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Ultrasoft Contribution to the Positronium Hyperfine Splitting

by

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Abstract

Positronium consists of an electron and positron in a bound state, a purely leptonic system and therefore an excellent test of QED (quantum electrodynamics). The ground state is characterized by two different spin configurations: spin-singlet and spin-triplet states. The difference between the corresponding energy levels is called the *hyperfine splitting*. Currently the discrepancy between theory and experiment is 3.9 standard deviations for this quantity. We are computing the *ultrasoft contribution* to the positronium hyperfine splitting. It represents the time-delayed exchange of a photon with energy of the order of the binding energy between the electron and positron. The full theoretical expression of the ultrasoft contribution was found using perturbation theory, and expansion of the positronium wavefunction at the origin about the Coulomb approximation. The expression was then evaluated using Mathematica and asymptotic approximations have been made when an exact numerical value could not be computed. The final result increases the discrepancy to 4.3 standard deviations. New experimental results are needed in order to solve the discrepancy.

Contents

List of Figures

List of Tables

1 Introduction

Positronium is a hydrogen-like and lightest known atom consisting of an electron and a positron, that is, an anti-electron. They form a bound state which survives long enough for experimentalists to measure the energy levels of such a system. Positronium is a purely leptonic system and therefore it constitutes a very good test of quantum electrodynamics (QED). Due to the smallness of the electron mass the strong and weak interaction effects are negligible and the positronium properties can be calculated perturbatively in QED as an expansion in the fine structure constant $\alpha \approx 1/137$ with very high precision only limited by the complexity of the calculations.

Positronium comes in two different states defined by the spin configuration of the electron and positron. In spin-singlet or *parapositronium* state the total spin S is zero, while in spin-triplet or *orthopositronium* state the total spin $S = 1$. The energy difference E_{HFS} between the triplet and the singlet configurations known as the *hyperfine splitting* is of considerable interest from both theoretical and experimental points of view. The ground state hyperfine splitting is the most precisely measured quantity in positronium spectroscopy [1]. At the same time it is known theoretically up to high orders in α. The experimentally observed quantity is the corresponding transition frequency $\nu = E_{HFS}/h$ where h is the Planck constant. The current status of the theoretical calculation is summarized by the following expression

$$\begin{aligned}\nu^{theo} = \nu_0 \cdot \Bigg\{ & 1 - \frac{\alpha}{\pi}\left(\frac{32}{21} + \frac{6}{7}\log 2\right) + \frac{5}{14}\alpha^2 \log\frac{1}{\alpha} + \left(\frac{\alpha}{2}^2\right) \\ & \cdot \left[\frac{1367}{378} - \frac{5197}{2016}\pi^2 + \left(\frac{6}{7} + \frac{221}{84}\pi^2\right)\log 2 - \frac{159}{56}\,\zeta(3)\right] \\ & - \frac{3}{2}\,\frac{\alpha^3}{\pi}\log^2\frac{1}{\alpha} + \left(\frac{62}{15} - \frac{68}{7}\log 2\right)\,\frac{\alpha^3}{\pi}\log\frac{1}{\alpha} + C\,\frac{\alpha^3}{\pi}\Bigg\} \end{aligned} \tag{1}$$

where

$$\nu_0 = \frac{7}{24\pi}\frac{m_e \alpha^4 c^2}{\hbar} \tag{2}$$

is the leading order result; m_e is the electron/positron mass, e is the electron charge, $\alpha = \frac{e^2}{\hbar c}$, $\hbar$ is the reduced Planck constant and c is the speed of light. The leading order ν_0 was calculated in Ref. [2] and is shown in some detail in Section 4 below. The first order correction was calculated in Ref. [3] and the $\alpha^6 \log(1/\alpha)$ term in Ref. [4, 5]. The $\mathcal{O}(\alpha^6)$ term with no logarithm includes the contribution due to the radiative correction to the Breit potential [6], the three-, two-, and one-photon annihilation contributions [7], the nonannihilation radiative

recoil contribution [8], and the pure recoil correction [9,10]. The $\alpha^7 \log^2(1/\alpha)$ has been calculated in [11]. The last known linear logarithmic third order term has been derived in [1]. The nonlogarithmic coefficient C remains unknown for positronium. In the much simpler case of muonium hyperfine splitting this coefficient is known [12,13] , $C_{\mu^+e^-} \approx 16$. The experimental value of the hyperfine splitting energy is $\nu^{exp} = 203.388\,65(67)\,GHz\,(3.3\,ppm)$ [15, 16], and the theoretical one, to date, is $\nu^{theo} = 203.391\,69(41)\,GHz\,(2.0\,ppm)$ [1, 17]. These numbers are illustrated in Fig.1, from Ref. [18]. The theoretical uncertainty value in Fig.1 reflects the contribution of the unknown coefficient C in Eq.(1) and the corresponding error bars are naively estimated by taking the muonium result for this coefficient.

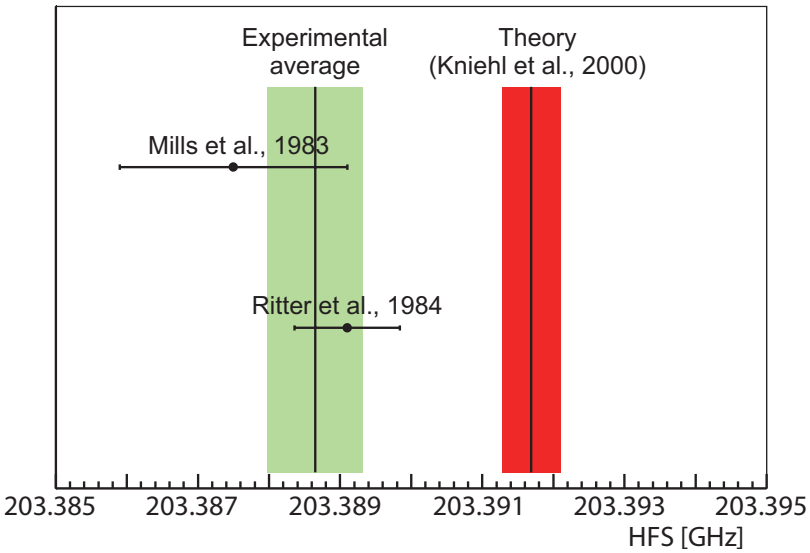

Figure 1: Current experimental and theoretical values of the positronium hyperfine splitting (HFS).

The above experimental and theoretical values differ by 3.9 standard deviations when the experimental average is considered. The deviation cannot be explained within the most popular extensions of the standard model of particle interactions such as supersymmetry because the corresponding effects are strongly suppressed by the tiny ratio of the electron mass to the mass of the supersymmetric particles. Thus, if unambiguously established the discrepancy may be a signal of an exotic "new physics" such as dark or mirror matter, hypothetical super-weakly interacting massless or fractionally charged particles. As a result the problem currently attracts much attention of the experimental community. New experiments are planned and have already been started [18–21] with the perspective of considerable reduction of the experimental errors. However, it is too early to draw any conclusion about a

possible contribution of new physics since the discrepancy can be covered by an abnormally large nonlogarithmic term of order α^3 of order ~ 200. The full calculation of C is one of the most challenging problems in perturbation theory and is beyond the reach of our current techniques. However, some typical contributions can be calculated to get an idea about the scale of the whole correction. A characteristic contribution which usually gives a bulk of the corrections in the perturbative analysis of the nonrelativistic bound states is the so-called ultrasoft correction related to the radiation and absorption of the virtual photons with the energy and momentum of the order of electron binding energy by the positronium state. The purpose of this work is to compute the ultrasoft contribution to the positronium hyperfine splitting.

In Section 2, I will begin by presenting the basic features of positronium. Section 3 consists of an overview of the derivation of the Hamiltonian with emphasis on the spin-spin interaction term relevant to the hyperfine splitting. Then in Section 4 I will present a step-by-step calculation of the leading order hyperfine structure. Section 5 is a discussion of Green's functions and perturbation theory and how one can extract information about the wavefunction correction as well as corrections to the energy levels to the desired order in α. The results, together with an example of the calculation, are presented in Section 6, and concluding remarks in Section 7. The complete expression that has been evaluated can be found in the Appendix.

2 Positronium - The Basics

Positronium is approximately a Coulomb state, but it differs from hydrogen in that the assumption of a stationary heavy nucleus does not hold anymore. Instead the two particles, electron and positron, are now orbiting their common center of mass [22]. The Hamiltonian and the energy levels differ from those of hydrogen in that the mass of the electron and that of the positron is replaced by the reduced mass[1]:

$$m_{red} = \frac{m_1 m_2}{m_1 + m_2} \tag{3}$$

and since the positron and electron have the same mass, $m_1 = m_2 = m$ and Eq.(3) simplifies to

$$m_{red} = \frac{m}{2} \tag{4}$$

Therefore the Hamiltonian of positronium

[1]We will use Gaussian i.e. CGS units in this section.

$$H = \frac{\mathbf{p}^2}{2m_{red}} + V, \tag{5}$$

with $\mathbf{p}$ being momentum and V the potential, in the leading Coulomb approximation reads

$$H_C = \frac{\mathbf{p}^2}{m} - \frac{e^2}{r} \tag{6}$$

where e is the electron charge, r is the distance between the electron and positron and the subscript C stands for *Coulomb*. The eigenstates of the Coulomb Hamiltonian are given by

$$H_C\,\psi_n(r) = E_{n_C}\,\psi_n(r) \tag{7}$$

and are the same as for hydrogen with $m \to m_{red}$:

$$E_{n_C} = -\frac{\alpha^2 mc^2}{4n^2} \tag{8}$$

Here the positronium wavefunction $\psi_n(r) = \psi_{n,l,m}(r,\theta,\phi)$ with $n = 0$, $l = 0$ is similar to the hydrogen wavefunction,

$$\psi_{n,l,m}(r) = \sqrt{\left(\frac{2}{na}\right)^3 \frac{(n-l-1)!}{2n[(n+1)!]^3}}\, e^{-\frac{r}{na}} \left(\frac{2r}{na}\right)^l \left[L^{2l+1}_{n-l-1}\left(\frac{2r}{na}\right)\right] Y^m_l(\theta,\phi) \tag{9}$$

with $m \to m/2$ yielding

$$a = \frac{2\hbar^2}{me^2} \tag{10}$$

which is twice the Bohr radius, and $L^p_{q-p}(x)$ the associated Laguerre polynomials. The spherical harmonics $Y^m_l(\theta,\phi)$ are functions of the Legendre polynomials $P^m_l(\cos\theta)$.

3 Corrections to the Coulomb Approximation

The Coulomb Hamiltonian is not exact and gets various corrections resulting in corrections to the positronium spectrum. The Hamiltonian which describes the dynamics of positronium can be written as

$$H = H_C + \delta H \tag{11}$$

In this section we consider the relativistic correction originating from the expansion of the Lorentz invariant fundamental Dirac equation in powers of $v/c \ll 1$ where v is the electron velocity in the positronium bound state. In order to find this δH we begin by considering the scattering and annihilation amplitudes, which make independent contributions to the interaction operator. The diagrams bellow illustrate these interactions between the electron and positron.

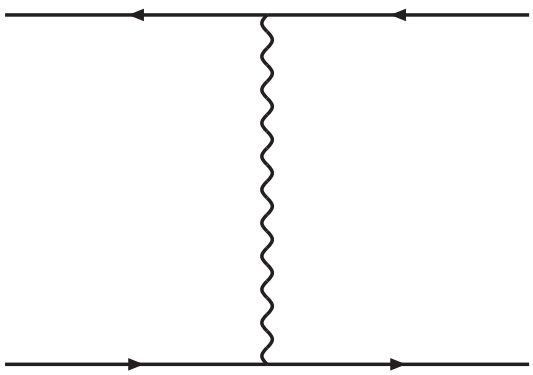

Figure 2a: Feynman diagram of electron-positron scattering. The arrows represent the electron and positron fields, the wavy line represents the photon propagator.

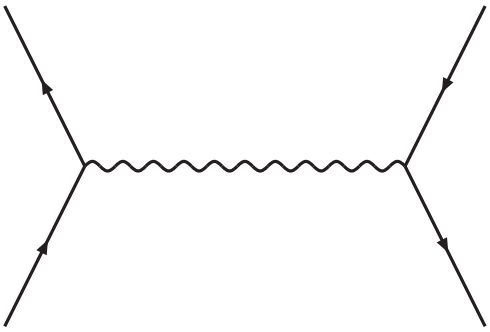

Figure 2b: Feynman diagram of electron-positron annihilation.

3.1 The Scattering Amplitude

In QED, the relativistic expression for the scattering amplitude of two particles with different masses m_1 and m_2 is [23]

$$M_{scat} = \pm e^2 \left(\overline{u_1^{'}}\gamma^{\mu} u_1\right) D_{\mu\nu}(\mathbf{k}) \left(\overline{u_2^{'}}\gamma^{\nu} u_2\right) \tag{12}$$

where e is the particle charge, $\mathbf{k} = \mathbf{p}_1^{'} - \mathbf{p}_1 = \mathbf{p}_2 - \mathbf{p}_2^{'}$ for particle momenta before ($\mathbf{p}_1^{'}$ and $\mathbf{p}_2^{'}$) and after ($\mathbf{p}_1$ and $\mathbf{p}_2$). In our case $m_1 = m_2 = m$. In order to see the meaning of the rest of Eq.(12), consider the Schrodinger equation

$$H\psi = (E - mc^2)\psi \tag{13}$$

with

$$H = \frac{\mathbf{p}^2}{2m} - \frac{\mathbf{p}^4}{8m^3c^2}, \tag{14}$$

which includes the next term in the expansion of the relativistic expression for the kinetic energy. Denote the solution w, the spinor amplitude of the plane wave (2 components). As $v/c \to 0$, the equation becomes the nonrelativistic Schrodinger equation with solution $w^{(0)}$, and in this limit $w \to w^{(0)}$. Now consider the Dirac equation for a spin - 1/2 particle:

$$i\hbar \frac{\partial}{\partial t}\psi(\mathbf{r}, t) = H_D \psi(\mathbf{r}, t) \tag{15}$$

and for a free particle,

$$H_D = c\boldsymbol{\alpha} \cdot \mathbf{p} + \beta mc^2 = \frac{\hbar}{i} c\boldsymbol{\alpha} \cdot \nabla + \beta mc^2 \tag{16}$$

where

$$\beta = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \end{bmatrix}, \quad \alpha^1 = \begin{bmatrix} 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{bmatrix} \tag{17}$$

$$\alpha^2 = \begin{bmatrix} 0 & 0 & 0 & -i \\ 0 & 0 & i & 0 \\ 0 & -i & 0 & 0 \\ i & 0 & 0 & 0 \end{bmatrix}, \quad \alpha^3 = \begin{bmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & -1 \\ 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \end{bmatrix} \tag{18}$$

Denote the solution u, the bispinor amplitude of the free particle (4 components). It can be expressed in terms of the Schrodinger amplitude w as

$$u = \sqrt{2m} \begin{bmatrix} \left(1 - \frac{\mathbf{p}^2}{8m^2c^2}\right) w \\ \\ \left(\frac{\boldsymbol{\sigma}\cdot\mathbf{p}}{2mc}\right) w \end{bmatrix} \tag{19}$$

This is the expression for u in Eq.(12). $\boldsymbol{\sigma}$ and $\boldsymbol{\gamma}$ are the Pauli Sigma and Dirac Gamma matrices, respectively: the Pauli sigma matrices are

$$\sigma^1 = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}, \quad \sigma^2 = \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix}, \quad \sigma^3 = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} \tag{20}$$

and the Dirac gamma matrices are

$$\gamma^0 = \beta, \quad \gamma^1 = \begin{bmatrix} 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \\ 0 & -1 & 0 & 0 \\ -1 & 0 & 0 & 0 \end{bmatrix}, \tag{21}$$

$$\gamma^2 = \begin{bmatrix} 0 & 0 & 0 & -i \\ 0 & 0 & i & 0 \\ 0 & i & 0 & 0 \\ -i & 0 & 0 & 0 \end{bmatrix}, \quad \gamma^3 = \begin{bmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & -1 \\ -1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \end{bmatrix} \tag{22}$$

such that $\gamma^i = \gamma^0\alpha^i$, $i = 1, 2, 3$ and

$$\alpha = \begin{bmatrix} 0 & \sigma \\ \sigma & 0 \end{bmatrix} \tag{23}$$

$D_{\mu\nu}$ is the propagator, and $+/-$ denotes same/opposite charges. Consider same charges for now. Choose the photon propagator in the Coulomb gauge [24]:

$$D_{ik} = \frac{4\pi}{\mathbf{k}^2 - k_0^2 - i0} \left(\delta_{ik} - \frac{\mathbf{k}_1\mathbf{k}_2}{\mathbf{k}^2}\right) \tag{24}$$

Then the scattering amplitude becomes

$$M_{scat} = e^2 \left[\left(\overline{u_1'}\gamma^0 u_1\right)\left(\overline{u_2'}\gamma^0 u_2\right) D_{00} + \left(\overline{u_1'}\gamma^i u_1\right)\left(\overline{u_2'}\gamma^k u_2\right) D_{ik}\right] \tag{25}$$

Note: keep c, use $\hbar = 1$ and put it back in at the end. We are neglecting all terms in v/c and so only the first term survives:

$$M_{scat} = -2m \cdot 2m \left(w_1^{(0)\prime *} w_1^{(0)} \right) \left(w_2^{(0)\prime *} w_2^{(0)} \right) U(\mathbf{k}) \tag{26}$$

where $U(\mathbf{k}) = \frac{4\pi\varepsilon_0}{\mathbf{k}^2}$ is the Fourier transform of the Coulomb potential $U(r) = \frac{e^2}{r}$ and $w_1^{(0)}$, $w_2^{(0)}$ are the two-component spinor amplitudes of the non-relativistic plane waves defined above. Using the expression for u in Eq.(19) we get the following results:

$$\overline{u_1^{'}} \gamma^0 u_1 = 2m w_1^{'*} \left(1 - \frac{\mathbf{k}^2}{8m^2c^2} + \frac{i\sigma \cdot \mathbf{k} \times \mathbf{p}_1}{4m^2c^2} \right) w_1 \tag{27}$$

and

$$\overline{u_1^{'}} \boldsymbol{\gamma} u_1 = \frac{1}{c} w_1^{'*} \left(i\boldsymbol{\sigma} \times \mathbf{p} + 2\mathbf{p}_1 + \mathbf{k} \right) w_1 \tag{28}$$

For u_2 terms, $1 \to 2$ and $\mathbf{k} \to -\mathbf{k}$. Now we can write (neglecting k_0 in D_{ik})

$$M_{scat} = -4m^2 \left[w_1^{'*} w_2^{'*} U_{scat}(\mathbf{p}_1, \mathbf{p}_2, \mathbf{k}) w_1 w_2 \right] \tag{29}$$

with the particle interaction operator, in the momentum representation, being

$$\begin{aligned} U_{scat}(\mathbf{p}_1, \mathbf{p}_2, \mathbf{k}) = 4\pi e^2 \Bigg[& \frac{1}{k^2} - \frac{2}{8m^2c^2} + \frac{(\mathbf{k} \cdot \mathbf{p}_1)(\mathbf{k} \cdot \mathbf{p}_2)}{m^2k^4} - \frac{\mathbf{p}_1 \cdot \mathbf{p}_2}{m^2k^2} + \frac{i\boldsymbol{\sigma}_1 \cdot \mathbf{k} \times \mathbf{p}_1}{4m^2c^2k^2} - \\ & - \frac{i\boldsymbol{\sigma}_1 \cdot \mathbf{k} \times \mathbf{p}_2}{2m^2c^2k^2} - \frac{i\boldsymbol{\sigma}_2 \cdot \mathbf{k} \times \mathbf{p}_2}{4m^2c^2k^2} + \frac{i\boldsymbol{\sigma}_2 \cdot \mathbf{k} \times \mathbf{p}_1}{2m^2c^2k^2} \\ & + \frac{(\boldsymbol{\sigma}_1 \cdot \mathbf{k})(\boldsymbol{\sigma}_2 \cdot \mathbf{k})}{4m^2c^2k^2} - \frac{\boldsymbol{\sigma}_1 \cdot \boldsymbol{\sigma}_2}{4m^2c_2} \Bigg] \end{aligned} \tag{30}$$

with $\boldsymbol{\sigma}_1$ acting on w_1 and $\boldsymbol{\sigma}_2$ on w_2. In the coordinate representation (put $\hbar$ in now), this corresponds to

$$
\begin{aligned}
U_{scat}(\mathbf{p}_1,\mathbf{p}_2,\mathbf{r}) = \frac{e^2}{r} - \frac{\pi e^2\hbar^2}{m^2c^2}\,\delta(\mathbf{r}) - \frac{e^2}{2m^2 2c^2 r}\left[\mathbf{p}_1\cdot\mathbf{p}_2 + \frac{\mathbf{r}\cdot(\mathbf{r}\cdot\mathbf{p}_1)\mathbf{p}_2}{r^2}\right] \\
- \frac{e^2\hbar^2}{4m^2c^2r^3}\,\mathbf{r}\times\mathbf{p}_1\cdot\boldsymbol{\sigma}_1 + \frac{e^2\hbar^2}{4m^2c^2r^3}\,\mathbf{r}\times\mathbf{p}_2\cdot\boldsymbol{\sigma}_2 \\
- \frac{e^2\hbar^2}{2m^2c^2r^3}\,(\mathbf{r}\times\mathbf{p}_1\cdot\boldsymbol{\sigma}_2 - \mathbf{r}\times\mathbf{p}_2\cdot\boldsymbol{\sigma}_1) \\
+ \frac{e^2\hbar^2}{4m^2c^2}\left[\frac{\boldsymbol{\sigma}_1\cdot\boldsymbol{\sigma}_2}{r^3} - 3\,\frac{(\boldsymbol{\sigma}_1\cdot\mathbf{r})(\boldsymbol{\sigma_2}\cdot\mathbf{r})}{r^5} - \frac{8\pi}{3}\,\boldsymbol{\sigma}_1\cdot\boldsymbol{\sigma}_2\,\delta(\mathbf{r})\right]
\end{aligned}
\tag{31}
$$

where $r = |\mathbf{r}|$.

3.2 The Annihilation Amplitude

In Eq.(11) we also need the annihilation term, δH_{ann}. The total amplitude M is the sum of the scattering and annihilation amplitudes:

$$
\begin{aligned}
M &= M_{scat} + M_{ann} \\
&= -e^2\left[\overline{u}(p_-^{'})\gamma^\mu u(p_-)\right] D_{\mu\nu}(p_- - p_-^{'})\left[\overline{u}(-p_+)\gamma^\mu u(-p_+^{'})\right] + \\
&+ e^2\left[\overline{u}(-p_+)\gamma^\mu u(p_-)\right] D_{\mu\nu}(p_- + p_+)\left[\overline{u}(p_-^{'})\gamma^\nu u(-p_+^{'})\right]
\end{aligned}
\tag{32}
$$

The first term will yield the same operator as found above in Section 3.1, but now with a minus sign (positron and electron have opposite charges). For the second term use the photon propagator in the ordinary gauge:

$$
D_{\mu\nu} = \frac{4\pi}{k^2}\,g_{\mu\nu} = \frac{4\pi}{k_0^2 - \mathbf{k}^2}\,g_{\mu\nu} \tag{33}
$$

where

$$
g_{\mu\nu} = \begin{bmatrix} -1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix} \tag{34}
$$

The Coulomb gauge was used for the first term (scattering) because it simplifies the calculation. Since the two terms are gauge independent, it does not matter which gauge is chosen

for the calculation of each. Here $\mathbf{k} = \mathbf{p}_+ + \mathbf{p}_-$ with $+/-$ for positron/electron. In the low velocity limit

$$k_0 = \frac{\omega^2}{c^2} \equiv \frac{(E_+ + E_-)^2}{c^2} \approx 4m^2c^2 \gg (\mathbf{p}_+ + \mathbf{p}_-)^2 \equiv \mathbf{k}^2 \tag{35}$$

so we can write

$$D_{\mu\nu} \approx \frac{\pi}{m^2c^2} g_{\mu\nu} \tag{36}$$

Because this already contains a factor of $1/c^2$, we can take the zero-order approximation in the amplitudes $u(p)$:

$$u(\mathbf{p}_-) = \sqrt{2m} \begin{bmatrix} w_- \\ 0 \end{bmatrix} \tag{37}$$

and

$$u(-\mathbf{p}_+) = \sqrt{2m} \begin{bmatrix} 0 \\ w \end{bmatrix} \tag{38}$$

where w_- and w are 3-component spinors [23]. Using the expressions for u in Eq.(37) and (38) we get the following results:

$$\bar{u}(-\mathbf{p}_+)\gamma^0 u(\mathbf{p}_-) = u^*(-\mathbf{p}_+)u(\mathbf{p}_-) = 0 \tag{39}$$

and

$$\bar{u}(-\mathbf{p}_+)\boldsymbol{\gamma} u(\mathbf{p}_-) = 2m(w^*\boldsymbol{\sigma}w_-) \tag{40}$$

Therefore the second (annihilation) term in M becomes

$$M_{ann} = -e^2 \frac{\pi}{m^2c^2}(2m)^2 (w^*\boldsymbol{\sigma}w_-)(w_-^{'*}\boldsymbol{\sigma}w^{'}) \tag{41}$$

$$M_{ann} = -4m^2 \left\{ w_-^{'*} w_+^{'*} \left[\frac{\pi e^2}{2m^2c^2}(3 + \boldsymbol{\sigma}_+ \cdot \boldsymbol{\sigma}_-) \right] w_- w_+ \right\} \tag{42}$$

with $\boldsymbol{\sigma}_+$ and $\boldsymbol{\sigma}_-$ acting on w_+ and w_-, respectively. From this we can deduce the second term of the interaction operator,

$$U_{ann} = \frac{\pi\hbar^2 e^2}{2m^2c^2} (3 + \boldsymbol{\sigma}_+ \cdot \boldsymbol{\sigma}_-) \, \delta(\mathbf{r}) \tag{43}$$

with $\mathbf{r} = \mathbf{r}_- - \mathbf{r}_+$.

3.3 The Spin-Spin Interaction Hamiltonian

From Sec. 3.1 and 3.2 we see that

$$U_{scat}(\mathbf{p}_1, \mathbf{p}_2, \mathbf{r}) = \frac{e^2}{r} + \delta H_{scat} \tag{44}$$

and

$$U_{ann} = \delta H_{ann} \tag{45}$$

Finally, putting the two terms together in the interaction operator and working in the center of mass frame with $\mathbf{p}_- = -\mathbf{p}_+ \equiv \mathbf{p}$, $\mathbf{p} = -i\hbar\nabla$, we have the total Hamiltonian for positronium described by Eq.(11):

$$H = H_C + \delta H \tag{46}$$

$$H = H_C + H_{scat} + H_{ann} \tag{47}$$

That is,

$$H = H_C + H_{HFS} + ... \tag{48}$$

where we have separated the term of interest: the spin-spin interaction potential given by[2]

$$H_{HFS} = 6\mu_0^2 \frac{1}{r^3} \left\{ \frac{(\mathbf{S}\cdot\mathbf{r})(\mathbf{S}\cdot\mathbf{r})}{r^2} - \frac{1}{3}\mathbf{S}^2 \right\} + 4\pi\mu_0^2 \frac{7}{3} \mathbf{S}^2 \delta(\mathbf{r}) \tag{49}$$

Here $\mu_0 = \frac{e\hbar}{2m}$, the Bohr magneton.

[2]In ordinary units.

4 Calculation of the Leading Order Hyperfine Splitting

The Hamiltonian in Eq.(49) has two eigenfunctions for $n = 1$ corresponding to the spin-triplet ${}_3S_1$ and spin-singlet ${}_1S_0$ configurations. The hyperfine splitting is the difference between the corresponding eigenvalues

$$\begin{aligned} E_{HFS} &= E({}_3S_1) - E({}_1S_0) \\ &= \langle {}_3S_1|H_{HFS}|{}_3S_1\rangle - \langle {}_1S_0|H_{HFS}|{}_1S_0\rangle \\ &= \langle {}_3S_1|H_{HFS}|{}_3S_1\rangle \end{aligned} \tag{50}$$

where the second term vanishes because the total spin is zero. H_{HFS} in Eq. (49) gives the leading order correction to the hyperfine splitting. We are interested in the positronium state with the quantum numbers $n = 1$, $l = 0$. The corresponding wavefunction is angular independent and can be decomposed into the radial and spin parts:

$$\psi = \psi_{1,0,0}(r) \cdot \psi_{spin} \tag{51}$$

with

$$\psi_{1,0,0}(r) = \frac{2}{\sqrt{\pi a^3}} e^{-\frac{r}{a}} \tag{52}$$

and

$$\psi_{spin} = \begin{cases} \left[\begin{array}{c} 1 \\ 0 \end{array}\right]_{e^-} \otimes \left[\begin{array}{c} 1 \\ 0 \end{array}\right]_{e^+} & for\ m_s = 1 \\ \frac{1}{\sqrt{2}} \left(\left[\begin{array}{c} 0 \\ 1 \end{array}\right]_{e^-} \otimes \left[\begin{array}{c} 1 \\ 0 \end{array}\right]_{e^+} + \left[\begin{array}{c} 1 \\ 0 \end{array}\right]_{e^-} \otimes \left[\begin{array}{c} 0 \\ 1 \end{array}\right]_{e^+} \right) & for\ m_s = 0 \\ \left[\begin{array}{c} 0 \\ 1 \end{array}\right]_{e^-} \otimes \left[\begin{array}{c} 0 \\ 1 \end{array}\right]_{e^+} & for\ m_s = -1 \end{cases} \tag{53}$$

where $\otimes$ is the direct product. Because of the spherical symmetry of the coordinate wavefunction with $l = 0$, after averaging over the angles we can replace in the matrix element

$$\frac{(\mathbf{S}\cdot\mathbf{r})(\mathbf{S}\cdot\mathbf{r})}{r^2} \to \frac{1}{3}\mathbf{S}^2 \tag{54}$$

and the first term in Eq.(49) vanishes. The remaining term gives the correction arising from the hyperfine structure:

$$\begin{aligned} E_{HFS} &= \left\langle \psi \left| 4\pi\mu_0^2 \frac{7}{3} \overline{\mathbf{S}}^2 \, \delta(\mathbf{r}) \right| \psi \right\rangle \\ &= \left\langle \psi_{1,0,0}(\mathbf{r}) \cdot \psi_{spin} \left| 4\pi\mu_0^2 \frac{7}{3} \overline{\mathbf{S}}^2 \, \delta(\mathbf{r}) \right| \psi_{1,0,0}(\mathbf{r}) \cdot \psi_{spin} \right\rangle \\ &= 4\pi\mu_0^2 \frac{7}{3} \left\langle \psi_{spin} \left| \overline{\mathbf{S}}^2 \right| \psi_{spin} \right\rangle \, |\psi_{1,0,0}(0)|^2 \end{aligned} \tag{55}$$

where in the last step the delta function integrated over $\psi_{1,0,0}(r)$ gives the square of the wavefunction at the origin. The spin part integrated over ψ_{spin} gives

$$\begin{aligned} \left\langle \psi_{spin} \left| \overline{\mathbf{S}}^2 \right| \psi_{spin} \right\rangle &= \left\langle \psi_{spin} \left| (\boldsymbol{\sigma}_+ + \boldsymbol{\sigma}_-)^2 \right| \psi_{spin} \right\rangle \\ &= S(S+1) \end{aligned} \tag{56}$$

which equals 2 since $S = 1$. The wavefunction at the origin is, from Eq.(52),

$$|\psi_{1,0,0}(0)|^2 = \frac{1}{2\pi} \left(\frac{\alpha mc}{\hbar} \right)^3 \tag{57}$$

So we get for the leading order hyperfine splitting [24]:

$$E_{HFS} = \frac{7}{12} m_e \alpha^4 c^2 \tag{58}$$

which corresponds to the leading order frequency ν_0 in Eq.(1).

5 General Structure of the Ultrasoft Contribution

5.1 Perturbation Theory

From Eq.(55) it can be seen that the hyperfine splitting energy is proportional to the wavefunction amplitude at the origin,

$$E_{HFS} \sim |\psi(0)|^2 \tag{59}$$

Thus, the perturbative corrections to the wavefunction at the origin result in the correction to the hyperfine splitting. Let us first consider the general structure of the perturbation theory for the wave function in the presence of a perturbation δH to the Coulomb Hamiltonian H_C. In this case the Coulomb spectrum and wavefunctions get the corrections

$$E_n = E_{n_C} + \delta E \tag{60}$$

$$\psi(\mathbf{r}) = \psi_C(\mathbf{r}) + \delta\psi(\mathbf{r}) \tag{61}$$

A powerful technique for computing the corrections is based on the Green's function method, indispensable in Perturbation Theory, which allows us to calculate almost anything in physics that can be expanded in a small parameter. In general,

$$(H - E)G(\mathbf{r}^{'}, \mathbf{r}; E) = \delta(\mathbf{r}^{'} - \mathbf{r}) \tag{62}$$

The Green's function that is the solution of Eq.(62) has the spectral representation

$$G(\mathbf{r}^{'}, \mathbf{r}; E) = \sum\!\!\!\!\!\!\int \frac{\psi_n^*(\mathbf{r}^{'})\psi_n(\mathbf{r})}{E_n - E} \tag{63}$$

The sum in Eq.(63) is taken over all discrete states, while the integral is over the continuum states. The ψ_n are the positronium wavefunctions described earlier in Eq.(9), with energies E_n corresponding to the n^{th} eigenstate of the system. The general expression for the expansion of the Green's function is

$$\begin{aligned} G(\mathbf{r}^{'}, \mathbf{r}; E) = G_C(\mathbf{r}^{'}, \mathbf{r}; E) - \int G_C(\mathbf{r}^{'}, \mathbf{r}^{''}; E)\, \delta H(\mathbf{r}^{''})\, G_C(\mathbf{r}^{''}, \mathbf{r}; E)\, d\mathbf{r}^{''} \\ + \int G_C(\mathbf{r}^{'}, \mathbf{r}^{''}; E)\, \delta H(\mathbf{r}^{''})\, G_C(\mathbf{r}^{''}, \mathbf{r}^{'''}; E)\, \delta H(\mathbf{r}^{'''})\, G_C(\mathbf{r}^{'''}, \mathbf{r}; E)\, d\mathbf{r}^{''}\, d\mathbf{r}^{'''} + \ldots \end{aligned} \tag{64}$$

Expanding Eq.(63) in δE and $\delta\psi(\mathbf{r})$ we get

$$\begin{aligned} G(\mathbf{r}^{'}, \mathbf{r}; E) = G_C(\mathbf{r}^{'}, \mathbf{r}; E) + \\ + \left[\sum\!\!\!\!\!\!\int \frac{\psi_{n_C}^*(\mathbf{r}^{'})\delta\psi_n(\mathbf{r}) + \delta\psi_n^*(\mathbf{r}^{'})\psi_{n_C}(\mathbf{r})}{E_{n_C} - E} - \sum\!\!\!\!\!\!\int \frac{\psi_{n_C}^*(\mathbf{r}^{'})\psi_{n_C}(\mathbf{r})}{(E_{n_C} - E)^2}\, \delta E_n \right] + \ldots \end{aligned} \tag{65}$$

where the dots represent higher order poles in $E_{n_C} - E$. The residues of the single and double poles in Eq.(65) determine the corrections to the wavefunction and energy levels,

respectively. Thus by matching the single pole residues of Eqs.(64) and (65) for $\mathbf{r} = \mathbf{r}' = 0$ one gets the correction to the square modulus of the wave function at the origin

$$\delta|\psi_n(0)|^2 = \psi^*_{nC}(0)\delta\psi_{nC}(0) + \delta\psi^*_{nC}(0)\psi_{nC}(0) \tag{66}$$

and hence to the hyperfine splitting. The expression in Eq.(65) above shows the leading order terms. The procedure can be repeated to the desired order in α. Since we are looking for the wavefunction correction, we are interested in the second term - the single pole. In our problem, the double pole giving the corrections to the energy levels has been subtracted.

5.2 The Ultrasoft Contribution

The dynamics of the positronium bound state is governed by several scales [1]: the three-momentum of nonrelativistic electron $|\mathbf{p}| \sim m_e v$ and its energy $E \sim m_e v^2$. In the positronium bound state the electron velocity is proportional to the fine structure constant $v \sim \alpha$ [3]. The three-momentum defines the characteristic size of the bound states - the Bohr radius $a \sim 1/(\alpha m_e)$ while the energy determines the characteristic time scale of bound state oscillations $t \sim 1/(\alpha^2 m_e)$. In QED the radiative corrections to the positronium parameters originate from the emission and absorption of virtual photons. An exchange of a *hard* photon with energy and momentum of order m_e results in an interaction localized in both space and time in comparison to the characteristic scales of positronium. Thus it can be described by a δ-function term in the nonrelativistic Hamiltonian (*e.g.* Eq.(43)). An exchange of a *soft* photon with energy and momentum of order $\alpha\, m_e$ results in an interaction localized in time and in general can be described by an instantaneous spatially non-local potential in the nonrelativistic Hamiltonian (*e.g.* the third term in Eq.(44)). Finally an exchange of an *ultrasoft* photon with energy and momentum of order $\alpha^2 m_e$ results in so-called retardation effects that are considered in this thesis. The concept of separating the contributions of different momentum regions is known as nonrelativistic effective field theory or potential nonrelativistic QED (pNRQED) [25, 26].

The leading order interaction of the ultrasoft photons with the positronium state is described by the standard electric dipole term in the Hamiltonian

$$\delta H_{US} = e\mathbf{E}\cdot\mathbf{r} \tag{67}$$

where e is the electron/positron charge, $\mathbf{E}$ is the electric field and $\mathbf{r}$ is distance between the electron and positron. Now the electric field is, in general,

[3] Through this section we adopt the system of units with $\hbar = c = 1$

$$\mathbf{E} = \partial_0 \mathbf{A} - \nabla A_0 \tag{68}$$

A_0 gives the static potential. Since we are interested in the propagation of dynamical, physical photons, for convenience we are using the Coulomb Gauge

$$\nabla \cdot \mathbf{A}(\mathbf{r}, t) = 0, \qquad A_0 = 0 \tag{69}$$

Therefore the expression for the electric field becomes

$$\mathbf{E} = \partial_0 \mathbf{A} \tag{70}$$

Graphically the ultrasoft exchange is given by the diagram in Fig.3: the positronium state radiates the ultrasoft photon through the dipole interaction, then propagates in the field of the ultrasoft photon for some time and finally absorbs it.

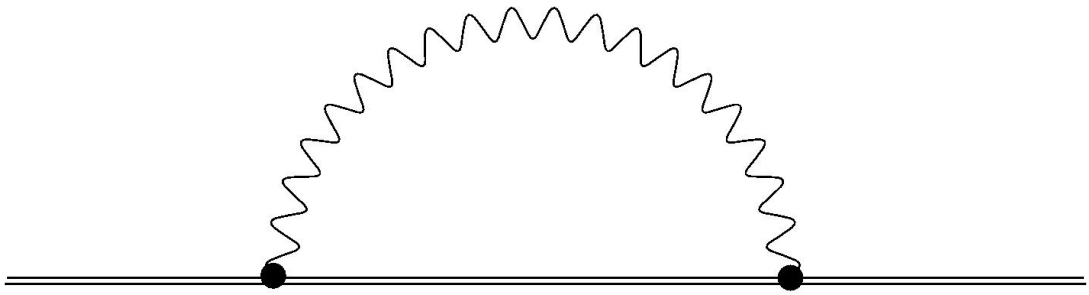

Figure 3: Feynman diagram of the ultrasoft exchange. The double line represents the positronium bound state, the wavy line represents the ultrasoft photon, the vertices represent the dipole interaction

We can now use perturbation theory to compute the corresponding correction to the wavefunction. This can be done by standard generalization of the time independent perturbation theory of the previous section to the time dependent perturbation. Since we are interested in virtual corrections in the absence of the external field the linear term in $\mathbf{A}$ vanishes. The quadratic term after vacuum averaging gives the photon propagator

$$\langle\, T\, \partial_0\, \mathbf{A}_i(\mathbf{r}'', t'')\, \partial_0\, \mathbf{A}_j(\mathbf{r}''', t''')\rangle = i \int \frac{d^4k}{(2\pi)^4} \frac{g_{ij} - \frac{\mathbf{k}_i \mathbf{k}_j}{\mathbf{k}^2}}{k^2 + i\epsilon}\, k_0^2\, e^{ik_0(t''-t''')}\, e^{-i\mathbf{k}(\mathbf{r}''-\mathbf{r}''')} \tag{71}$$

where T stands for the time ordered product. Since for the ultrasoft photon $\mathbf{kr} \ll 1$ we can substitute $e^{i\mathbf{kr}}$ by 1 to the leading order. After substituting the propagator into Eq.(64) and integrating over $t'' - t'''$ one gets the final expression for the correction to the Green's function at the origin

$$\delta G_{US}(0,0;E) = ie^2 \int d^3\mathbf{r} d^3\mathbf{r}^{'} \int \frac{d^4k}{(2\pi)^4} \Bigg[\frac{k_0^2 \mathbf{r}\mathbf{r}^{'} - (\mathbf{r}\mathbf{k})(\mathbf{r}^{'}\mathbf{k})}{k^2 + i\varepsilon} \times$$
$$\times G_C(0,\mathbf{r};E) G_C(\mathbf{r},\mathbf{r}^{'};E-k_0) G_C(\mathbf{r}^{'},0;E) \Bigg] \qquad (72)$$

Note that the argument of the intermediate Green's function is shifted from E to $E - k_0$ which is the result of the time dependent exponential factor in Eq.(71) and simply reflects the energy conservation. With the Green's function correction at hand it is straightforward to get the ultrasoft correction to the wavefunction at the origin. Technically it is convenient to use the following representation for the Coulomb Green's function where the dependence on $\mathbf{r}$ and $\mathbf{r}'$ is factorized:

$$G_C(\mathbf{r},\mathbf{r}',k) = \sum_{l=0}^{\infty} (2l+1) G_l(r,r',k) P_l((\mathbf{r}\mathbf{r}')/rr')$$

$$G_l(r,r',z) = \frac{m_e k}{2\pi} (2kr)^l (2kr')^l e^{-k(r+r')} \sum_{m=0}^{\infty} \frac{L_m^{2l+1}(2kr) L_m^{2l+1}(2kr') m!}{[m+l+1-\alpha m/(4k)](m+2l+1)!} \qquad (73)$$

with m_e the electron mass, $P_l(z)$ the Legendre polynomial and $L_m^{\alpha}(z)$ the associated Laguerre polynomial. Since the dipole interaction is proportional to $\mathbf{r}$ only the $l = 1$ P-wave component of Eq.(73) contributes to the intermediate state Green's function in Eq.(72). The integral over k_0 in Eq.(73) can be taken by residues. After integrating over $\mathbf{r}$ and $\mathbf{r}'$ one finally gets the correction to the wave function in the form of at most three-fold sum of one-parametric integral resulting from the integration over $|\mathbf{k}|$, which is evaluated in the next section.

In our analysis we use the expressions for the ultrasoft corrections to the Green's function obtained for the quarkonium bound state in quantum chromodynamics in Ref. [27]. The structure of the Green's function in QED however is different. In particular the emission of an ultrasoft gluon changes the quark-antiquark pair state to color-octet which does not have bound states since the corresponding potential is repulsive. This does not happen in QED and independent analysis of the corrections is necessary.

5.3 Dimensional Regularization

The above expression for the ultrasoft contribution is formally infinite since the integral over the three-momentum of the ultrasoft gluon is ultraviolet divergent. This spurious divergence reflects the breakdown of the nonrelativistic expressions for the vertices and the Green's

functions in the region of large $|\mathbf{k}|$ where they are not applicable and have to be replaced by the relativistic expressions. Formally one has to impose a cutoff $\alpha^2 m_e \ll \Lambda \ll \alpha m_e$ on the virtual momentum to separate the ultrasoft contribution from the soft and hard one, treat every contribution separately and add them up at the end to the final result where the dependence on the auxiliary cutoff cancels out.

To deal with the spurious divergences we adopt a modern approach based on dimensional regularization [28]. It consists of formal analytical continuation of the divergent integrals to a noninteger number of spatial dimensions $D = 3 - 2\varepsilon$. Then the divergences show up as poles in $1/\varepsilon$ in the physical limit $D \to 3$. It has been shown that in the sum of the contributions of all the momentum regions the poles of different contributions cancel each other out and the correct total result is recovered for $\varepsilon = 0$ [10, 29, 30]. The use of dimensional regularization has a significant advantage over an explicit momentum cutoff since it preserves gauge and Lorentz invariance at the intermediate steps of the calculation.

We consider the ultrasoft contribution separately and subtract the divergent part of the integral according to the $\overline{\text{MS}}$ prescription [31]. This implies that the contributions from the soft and hard contribution have to be treated in the same way.

6 Calculation of the Ultrasoft Contribution

6.1 Overview of the Calculation

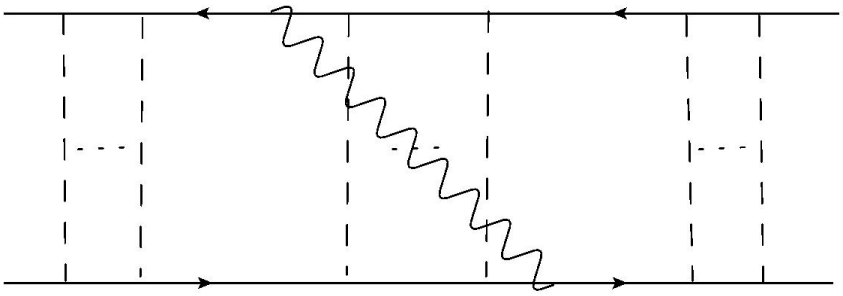

Figure 4a: Feynman diagram of a type I contribution with two or more Coulomb photons inside the ultrasoft exchange. The dots stand for an arbitrary number of Coulomb photons.

The leading ultrasoft contribution is of order $\mathcal{O}(\alpha^3)$. Indeed every dipole interaction is suppressed by the electron velocity $v \sim \alpha$ and the remaining power of α comes explicitly from two electron-photon vertices. Thus the ultrasoft correction to the wave function at the origin can be parametrized as follows

$$|\psi(0)|^2 = |\psi_C(0)|^2 \left(1 + \frac{\alpha^3}{\pi} C_{US}\right) \tag{74}$$

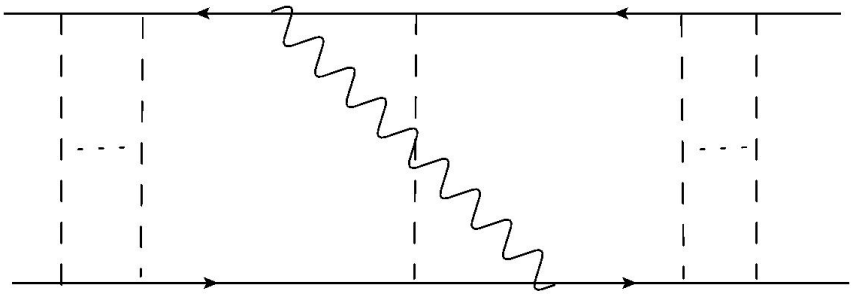

Figure 4b: Feynman diagram of a type II contribution with one Coulomb photon inside the ultrasoft exchange.

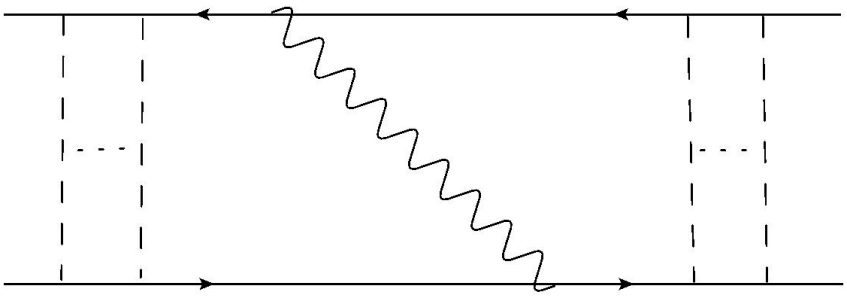

Figure 4c: Feynman diagram of a type III contribution with zero Coulomb photons inside the ultrasoft exchange.

where C_{US}, determines the ultrasoft contribution to the coefficient C in Eq.(1). It is precisely this C_{US} that we are calculating.

We split the correction to the wave function in four parts according to the their ultraviolet renormalization properties. Characteristic contributions of each type are graphically presented on Figs. 4a-4d. In Type II and III the factorized three loop diagram with one ultrasoft and two Coulomb photons is subtracted and denoted Type IV. The ultrasoft correction to the wave function then has the following decomposition

$$C_{US} = \delta\psi^{I} + \delta\psi^{II,a} + \delta\psi^{II,b} + \delta\psi^{III,a} + \delta\psi^{III,b} + \delta\psi^{IV} \tag{75}$$

The roman numerals correspond to the four different types of contributions. The analytical results for the different terms of Eq.(75) are of the following general form

$$\delta\psi^{i} = \sum_{j} \delta\psi^{i}_{j} \tag{76}$$

where $\delta\psi^{i}_{j}$ are presented in Appendix A and are of the following general form:

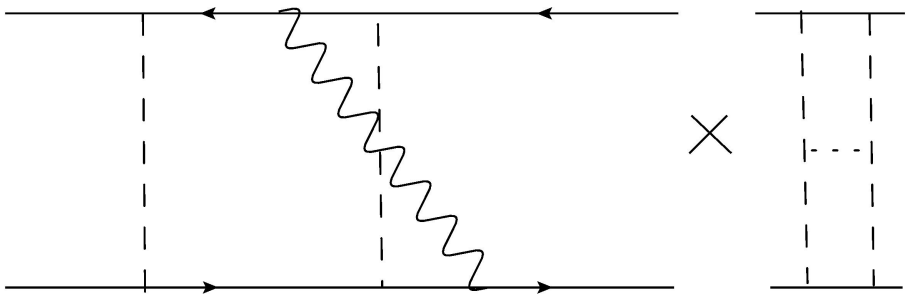

Figure 4d: Feynman diagram of a type IV contribution with factorized three-loop corrections with one ultrasoft and two Coulomb photons.

$$\delta\psi_j^i = \sum_{n=0}^{\infty} a_n \tag{77}$$

with the a_n terms given by a single integral of a complicated function which cannot be evaluated analytically, resulting from integration over k in Eq.(72) (the indices i and j of these coefficients are suppressed). See as an example Eq.(100) to (104). The main problem in getting a reliable numerical result for the ultrasoft correction is that the series in Eq.(76) is very slowly convergent so one has to take into account a large number of terms. At the same time large n means the integrand in a_n becomes rapidly oscillating and the numerical programs fail to integrate it with sufficient precision. To overcome this difficulty we elaborate a technique based on the asymptotic resummation of the series. First we determine the asymptotic behavior of the series numerically in the region of $n < N$ where N is the critical order where numerical integration starts to fail. The most general asymptotic of the coefficients found is

$$a_n \sim [c_0 + c_1 \log(n)]/n^b \tag{78}$$

with $b = 2$ or 3 and c_i being numerical coefficients. The sum is split into the "head" and "tail" parts according to

$$\sum_{n=0}^{\infty} a_n = \sum_{n=0}^{N} a_n + \sum_{n=N+1}^{\infty} a_n \equiv \sum\nolimits_H^N + \sum\nolimits_T^N \tag{79}$$

Then the head of the series is computed exactly while for the tail of the series we use the asymptotic expression for the coefficients in Eq.(78). The all-order summation of the tail can be easily performed by using the following relations

$$\sum_{n=1}^{\infty} \frac{1}{n^p} = \zeta(p), \tag{80}$$

where $\zeta(p)$ is the Riemann zeta-function, $\zeta(2) = 1.644934...$, $\zeta(3) = 1.202056...$, and

$$\begin{aligned} \sum_{n=1}^{\infty} \frac{\log(n)}{n^2} &= -\frac{1}{6}\pi^2(\gamma + \log 2 - 12\log A + \log \pi) \\ &= 0.937548... \end{aligned} \tag{81}$$

where γ is Euler's Gamma, $\gamma = 0.577216...$; A is Glaisher's constant, $A = 1.28243...$; and

$$\begin{aligned} \sum_{n=1}^{\infty} \frac{\log(n)}{n^3} &= -\zeta'(3) \\ &= 0.198126... \end{aligned} \tag{82}$$

Numerical evaluation of the coefficients a_n and fitting of the asymptotic coefficients c_i has been done with the help of the Mathematica 7.1 program. The results of the analysis are summarized in Table 1. The final results for the individual terms in Eq.(75) are given in Table 2. In the next section we present the details of a typical calculation.

$\delta\psi_j^i$	c_0	c_1	b	N	c_e
$\delta\psi_1^I$	13.15	2.10	3	52 (even)	0.11
$\delta\psi_2^I$	-4.46	-0.68	3	51(odd)	0.11
$\delta\psi_3^I$	4.44	0.69	3	51	0.24
$\delta\psi_4^I$	5.93	0.35	3	121	0.080
$\delta\psi_5^I$	0.0032	-0.0071	3	41	0.00021
$\delta\psi^{II,a}$	-8.02	-8.38	2	60	0.039
$\delta\psi^{III,a}$	1.46	0.11	3	74	0.094
$\delta\psi_1^{III,b}$	0.23	3.76	2	11	0.094
$\delta\psi_2^{III,b}$	0.69	1.56	2	11	14

Table 1: Asymptotic structure of the corrections

$\delta\psi^i$	result	uncertainty
$\delta\psi^I$	1.358546	0.000001
$\delta\psi^{II,a}$	41.85481	0.00003
$\delta\psi^{II,b}$	-7.05	0
$\delta\psi^{III,a}$	-4.4446672	0.0000004
$\delta\psi^{III,b}$	-20.906	0.002
$\delta\psi^{IV}$	8.051	0

Table 2: Numerical result for individual contributions

6.2 Example Calculation

Let us consider the calculation of the integral part of $\delta\psi^{II,a}$, call it $\delta\psi_{int}$. In this case $N = 60$. The exact evaluation of the first 59 terms with 100-digit precision took about 4 hours on one of the cores of an Intel Core2 Duo CPU E6550 (2.33GHz) computer with the result

$$\sum\nolimits_H^{60} = -18.8808... \tag{83}$$

The maximum computing time for such a calculation was around 7 hours. The next step of our procedure is finding the asymptotic coefficients c_i and b of Eq.(78). We found

$$\begin{aligned} c_0 &= -8.01677... \\ c_1 &= -8.38457... \\ b &= 2 \end{aligned} \tag{84}$$

The exact result for the coefficients a_n versus the asymptotic are plotted in Fig.5 which clearly shows the quality of the fit. It took about 18 hours of computing time to make this plot, with a maximum of 65 hours for this kind of calculation. The result for the asymptotic tail of the sum then reads

$$\sum\nolimits_T^{60} = -0.851422... \tag{85}$$

Finally we obtain

$$\begin{aligned} \delta\psi_{int} &= \sum\nolimits_H^{60} + \sum\nolimits_T^{60} \\ &= -19.7322... \end{aligned} \tag{86}$$

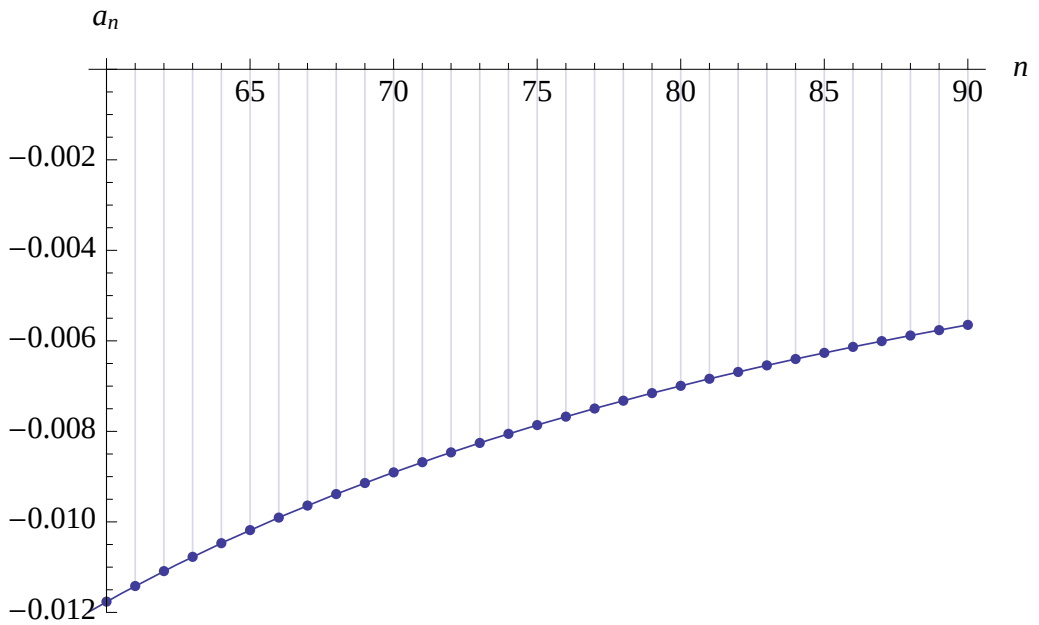

Figure 5: The exact result for the coefficients a_n (dots) with the asymptotic result, Eq.(78), as functions of n

Increasing the working precision was another way of getting exact results for heads of these sums up to the highest n possible. Most of the terms have thus been calculated with a precision of 100 digits.

6.3 Numerical Error Estimate

Our method is approximate and it is very important to control the numerical uncertainty of the result. The error comes from the neglected terms in Eq.(78) suppressed by higher powers of n. Let us estimate the effect of such terms. It is maximal for the lowest n when the approximation is used *i.e.* for $n = N + 1$. We then write

$$a_{N+1} = c_0 \frac{1}{(N+1)^b} + c_1 \frac{\log(N+1)}{(N+1)^b} + c_e \frac{\log(N+1)}{(N+1)^{b+1}} \tag{87}$$

Then we get

$$c_e = a_{N+1} \frac{(N+1)^{b+1}}{\log(N+1)} - c_0 \frac{(N+1)}{\log(N+1)} - c_1 (N+1) \tag{88}$$

Then the uncertainty of the result for $\delta\psi$ is

$$\sum_{n=N+1}^{\infty} c_e \frac{\log(n)}{n^{b+1}} \tag{89}$$

The numerical results for the coefficients c_e are given in Table 1. The $1/n^3$ terms in the fits already give very small contributions, therefore the corresponding error of order $1/n^4$ is negligible but was calculated nonetheless. To find the total error, all the errors of the individual approximations were added in order to avoid underestimating. Two significant digits have been kept for the final value.

6.4 The Final Result

Adding up all individual contributions, the final result was found to be

$$C_{US} = 18.8646 \pm 0.0017 \tag{90}$$

Therefore we have

$$\nu_{new}^{theo} = \nu^{theo} + \delta\nu_{US} \tag{91}$$

where

$$\delta\nu_{US} = \nu_0 \frac{\alpha^3}{\pi} C_{US} \tag{92}$$

And so the order α^3 contribution is

$$\frac{\alpha^3}{\pi} C_{US} = 2.33 \cdot 10^{-6} \tag{93}$$

which makes

$$\delta\nu_{US} = 0.000\,474\,600(42)\ GHz \tag{94}$$

This is added to the current theoretical result ν^{theo}. Therefore the new theoretical value for the positronium hyperfine splitting is

$$\nu_{new}^{theo} = 203.392\,17(47)\,GHz \tag{95}$$

7 Conclusion

In this thesis the $\mathcal{O}(\alpha^3)$ ultrasoft contribution to the positronium hyperfine splitting has been evaluated. The calculation required the use of nontrivial resummation techniques to get a reliable numerical result. Our new theoretical prediction reads

$$\nu_{new}^{theo} = 203.392\,17(47)\,GHz \tag{96}$$

which should be compared to the previous theoretical result [1, 17]

$$\nu^{theo} = 203.391\,69(41)\,GHz \tag{97}$$

and the experimentally measured value

$$\nu^{exp} = 203.388\,65(67)\,GHz \tag{98}$$

As we see the ultrasoft contribution increases the difference between theory and experiment to 4.3 σ. As an estimate of the uncertainty due to yet unknown parts of the third order correction we use the value of the ultrasoft contribution itself. It can be seen that it is in very good agreement with the naive estimate based on the result for the muonium hyperfine splitting.

Our analysis is the first step towards the full calculation of the third order QED corrections to the positronium hyperfine splitting. However, our result gives a strong indication that the existing discrepancy between theory and experiment cannot be explained by abnormally large radiative corrections. Thus the reduction of the experimental error is now crucial to remove or unambiguously establish the discrepancy and therefore a possible sign of "new physics".

New experiments are being designed to improve the measurement accuracy of the hyperfine splitting energy of positronium. Three papers all published in 2010 came up with various methods of doing this: using the Zeeman effect and Thermalization effect [18], sub-THz high power radiation [19], and quantum oscillation where the interference between the energy eigensates in the quantum system results in oscillations with frequency proportional to the hyperfine splitting energy [20]. The latest paper [21] points out probable systematic errors in past experiments and a direct measurement method. No new experimental or theoretical results have been published since. We are looking forward to the next generation of upcoming experiments which may shed some light on the positronium hyperfine splitting puzzle.

Acknowledgements

I would like to thank my supervisor Dr. Alexander Penin for all the help and advice provided since the beginning of this project, as well as the University of Alberta Theoretical Particle Physics group for their help whenever I needed it. I would also like to thank my parents and my sister who supported me always.

A Appendix

Here we present the analytical result for the corrections to the wavefunction before the numerical integration and summation are performed. They are obtained by inserting the Coulomb Green's function Eq.(73) into Eq.(72) and matching the result to the spectral representation Eq.(63). The result of the spatial integration and renormalization in Eq.(72) is obtained in [27, 32].

A.1 Type I - Two or More Coulomb Photons Inside the Ultrasoft Exchange

This contribution is obtained by plugging into the Eq.(72) the Green's function Eq.(73) with the first two terms of the expansion in α subtracted. We have

$$\delta\psi^I = \delta\psi_1^I + \delta\psi_2^I + \delta\psi_3^I + \delta\psi_4^I + \delta\psi_5^I \tag{99}$$

Where:

$$\delta\psi_1^I = \int_{\nu=0}^{1} d\nu \sum_{n=0}^{\infty} \left[F\left(3, n, 0, \frac{2}{\nu+1}, \frac{2\nu}{\nu+1}\right) \cdot (n+2-\nu) + F\left(4, n, 0, \frac{2}{\nu+1} \cdot \frac{2\nu}{\nu+1}\right) \cdot \frac{\nu^2}{4} \right] \cdot \frac{1-\nu^2}{6\nu} \cdot K1(n,1,\nu) \cdot \frac{(n+3)(n+1)}{(n+2)^2} \cdot \frac{1}{1-\frac{\nu}{n+2}} \tag{100}$$

$$\delta\psi_2^I = \int_{\nu=0}^{1} d\nu \sum_{n=0}^{\infty} \left\{ \left[Z2(n,2) + Z3(n,2) + (\log(\nu)+\gamma) \cdot F\left(3, n, 0, \frac{2}{\nu+1}, \frac{2\nu}{\nu+1}\right) \right] \cdot (n+2-\nu) + \left[Z2(n,2) + Z3(n,2) + (\log(\nu)+\gamma) \cdot F\left(3, n, 0, \frac{2}{\nu+1}, \frac{2\nu}{\nu+1}\right) \right] \cdot \frac{\nu^2-1}{4} \right\} \cdot \frac{1-\nu^2}{6\nu} \cdot K1(n,1,\nu) \cdot \frac{(n+3)(n+1)}{(n+2)^2} \cdot \frac{1}{1-\frac{\nu}{n+2}} \tag{101}$$

$$\delta\psi_3^I = \int_{\nu=0}^{1} d\nu \sum_{n=0}^{\infty} \left[-\frac{1}{2} K1(n,1,\nu) \cdot \frac{1}{1-\frac{\nu}{n+2}} + \frac{1}{2} K(n,1,\nu) + 2 \cdot K2(n,1,\nu) \right] \cdot (1-\nu)^2 \cdot K1(n,1,\nu) \cdot \frac{(n+3)(n+1)}{6(n+2)^2} \cdot \frac{1}{1-\frac{\nu}{n+2}} \tag{102}$$

$$\delta\psi_4^I = \int_{\nu=0}^{1} d\nu \sum_{n=0}^{\infty} \sum_{l=0}^{m-2} \left[K1(n,1,\nu) \cdot F\left(4,n,l,\frac{2}{\nu+1},\frac{2\nu}{\nu+1}\right) \cdot (n+2-\nu) \right.$$
$$\left. + K1(n,m,\nu) \cdot F\left(5,n,l,\frac{2}{\nu+1},\frac{2\nu}{\nu+1}\right) \cdot \frac{\nu^2-1}{4} \right] \cdot \frac{(1-\nu^2)(n+3)(n+1)}{6(n+2)^2}$$
$$\cdot \frac{1}{1+m\cdot d\cdot \frac{\nu}{n+2}} \cdot \frac{m^2}{(l+1)^2} \cdot \frac{1}{(l+1-m)} \tag{103}$$

$$\delta\psi_5^I = \int_{\nu=0}^{1} d\nu \sum_{n=0}^{\infty} \sum_{l=1}^{\infty} \left[K1(n,1,\nu) \cdot F\left(4,n,l,\frac{2}{\nu+1},\frac{2\nu}{\nu+1}\right) \cdot (n+2-\nu) \right.$$
$$\left. + K1(n,1,\nu) \cdot F\left(5,n,l,\frac{2}{\nu+1},\frac{2\nu}{\nu+1}\right) \cdot \frac{\nu^2-1}{4} \right] \cdot \frac{(1-\nu^2)(n+3)(n+1)}{6(n+2)^2}$$
$$\cdot \frac{1}{1-\frac{\nu}{n+2}} \cdot \frac{1}{l(l+1)^2} \tag{104}$$

And:

$$(a)_k = a(a+1)...(a+k-1) \tag{105}$$

$${}_2F_1(a,b;c;z) = \sum_{k=0}^{\infty} \frac{(a)_k (b)_k}{(c)_k} \frac{z^k}{k!} \tag{106}$$

$$F(a,b,c,x,y) = \frac{2^a (a-1)!}{(\nu+1)^a} \frac{c+1}{3!} \sum_{m=0}^{b+1} \sum_{n=0}^{c+1} \frac{(a)_{m+n} (-b)_m (-c)_n}{(4)_m (2)_n m!\, n!\, x^m y^n} \tag{107}$$

$$X(n,l,x) = \frac{\partial^l}{\partial x^l} \frac{(x-1)^n}{x^{n+4}} \tag{108}$$

$$K1(n,m,\nu) = -\sum_{l=0}^{m-1} \frac{(m-1)!}{(m-1-l)!\,(l+1)!\,l!} X\left(n,l,\frac{1+\nu}{2}\right) \cdot m \cdot \nu^{l+1} \tag{109}$$

$$K2(n,m,\nu) = \frac{1}{2} \sum_{l=0}^{m-1} \frac{(m-1)!}{(m-1-l)!\,(l+1)!\,l!} X\left(n,l,\frac{1+\nu}{2}\right) \cdot m \cdot \nu^{l+1} \tag{110}$$

$$Z1(a,\nu) = \frac{(a-1)!\,2^a}{a(1+\nu)^a}\,{}_2F_1\left(a,1;a+1;\frac{1-\nu}{1+\nu}\right) \tag{111}$$

$$Z2(n,p) = \frac{1}{(n+1)(n+2)(n+3)}\sum_{l=0}^{n}\frac{(-1)^l(n+3)!}{(n-l)!\,(3+l)!\,l!}\cdot Z1(l+1+p,\nu) \tag{112}$$

$$Z3 = \frac{\partial}{\partial r}F\left(p+1,n,0,\frac{2}{\nu+1},\frac{2\nu}{\nu+1}\right) \tag{113}$$

$$Z4 = \frac{\partial}{\partial r}F(p+1,n,0,2,1) \tag{114}$$

A.2 Type II - One Coulomb Photon Inside the Ultrasoft Exchange

This contribution is obtained by plugging into the Eq.(72) the $\mathcal{O}(\alpha^1)$ term in the expansion of the Green's function Eq.(73). The factorized three loop correction has been subtracted and included in Type IV. We have

$$\delta\psi^{II} = \delta\psi^{II,a} + \delta\psi^{II,b} \tag{115}$$

Where:

$$\begin{aligned}
\delta\psi^{II,a} = &-\int_{\nu=0}^{\infty}d\nu\Bigg(\sum_{n=0}^{m-1}\left[I4(n)-\frac{I1(n)}{2}\right]\cdot\left[I4(0)-\frac{I1(0)}{2}\right]\\
&\cdot\frac{\nu^2+1}{\nu^6}\cdot\log\left[\frac{\nu^2}{\nu^2+1}\right]\cdot\frac{1}{3\pi}\cdot\left(\frac{1}{n+1}\right)^2\cdot\frac{1}{n}\\
&-\sum_{n=1}^{\infty}\left[I4(n)-\frac{I1(n)}{2}\right]\cdot\left[I4(0)-\frac{I1(0)}{2}\right]\\
&\cdot\frac{\nu^2+1}{\nu^6}\cdot\log\left[\frac{\nu^2}{\nu^2+1}\right]\cdot\frac{4}{3\pi}\cdot\left(\frac{1}{n+1}\right)^2\cdot\frac{1}{n}\Bigg)\\
&+\int_{\nu=0}^{\infty}d\nu\left[I4(0)-\frac{I1(0)}{2}\right]^2\cdot\left(\frac{\nu^2+1}{\nu^6}\right)\cdot\frac{1}{3\pi}\\
&-\int_{\nu=0}^{\infty}d\nu\left[I4(0)-\frac{I1(0)}{2}\right]^2\cdot\frac{\nu^2+1}{\nu^6}\cdot\log\left[\frac{\nu^2}{\nu^2+1}\right]\cdot\frac{1}{3\pi}
\end{aligned} \tag{116}$$

$$\delta\psi^{II,b} = \sum_{n=1}^{\infty} \Bigg(\int_{x=0}^{1/2} dx \int_{\nu=0}^{\infty} d\nu \, 4 \cdot \left[I5(n) - \frac{I2(n)}{2} \right] \cdot \left[I6(0) - \frac{I3(0)}{2} \right] \cdot \frac{1}{\nu^5 x^3 (1-x)^3}$$
$$\cdot \left[\frac{x^2 + (1-x)^2}{x(1-x)} \cdot \log\left(\frac{1}{1-2x} \right) - 2 \right] \cdot \left\{ \log\left[\frac{x^2\nu^2}{x^2\nu^2+1} \right] \cdot \frac{x^2\nu^2+1}{x^2} \right.$$
$$\left. - \log\left[\frac{(1-x)^2\nu^2}{(1-x)^2\nu^2+1} \right] \cdot \frac{(1-x)^2\nu^2+1}{(1-x)^2} \right\} \cdot \frac{(1-x)^2 x^2}{(1-x)^2 - x^2}$$

$$+ \int_{x=1/2}^{1} dx \int_{\nu=0}^{\infty} d\nu \, 4 \cdot \left[I5(n) - \frac{I2(n)}{2} \right] \cdot \left[I6(0) - \frac{I3(0)}{2} \right] \cdot \frac{1}{\nu^5 x^3 (1-x)^3}$$
$$\cdot \left[\frac{x^2 + (1-x)^2}{x(1-x)} \cdot \log\left(\frac{1}{2x-1} \right) - 2 \right] \cdot \left\{ \log\left[\frac{x^2\nu^2}{x^2\nu^2+1} \right] \cdot \frac{x^2\nu^2+1}{x^2} \right.$$
$$\left. - \log\left[\frac{(1-x)^2\nu^2}{(1-x)^2\nu^2+1} \right] \cdot \frac{(1-x)^2\nu^2+1}{(1-x)^2} \right\} \cdot \frac{(1-x)^2 x^2}{(1-x)^2 - x^2} \Bigg)$$
$$\cdot \frac{1}{12\pi^2 n} \left(\frac{1}{n+1} \right)^2$$

$$+ \Bigg(\int_{x=0}^{1/2} dx \int_{\nu=0}^{\infty} d\nu \, \left[I5(0) - \frac{I2(0)}{2} \right] \cdot \left[I4(0) - \frac{I6(0)}{2} \right]$$
$$\cdot \frac{1}{\nu^5 x^3 (1-x)^3} \cdot \left[\frac{x^2 + (1-x)^2}{x(1-x)} \cdot \log\left(\frac{1}{1-2x} \right) - 2 \right]$$
$$\cdot \left[-\frac{x^2\nu^2+1}{x^2} + \frac{(1-x)^2\nu^2+1}{(1-x)^2} \right] \cdot \frac{(1-x)^2 x^2}{(1-x)^2 - x^2}$$

$$+ \int_{x=1/2}^{1} dx \int_{\nu=0}^{\infty} d\nu \, \left[I5(0) - \frac{I2(0)}{2} \right] \cdot \left[I4(0) - \frac{I6(0)}{2} \right] \cdot \frac{1}{\nu^5 x^3 (1-x)^3}$$
$$\cdot \left[\frac{x^2 + (1-x)^2}{x(1-x)} \cdot \log\left(\frac{1}{2x-1} \right) - 2 \right] \cdot \left[-\frac{x^2\nu^2+1}{x^2} + \frac{(1-x)^2\nu^2+1}{(1-x)^2} \right]$$
$$\cdot \frac{(1-x)^2 x^2}{(1-x)^2 - x^2} \Bigg) \cdot \frac{1}{3\pi^2}$$

$$+\left(\int_{x=0}^{1/2} dx \int_{\nu=0}^{\infty} d\nu \left[I5(0) - \frac{I2(0)}{2}\right] \cdot \left[I6(0) - \frac{I3(0)}{2}\right]\right.$$
$$\cdot \frac{1}{\nu^5 x^3 (1-x)^3} \cdot \left[\frac{x^2 + (1-x)^2}{x(1-x)} \cdot \log\left(\frac{1}{1-2x}\right) - 2\right] \cdot \left\{\log\left[\frac{x^2\nu^2}{x^2\nu^2+1}\right] \cdot \frac{x^2\nu^2+1}{x^2}\right.$$
$$\left.\left. - \log\left[\frac{(1-x)^2\nu^2}{(1-x)^2\nu^2+1}\right] \cdot \frac{(1-x)^2\nu^2+1}{(1-x)^2}\right\} \cdot \frac{(1-x)^2 x^2}{(1-x)^2 - x^2}\right.$$

$$+\int_{x=1/2}^{1} dx \int_{\nu=0}^{\infty} d\nu \left[I5(0) - \frac{I2(0)}{2}\right] \cdot \left[I6(0) - \frac{I3(0)}{2}\right]$$
$$\cdot \frac{1}{\nu^5 x^3 (1-x)^3} \cdot \left[\frac{x^2 + (1-x)^2}{x(1-x)} \cdot \log\left(\frac{1}{2x-1}\right) - 2\right] \cdot \left\{\log\left[\frac{x^2\nu^2}{x^2\nu^2+1}\right]\right.$$
$$\left. \cdot \frac{x^2\nu^2+1}{x^2} - \log\left[\frac{(1-x)^2\nu^2}{(1-x)^2\nu^2+1}\right] \cdot \frac{(1-x)^2\nu^2+1}{(1-x)^2}\right\}$$
$$\left. \cdot \frac{(1-x)^2 x^2}{(1-x)^2 - x^2}\right) \cdot \frac{1}{3\pi^2} \tag{117}$$

And:

$$I1(n) = \sum_{l=0}^{n} \frac{(-1)^l (n+1)!\,(l+0)!}{(n-l)!\,(l+1)!\,l!} \cdot \frac{(2\nu)^{1+l}}{(1+\nu^2)^{\frac{1}{2}+\frac{l}{2}}} \cdot 4\nu^2 \sin\left[-(1+l)\arctan\left(\frac{1}{\nu}\right)\right]$$
$$+ \sum_{l=0}^{n} \frac{(-1)^l (n+1)!\,(l+1)!}{(n-l)!\,(l+1)!\,l!} \cdot \frac{(2\nu)^{2+l}}{(1+\nu^2)^{\frac{2}{2}+\frac{l}{2}}}$$
$$\cdot 2\nu \cos\left[-(2+l)\arctan\left(\frac{1}{\nu}\right)\right] \tag{118}$$

$$I2(n) = \sum_{l=0}^{n} \frac{(-1)^l (n+1)!\,(l+0)!}{(n-l)!\,(l+1)!\,l!} \cdot \frac{(2x\nu)^{1+l}}{(1+x^2\nu^2)^{\frac{1}{2}+\frac{l}{2}}} \cdot 4x^2\nu^2 \sin\left[-(1+l)\arctan\left(\frac{1}{x\nu}\right)\right]$$
$$+ \sum_{l=0}^{n} \frac{(-1)^l (n+1)!\,(l+1)!}{(n-l)!\,(l+1)!\,l!} \cdot \frac{(2x\nu)^{2+l}}{(1+x^2\nu^2)^{\frac{2}{2}+\frac{l}{2}}}$$
$$\cdot 2x\nu \cos\left[-(2+l)\arctan\left(\frac{1}{x\nu}\right)\right] \tag{119}$$

$$I3(n) = \sum_{l=0}^{n} \frac{(-1)^l (n+1)!\,(l+0)!}{(n-l)!\,(l+1)!\,l!} \cdot \frac{[2(1-x)\nu]^{1+l}}{[1+(1-x)^2\nu^2]^{\frac{1}{2}+\frac{l}{2}}} \cdot 4(1-x)^2\nu^2$$
$$\cdot \sin\left[-(1+l)\arctan\left(\frac{1}{(1-x)\nu}\right)\right]$$
$$+ \sum_{l=0}^{n} \frac{(-1)^l (n+1)!\,(l+1)!}{(n-l)!\,(l+1)!\,l!} \cdot \frac{[2(1-x)\nu]^{2+l}}{[1+(1-x)^2\nu^2]^{\frac{2}{2}+\frac{l}{2}}} \cdot 2(1-x)\nu$$
$$\cdot \cos\left[-(2+l)\arctan\left(\frac{1}{(1-x)\nu}\right)\right] \tag{120}$$

$$I4(n) = \sum_{l=0}^{n} \frac{(-1)^{l+1} (n+1)!\,(l+0)!}{(n-l-1)!\,(l+2)!\,l!} \cdot \frac{(2\nu)^{1+l}}{(1+\nu^2)^{\frac{1}{2}+\frac{l}{2}}} \cdot 4\nu^2 \sin\left[-(1+l)\arctan\left(\frac{1}{\nu}\right)\right]$$
$$+ \sum_{l=0}^{n-1} \frac{(-1)^{l+1} (n+1)!\,(l+1)!}{(n-l-1)!\,(l+2)!\,l!} \cdot \frac{(2\nu)^{2+l}}{(1+\nu^2)^{\frac{2}{2}+\frac{l}{2}}}$$
$$\cdot 2\nu \cos\left[-(2+l)\arctan\left(\frac{1}{\nu}\right)\right] \tag{121}$$

$$I5(n) = \sum_{l=0}^{n} \frac{(-1)^{l+1} (n+1)!\,(l+0)!}{(n-l-1)!\,(l+2)!\,l!} \cdot \frac{(2x\nu)^{1+l}}{(1+x^2\nu^2)^{\frac{1}{2}+\frac{l}{2}}} \cdot 4x^2\nu^2 \sin\left[-(1+l)\arctan\left(\frac{1}{x\nu}\right)\right]$$
$$+ \sum_{l=0}^{n} \frac{(-1)^{l+1} (n+1)!\,(l+1)!}{(n-l-1)!\,(l+2)!\,l!} \cdot \frac{(2x\nu)^{2+l}}{(1+x^2\nu^2)^{\frac{2}{2}+\frac{l}{2}}}$$
$$\cdot 2x\nu \cos\left[-(2+l)\arctan\left(\frac{1}{x\nu}\right)\right] \tag{122}$$

$$I6(n) = \sum_{l=0}^{n} \frac{(-1)^{l+1} (n+1)!\,(l+0)!}{(n-l-1)!\,(l+2)!\,l!} \cdot \frac{[2(1-x)\nu]^{1+l}}{[1+(1-x)^2\nu^2]^{\frac{1}{2}+\frac{l}{2}}} \cdot 4(1-x)^2\nu^2$$
$$\cdot \sin\left[-(1+l)\arctan\left(\frac{1}{(1-x)\nu}\right)\right]$$
$$+ \sum_{l=0}^{n} \frac{(-1)^{l+1} (n+1)!\,(l+1)!}{(n-l-1)!\,(l+2)!\,l!} \cdot \frac{[2(1-x)\nu]^{2+l}}{[1+(1-x)^2\nu^2]^{\frac{2}{2}+\frac{l}{2}}} \cdot 2(1-x)\nu$$
$$\cdot \cos\left[-(2+l)\arctan\left(\frac{1}{(1-x)\nu}\right)\right] \tag{123}$$

A.3 Type III - Zero Coulomb Photons Inside the Ultrasoft Exchange

This contribution is obtained by plugging into the Eq.(72) the $\mathcal{O}(\alpha^0)$ term in the expansion of the Green's function Eq.(73). The factorized three loop correction has been subtracted and included in Type IV. We have

$$\delta\psi^{III} = \delta\psi^{III,a} + \delta\psi^{III,b} \tag{124}$$

and

$$\delta\psi^{III,b} = \delta\psi_1^{III,b} + \delta\psi_2^{III,b} + \delta\psi_3^{III,b} \tag{125}$$

Where:

$$\begin{aligned}
\delta\psi^{III,a} = & -4 \cdot \sum_{n=0}^{\infty} \int_{\nu=0}^{\infty} d\nu \left[I4(n) - \frac{I1(n)}{2} \right] \\
& \cdot \left\{ (-2) \cdot \left[I4(0) - \frac{I1(0)}{2} \right] \cdot \frac{\nu^2+1}{\nu^6} + \frac{16}{\nu^3} \right\} \cdot \log\left[\frac{\nu^2}{\nu^2+1} \right] \cdot \frac{1}{16\pi} \cdot \left(\frac{1}{n+1} \right)^2 \\
& - \int_{\nu=0}^{\infty} d\nu \left[-\frac{I7(m)}{4\nu^2} - 1 \right] \cdot \frac{1}{1+\nu^2} \cdot \left[1 + \frac{1+\nu^2}{\nu} \cdot \operatorname{arccsc}(\sqrt{1+\nu^2}) \right] \cdot \frac{16}{\pi} \\
& - \int_{\nu=0}^{\infty} d\nu \left[I10 - \frac{I8}{2} \right] \cdot \left[I4(0) - \frac{I1(0)}{2} \right] \cdot \frac{\nu^2+1}{\nu^4} \cdot \log\left[\frac{\nu^2}{\nu^2+1} \right] \cdot \frac{1}{2\pi} \\
& + \int_{x=0}^{1} dx \int_{\nu=0}^{\infty} d\nu \cdot \nu \cdot \frac{x^{-1/2}}{1+\nu^2} \cdot (\nu^2+1-x)^{-1/2} \cdot \log\left[\frac{4(\nu^2+1-x)}{\nu^2} \right] \cdot \frac{8}{\pi}
\end{aligned} \tag{126}$$

$$\delta\psi_1^{III,b} = \sum_{n=0}^{\infty} \int_{x=0}^{1/2} dx \int_{\nu=0}^{\infty} d\nu \left[I5(n) - \frac{I2(n)}{2} \right] \cdot \left[I6(0) - \frac{I3(0)}{2} \right]$$
$$\cdot \frac{1}{\nu^5 x^3 (1-x)^3} \cdot \left[\frac{x^2 + (1-x)^2}{x(1-x)} \cdot \log\left(\frac{1}{1-2x} \right) - 2 \right] \cdot \left\{ \log\left[\frac{x^2\nu^2}{x^2\nu^2+1} \right] \cdot \frac{x^2\nu^2+1}{x^2} \right.$$
$$\left. - \log\left[\frac{(1-x)^2\nu^2}{(1-x)^2\nu^2+1} \right] \cdot \frac{(1-x)^2\nu^2+1}{(1-x)^2} \right\} \cdot \frac{(1-x)^2 x^2}{(1-x)^2 - x^2}$$
$$\cdot \frac{1}{3\pi^2} \cdot \frac{1}{(n+1)^2} \tag{127}$$

$$\delta\psi_2^{III,b} = \sum_{n=0}^{\infty} \int_{x=1/2}^{1} dx \int_{\nu=0}^{\infty} d\nu \left[I5(n) - \frac{I2(n)}{2} \right] \cdot \left[I6(0) - \frac{I3(0)}{2} \right]$$
$$\cdot \frac{1}{\nu^5 x^3 (1-x)^3} \cdot \left[\frac{x^2 + (1-x)^2}{x(1-x)} \cdot \log\left(\frac{1}{2x-1} \right) - 2 \right] \cdot \left\{ \log\left[\frac{x^2\nu^2}{x^2\nu^2+1} \right] \cdot \frac{x^2\nu^2+1}{x^2} \right.$$
$$\left. - \log\left[\frac{(1-x)^2\nu^2}{(1-x)^2\nu^2+1} \right] \cdot \frac{(1-x)^2\nu^2+1}{(1-x)^2} \right\} \cdot \frac{(1-x)^2 x^2}{(1-x)^2 - x^2}$$
$$\cdot \frac{1}{3\pi^2} \cdot \frac{1}{(n+1)^2} \tag{128}$$

$$\delta\psi_3^{III,b} = -\left(\int_{x=0}^{1/2} dx \int_{\nu=0}^{\infty} d\nu \left[I11 - \frac{I9}{2} \right] \left\{ (-2) \left[I6(0) - \frac{I3(0)}{2} \right] \right.\right.$$
$$\left.\left. + 16 \frac{(1-x)^3\nu^3}{1+\nu^2(1-x)^2} \right\} \cdot \frac{1}{\nu^5 x^3 (1-x)^3} \cdot \left[\frac{x^2 + (1-x)^2}{x(1-x)} \cdot \log\left(\frac{1}{1-2x} \right) - 2 \right] \right.$$
$$\left. \cdot \left\{ \log\left[\frac{x^2\nu^2}{x^2\nu^2+1} \right] \cdot \frac{x^2\nu^2+1}{x^2} - \log\left[\frac{(1-x)^2\nu^2}{(1-x)^2\nu^2+1} \right] \cdot \frac{(1-x)^2\nu^2+1}{(1-x)^2} \right\} \right.$$
$$\left. \cdot \frac{(1-x)^2 x^2}{(1-x)^2 - x^2} \right.$$

$$
\begin{aligned}
&- \int_{x=1/2}^{1} dx \int_{\nu=0}^{\infty} d\nu \left[I11 - \frac{I9}{2} \right] \left\{ (-2) \left[I6(0) - \frac{I3(0)}{2} \right] \right. \\
&\left. + 16 \frac{(1-x)^3 \nu^3}{1+\nu^2(1-x)^2} \right\} \cdot \frac{1}{\nu^5 x^3 (1-x)^3} \cdot \left[\frac{x^2 + (1-x)^2}{x(1-x)} \cdot \log\left(\frac{1}{2x-1} \right) - 2 \right] \\
&\cdot \left\{ \log\left[\frac{x^2\nu^2}{x^2\nu^2+1} \right] \cdot \frac{x^2\nu^2+1}{x^2} - \log\left[\frac{(1-x)^2\nu^2}{(1-x)^2\nu^2+1} \right] \cdot \frac{(1-x)^2\nu^2+1}{(1-x)^2} \right\} \\
&\cdot \frac{(1-x)^2 x^2}{(1-x)^2 - x^2} \Bigg) \cdot \frac{1}{6\pi^2} \\
&- \frac{35}{9} - \frac{62 \log 2}{9} - \frac{8 \log^2 2}{3}
\end{aligned}
\tag{129}
$$

And:

$$
\begin{aligned}
I1(n) = &\sum_{l=0}^{n} \frac{(-1)^l (n+1)! \, (l+0)!}{(n-l)! \, (l+1)! \, l!} \cdot \frac{(2\nu)^{l+1}}{(1+\nu^2)^{\frac{1}{2}+\frac{l}{2}}} \cdot 4\nu^2 \sin\left[-(l+1) \arctan\left(\frac{1}{\nu} \right) \right] \\
&+ \sum_{l=0}^{n} \frac{(-1)^l (n+1)! \, (l+1)!}{(n-l)! \, (l+1)! \, l!} \cdot \frac{(2\nu)^{l+2}}{(1+\nu^2)^{\frac{2}{2}+\frac{l}{2}}} \\
&\cdot 2\nu \cos\left[-(l+2) \arctan\left(\frac{1}{\nu} \right) \right]
\end{aligned}
\tag{130}
$$

$$
\begin{aligned}
I2(n) = &\sum_{l=0}^{n} \frac{(-1)^l (n+1)! \, (l+0)!}{(n-l)! \, (l+1)! \, l!} \cdot \frac{(2x\nu)^{l+1}}{(1+x^2\nu^2)^{\frac{1}{2}+\frac{l}{2}}} \cdot 4x^2\nu^2 \sin\left[-(l+1) \arctan\left(\frac{1}{x\nu} \right) \right] \\
&+ \sum_{l=0}^{n} \frac{(-1)^l (n+1)! \, (l+1)!}{(n-l)! \, (l+1)! \, l!} \cdot \frac{(2x\nu)^{l+2}}{(1+x^2\nu^2)^{\frac{2}{2}+\frac{l}{2}}} \\
&\cdot 2x\nu \cos\left[-(l+2) \arctan\left(\frac{1}{x\nu} \right) \right]
\end{aligned}
\tag{131}
$$

$$I3(n) = \sum_{l=0}^{n} \frac{(-1)^l (n+1)!\,(l+0)!}{(n-l)!\,(l+1)!\,l!} \cdot \frac{[2(1-x)\nu]^{l+1}}{[1+(1-x)^2\nu^2]^{\frac{1}{2}+\frac{l}{2}}} \cdot 4(1-x)^2\nu^2$$
$$\cdot \sin\left[-(l+1)\arctan\left(\frac{1}{(1-x)\nu}\right)\right]$$
$$+ \sum_{l=0}^{n} \frac{(-1)^l (n+1)!\,(l+1)!}{(n-l)!\,(l+1)!\,l!} \cdot \frac{[2(1-x)\nu]^{l+2}}{[1+(1-x)^2\nu^2]^{\frac{2}{2}+\frac{l}{2}}} \cdot 2(1-x)\nu$$
$$\cdot \cos\left[-(l+2)\arctan\left(\frac{1}{(1-x)\nu}\right)\right] \tag{132}$$

$$I4(n) = \sum_{l=0}^{n} \frac{(-1)^{l+1} (n+1)!\,(l+0)!}{(n-l-1)!\,(l+2)!\,l!} \cdot \frac{(2\nu)^{l+1}}{(1+\nu^2)^{\frac{1}{2}+\frac{l}{2}}} \cdot 4\nu^2 \sin\left[-(l+1)\arctan\left(\frac{1}{\nu}\right)\right]$$
$$+ \sum_{l=0}^{n-1} \frac{(-1)^{l+1} (n+1)!\,(l+1)!}{(n-l-1)!\,(l+2)!\,l!} \cdot \frac{(2\nu)^{l+2}}{(1+\nu^2)^{\frac{2}{2}+\frac{l}{2}}}$$
$$\cdot 2\nu \cos\left[-(l+2)\arctan\left(\frac{1}{\nu}\right)\right] \tag{133}$$

$$I5(n) = \sum_{n=0}^{n} \frac{(-1)^{l+1} (n+1)!\,(l+0)!}{(n-l-1)!\,(l+2)!\,l!} \cdot \frac{(2x\nu)^{l+1}}{(1+x^2\nu^2)^{\frac{1}{2}+\frac{l}{2}}} \cdot 4x^2\nu^2 \sin\left[-(l+1)\arctan\left(\frac{1}{x\nu}\right)\right]$$
$$+ \sum_{l=0}^{n} \frac{(-1)^{l+1} (n+1)!\,(l+1)!}{(n-l-1)!\,(l+2)!\,l!} \cdot \frac{(2x\nu)^{l+2}}{(1+x^2\nu^2)^{\frac{2}{2}+\frac{l}{2}}}$$
$$\cdot 2x\nu \cos\left[-(l+2)\arctan\left(\frac{1}{x\nu}\right)\right] \tag{134}$$

$$I6(n) = \sum_{l=0}^{n} \frac{(-1)^{l+1} (n+1)!\,(l+0)!}{(n-l-1)!\,(l+2)!\,l!} \cdot \frac{[2(1-x)\nu]^{l+1}}{[1+(1-x)^2\nu^2]^{\frac{1}{2}+\frac{l}{2}}} \cdot 4(1-x)^2\nu^2$$
$$\cdot \sin\left[-(l+1)\arctan\left(\frac{1}{(1-x)\nu}\right)\right]$$
$$+ \sum_{l=0}^{n} \frac{(-1)^{l+1} (n+1)!\,(l+1)!}{(n-l-1)!\,(l+2)!\,l!} \cdot \frac{[2(1-x)\nu]^{l+2}}{[1+(1-x)^2\nu^2]^{\frac{2}{2}+\frac{l}{2}}} \cdot 2(1-x)\nu$$
$$\cdot \cos\left[-(l+2)\arctan\left(\frac{1}{x(1-)\nu}\right)\right] \tag{135}$$

$$I7(n) = \sum_{l=0}^{n} \frac{(-1)^l (n+1)!\,(l+0)!}{(n-l)!\,(l+1)!\,l!} \cdot \frac{(2\nu)^{l+1}}{(1+\nu^2)^{\frac{1}{2}+\frac{l}{2}}} \cdot 2\nu \sin\left[-(l+1)\arctan\left(\frac{1}{\nu}\right)\right] \tag{136}$$

$$I8 = \frac{(2\nu)^2\nu}{\nu^2+1} - (2\nu)^2 \arctan\left(\frac{1}{\nu}\right) \tag{137}$$

$$I9 = \frac{(2x\nu)^2 x\nu}{x^2\nu^2+1} - (2x\nu)^2 \arctan\left(\frac{1}{x\nu}\right) \tag{138}$$

$$I10 = -(2\nu) \cdot \left[-1 + \nu \arctan\left(\frac{1}{\nu}\right)\right] \tag{139}$$

$$I11 = -(2\nu x) \cdot \left[-1 + \nu x \arctan\left(\frac{1}{x\nu}\right)\right] \tag{140}$$

A.4 Type IV - Factorized Three-Loop Corrections With One Ultrasoft and Two Coulomb Photons

These corrections include the subtracted terms from Type II and III which are of the form $\psi_C(0) \times (\textit{three loop subdiagram})$. We have

$$\delta\psi^{IV} = \frac{436}{27} - \frac{3\pi^2}{8} - \frac{55\log(2)}{9} - \log(2)^{2/3} \tag{141}$$

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