A., Graf T. H., Hänsch T. W., Indelicato P., Julien L., Liu Y.-W., Lopes J. A. M., Ludhova L., Monteiro C. M. B., Mulhauser F., Nebel T., Nez F., Rabinowitz P., Santos J. M. F. dos, Schaller L. A., Schuhmann K., Schwob C., Taqqu D., Veloso J. F. C. A. and Pohl R., *Journ. of Phys.: Conf. ser.* **312** (2010), 032002
- [3] Biedenharn L. C., *Phys. Rev.* **126** (1962), 845
- [4] Borie E. and Rinker G. A., *Rev Mod. Phys.* **54** (1982), 67
- [5] Bouchiat M. A. and Bouchiat C., *Rep. Prog. Phys.* **60** (1997), 1351
- [6] COMMINS E. D., P. H. BUCKSBAUM: *Weak interactions of leptons and quarks*, Cambridge University Press, Cambridge, 1983
- [7] Ginges J. S. M., Flambaum V. V., *Phys. Rep.* **397** (2004), 63
- [8] GREINER W., J. REINHARDT: *Quantum Electrodynamics*, Springer-Verlag, Berlin, 2003
- [9] Grotch H. and Yennie D. R., *Rev. Mod. Phys.* **41** (1969), 350
- [10] LANDAU L. D., E. M. LIFSHITZ: *Quantum Mechanics – Non-relativistic Theory*, Pergamon Press, Oxford, 1977
- [11] Mohr P. J., Taylor B. N. and Newell B. D., *Rev. Mod. Phys.*, **84** (2012), 1527
- [12] PATKÓŠ V.: *Radiační korekce k atomovým spektrům*, Master thesis, Charles University, 2010
- [13] Prescott C. Y., Atwood W. B., Cottrell R. L. A., DeStaebler H., Garwin E. L., Gonidec A., Miller R. H., Rochester L. S., Sato T., Sherden D. J., Sinclair C. K., Stein S., Taylor R. E., Clendenin J. E., Hugnes V. W., Sasao N., Schüler K. P., Borghini M. G., Lübelsmeyer K. and Jentschke W., *Phys. Lett. B* **77** (1978), 347

- [14] Prescott C. Y., Atwood W. B., Cottrell R. L. A., DeStaebler H., Garwin E. L., Gonidec A., Miller R. H., Rochester L. S., Sato T., Sherden D. J., Sinclair C. K., Stein S., Taylor R. E., Young C., Clendenin J. E., Hugnes V. W., Sasao N., Schüler K. P., Borghini M. G. and Lübelmeyer K., Phys. Lett. B **84** (1979), 524
- [15] Salpeter E. E. and Bethe H. A., Phys. Rev. **84** (1951), 1232
- [16] SCHWEBER S. S.: *An Introduction to Relativistic Quantum Field Theory*, Harper & Row, New York, 1962
- [17] Soff G. and Mohr P. J., Phys. Rev. A **38** (1988), 5066
- [18] Tsigutkin K., Dounas-Frazer D., Family A., Stalnaker J. E., Yashchuk V. V. and Brudker D., Phys. Rev. Lett. **103** (2009), 071601
- [19] Uehling E. A., Phys. Rev. **48** (1935), 55
- [20] Weinberg S., Phys. Rev. D **5** (1972), 1412
- [21] Wichmann E. H. and Kroll N. M., Phys. Rev. **101** (1956), 843
- [22] Wood C. S., Bennett S. C., Cho D., Masterson B. P., Roberts J. L., Tanner C. E. and Wiemann C. E., Science, **275** (1997), 1759
- [23] Zamastil J.: *Kvantová teorie*, lecture notes, to be published
- [24] Zamastil J., Ann. of Phys. **327** (2012), 297