Study of leptonic systems and loop calculation techniques

by

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Abstract

In the first part of this thesis, proper handling of divergent integrals is presented, first with the example of the photon-photon scattering. The classic result of this process was questioned, because the necessity of regularization in the classic calculation was not clear. This challenge has its counterpart. The standard result for the decay of the Higgs boson into two photons was also questioned for a similar reason. We have verified the classic result of the photon-photon scattering, and have confirmed the necessity of regularization. The need to implement the regularization procedure in the calculation of the Higgs decay process is tested with multiple calculational approaches. We find once again the standard result to be correct.

In the second part of the thesis, we numerically study properties of leptonic systems. The first system is the positronium ion, a three-body system consisting of two electrons and a positron. The gyromagnetic factor of the positronium ion is determined with first relativistic corrections. We calculate the modified g-factor of this system for the first time. Our final topic is the computation of the spin asymmetry of the muon decay $\mu \to e\bar{\nu}_e\nu_\mu$ through $\mathcal{O}(\alpha^2)$ in perturbative QED. We point out that at $\mathcal{O}(\alpha^2)$ the asymmetry requires a careful definition due to multi-lepton final states and suggest to use familiar QCD techniques to define it in an infra-red safe way. We find that the TWIST measurement of the asymmetry is in excellent agreement with the Standard Model.

Preface

Chapter 2 of this thesis has been published as Yi Liang and Andrzej Czarnecki, "Theoretical Responses to Rays in the Gamma System," Canadian Journal of Physics, vol. 90, 11. I was responsible for the calculation as well as the manuscript composition. Porfessor Andrzej Czarnecki was the supervisory author. He assisted with the concept formation, the interpretation of results, and contributed to manuscript edits.

Chapter 5 of this thesis has been submitted as Yi Liang, Paul McGrath, and Andrzej Czarnecki, "Anomalous magnetic moment of the positronium ion," to New Journal of Physics. This paper was accepted for publication. The calculation procedure discussed in Chapter 5 was found by me. I also contributed to the manuscript composition. The code used to do the calculation was developed by me based on a program written by Doctor Paul McGrath. Professor Andrzej Czarnecki was the supervisory author. He assisted with the concept formation, and contributed to manuscript edits.

The research conducted for the Chapter 6 of this thesis forms part of an international research collaboration, led by Professor Kirill Melnikov at he Johns Hopkins University, with Professor Andrzej Czarnecki being the lead collaborator at the University of Alberta. The calculation discussed in this chapter was done by me and Doctor Robert Szafron, with the assistance of Doctor Fabrizio Caola, Professor Kirill Melnikov and Professor Andrzej Czarnecki.

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Chapter 1

Introduction

This thesis has two main topics. The **first** topic is the discussion of the calculation of Feynman diagrams at the one loop level. This work roots in the recent question on the standard result of the low-energy cross section of the photon-photon scattering process [1, 2], and the classic calculation of the Higgs boson decay to two photons [3, 4]. Theses authors claimed the classic results are problematic, because dimensional regularization is improper to be used in these kind of calculation. Since the processes discussed here are very fundamental and important in the current study of physics, both theoretically and experimentally, it is necessary to have a closer look at these debates.

In Chapter 2 we discuss the calculation of the photon-photon scattering. The authors in [1, 2] claimed that the low energy differential cross section of the photon-photon scattering is inversely proportional to the square of the energy of the photon, while in the classic result, it is proportional to the photon's energy to the 6th power. The reason that these authors obtained a different result is that they abandoned the regularization procedure in their calculation. We point out in Chapter 2, that the regularization is necessary in the calculation of this process. We show in addition that if their result were true, the mean free path of visible light due to the scattering on the cosmic microwave background radiation would be less than the distance between Earth and Jupiter. Obviously, the new proposed low-energy differential cross section is incorrect. The discussion presented in Chapter 2 is published in Canadian Journal of Physics (CJP) [5], and won the award for "Best Paper" of the year.

As we mentioned above, another group questioned the standard result of the decay of Higgs to two photons through W boson loop [3, 4]. These authors also claimed that there is no need for the regularization procedure. In order to see if their argument makes sense, we apply two approaches to calculate this process. In Chapter 3, we use the method called expansion by regions to calculate the decay amplitude in the limit $m^2/M^2 \ll 1$, where m is the mass of the particle in the loop, and M is the mass of Higgs. The result obtained by this method is a series of m^2/M^2. In the expansion by regions method, a procedure called auxiliary analytic regularization was employed. We compare the result from our calculation with the result calculated directly with the dimension regularization. The two results agree with each other.

In Chapter 4, in order to find out if the regularization procedure does introduce error to the decay amplitude as claimed by the authors in [3, 4], we use dispersion relations to calculate the decay of Higgs to two photons. The dispersion relation can be generally derived from Cauchy's residue theorem. Using the dispersion relations, one can obtain the full expression of the form factor and henceforth the decay amplitude, starting from the imaginary part of the form factor. The imaginary part of the form factor can be calculated with the Cutkosky rules. Since one will not encounter any divergence in this calculation, there is no need to introduce the regularization. We also present a discussion of the applicable condition of the unsubtracted

and the once subtracted dispersion relations in a later part of Chapter 4.

The **second** main topic of this thesis is studying the properties of leptonic systems, including the single electron or positron, and systems composed of several electrons and positrons, which are called polyelectron systems. Now let us have a look at what these systems are.

In 1928, Dirac [6] discovered an equation describing spin-1/2 particles such as electrons. Its negative-energy solutions were interpreted as anti-electrons. Soon, in 1932 Anderson confirmed that prediction. He discovered the existence of positron, which is the anti-particle of the electron, using a cloud chamber as a detector of cosmic rays. The positronium system is composed of one electron and its antiparticle with a positive charge. The internal interaction of this atom follows the rules of Quantum Electrodynamics (QED), and the precision of the theoretical description is only limited by people's ability to calculate rather than by nuclear uncertainties. This fact makes positronium an ideal testing ground for QED [7], and it is a very important research tool in various areas of physics.

The idea that positrons could substitute nuclei in more complex atoms and molecules was proposed and investigated even before the experimental discovery of positronium. These kinds of systems contain at least three particles, which makes finding an analytical solution for their wave function impossible. A solution can only be achieved by doing a large-scale variational calculation. It was first proved by Wheeler [8] in 1946 that a positronium can bind an extra electron to form a state called positronium ion. The existence of positronium ion was experimentally confirmed much later by Mills [9]. Positronium ion has many similarities with the hydrogen ion H^-; it is weakly bound with a binding energy of 0.012 a.u. (where the atomic unit is 1 a.u. $= \alpha^2 m_e c^2$). To minimize the energy, the two electrons in the ground state of positronium ion form a symmetric spatial part of the wave function, and consequently they have to be in spin singlet state to fulfill the Fermi-Dirac statistics. Therefore, the positron can form both a spin singlet and a triplet state with the electrons, making the decay channels of the positronium ion very interesting. It can decay into both even and odd numbers of photons, and even a single-photon decay is possible [10, 11].

In Chapter 5, a numerical calculation of the magnetic moment of the positronium ion system is presented. This is the first time that the anomalous magnetic moment of this system is calculated. A brief review of the magnetic moment of some other leptonic systems, including the positronium, the hydrogen, and the hydrogen like ion systems is given in this chapter as well. We derive the expression of the magnetic moment of the positronium ion system and calculate its value by using a Gaussian like trial function. A numerical optimization procedure is implemented in the calculation. The paper of this work is accepted by New Journal of Physics (NJP) [12].

In Chapter 6, the asymmetry of a polarized muon decay is studied. Muon is a lepton, which has the same electric charge and spin as electron, but with a much larger mass (105.7 MeV). The muon decay is a paradigm for all charged current flavor transformations. The properties of this pure leptonic process $\mu \to e\bar{\nu}_e\nu_\mu$ can be theoretically predicted with very high precision. Measurements of its lifetime [13] and distributions of the daughter electron [14, 15, 16] determine fundamental parameters of the Standard Model and probe its extensions. The radiative decay of a polarized muon is important for controlling the background to the search of $\mu \to e\gamma$, and the need for such a correction has recently been pointed out [17]. The spin asymmetry of the muon decay $\mu \to e\bar{\nu}_e\nu_\mu$ is computed through $\mathcal{O}(\alpha^2)$ in perturbative QED in Chapter 6. These two-loop corrections are about a factor five (twenty) smaller than the current statistical (systematic) uncertainty of the most precise measurement, performed by the TWIST collaboration. We point out that at $\mathcal{O}(\alpha^2)$ the asymmetry requires a careful definition due to multi-lepton final states and suggest to use familiar QCD techniques to define it in an infra-red safe way. We find that the TWIST measurement of the asymmetry is in excellent agreement with the Standard Model.

A document of the study in this chapter can also be found in [18].

Chapters 7 to 10 are appendices, with more details and some necessary techniques of our calculations.

Chapter 2

Photon-photon Scattering

2.1 Introduction

After Dirac proposed the theory of negative energy solutions of his equation [19], it was realized that photons can interact with other photons by polarizing the vacuum. Photon-photon scattering was qualitatively considered in this context by Halpern [20], and its cross section, for the case of photon energies low compared to the electron mass, was determined by Euler and Kockel in 1935 [21, 22]. If the energy of each of the colliding photons is ω in the frame in which their total momentum vanishes, the low-energy differential cross section is

$$\frac{d\sigma}{d\Omega} = \frac{139\alpha^4}{(180\pi)^2}\frac{\omega^6}{m^8}\left(3+\cos^2\theta\right)^2, \tag{2.1.1}$$

where $\alpha \simeq 1/137$ is the fine structure constant and m is the electron mass. High energy scattering was considered soon afterward [23, 24]. A thorough analysis of the scattering at all energies, including partial cross sections for various polarization states, was carried out in [25, 26], using the then new diagrammatic technique of Feynman.

These results were reproduced in a more compact form by Tollis [27, 28], using the double-dispersive representation and the dispersion relation techniques. In those papers, the cross section as a function of the energy, as well as a discussion of the angular distribution of photons was presented. The result of Karplus and Neuman was further explored [29], and it was shown that the scattering amplitude can be constructed with a certain set of tensors, which maintain the symmetry of being closed under the permutation of the tensor indices and of the momenta. In 1974, the so called "Null-plane" coordinates were introduced [30] in order to make the calculation simpler. The method called dimensional-regularization was adopted in this work, and appeared to be superior to the standard Pauli–Villars regularization in the case of forward photon-photon scattering of linearly polarized light.

The result of photon-photon scattering can also be represented in terms of the hyper-geometric representations [31], which can be analytically continued from one variable region to the other. In order to discuss the experimental possibility on the observation of the process involving photon-photon scattering at the Photon Linear Collider (PLC), the scattering amplitude of the photon-photon process in the full electroweak Standard Model was calculated [32]. A cross section of unpolarized and polarized photons in the MeV energy region was obtained, as well as the unpolarized cross section in the GeV, and up to more than 10 TeV regions. Later, a new calculation of the photon-photon scattering process in the electroweak Standard Model was done to investigate the possible observation of photon-photon scattering in PLC [33]. This calculation was done both in the 't Hooft-Feynman gauge and non-linear R_ξ gauge,

including the contribution from W boson loop. The calculation was accomplished with symbolic manipulation program FORM. A reduction algorithm [34] was adopted in their derivations. A few years later, it was realized that the scattering cross section of photon-photon scattering process may also be derived with the effective-action approach [35], in low and high energy limits. In that calculation, QED corrections of higher-order were computed in the high energy limit.

Two loop QCD and QED corrections to the photon-photon scattering process were first introduced by Bern et al. [36], where the ultrarelativistic limit was taken, and it was assumed that the kinematic invariants were much larger than the masses of the charged fermions. In the next year, the loop corrections were obtained with an n-dimensional projection method [37], where an extension of calculation to the supersymmetric QED was done in massless theory. Later, it was argued that at an energy level as high as that of LHC, which is about 14 TeV, the effect of the mass of heavy quark t is not negligible. An effort was made to explain how to use a so called unitarity-cut methods in the case of massive theories [38]. Soon it was shown that the cross section in the electroweak Standard Model may be calculated generally, through fermion and boson loops. This calculation was done in the framework of SANC system [39]. SANC is a software for the semi-automatic computation of realistic and pseudo-realistic observables at one-loop precision, for various processes of elementary particle interactions. The author obtained the helicities amplitudes expressions of general massive loop particles in high energy limit. Results obtained up to 1971 are reviewed in [40] and more recent developments are summarized in [41].

Measurements [42, 43] of the scattering cross section have been done in order to find the evidence of new light particles. The result, limited by the accuracy of the experiment, gave only an upper limit of the cross section, but it could be a good direction of looking for a deviation from QED. In order to make sure that the scattering amplitudes satisfy the gauge invariance, or the so called Ward–Takahashi identity, we have adopted regularization procedure in our calculations to remove the finite non-gauge-invariant term. This topic was discussed by Khare [44] in 1976. Both of the Pauli-Villars regularization and the dimensional regularization procedure are introduced to our program, and the results obtained from these two methods are identical. Therefore our calculation confirms Khare's conclusion, that the dimensional regularization works well in getting rid of the finite non-gauge-invariant terms.

In 2011, the classic result for the low-energy cross section (2.1.1) has been questioned [1, 2]. In those papers, the cross section is found to be many orders of magnitude larger, since it is not suppressed by powers of (ω/m), but is proportional to $1/\omega^2$,

$$\frac{d\sigma_{\mathrm{FK}}}{d\Omega} = \frac{\alpha^4}{(12\pi)^2\,\omega^2}\left(3 + 2\cos^2\theta + \cos^4\theta\right). \tag{2.1.2}$$

As we will demonstrate in this paper, this claim is incorrect. It has already been pointed out [45] that it contradicts existing laboratory bounds on the the photon-photon cross section, obtained by colliding laser beams. We show in addition that a cross section increasing with the inverse squared energy of the colliding photons limits the mean free path of visible light due to collisions with the cosmic microwave background radiation (CMBR) to less than the distance between Earth and Jupiter. Thus the fact that we can sharply see much more distant astronomical objects proves that the low-energy photon-photon scattering must be significantly suppressed, as predicted by eq. (2.1.1).

The matrix element for the photon-photon scattering is absent at the tree level since photons are neutral. It arises only at the loop level. The sum of all contributing loop diagrams must be finite since there is no parameter in the QED Lagrangian whose renormalization could absorb a divergence. Refs. [1, 2] found an incorrect result because of the assumption that if the sum

of those diagrams is finite, they can be calculated without any regularization. In fact, even though the sum of the diagrams is finite, each of them separately is divergent. Calculating the sum is somewhat delicate and is easiest done with regularized loop integrals (see, however, an alternative calculation in [46] and another point of view on avoiding regularization in [47]).

Interestingly, a similar error [3, 4] has recently cast doubt over the rate of the Higgs boson decay into two photons. That process, too, is loop induced, and the sum of contributing loops is finite. But individual loop integrals are divergent and must be regularized, as has already been thoroughly discussed in this context [48, 49, 50, 51, 52].

2.2 Mean free path of photons in a microwave background

The CMBR is a gas of photons with the spectrum of a black body at a temperature of $1/\beta = 2.725$ K. Here we want to compute how far a visible-light photon with energy $E_\gamma \simeq 2.5$ eV can travel in such a gas before scattering, from the point of view of an observer in whose frame the CMBR is isotropic. (We will call it the LAB frame. For the purposes of this discussion an Earth-based observer is a good approximation.) Consider one mode of the CMBR radiation, characterized by its energy E and inclination angle θ with respect to the direction from which the visible photon is incident. Writing in the plane coordinate, we may choose that one of the photons are travelling along the y direction with a velocity $\vec{v}_1 = (1,0)$, henceforth the other one has a velocity $\vec{v}_2 = (-\cos\theta, \sin\theta)$ (we use the units $c = \hbar = k_B = 1$). The relative velocity of the two photons (as seen in the LAB frame) is $\vec{v}_1 - \vec{v}_2 = (1+\cos\theta, -\sin\theta)$, $|\vec{v}_1 - \vec{v}_2| = 2\cos\frac{\theta}{2}$. In the frame where the total momentum of the photons vanishes, each has the energy ω given by

$$\omega = \frac{1}{2}\sqrt{2EE_\gamma\left(1+\cos\theta\right)} = \cos\frac{\theta}{2}\sqrt{EE_\gamma}. \tag{2.2.1}$$

That energy determines the scattering cross section. Collisions with photons in this particular mode will occur at the rate

$$\mathrm{d}\Gamma_{E\theta} = \left|\vec{v}_1 - \vec{v}_2\right| \sigma \mathrm{d}\rho\left(E\right) \tag{2.2.2}$$

where

$$\mathrm{d}\rho\left(E\right) = \frac{E^2}{2\pi^2}\frac{\mathrm{d}E\mathrm{d}\cos\theta}{\exp\left(\beta E\right)-1} \tag{2.2.3}$$

is the density of CMBR photons with energy E, and σ is the scattering cross section. Integrating over the energies and directions of the CMBR photons we find the mean free path. Between collisions, the visible-light photon will travel on average the distance

$$\lambda = \pi^2\left[\int_0^\infty \mathrm{d}E\int_{-1}^1 \mathrm{d}\cos\theta\cos\frac{\theta}{2}\frac{E^2\sigma}{\exp\left(\beta E\right)-1}\right]^{-1}. \tag{2.2.4}$$

We now consider the two formulas for the low-energy cross section. If we use the classical result (2.1.1), we find the total cross section

$$\sigma\left(\gamma\gamma\to\gamma\gamma\right) = \frac{973\alpha^4\omega^6}{10125\pi m^8}, \tag{2.2.5}$$

and the mean free path

$$\begin{aligned}\lambda &= \pi^2\left[\frac{973\alpha^4E_\gamma^3}{10125\pi m^8}\int_{-1}^1 \mathrm{d}\cos\theta\cos^7\frac{\theta}{2}\int_0^\infty \mathrm{d}E\frac{E^5}{\exp\left(\beta E\right)-1}\right]^{-1}\\ &= \pi^2\left[\frac{973\alpha^4E_\gamma^3}{10125\pi m^8}\cdot\frac{4}{9}\cdot\frac{8\pi^6}{63\beta^6}\right]^{-1} = \frac{820125m^8\beta^6}{4448\pi^3\alpha^4E_\gamma^3}.\end{aligned} \tag{2.2.6}$$

Using $m = 0.511$ MeV we find $\lambda \simeq 7 \cdot 10^{68}$ meters, a distance that would take light about 10^{43} times more time to travel than the age of the Universe. In other words, the CMBR is a rather transparent medium at visible frequencies.

However, if we take instead the cross section suggested in [1, 2], we find from eq. (2.1.2)

$$\sigma_{\rm FK} = \frac{29\alpha^4}{540\pi\omega^2}, \tag{2.2.7}$$

which gives a much shorter mean free path,

$$\begin{aligned} \lambda_{\rm FK} &= \pi^2 \left[\frac{29\alpha^4}{540\pi E_\gamma} \int_{-1}^{1} \frac{{\rm d}\cos\theta}{\cos\frac{\theta}{2}} \int_0^\infty {\rm d}E \frac{E}{\exp(\beta E) - 1} \right]^{-1} \\ &= \pi^2 \left[\frac{29\alpha^4}{540\pi E_\gamma} \cdot 4 \cdot \frac{\pi^2}{6\beta^2} \right]^{-1} = \frac{810\pi\beta^2 E_\gamma}{29\alpha^4}, \end{aligned} \tag{2.2.8}$$

or $\lambda_{\rm FK} = 3 \cdot 10^{11}$ meters, equivalent to about 15 light minutes. For comparison, the orbital radius of Jupiter is about $8 \cdot 10^{11}$ meters. If the mean free path of the visible light were so much shorter than even the radius of Jupiter's orbit, no stars would be visible on the night sky. Clearly, the result eq. (2.1.2) is at odds with experience.

The situation with eq. (2.1.2) is actually even worse. Since the cross section is not suppressed by the mass of the electron, there would be additional positive contributions from other charged fermions that would differ only by the coupling constant, and would further decrease the mean free path. This lack of suppression by the inverse mass of the loop particle contradicts the Appelquist-Carazzone decoupling theorem [53].

2.3 Determination of the photon-photon scattering

In this section we present a derivation of the photon-photon scattering matrix element in two regularization schemes: dimensional and Pauli-Villars. We consider the box diagram shown in Fig. 2.1. External photons carry momenta $k_1, \ldots, k_4$ which we will consider as incoming, $k_1 + k_2 + k_3 + k_4 = 0$.

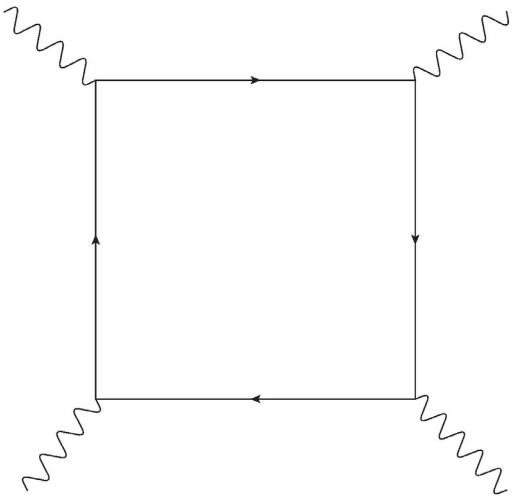


Figure 2.1: Virtual electron loop inducing the four-photon coupling.

There are six ways in which the four momenta can be arranged around the oriented electron loop. However, diagrams that differ only by the direction of the electron line give identical

results so it is enough to compute three of them, corresponding to three cyclic permutations of k_1, k_2, and k_3. (If there was an odd number of photons coupling to the electron loop, the diagrams differing by the direction of the electron would cancel one other, resulting in a vanishing amplitude. This is the theorem due to Furry [54].)

At low energies of external photons it is especially easy to compute the diagrams in Fig. 2.1. We simply Taylor-expand the electron propagators in the external momenta, so that each propagator's denominator becomes simply $(\not{q} - m)^{-1} = (\not{q} + m) / (q^2 - m^2)$ where q is the loop momentum. Such expansion does not lead to any spurious divergences, and commutes with the integration over q. We now explain how this integration is performed in two regularization schemes.

2.3.1 Dimensional regularization

Now that q is present in the denominators only through q^2, also in the numerator we can replace all scalar products of q with other vectors by powers of q^2 times products not involving q,

$$q^{\mu_1} \dots q^{\mu_{2n}} \to \frac{\Gamma\left(\frac{D}{2}\right)}{2^n \Gamma\left(\frac{D}{2}+n\right)} \left(q^2\right)^n S\left(g^{\mu_1\mu_2} \dots g^{\mu_{2n-1}\mu_{2n}}\right). \tag{2.3.1}$$

Here D is the space-time dimension and $S\left(g^{\mu_1\mu_2} \dots g^{\mu_{2n-1}\mu_{2n}}\right)$ is a sum of products of n metric tensors g, totally symmetric in all indices μ_i; it has $(2n-1)!!$ terms. Terms odd in q vanish upon integration.

The powers of q^2 resulting from (2.3.1) can be canceled against the denominators and the loop integration can be completed using

$$\int \frac{\mathrm{d}^D q}{(2\pi)^D} \frac{1}{\left(q^2 - m^2 + i0\right)^a} = \frac{(-1)^a\, i}{(4\pi)^{D/2}} m^{D-2a} \frac{\Gamma\left(a - \frac{D}{2}\right)}{\Gamma(a)}. \tag{2.3.2}$$

Each of the three diagrams contains terms with the exponent $a = 2$, leading to a divergence $\Gamma\left(2 - \frac{D}{2}\right) \sim 1/(D-4)$. The divergences cancel when we add all three contributions. But individual diagrams containing singularities $1/(D-4)$ have also D-dependent factors, arising from the averaging in eq. (2.3.1). The resulting finite contributions *do not* cancel among themselves.

How do these remaining terms depend on m? We remember that they arise from the $a = 2$ sector, therefore they scale like m^0 (the overall dimension of the $\gamma\gamma \to \gamma\gamma$ amplitude). There are other terms that scale with this power, arising from convergent integrals like $m^2 \int \mathrm{d}^4 q / \left(q^2 - m^2\right)^3$. The essential point is that the sum of all m^0 terms, including the remnants of singularities, adds up to zero. The total result for the amplitude turns out to be suppressed by four powers of $1/m$.

2.3.2 Pauli-Villars regularization

Another way of carrying out this calculation is to stay in four dimensions but add another amplitude, with the electron replaced by a very heavy particle of mass M, and with an opposite sign than the electron loop. The calculation proceeds very similarly to the case of dimensional regularization, with two changes. In averaging over the loop momentum directions (2.3.1) we replace $\frac{\Gamma(D+2n-1)}{\Gamma(D)}$ by its value at $D = 4$, $(2n+2)!/6$. The formula for the loop integration (2.3.2) is also replaced by its $D = 4$ value, except in the divergent case $a = 2$. In the dimensional

regularization, this divergent integral gives $m^{D-4}\Gamma\left(2-\frac{D}{2}\right) \to \frac{2}{4-D} - \ln m^2$. In the Pauli-Villars approach one finds a convergent combination

$$\int \frac{\mathrm{d}^4 q}{(2\pi)^4} \left[\frac{1}{\left(q^2 - m^2 + i0\right)^2} - \frac{1}{\left(q^2 - M^2 + i0\right)^2} \right] = \frac{i}{16\pi^2} \ln \frac{M^2}{m^2}. \tag{2.3.3}$$

When the three diagrams are added, this logarithm cancels, but now there are no finite remnants of the singularities. Instead, the m^0 terms from the convergent diagrams are canceled by the M^0 terms from the Pauli-Villars subtraction. Since they are independent of the electron mass, they are the same in the amplitudes with the electron and with the very heavy particle, and cancel in the difference.

In both regularization schemes, the only remaining result is suppressed by the electron mass.

2.3.3 Potential error from neglecting regularization

We have just seen that the regularization is crucial in computing the photon-photon scattering amplitude, even though the final result does not contain divergences. We now want to inspect more closely the part of the amplitude that does not contain external photon momenta, and thus scales like the zeroth power of the electron mass,

$$\begin{aligned} \mathcal{M}_{m^0} \;\sim\; & \int \frac{\mathrm{d}^D q}{\left(q^2 - m^2 + i0\right)^4} \Big[m^4 S_1^{\mu\nu\rho\sigma} + 2m^2 \left(2S_2^{\mu\nu\rho\sigma} - q^2 S_1^{\mu\nu\rho\sigma} \right) \\ & + 24 q^\mu q^\nu q^\rho q^\sigma + \left(q^2\right)^2 S_1^{\mu\nu\rho\sigma} - 4q^2 S_2^{\mu\nu\rho\sigma} \Big] \epsilon_{1\mu} \epsilon_{2\nu} \epsilon_{3\rho} \epsilon_{4\sigma}, \end{aligned} \tag{2.3.4}$$

with

$$\begin{aligned} S_1^{\mu\nu\rho\sigma} &= g^{\mu\nu} g^{\rho\sigma} + g^{\mu\rho} g^{\nu\sigma} + g^{\mu\sigma} g^{\rho\nu}, \\ S_2^{\mu\nu\rho\sigma} &= g^{\mu\nu} q^\rho q^\sigma + \text{five other terms}, \end{aligned}$$

where the terms not shown in S_2 have the other five distributions of indices so that both S_1 and S_2 are totally symmetric in μ, ν, ρ, σ. The second line in (2.3.4) contains four powers of the loop momentum q and thus represents divergent integrals. Without regularization, these divergent integrals simply do not have a meaning. If we apply the averaging procedure (2.3.1) to these terms, we find

$$\begin{aligned} \left\langle S_2^{\mu\nu\rho\sigma} \right\rangle &= \frac{2q^2}{D} S_1^{\mu\nu\rho\sigma}, \\ \left\langle q^\mu q^\nu q^\rho q^\sigma \right\rangle &= \frac{\left(q^2\right)^2}{D\left(D+2\right)} S_1^{\mu\nu\rho\sigma}, \end{aligned} \tag{2.3.5}$$

so that if $D = 4$, the second line of (2.3.4) vanishes, as does the term $\sim m^2$ in its first line. Thus, if the regularization is neglected, one is left with only the first term $m^4 S_1$ which, after the q integration, gives a result independent of the electron mass, scaling like m^0,

$$i\mathcal{M}_{m^0} = -\frac{4}{3}\alpha^2 S_1^{\mu\nu\rho\sigma} \epsilon_{1\mu} \epsilon_{2\nu} \epsilon_{3\rho} \epsilon_{4\sigma} \tag{2.3.6}$$

$$= -\frac{4}{3}\alpha^2 \left(\epsilon_1 \cdot \epsilon_2 \, \epsilon_3 \cdot \epsilon_4 + \epsilon_1 \cdot \epsilon_3 \, \epsilon_2 \cdot \epsilon_4 + \epsilon_1 \cdot \epsilon_4 \, \epsilon_2 \cdot \epsilon_3 \right), \tag{2.3.7}$$

where ϵ_i are the polarization vectors of the four photons. This dependence of the amplitude only on the polarization vectors (and not on the photon momenta) means that the induced coupling of the photons involves only their vector potential (the induced effective operator is proportional to $(A^2)^2$), and not its derivatives. It is not possible to construct such a coupling in a gauge invariant way.

This violation of gauge invariance may also generate photon's mass. For example, if two of the external photon lines in Fig. 2.1 are contracted, the resulting two-loop diagram generates an operator $\sim A^2$, thus giving the photon a mass.

In order to see how the cross section in eq. (2.1.2) follows from the amplitude (2.3.7), we define two transverse polarization vectors for each photon, $\vec{\epsilon}_i^{\,1,2}$, with $\vec{\epsilon}^{\,1}$ perpendicular to the scattering plane and $\vec{\epsilon}^{\,2}$ lying in that plane. We do not include here the longitudinal photon polarizations, present if the photon becomes massive, even though they may dominate the cross section; however, our goal here is merely to explain how the result (2.1.2) is related to the gauge-invariance violating amplitude (2.3.7). For the eq. (2.3.7) to give a non-zero result, each polarization must be represented an even number of times (otherwise there will always be a factor 0 in every term). There are eight possible such polarization assignments, giving the following values of the three terms in (2.3.7),

$$\begin{aligned}
\mathcal{M}_{1111} &\sim 1+1+1, \\
\mathcal{M}_{2222} &\sim 1+\cos^2\theta+\cos^2\theta, \\
\mathcal{M}_{1122} &\sim 1+0+0, \\
\mathcal{M}_{1212} &\sim 0+\cos\theta+0, \\
\mathcal{M}_{1221} &\sim 0+0+\cos\theta,
\end{aligned}$$

and the last three amplitudes enter with a weight factor of 2, due to the symmetry $1 \leftrightarrow 2$. The various amplitudes differ by the polarization of some photons, so they do not interfere. The sum of their squares gives $3^2+(1+2\cos^2\theta)^2+2+4\cos^2\theta = 4\,(3+2\cos^2\theta+\cos^4\theta)$, the angular structure of the (incorrect) result quoted in (2.1.2). In fact, a sum over the polarizations of the final state photons and an average over the polarizations of the initial state photons, leads to the cross section given in eq. (2.1.2).

What went wrong in the above procedure? The formulas (2.3.5) cannot be applied to the divergent integrals in the second line of (2.3.4) in $D=4$, without regularization. If we stay in D dimensions, the terms we found to be zero in the $D \to 4$ limit given finite contributions that cancel against the first term of the integrand, $\sim m^4 S_1$. In this correct treatment the resulting amplitude is suppressed by four powers of $1/m$.

The recent incorrect claim about the decay $H \to \gamma\gamma$ [3, 4] originated with a similar, but somewhat simpler integral. An example of a contribution to that process is shown in Fig. (2.2). There are only three propagators, and the divergent integrals are present in the combination [4]

$$I_{\mu\nu}(D) = \int \mathrm{d}^D q \frac{q^2 g_{\mu\nu} - 4 q_\mu q_\nu}{\left(q^2 - m^2 + i0\right)^3}. \tag{2.3.8}$$

Without dimensional regularization, if we take $D=4$, it seems that this integral vanishes after averaging over q with help of (2.3.1). As we have seen with the example of $\gamma\gamma$ scattering, and as has already been discussed in the literature [50, 48, 47], such manipulations with unregulated, divergent integrals are unjustified. In the case of the Higgs decay, they lead to the incorrect conclusion that $I_{\mu\nu}(D \to 4)$ vanishes. In fact, in the limit of a very heavy Higgs boson, the correct finite result of $I_{\mu\nu}$ gives the most important contribution.

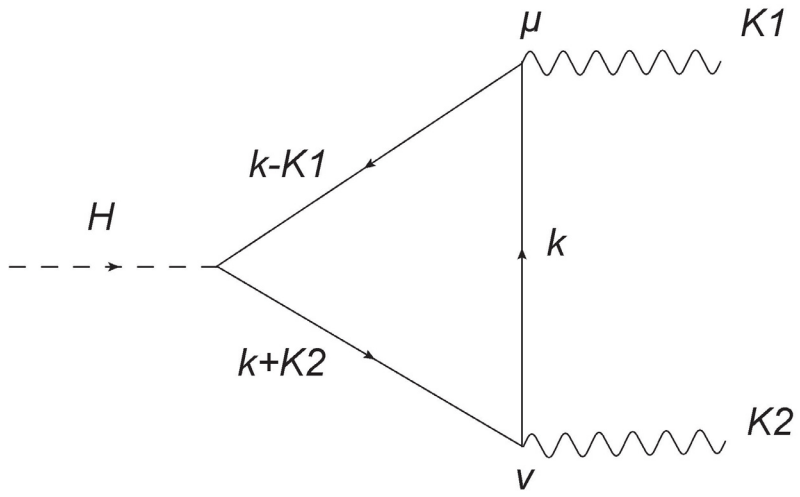


Figure 2.2: An example of a W boson loop mediating the Higgs boson decay into two photons.

2.3.4 Results for polarized photons

The correct result of the loop integration in the $\gamma\gamma \to \gamma\gamma$ amplitude contains scalar products among photon momenta k_i, in addition to the polarization vectors ϵ_i^λ. The effective photon-photon coupling induced in this way is described by operators involving the electromagnetic field tensor and is gauge invariant. We know calculate the scattering cross sections for various polarization situations. Instead of the linear polarizations we have just considered, the scattering amplitudes will be presented in terms of circular polarization states. Thus we introduce

$$\vec{\epsilon}^{\pm} = \frac{1}{\sqrt{2}}\left(\vec{\epsilon}^{1} \pm i\vec{\epsilon}^{2}\right), \tag{2.3.9}$$

describing right- and left-handed polarization states, respectively. There are four possible initial polarization states, but it is sufficient to consider just two of them, $++$ and $+-$. We get three independent scattering amplitudes, $\mathcal{M}_{++++}$, $\mathcal{M}_{+++-}$, and $\mathcal{M}_{++--}$. We describe kinematics in terms of Mandelstam variables $s = (k_1 + k_2)^2 = 4E^2$ and $t = (k_1 + k_3)^2 = -2E^2(1 - \cos\theta)$ and find

$$\begin{aligned} i\mathcal{M}_{++++} &= \frac{2\alpha^2(s^2 + st + t^2)}{15m^4} = \frac{8\alpha^2\omega^4(3 + \cos^2\theta)}{15m^4}, \\ i\mathcal{M}_{+++-} &= -\frac{\alpha^2 st(s + t)}{315m^6} = -\frac{16\alpha^2 \sin^2\theta\omega^6}{315m^6}, \\ i\mathcal{M}_{++--} &= -\frac{11\alpha^2 s^2}{45m^4} = -\frac{176\alpha^2\omega^4}{45m^4}. \end{aligned} \tag{2.3.10}$$

We note that the amplitude $\mathcal{M}_{+++-}$ vanishes at the leading order in E/m expansion at which the other amplitudes are finite. In order to compute it, we have to evaluate two more terms in the Taylor expansion.

All other amplitudes can be obtained from eq. (2.3.10) using space and/or time reversal and the crossing symmetry. For example, $i\mathcal{M}_{+-+-} = -\frac{11\alpha^2 t^2}{45m^4}$ and $i\mathcal{M}_{+--+} = -\frac{11\alpha^2(s+t)^2}{45m^4}$

2.3.5 Total cross section

Once the polarized amplitudes have been evaluated, the unpolarized cross section can be easily found. We quote here only the leading low-energy result (thus we neglect $\mathcal{M}_{+++-}$ and seven amplitudes related to it) for the cross section averaged over initial and summed over final polarizations,

$$\frac{\mathrm{d}\sigma\left(\gamma\gamma\to\gamma\gamma\right)}{\mathrm{d}\Omega} = \frac{1}{256\pi^2\omega^2}\cdot\frac{\left|\mathcal{M}_{++++}\right|^2+\left|\mathcal{M}_{++--}\right|^2+\left|\mathcal{M}_{+-+-}\right|^2+\left|\mathcal{M}_{+--+}\right|^2}{2} \quad (2.3.11)$$

$$= \frac{139\alpha^4\omega^6}{\left(180\pi\right)^2 m^8}\left(3+\cos^2\theta\right)^2, \quad (2.3.12)$$

in agreement with the classic result (2.1.1). When integrated over both θ and ϕ from 0 to π (we integrate only over one hemisphere since the two final-state photons are identical), this gives the total photon-photon scattering cross section,

$$\sigma\left(\gamma\gamma\to\gamma\gamma\right) = \frac{973\alpha^4\omega^6}{10125\pi m^8}, \quad (2.3.13)$$

in agreement with [55]. Other texts seem to have misprints in these results [56, 57].

2.4 Conclusions

We have demonstrated that the recently claimed result for the $\gamma\gamma\to\gamma\gamma$ scattering cross-section (2.1.2) must be wrong. The photon-photon coupling is induced by virtual loops with charged particles and is suppressed at low photon energy by the inverse power of the electron mass. The result (2.1.2) lacks this suppression and yields a very large cross-section, therefore a short mean free path of visible photons even in the rare cosmic microwave radiation background. Such short path would obscure all astronomical objects as close as Jupiter.

We have showed that the error resulted from manipulating unregulated divergent integrals. A similar error misled the authors of [3, 4] in the context of the Higgs decay to two photons. Both processes arise only at the loop level and their amplitudes must be finite, since there are no parameters in the Lagrangian that could absorb a divergence. However, both processes are usually computed from a sum of several diagrams, among which some are divergent. For this reason, a regularization of individual contributions is necessary.

Interestingly, the mistakes in these recent studies of $\gamma\gamma\to\gamma\gamma$ and $H\to\gamma\gamma$ led to confusions about various types of decoupling. The correct result for the former process does respect Appelquist-Carazzone decoupling theorem in the limit of low photon energies or large electron mass, whereas the incorrect result of [1, 2] does not. On the other hand, the correct result for the Higgs decay does not vanish, as one could naively expect, in the limit of large Higgs mass [48] (or, equivalently, low W boson mass; this type of decoupling affects for example quarks but not the longitudinal W components), while part of the reason why [3, 4] believed their result was that it did vanish in that limit.

We have also shown how the $\gamma\gamma\to\gamma\gamma$ amplitude can be calculated in the low-energy regime, and how an expansion in powers of the photon energy to the electron mass ratio can be organized. This tutorial illustrates useful techniques of loop calculations: averaging over loop momentum direction, loop momentum integration, and various regularizations. We hope it will be helpful for other similar loop calculations.

Chapter 3

Expansion by regions

3.1 Introduction

In particle physics when we do the calculations in the framework of perturbation theory, the calculation of a Feynman loop diagram might turn out to be complicated. Usually an amplitude of a process which involves particles cannot be completely treated perturbatively. Fortunately, it has been pointed out [58] that the amplitude can be factorized as a product of factors, which are responsible for contributions of different scales. By an asymptotic expansion of Feynman integrals in the limit of momenta and masses determined by the process condition, one can conveniently factorize the amplitude. In this chapter, we are going to introduce a factorization method based on the expansion by regions strategy. According to this method, a Feynman integral depending on several scales can be calculated by summing the first terms of corresponding expansions. Each term can be written as a product of factors of different scales. In this chapter, we will first get warmed up with two toy examples. In this chapter we first examine the photon self-energy problem, then we will see how the expansion by regions works with a scalar triangle loop. More details concerning the method of expansion by regions can be found in the books [59, 60]. We start from some basic techniques of the calculation of a Feynman loop diagram.

3.2 Feynman parameters

It is quite natural that we encounter a denominator composed of several factors in an integral of a loop diagram calculation. In order to solve the integral, we introduce a method named after Feynman, called Feynman parametrization. The idea of Feynman parametrization is based on the identity

$$\frac{1}{A_1^{m_1} A_2^{m_2}} = \int_0^1 dx\, x^{m_1-1} (1-x)^{m_2-1} \frac{\Gamma(m_1+m_2)}{\Gamma(m_1)\Gamma(m_2)} \frac{1}{(xA_1+(1-x)A_2)^{m_1+m_2}} \tag{3.2.1}$$

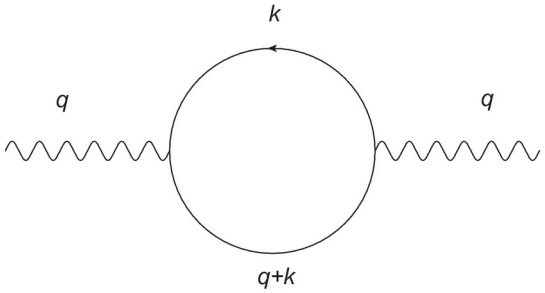
where we may replace the variable x with $\lambda = \frac{1-x}{x}$, and the above equation can be written as

$$\frac{1}{A_1^{m_1} A_2^{m_2}} = \int_0^\infty \frac{\Gamma(m_1+m_2)}{\Gamma(m_1)\Gamma(m_2)} \frac{\lambda^{m_2-1}}{(A_1+\lambda A_2)^{m_1+m_2}} d\lambda \tag{3.2.2}$$

A_1 and A_2 are some propagators in a loop integral calculation. There is only one factor in the denominator of the integrand on the right hand side of above formulas. Therefore the integral can be done more conveniently.

3.3 Photon self-energy

A simple example that will be demonstrated in this section is the calculation of the photon self-energy. A photon self-energy is shown in the diagram below to the first order. The loop is composed of two electron propagators.



The amplitude of this diagram corresponds to the following function

$$i\Pi_2^{\mu\nu}(q) = -(ie)^2 \int \frac{d^D k}{(2\pi)^D} \mathrm{Tr}\left[\gamma^\mu \frac{i(\not{k}+m)}{k^2-m^2} \gamma^\nu \frac{i(\not{k}+\not{q}+m)}{(k+q)^2-m^2}\right], \tag{3.3.1}$$

where e is the charge of the electron. The slashed momenta $\not{k} = \gamma^\mu k_\mu$ and $\not{q} = \gamma^\mu q_\mu$. Tr means taking the trace of the expression in the brackets. In order to compute the finite contribution from this integral, we introduce a trick called asymptotic expansion.

3.3.1 Asymptotic expansion

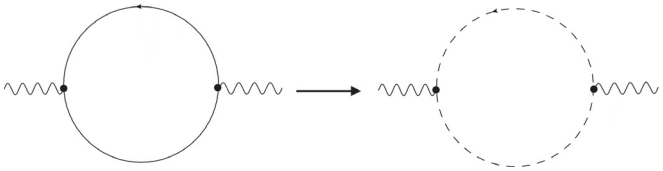
We first consider the region $k \sim q \gg m$, where m is the mass of electron. The next step is to perform a Taylor expansion in the denominator. For the first propagator in (3.3.1) we obtain

$$\frac{1}{k^2-m^2} = \frac{1}{k^2}\left[1 + \frac{m^2}{k^2} + \ldots\right] \tag{3.3.2}$$

For the second propagator, the Taylor expansion is

$$\frac{1}{(k+q)^2 - m^2} = \frac{1}{(k+q)^2}\left[1 + \frac{m^2}{(k+q)^2} - \ldots\right] \tag{3.3.3}$$

Notice that we get rid of the mass term in the denominator, and turn it into a series of massless propagators with positive powers of mass as the coefficients. This procedure can also be demonstrated by the topology below



where the second diagram is the representation of the photon self-energy with massless propagators. Doing the integration using general integral formulae, and the aid of dimensional regularization, we obtain the contribution of this region

$$\Pi^{\mu\nu}_{2a}(q) = \Pi^a\left(q^2\right)\left(g_{\mu\nu} - \frac{q_\mu q_\nu}{q^2}\right), \tag{3.3.4}$$

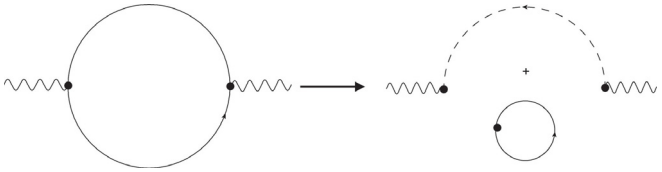
where if we keep only terms up to the forth power of m

$$\Pi^a\left(q^2\right) = \frac{\alpha}{4\pi}\left(-\frac{4}{3}\frac{q^2}{\epsilon} - \frac{20}{9}q^2 + \frac{8}{3}\ln q\, q^2 - 8m^2 + \frac{8m^4}{q^2\epsilon} + \frac{8m^4}{q^2} - 16\ln q\frac{m^4}{q^2}\right) \tag{3.3.5}$$

Notice that the expression of the amplitude (3.3.4) satisfies the Ward identity. Next, let us compute the integral in the region $k \sim m \ll q$. Similarly, we perform a Taylor expansion on the denominator. Since both k and m are small quantities, the first propagator $\frac{1}{k^2-m^2}$ in (3.3.1) need not be expanded. The second propagator can be expanded as follows

$$\frac{1}{(k+q)^2 - m^2} = \frac{1}{q^2}\left[1 - \frac{k^2 + 2k\cdot q - m^2}{q^2} + \ldots\right] \tag{3.3.6}$$

This Taylor expansion can also be represented by following topologies



The amplitude in this region is

$$\Pi^{\mu\nu}_{2b}(q) = \Pi^b\left(q^2\right)\left(g_{\mu\nu} - \frac{q_\mu q_\nu}{q^2}\right), \tag{3.3.7}$$

where if we keep only terms up to the forth power of m

$$\Pi^b\left(q^2\right) = \frac{\alpha}{4\pi}\left(-4\frac{m^4}{q^2\epsilon} - 6\frac{m^4}{q^2} + 8\ln m\frac{m^4}{q^2}\right) \tag{3.3.8}$$

Since there are two propagators, we have two ways to decouple the loop. Therefore, the amplitude from the second limit needs to be multiplied by 2. We then obtain the expression of the total amplitude

$$\begin{aligned}
\Pi^{\mu\nu}_2(q) &= \left(\Pi^a\left(q^2\right) + 2\Pi^b\left(q^2\right)\right)\left(g_{\mu\nu} - \frac{q_\mu q_\nu}{q^2}\right) \\
&= \frac{\alpha}{4\pi}\left[-\frac{4}{3}\frac{q^2}{\epsilon} - \frac{4m^4}{q^2} - \frac{20}{9}q^2 - 8m^2 - 8\frac{m^4}{q^2}\ln\frac{q^2}{m^2} + \frac{8}{3}\ln m\, q^2\right]\left(g_{\mu\nu} - \frac{q_\mu q_\nu}{q^2}\right) \\
&= \Pi^2\left(q^2\right)\left(g_{\mu\nu} - \frac{q_\mu q_\nu}{q^2}\right)
\end{aligned} \tag{3.3.9}$$

Notice there still is one divergent term in this expression. In order to remove this divergence, we need to introduce the renormalization procedure.

3.3.2 Renormalization

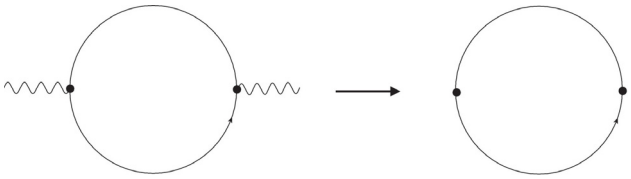
In order to renormalize the amplitude, we replace the $\Pi_2(q^2)$ by the following renormalized expression [57]

$$\Pi_{2R}(q^2) = \Pi_2(q^2) - \Pi_2(0) - q^2 \left(\frac{\partial \Pi_2^2(q^2)}{\partial q^2}\right)_{q^2=0} \tag{3.3.10}$$

In order to find out the expressions for $\Pi_2^2(0)$ and $q^2 \left(\frac{\partial \Pi_2^2(q^2)}{\partial q^2}\right)_{q^2=0}$, we may start with the general integral (3.3.1) of $\Pi_2(q^2)$, with the aid of a Taylor expansion in q^2. The first and second terms are just $\Pi_2(0)$ and $q^2 \left(\frac{\partial \Pi_2^2(q^2)}{\partial q^2}\right)_{q^2=0}$. This can be achieved by doing a Taylor expansion on the denominator

$$\frac{1}{(k+q)^2 - m^2} = \frac{1}{k^2 - m^2}\left[1 - \frac{2k\cdot q + q^2}{k^2 - m^2} + \ldots\right], \tag{3.3.11}$$

which corresponds to a following topology



The amplitude obtained after this expansion is

$$\Pi_{2\,\mu\nu}(q^2) \simeq \frac{\alpha}{4\pi}\left(-\frac{4}{3}\frac{q^2}{\epsilon} + \frac{8}{3}\ln m\, q^2\right)\left(g_{\mu\nu} - \frac{q_\mu q_\nu}{q^2}\right) \tag{3.3.12}$$

Hence $\Pi_2(0) = 0$, and $q^2 \left(\frac{\partial \Pi_2^2(q^2)}{\partial q^2}\right)_{q^2=0} = \frac{q^2\alpha}{3\pi\epsilon}$.

3.3.3 Results

According to (3.3.9) and (3.3.10), we obtain the renormalized amplitude

$$\Pi_{2R}(q^2) = \frac{\alpha}{4\pi}\left(-\frac{4m^4}{q^2} - \frac{20}{9}q^2 - 8m^2 - 8\frac{m^4}{q^2}\ln\frac{q^2}{m^2} + \frac{8}{3}\ln\frac{q}{m}\,q^2\right) \simeq \frac{\alpha}{3\pi}\left(\ln\frac{q^2}{m^2}\,q^2 - \frac{5}{3}q^2\right) \tag{3.3.13}$$

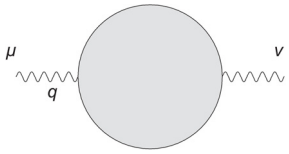
Therefore, we have a finite form of the amplitude for the photon self-energy

$$\begin{aligned}\Pi_{2\,\mu\nu}(q) &= \Pi_{2R}(q^2)\left(g_{\mu\nu} - \tfrac{q_\mu q_\nu}{q^2}\right)\\ &\simeq \tfrac{\alpha}{3\pi}\left(\ln\tfrac{q^2}{m^2}\,q^2 - \tfrac{5}{3}q^2\right)\left(g_{\mu\nu} - \tfrac{q_\mu q_\nu}{q^2}\right)\end{aligned} \tag{3.3.14}$$

which agrees with the result from text books [57].

3.3.4 Interpretation: running coupling constant

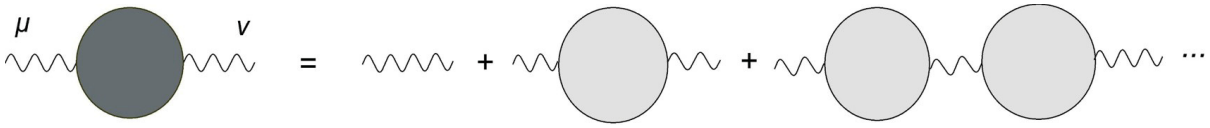
In order to find the total contribution to the photon self-energy, we need to sum all 1-particle-irreducible insertions into the photon propagator. Now let us define the general self-energy insertions as $i\Pi^{\mu\nu}\left(q^2\right)$, which corresponds to a diagram



The $\Pi_{2\,\mu\nu}\left(q^2\right)$ we discussed previously is the electron second-order contribution to the $\Pi_{\mu\nu}\left(q^2\right)$. Similar to what happens in the electron loop, the tensor structure of the $\Pi_{\mu\nu}$ has the form

$$\Pi_{\mu\nu}\left(q^2\right)=\Pi\left(q^2\right)\left(g_{\mu\nu}-\frac{q_\mu q_\nu}{q^2}\right) \tag{3.3.15}$$

The exact photon two-point function can be written as a series of $\Pi\left(q^2\right)$ as shown by the following graph



The right hand side of the above graph can be expressed in the following way

$$\begin{aligned}&\frac{-ig_{\mu\nu}}{q^2}+\frac{-ig_{\mu\rho}}{q^2}\left(g^{\rho\sigma}-\frac{q_\rho q_\sigma}{q^2}\right)i\Pi\left(q^2\right)\frac{-ig_{\sigma\nu}}{q^2}+\cdots\\&=\frac{-ig_{\mu\nu}}{q^2}+\frac{-ig_{\mu\rho}}{q^2}\Delta_\nu^\rho\frac{\Pi\left(q^2\right)}{q^2}+\frac{-ig_{\mu\rho}}{q^2}\Delta_\sigma^\rho\Delta_\nu^\sigma\left(\frac{\Pi\left(q^2\right)}{q^2}\right)^2,\end{aligned} \tag{3.3.16}$$

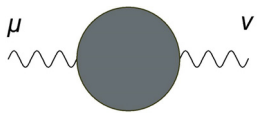
where

$$\Delta_\nu^\rho\equiv g_\nu^\rho-\frac{q^\rho q_\nu}{q^2} \tag{3.3.17}$$

Since $\Delta_\sigma^\rho\Delta_\nu^\sigma=\Delta_\nu^\rho$, we may write (3.3.16) into a more compact form

$$\begin{aligned}&\tfrac{-ig_{\mu\nu}}{q^2}+\tfrac{-ig_{\mu\rho}}{q^2}\left(g_\nu^\rho-\tfrac{q^\rho q_\nu}{q^2}\right)\left[\tfrac{\Pi\left(q^2\right)}{q^2}+\left(\tfrac{\Pi\left(q^2\right)}{q^2}\right)^2+\cdots\right]\\&=\tfrac{-i}{q^2\left(1-\frac{\Pi\left(q^2\right)}{q^2}\right)}\left(g_{\mu\nu}-\tfrac{q_\mu q_\nu}{q^2}\right)+\tfrac{-i}{q^2}\left(\tfrac{q_\mu q_\nu}{q^2}\right)\end{aligned}$$

At least one end of this propagator is connected to a fermion line in a S-matrix element. According to the Ward identity, the summation of the propagator over all places along the line removes all the terms proportional to q_μ and q_ν. Hence, in the computation of the S-matrix element, we may introduce an abbreviated expression of the exact photon two-point function $\frac{-ig_{\mu\nu}}{q^2(1-\Pi(q^2))}$ corresponding to the following diagram



Now let us see how the fine structure constant α in QED is altered by the vacuum polarizations. Suppose that we only take the leading order in α by taking $\Pi\left(q^2\right)\simeq\Pi_2\left(q^2\right)$. Then the amplitude of the process is proportional to

$$\frac{-ig_{\mu\nu}}{q^2}\frac{e_0^2}{\left(1-\frac{\Pi(q^2)}{q^2}\right)}, \tag{3.3.18}$$

where e_0 is the so called "bare" charge. This can be interpreted as the effect of replacing the original fine structure constant with an effective $\alpha_{\text{eff}}(q^2)$ as a function of q^2

$$\alpha_0 \to \alpha_{\text{eff}}\left(q^2\right) = \frac{e_0^2/4\pi}{1-\frac{\Pi_R^2(q^2)}{q^2}} = \frac{\alpha}{1-\frac{1}{q^2}\left(\Pi^2(q^2)-\Pi^2(0)-q^2\left(\frac{\partial\Pi^2(q^2)}{\partial q^2}\right)_{q^2=0}\right)}$$
$$= \frac{\alpha}{1-\frac{1}{q^2}\frac{\alpha}{3\pi}\left(\ln\frac{q^2}{m^2}q^2-\frac{5}{3}q^2\right)} = \frac{\alpha}{1-\frac{\alpha}{3\pi}\left(\ln\frac{q^2}{m^2}-\frac{5}{3}\right)}, \tag{3.3.19}$$

where we have used the expression for $\Pi_R^2(q^2)$ in the large q limit (3.3.14)

3.3.5 Effective fine structure constant

Considering the second order QED and QCD corrections to the fine structure constant α, we include loops composed with the following particles

Name	Mass [MeV]	Charge Q	Color factor N_c
e	0.511	-1	1
μ	106	-1	1
τ	1770	-1	1
u	300	$+\frac{2}{3}$	3
d	300	$-\frac{1}{3}$	3
s	490	$-\frac{1}{3}$	3
c	1550	$+\frac{2}{3}$	3
b	4700	$-\frac{1}{3}$	3

Table 3.1: Fermions contributing to the photon self-energy

where the masses of the quarks are the effective masses [61]. A common laboratory energy scale is the rest mass of Z^0 boson, which is 91 GeV. In order to calculate an α_{eff} value as an example, we take q^2 equals to 91 GeV, and sum all these contributions. According to (3.3.19), we obtain the effective fine structure constant

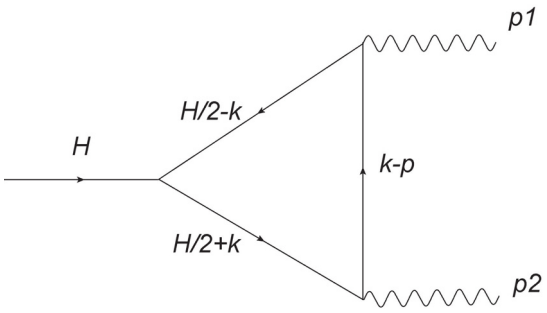
$$\alpha_{\text{eff}}(q^2) = \frac{\alpha}{1-\frac{\alpha}{3\pi}\sum_f N_{cf}Q_f^2\ln\frac{q^2}{m_f^2}} \approx \alpha\left(1+\frac{\alpha}{3\pi}\sum_f N_{cf}Q_f^2\ln\frac{q^2}{m_f^2}\right) \tag{3.3.20}$$

Note that the summation is over all kinds of particles listed in the tables above. The factor Q_f^2 comes from the fact that the loop correction from a certain particle is proportional to Q_f^2, according to the general formula for computation of the photon self-energy (3.3.1). Now taking the energy of the photon to be 91 GeV, then the α_{eff} at this energy is

$$\alpha_{\text{eff}}(91\,\text{GeV}) = \frac{1}{128.9} \tag{3.3.21}$$

3.4 Scalar loop

In Chapter 4, we will study the decay of the Higgs into photons. In order to prepare for it, we present in this Section a calculation of the Feynman diagram that we will need. We use the calculation of a scalar triangular loop as our second example. The Feynman diagram of this process is presented in the following graph



In order to make our argument simpler, we make an assumption that the masses of all the three propagators are identical. These masses are denoted as m. We further assume that the mass of the incoming particle is much larger than the mass of the loop particle $M \gg m$, and the two out-going particles are massless, which means we have $p_1^2 = 0$ and $p_2^2 = 0$. k is the loop momentum. Henceforth, the integrand of this diagram can be written as

$$D_0 \equiv \frac{1}{\left(k^2 - m^2 + i0\right)\left[(k+p_2)^2 - m^2 + i0\right]\left[(k-p_1)^2 - m^2 + i0\right]} \tag{3.4.1}$$

according to our Feynman diagram. The next step is doing the Feynman parametrization (3.2.1). We combine the last two factors of the denominator

$$\begin{aligned}
&\frac{1}{\left[(k+p_2)^2 - m^2 + i0\right]\left[(k-p_1)^2 - m^2 + i0\right]} \\
&= \int_0^1 dx \, \frac{1}{\left(x\left[(k+p_2)^2 - m^2 + i0\right] + (1-x)\left[(k-p_1)^2 - m^2 + i0\right]\right)^2} \\
&= \int_0^1 dx \, \frac{1}{\left(k^2 + 2xk\cdot(p_2+p_1) - 2k\cdot p_1 - m^2 + i0\right)^2}
\end{aligned}$$

Then the total expression may be further derived with the aid of another form of Feynman parameters (3.2.2)

$$\begin{aligned}
D_0 &= \frac{1}{\left(k^2 - m^2 + i0\right)\left[(k+p_2)^2 - m^2 + i0\right]\left[(k-p_1)^2 - m^2 + i0\right]} \\
&= \int_0^1 dx \, \frac{1}{\left(k^2 - m^2 + i0\right)\left(k^2 + 2xk\cdot(p_2+p_1) - 2k\cdot p_1 - m^2 + i0\right)^2} \\
&= \frac{1}{B(2,1)} \int_0^1 dx \int_0^1 dy \frac{y}{\left\{y\left[k^2 + 2xk\cdot(p_2+p_1) - 2k\cdot p_1 - m^2 + i0\right] + (1-y)\left(k^2 - m^2 + i0\right)\right\}^3} \\
&= \frac{1}{B(2,1)} \int_0^1 dx \int_0^1 dy \frac{y}{\left(K^2 - U^2 + i0\right)^3},
\end{aligned}$$

where we have introduced a group of new variables

$$K = k + Q; \tag{3.4.2}$$

$$Q = xy(p_2 + p_1) - yp_1; \tag{3.4.3}$$

$$U^2 = Q^2 + m^2 = m^2 - x(1-x)y^2M^2. \tag{3.4.4}$$

Therefore, the general integral with D is

$$
\begin{aligned}
I &\equiv \int \frac{d^D k}{(2\pi)^D} D_0 \\
&= \frac{1}{B(2,1)} \int \frac{d^D k}{(2\pi)^D} \int_0^1 dx \int_0^1 dy \frac{y}{\left(K^2 - U^2 + i0\right)^3} \qquad (3.4.5) \\
&= -i \frac{1}{B(2,1)} \int \frac{d^D k}{(2\pi)^D} \int_0^1 dx \int_0^1 dy \frac{y}{\left(K^2 + U^2 - i0\right)^3} \\
&= -i \frac{1}{B(2,1)} \int_0^1 dx \int_0^1 dy\, y \frac{1}{(4\pi)^{D/2}} \frac{\Gamma\left(3 - \frac{D}{2}\right)}{\Gamma(3)} \left(\frac{1}{U^2 - i0}\right)^{3-\frac{D}{2}} \qquad (3.4.6) \\
&= -i \frac{\Gamma(1+\epsilon)}{(4\pi)^{D/2}} \int_0^1 dx \int_0^1 dy \frac{y}{\left(m^2 - x(1-x) y^2 M^2\right)^{1+\epsilon}} \qquad (3.4.7) \\
&= \frac{-i}{(4\pi)^2 m^2} \int_0^1 dx \int_0^1 dy \frac{y}{1 - x(1-x) y^2 \frac{M^2}{m^2} - i0} \qquad (3.4.8)
\end{aligned}
$$

Then the denominator with a small factor $i0$ of the integrand can be written into a principle term plus a imaginary term as following

$$
\frac{1}{1 - x(1-x) y^2 \frac{M^2}{m^2} - i0} = PV \frac{1}{1 - x(1-x) y^2 \frac{M^2}{m^2}} + i\pi\delta\left(1 - x(1-x) y^2 \frac{M^2}{m^2}\right) \qquad (3.4.9)
$$

3.4.1 The principal value

We first consider the real part of the calculation, which can be calculated by integral of the principle value of the denominator given in (3.4.9). In order to simplify the calculation, we may introduce a new set of parameters by letting $a = \frac{M^2}{m^2}$, and $\beta = \frac{4m^2}{M^2} = \frac{4}{a}$. Since we are assuming $M^2 \gg m^2$, we know that $\beta \leq 1 \Longleftrightarrow a \geq 4$. Then the integral with x and y can be written into

$$
\int_0^1 dx \int_0^1 dy \frac{y}{1 - x(1-x) y^2 \frac{M^2}{m^2}} = \frac{1}{2} \int_0^1 dx \int_0^1 dy^2 \frac{1}{1 - ax(1-x) y^2}
$$

Setting $z = y^2$ we may write the integral of $\int_0^1 dy^2$ as

$$
\int_0^1 dy^2 \frac{1}{1 - ax(1-x) y^2} = \frac{1}{ax(x-1)} \ln \left| ax(1-x) z - 1 \right|_{z=0}^1 ,
$$

Now let the denominator equal to zero, and solve the corresponding equation

$$
ax(1-x) - 1 = 0 \qquad (3.4.10)
$$

The solutions corresponding to two poles are

$$
\begin{cases}
x_+ = \frac{1 + \sqrt{1 - \frac{4}{a}}}{2} \\
x_- = \frac{1 - \sqrt{1 - \frac{4}{a}}}{2},
\end{cases}
$$

The integration interval is divided by these values into three regions, $(0,\, x_1)$, $(x_1,\, x_2)$, and $(x_2,\, 1)$. First, notice if $x \in (0,\, x_1)$ or $x \in (x_2,\, 1)$, then $ax(1-x) < 1$. Hence, $ax(1-x) z - 1$ is always negative, and there is no restriction on the integral interval of dy. The integral can be obtained easily as

$$
\int_0^1 dy^2 \frac{1}{1 - ax(1-x) y^2} = \frac{1}{ax(x-1)} \ln\left[1 - ax(1-x)\right] \qquad (3.4.11)
$$

However, if $x \in (x_1,\, x_2)$, then $ax\,(1-x) \geq 1$, it is possible that $0 < \frac{1}{ax(1-x)} \leq z < 1$. This means that there is a pole of the integral with $dz = dy^2$. In order to calculate a finite value from this integration, we introduce a small value parameter ϵ to shift the integral boundary at the pole. Then this parameter will be cancelled in the summation of the contributions from the two regions, and a finite result will be obtained

$$\begin{aligned}
&\int_0^1 \frac{dy^2}{1-ax\,(1-x)\,y^2} = \lim_{\epsilon\to 0}\left(\int_0^{l-\epsilon} + \int_{l+\epsilon}^1\right)\frac{dy^2}{1-ax\,(1-x)\,y^2} \\
&= \lim_{\epsilon\to 0}\left(\frac{1}{ax\,(x-1)}\ln\left[1-ax\,(1-x)\,z\right]\Big|_{z=0}^{l-\epsilon} + \frac{1}{ax\,(x-1)}\ln\left[ax\,(1-x)\,z-1\right]\Big|_{z=l+\epsilon}^{1}\right) \\
&= \frac{1}{ax\,(x-1)}\ln\left[ax\,(1-x)\,\epsilon\right] + \frac{1}{ax\,(x-1)}\ln\left[\frac{ax\,(1-x)-1}{ax\,(1-x)\,\epsilon}\right] \\
&= \frac{1}{ax\,(x-1)}\ln\left[ax\,(1-x)-1\right], \qquad (3.4.12)
\end{aligned}$$

where $l = \frac{1}{ax(1-x)}$ is the pole of the integral with dy^2. In the end, the double integral is calculated by a summation over all three zones

$$\begin{aligned}
&\int_0^1 dx\int_0^1 dy\frac{y}{1-x\,(1-x)\,y^2\frac{M^2}{m^2}} = \frac{1}{2}\int_0^1 dx\int_0^1 dy^2\frac{1}{1-ax\,(1-x)\,y^2} \\
&= \frac{1}{2}\left\{\left(\int_0^{x_1} dx + \int_{x_2}^1 dx\right)\frac{1}{ax\,(x-1)}\ln\left[1-ax\,(1-x)\right] + \int_{x_1}^{x_2}\frac{1}{ax\,(x-1)}\ln\left[ax\,(1-x)-1\right]\right\} \qquad (3.4.13)
\end{aligned}$$

The result of this integral can be computed in Mathematica. It is

$$\begin{aligned}
I_R &= \frac{-1}{(4\pi)^2 m^2}\frac{-\beta}{2}\left(\frac{1}{4}\ln^2\left[\frac{1-\sqrt{1-\beta}}{1+\sqrt{1-\beta}}\right]\right) + \frac{7\beta}{48}\pi^2 + \frac{\beta}{16}\ln^2\left[\frac{4}{\beta}\left(\frac{1-\sqrt{1-\beta}}{2}\right)^2\right] \\
&- \frac{\beta}{16}\ln^2\left[\frac{1+\sqrt{1-\beta}}{2}\right] - \frac{\beta}{16}\ln^2\left[\frac{4}{\beta}\frac{1+\sqrt{1-\beta}}{2}\right] \\
&- \frac{\beta}{8}\left(\mathrm{Li}_2\left[\frac{1+\sqrt{1-\beta}}{2}\right] + \mathrm{Li}_2\left[\frac{\beta}{2\left(1+\sqrt{1-\beta}\right)}\right]\right) \\
&= \frac{-1}{(4\pi)^2 m^2}\left(\frac{\pi^2\beta}{8} - \frac{\ln^2 4}{8}\beta + \frac{\ln 4}{8}\beta^2 - \frac{\beta^3}{32} + \frac{3}{64}\ln 4\beta^3\right. \\
&\left. + \frac{\ln 4}{4}\beta\ln\beta - \frac{1}{8}\ln\beta\beta^2 - \frac{3}{64}\ln\beta\beta^3 - \frac{1}{8}\beta\ln^2\beta + \cdots\right) \\
&= \frac{-1}{(4\pi^2)\,M^2}\left[\frac{\pi^2}{2} - \frac{1}{8}\left(2\ln\frac{4}{\beta} - \beta\right)^2 + \frac{3}{16}\beta^2\ln\frac{4}{\beta} + \cdots\right] \\
&= \frac{-1}{2\,(4\pi^2)\,M^2}\left[\pi^2 - \ln^2\frac{m^2}{M^2} - 4\frac{m^2}{M^2}\ln\frac{m^2}{M^2} - 4\left(\frac{m^2}{M^2}\right)^2 + \cdots\right] \qquad (3.4.14)
\end{aligned}$$

3.4.2 The $i\pi\delta\left(1-x\left(1-x\right)y^2\frac{M^2}{m^2}\right)$ integral

Adopting the same procedure, the integral with the delta function can be written

$$\begin{aligned}
&\frac{1}{\left(4\pi\right)^2 m^2} i\pi \int_0^1 dx \int_0^1 dy \delta\left(1-x\left(1-x\right)y^2\frac{M^2}{m^2}\right) y \\
&= \frac{1}{\left(4\pi\right)^2 m^2} \frac{i\pi}{2} \int_0^1 dx \int_0^1 dz \delta\left(1-x\left(1-x\right)az\right) \\
&= \frac{i\pi}{2} \frac{1}{\left(4\pi\right)^2 m^2} \int_0^1 dx \int_0^1 dz \frac{\delta\left(z-z_0\right)}{x\left(1-x\right)a},
\end{aligned} \tag{3.4.15}$$

where $z_0 = \frac{1}{x(1-x)a}$, and $0 < z_0 < 1$ only if $x \in (x_1,\, x_2)$. So the integral turns out to be

$$\begin{aligned}
&\frac{-1}{\left(4\pi\right)^2 m^2} \frac{i\pi}{2} \int_0^1 dx \int_0^1 dz \frac{\delta\left(z-z_0\right)}{x\left(1-x\right)a} = \frac{i\pi}{2} \int_{x_1}^{x_2} dx \frac{1}{x\left(1-x\right)a} \\
&= \frac{-1}{\left(4\pi\right)^2 m^2} \frac{i\pi}{a} \ln\frac{x_2}{x_1} = \frac{i\pi\beta}{4} \ln\frac{1+\sqrt{1-\beta}}{1-\sqrt{1-\beta}} \\
&= \frac{-i}{\left(4\pi\right)^2 m^2} \left(\frac{\beta\pi}{4}\ln 4 - \frac{\beta\pi}{4}\ln\beta - \frac{\beta^2\pi}{8} - \frac{3\beta^3\pi}{64} + \cdots\right) \\
&= \frac{-i}{4\pi^2 M^2} \left(\frac{\pi}{4}\ln\frac{4}{\beta} - \frac{\beta\pi}{8} - \frac{3\pi\beta^2}{64} + \cdots\right) \\
&= \frac{i}{\left(4\pi\right)^2 M^2} \left(\pi\ln\frac{m^2}{M^2} + \frac{2\pi m^2}{M^2} + \frac{3\pi m^4}{M^4} + \cdots\right)
\end{aligned} \tag{3.4.16}$$

3.5 Verification of the result with FF

FF [62] is a package created for the calculation of one-loop integrals in the calculation of the radiative corrections. It is a library based on FormF by M.Veltman [63]. We use FF to verify our derivations above.

The FF package basically contains four kind of routines. The first kind of them is the high-level callable routine, such as $ffxd0$. Then there are routines specially designed for dot production, such as $ffdot4$. There are also the determinant routines, which are the routines for obtaining combinations of dilogarithms. The third kind of routines are called low-level routines, for example the logarithms, dilogarithms functions. The last kind of routines are called support routines, for instance, the initialization, and the error and warning system etc.

3.5.1 Scalar n-point functions

There are two types of functions in the evaluation of the scalar loop. One was designed for the situation where all the parameters are real, the other was designed for the amplitude with one or more complex parameters. The one-point function $ca0 = A_0\left(m^2\right) = \frac{1}{i\pi^2}\int d^nQ/\left(Q^2-m^2\right)$ is a trivial function with only one argument. Likewise, the two-point function $cb0 = B_0\left(m_a^2, m_b^2, k^2\right)$ is a function with three variables. In our calculation of the scalar loop, what we are interested in is the three point function $cc0 = C_0\left(m_1^2, m_2^2, m_3^2, p_1^2, p_2^2, p_3^2\right)$.

The array xpi should contain the internal masses squared in positions 1–3, and the external momenta squared in 4–6. The momentum xpi(4) = p21 is the one between xpi(1) = m21 and

xpi(2) = m22 , and so on cyclically. The routine rotates the diagram to the best position. Thus only the swap between m21 & m23 , and p21 & p22 can be used to test the accuracy. Here is the main file of the FF code we use to do the check,

```
 program testff include 'ff.h' call form end subroutine
FORM implicit DOUBLE PRECISION (A-H,O-Z) DOUBLE COMPLEX TADMU DOUBLE
COMPLEX AA0,B0,B0PM,B1,B1PM,B2,C0,C1,C2,C3,D0,D1,D2,D3,D4 COMMON PX(6),RM(4),DEL
COMMON B0,B0PM,B1,B1PM,B2(2),C0,C1(2),C2(4),C3(6) COMMON D0,D1(3),D2(7),D3(13),D4(22)
integer ier DOUBLE COMPLEX cc0, cpi(6) DOUBLE PRECISION xpi(6)\par xpi(1)=1.d0
xpi(2)=1.d0 xpi(3)=1.d0 xpi(4)=0.d0 xpi(5)=10.d0 xpi(6)=0.d0 cpi(1)=1.d0
cpi(2)=1.d0 cpi(3)=1.d0 cpi(4)=0.d0 cpi(5)=10.d0 cpi(6)=0.d0\par CALL
ffcc0(cc0,cpi,ier) PRINT {*},cc0 CALL ffexi STOP END
```

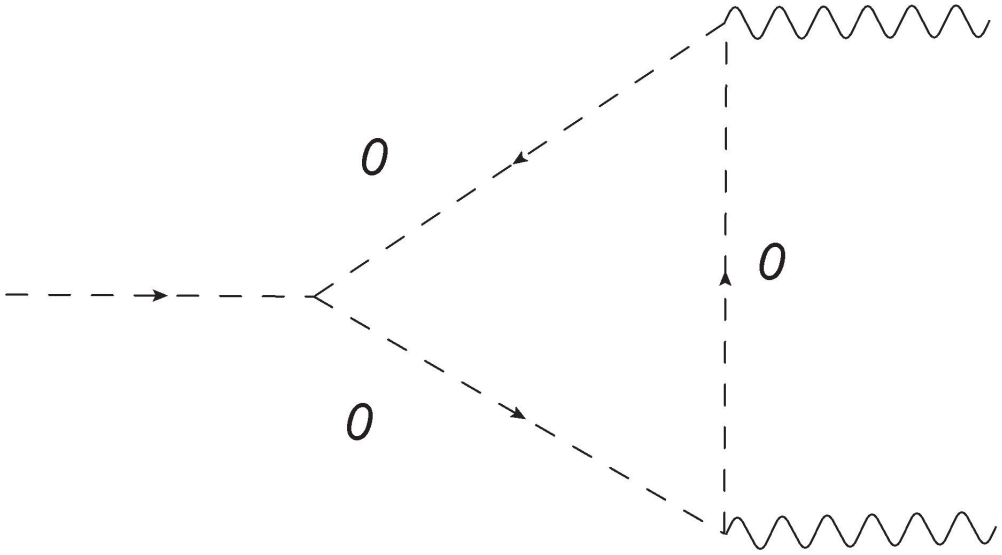
The result given by FF does agree with the result derived in above sections.

3.6 Expansion by regions

Now, after practice our calculation skill with two examples, we want to introduce the expansion by regions method in this section. We would like to reproduce the exact solution of the triangular loop obtained in last section, using expansions.

3.6.1 The hard region

Our primary task is to find out all relevant regions in the problem. Let us start with the hard region, where the propagator momentum are much larger than its mass m, which allow us to do the Taylor expansion with m. The leading term corresponds to the following Feynman diagram



In order to make our illustration more straightforward, we will only present the calculations of the leading term of each region from now on. The more general calculations for other terms can be easily obtained by extending our derivation of leading terms. In the hard region, we expand the three factors in the denominator separately to calculate a full expansion

$$\begin{aligned}
\frac{1}{k^2-m^2+i0} &= \frac{1}{k^2+i0}\left[1+\frac{m^2}{k^2+i0}+\cdots\right] \\
\frac{1}{(k-p_1)^2-m^2+i0} &= \frac{1}{(k-p_1)^2+i0}\left[1+\frac{m^2}{(k-q)^2+i0}+\cdots\right] \\
\frac{1}{(k+p_2)^2-m^2+i0} &= \frac{1}{(k+p_2)^2+i0}\left[1+\frac{m^2}{(k+p_2)^2+i0}+\cdots\right],
\end{aligned}$$

The leading term of the integrand is in the following form (considering $p_1^2=p_2^2=0$)

$$D_h = \frac{1}{[k^2-2p_1\cdot k+i0]\,[k^2+2p_2\cdot k+i0]\,[k^2+i0]} \tag{3.6.1}$$

Now using the Feynman parameter that we introduced in (3.2.1), the first two factors can be combined

$$\begin{aligned}
&\frac{1}{[k^2-2p_1\cdot k+i0]\,[k^2+2p_2\cdot k+i0]} \\
&= \int_0^1 dx\,\frac{1}{[x\,(k^2-2k\cdot p_1+i0)+(1-x)\,(k^2+2p_2\cdot k+i0)]} \\
&= \int_0^1 dx\,\frac{1}{[k^2-2xk\cdot p_1+2\,(1-x)\,p_2\cdot k+i0]^2}.
\end{aligned} \tag{3.6.2}$$

Then again we Feynman parametrize the new denominator with the third factor, with the relation (3.2.1)

$$\begin{aligned}
&\frac{1}{\left[k^2-2p_1\cdot k+i0\right]\left[k^2+2p_2\cdot k+i0\right]\left[k^2+i0\right]}\\
&=\int_0^1 dx\,\frac{1}{\left[k^2-2xk\cdot p_1+2\left(1-x\right)p_2\cdot k+i0\right]^2\left[k^2+i0\right]}\\
&=2\int_0^1 dx\int_0^1 dy\,y\frac{1}{\left[k^2-2\left(xyp_1-y\left(1-x\right)p_2\right)\cdot k+i0\right]^3}\\
&=2\int_0^1 dx\int_0^1 dy\,y\frac{1}{\left[K^2-Q^2+i0\right]^3},
\end{aligned}\tag{3.6.3}$$

where we have introduced a group of new variables

$$K=k-Q,\tag{3.6.4}$$

$$Q=xyp_1-y\left(1-x\right)p_2,\tag{3.6.5}$$

$$Q^2=-x\left(1-x\right)y^2M^2.\tag{3.6.6}$$

Finally, we can write the integral of the leading term as

$$F_h=\int\frac{d^DK}{\left(2\pi\right)^D}2\int_0^1 dx\int_0^1 dy\,y\frac{1}{\left[K^2-Q^2+i0\right]^3},$$

Doing the Wick rotation $K_0\to iK_0$, the integral is transferred from the Minkowski space to the Euclidean space:

$$\begin{aligned}
F_h&=i\int\frac{d^DK}{\left(2\pi\right)^D}2\int_0^1 dx\int_0^1 dy\,y\frac{1}{\left[-K^2-Q^2+i0\right]^3}\\
&=-i\int\frac{d^DK}{\left(2\pi\right)^D}2\int_0^1 dx\int_0^1 dy\,y\frac{1}{\left[K^2+Q^2-i0\right]^3}\\
&=-i\frac{1}{\left(4\pi\right)^{D/2}}\Gamma\left(1+\epsilon\right)\int_0^1 dx\int_0^1 dy\,y\frac{1}{\left[Q^2-i0\right]^{1+\epsilon}}.
\end{aligned}\tag{3.6.7}$$

Here we notice the denominator of the integrand is $\frac{1}{\left[Q^2-i0\right]^{1+\epsilon}}$. If we want to take the real part out of the brackets, there will be a complex number with a non-integer power. By employing a trick which we will discuss in more details in next section 3.8. We can accomplish integral as follows

$$\begin{aligned}
F_h&=-i\frac{1}{\left(4\pi\right)^{D/2}}\Gamma\left(1+\epsilon\right)\int_0^1 dx\int_0^1 dy\,y\frac{1}{\left[-x\left(1-x\right)y^2M^2-i0\right]^{1+\epsilon}}\\
&=\frac{-i}{\left(4\pi\right)^{D/2}}\Gamma\left(1+\epsilon\right)\int_0^1 dx\int_0^1 dy\,y\frac{1}{\left[x\left(1-x\right)y^2M^2\right]^{1+\epsilon}}\frac{1}{\left[-1-i0\right]^{1+\epsilon}}\\
&=\frac{-i}{\left(4\pi\right)^{D/2}}\Gamma\left(1+\epsilon\right)\left(\frac{1}{M^2}\right)^{1+\epsilon}\frac{\Gamma^2\left(-\epsilon\right)}{\Gamma\left(1-2\epsilon\right)}\left(-e^{i\pi\epsilon}\right),
\end{aligned}\tag{3.6.8}$$

where we have used the relation

$$\frac{1}{\left[-1-i0\right]^{1+\epsilon}}=\left(e^{-i\pi}\right)^{-1-\epsilon}=-e^{i\pi\epsilon}.$$

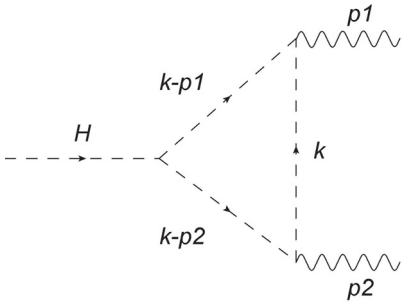
The result can be further written as a polynomial of ϵ

$$F_h=\frac{1}{\left(4\pi\right)^2M^2}\left(\frac{1}{\epsilon^2}+\frac{i\pi}{\epsilon}-\frac{2\pi^2}{3}-\frac{2}{\epsilon}\ln M-2\pi i\ln M+2\ln^2 M\right)\tag{3.6.9}$$

We can see that this integral is divergent. Therefore, the result from the hard region (3.6.8) is not the whole result. This is because the Taylor expansion that we have used here is valid only in the large k limit.

3.6.2 The soft and the ultra soft region

We now look for other possible regions. For the soft region, we have $k^2 \sim m^2$, we need to expand the denominator in another way. However, it can be proved that the contributions from the soft and ultra soft regions are zero. Let me prove this now. Recall our graph corresponds to the scalar loop,



According to this diagram, we may write the general integral

$$F\left(H^2, m, M; D\right) = \int \frac{d^D k}{\left[k^2 - 2p_1 \cdot k - m^2 + i0\right]\left[k^2 - 2p_2 \cdot k - m^2 + i0\right]\left[k^2 - m^2 + i0\right]} \tag{3.6.10}$$

Now we introduce a group of loop momentums, $k^{\pm} = k^0 \pm k^z$, and henceforth $k^2 = k^+ k^- - k_\perp^2$, where $k_\perp^2 = k_x^2 + k_y^2$. On one hand, in the soft region, we have $k^2 \sim m^2$. Taking $H = (M, \mathbf{0})$ and $p_{1,2} = \left(\pm\frac{M}{2}, 0, 0, -\frac{M}{2}\right)$, the leading order term of the integral is

$$\begin{aligned} F^{(s)} &= \int \frac{d^D k}{\left[-2p_1 \cdot k + i0\right]\left[-2p_2 \cdot k + i0\right]\left[k^2 - m^2 + i0\right]} \\ &= \int \frac{dk_+ dk_- d^{D-2} k_\dagger}{\left[-k_+ M + i0\right]\left[k_- M + i0\right]\left[k_+ k_- - k_\perp^2 - m^2 - i0\right]} \\ &= \int \frac{dk_+ d^{D-2} k_\perp}{\left[k_+ + i0\right]\left[-k_\perp^2 - m^2 - i0\right]} = \int \frac{dk_+}{k_+} \int \frac{d^{D-2} k_\perp}{k_\perp^2 + m^2} = 0 \end{aligned} \tag{3.6.11}$$

where the integral over k_+ is set to be zero, because it is an integral without scale. On the other hand, in the ultra soft region, we have $k^2 \sim m^2 \frac{m^2}{M^2}$. Thus the leading order term of the integral is

$$\begin{aligned} F^{(us)} &= \int \frac{d^D k}{\left[2p_1 \cdot k + m^2 - i0\right]\left[2p_2 \cdot k + m^2 + -i0\right] m^2} \\ &= \frac{1}{m^2} \int \frac{dk_+ dk_- d^{D-2} k_\perp}{\left[k_+ M + m^2 - i0\right]\left[k_- M + m^2 - i0\right]} = 0 \end{aligned} \tag{3.6.12}$$

The integral is also set to be zero, since the scale of the integration over $k_\perp$ is zero.

3.6.3 Collinear region

It might be a good idea to consider the region where $k^2 \sim m^2$, without the last propagator being expanded. We may choose the values of the external momentums as

$$p_1 = \left\{ \begin{pmatrix} \frac{M}{2} \\ 0 \\ 0 \\ -\frac{M}{2} \end{pmatrix}, \quad p_2 = \left\{ \begin{pmatrix} \frac{M}{2} \\ 0 \\ 0 \\ \frac{M}{2} \end{pmatrix} \right. \right. . \tag{3.6.13}$$

Still, the integrand is

$$\frac{1}{[k^2 - 2p_1 \cdot k - m^2 + i0]\,[k^2 + 2p_2 \cdot k - m^2 + i0]\,[k^2 - m^2 + i0]} \tag{3.6.14}$$

If we set a limit for each of the factors in the denominator, we may obtain them to different levels of magnitude in different regions, and expand them accordingly. There are two regions that satisfy our expectation.

3.6.3.1 The first region

In the first region, we assume that the conditions

$$\begin{aligned} k_\perp &\sim m; \\ k^+ &\sim \frac{m^2}{M}; \\ k^- &\sim M. \end{aligned} \tag{3.6.15}$$

are satisfied. Now let us look at the three propagators

$\mathbf{(k - p_1)^2 - m^2}$

$$(k + p_1)^2 - m^2 = k^+k^- - k_\perp^2 + Mk^+ - m^2 \tag{3.6.16}$$

Since $k^+k^- \sim m^2$, $k_\perp^2 \sim m^2$, $Mk^+ \sim m^2$, there is no need to do expansion of this term.

$\mathbf{k^2}$

$$k^2 = k^+k^- - k_\perp^2 \tag{3.6.17}$$

Since $k^+k^- \sim m^2$, $k_\perp^2 \sim m^2$, again, there is no need for expansion.

$\mathbf{(k + p_2)^2 - m^2}$ This term can be written as

$$\begin{aligned} &(k + p_2)^2 - m^2 = k^+k^- - k_\perp^2 + Mk^- - m^2 \\ &\text{which leads to} \rightarrow Mk^- = 2p_2 \cdot k \sim M^2 \end{aligned} \tag{3.6.18}$$

Hence $\frac{1}{(k+p_2)^2 - m^2}$ should be expanded with $\frac{1}{2p_2 \cdot k}$.

3.6.3.2 The second region

In the second region, we switch the limits of $k^+$and k^-in the first region and obtain

$$\begin{aligned} k_\perp &\sim m; \\ k^+ &\sim M; \\ k^- &\sim \frac{m^2}{M}. \end{aligned}$$

Now let us look at the three factors in the denominator

$\mathbf{(k-p_1)^2-m^2}$ The first factor can be written into

$$(k-p_1)^2-m^2=k^+k^--k_\perp^2-Mk^+-m^2 \tag{3.6.19}$$

Since $k^+k^-\sim m^2$, $k_\perp^2\sim m^2$, $Mk^+\sim M^2$, we will expand this factor with $\frac{1}{2p_1\cdot k}$ in this region.

$\mathbf{k^2}$ The second factor can be written into

$$k^2=k^+k^--k_\perp^2 \tag{3.6.20}$$

Since $k^+k^-\sim m^2$, $k_\perp^2\sim m^2$, there is need for expansion.

$\mathbf{(k+p_2)^2-m^2}$ The third factor can be written into

$$\begin{aligned}(k+p_2)^2 \quad & -m^2=k^+k^--k_\perp^2+Mk^--m^2\\ \to \quad & Mk^-=2p_2\cdot k\sim m^2\end{aligned} \tag{3.6.21}$$

There is no need for expansion of this factor in the second region. Now, we know which factor needs to be expanded in each region. However, we found if we perform the integral in the two regions, both of them would contribute a divergence that are not dimensionally regularized. In order to get rid of these divergences, we consider the powers of the first two propagators to be $1+\delta_1$ and $1+\delta_2$, with $\delta_1\neq\delta_2$ and both $\delta_1,\delta_2\ll\epsilon$. This is called **auxiliary analytic regularization**. So the general integrand has the following form

$$\frac{1}{\left[k^2-2p_1\cdot k-m^2+i0\right]^{1+\delta_1}\left[k^2+2p_2\cdot k-m^2+i0\right]^{1+\delta_2}\left[k^2-m^2+i0\right]}. \tag{3.6.22}$$

What we will do next is calculating the two regions separately, then adding them up, and letting δ_1 and δ_2 goes to zero.

3.6.4 How to do the expansions

In order to do the integrations of each of the collinear regions, we first need to know how to expand the propagators. Notice that the power of the propagator yet to be expanded is non-integer. Hence, we cannot use the usual Taylor expansion formula. Instead, we may expand these factors with the aid of Gamma functions. Particularly, for the first region, we need to expand the propagator

$$\begin{aligned}&\frac{1}{\left[(k+p_2)^2-m^2\right]^{1+\delta_2}}=\frac{1}{\left[2p_2\cdot k-(m^2-k^2)+i0\right]^{1+\delta_2}}\\ &=\frac{1}{(2k\cdot p_2+i0)^{1+\delta_2}}\sum_{n=0}^{\infty}\frac{\Gamma(1+\delta_2+n)}{\Gamma(1+\delta_2)\,n!}\left(\frac{m^2-k^2}{2p_2\cdot k+i0}\right)^n\\ &=\sum_{n=0}^{\infty}\frac{\Gamma(1+\delta_2+n)}{\Gamma(1+\delta_2)\,n!}\frac{(m^2-k^2)^n}{(-2p_2\cdot k)^{n+1+\delta_2}}\frac{1}{(-1-i0)^{n+1+\delta_2}},\end{aligned} \tag{3.6.23}$$

where we have assumed the relation $2p_2\cdot k>0$, and we can take the $-2p_2\cdot k$ out leaving the sign of $i0$ changed to negative

$$\frac{1}{(2p_2\cdot k+i0)^{n+1+\delta_2}}\to\frac{1}{(-2p_2\cdot k)^{n+1+\delta_2}(-1-i0)^{n+1+\delta_2}}. \tag{3.6.24}$$

Let us prove it is the only case that needs to be considered now. As stated in previous sections, the propagator can be written in terms of k_+, k_-, and $k_\perp$ as following

$$\frac{1}{\left(k_+k_- - k_\perp^2 - k_+M - m^2 + i0\right)\left(k_-M + i0\right)\left(k_+k_- - k_\perp^2 - m^2 + i0\right)}. \tag{3.6.25}$$

If we do the integral with k, we have

$$F^{c1} = \int \frac{d^dk}{\left(k_+k_- - k_\perp^2 - k_+M - m^2 + i0\right)\left(k_-M + i0\right)\left(k_+k_- - k_\perp^2 - m^2 + i0\right)} \tag{3.6.26}$$

Notice both residues of k_+

$$\frac{k_\perp^2 + m^2 - i0}{k_- - M},\ \frac{k_\perp^2 + m^2 - i0}{k_-} \tag{3.6.27}$$

would be in the upper half-plane of the complex variable k_+ if $k_- < 0$. In this case, we would obtain a zero F^{c1} by choosing the contour in the lower half-plane. Therefore, only in the situation of $0 < k_- < M$, we have the poles in both the upper and the lower half-plane, and a none-zero contribution will be obtained. Since $2p_2 \cdot k = k_-M$, we have proved our assumption. Similarly, we may prove that $2p_1 \cdot k = k_+M < 0$, and do the expansion in the second collinear region as

$$\begin{aligned}
&\frac{1}{\left[\left(k-p_1\right)^2 - m^2 + i0\right]^{1+\delta_1}} = \frac{1}{\left[-2p_1\cdot k - \left(m^2-k^2\right) + i0\right]^{1+\delta_1}} \\
&= \frac{1}{\left(-2k\cdot p_2 + i0\right)^{1+\delta_1}} \sum_{n=0}^{\infty} \frac{\Gamma\left(1+\delta_1+n\right)}{\Gamma\left(1+\delta_1\right)n!} \left(\frac{m^2-k^2}{-2p_1\cdot k + i0}\right)^n \\
&= \sum_{n=0}^{\infty} \frac{\Gamma\left(1+\delta_1+n\right)}{\Gamma\left(1+\delta_1\right)n!} \frac{\left(m^2-k^2\right)^n}{\left(2p_1\cdot k\right)^{n+1+\delta_1}} \frac{1}{\left(-1-i0\right)^{n+1+\delta_1}},
\end{aligned} \tag{3.6.28}$$

3.6.5 Leading term of the two regions

Following the steps presented above, we may calculate the leading term contributions of the two regions. In the first region, we have the leading term

$$\frac{i}{\left(4\pi\right)^{D/2}} \left(\frac{1}{m}\right)^{\delta_1+\epsilon} \left(\frac{1}{M^2}\right)^{1+\delta_2} \frac{\Gamma\left(\delta_1+\epsilon\right)\Gamma\left(\delta_1-\delta_2\right)}{\Gamma\left(1+\delta_1\right)\Gamma\left(1+\delta_1-\delta_2\right)} \left(e^{i\pi\delta_2}e^{-i\pi\delta_1}e^{-i\pi\delta_2}\right), \tag{3.6.29}$$

In the second region, we have the leading term

$$\frac{i}{\left(4\pi\right)^{D/2}} \left(\frac{1}{m}\right)^{\delta_2+\epsilon} \left(\frac{1}{M^2}\right)^{1+\delta_1} \frac{\Gamma\left(\delta_2+\epsilon\right)\Gamma\left(\delta_2-\delta_1\right)}{\Gamma\left(1+\delta_2\right)\Gamma\left(1+\delta_2-\delta_1\right)} \left(e^{i\pi\delta_1}e^{-i\pi\delta_1}e^{-i\pi\delta_2}\right). \tag{3.6.30}$$

By adding the results from the two regions, and letting $\delta_1, \delta_2 \to 0$ before we let ϵ go to zero, we find the leading order contribution from the collinear region. The expression is written as a polynomial of ϵ

$$\frac{1}{\left(4\pi\right)^2 M^2} \left(-\frac{1}{\epsilon^2} - \frac{i\pi}{\epsilon} + \frac{\pi^2}{6} + \frac{2}{\epsilon}\ln M + 2\pi i \ln m + 2\ln^2 m - 4\ln M \ln m\right). \tag{3.6.31}$$

The divergent terms happen to cancel with the divergent terms from the hard region (3.6.19). this is a good sign that we are doing things correctly.

3.7 Summary

The results from exact calculation and the asymptotic expansion method are presented here for comparison. The real and imaginary parts of the exact solution are summarized in the table 3.2. The result obtained from expansion by regions is presented in table 3.3.

	Real part	Imaginary part
Exact solution	$\frac{-1}{2(4\pi)^2M^2}\left(\pi^2-\ln^2\frac{m^2}{M^2}\right)$	$\frac{i}{(4\pi)^2M^2}\pi\ln\frac{m^2}{M^2}$

Table 3.2: Real and imaginary parts of the exact solution

	Results from integral by regions
Hard region	$\frac{1}{(4\pi)^2M^2}\left(\frac{1}{\epsilon^2}+\frac{i\pi}{\epsilon}-\frac{2\pi^2}{3}-\frac{2}{\epsilon}\ln M-2\pi i\ln M+2\ln^2 M\right)$
Collinear region	$\frac{1}{(4\pi)^2M^2}\left(-\frac{1}{\epsilon^2}-\frac{i\pi}{\epsilon}+\frac{\pi^2}{6}+\frac{2}{\epsilon}\ln M+2\pi i\ln m+2\ln^2 m-4\ln M\ln m\right)$
In total	$\frac{-1}{2(4\pi)^2M^2}\left(\pi^2-\ln^2\frac{m^2}{M^2}-2i\pi\ln\frac{m^2}{M^2}\right)$

Table 3.3: Results obtained from expansion by regions

We can see that the results from integral by regions agree with the exact result obtained analytically.

3.8 Imaginary terms

Now let us have a closer look at the trick, that we used to obtain the imaginary part of the integral in previous subsections. Take the factor that we encountered in the first collinear region for example

$$\frac{1}{(-2p_1\cdot k+i0)^{n+1+\delta_1}}=\frac{1}{(2p_1\cdot k)^{n+1+\delta_1}(-1-i0)^{n+1+\delta_1}}\qquad(for\ 2p_1\cdot k<0)\tag{3.8.1}$$

where we have factored out $2p_1\cdot k$, which is negative. We now examine the second factor

$$(-1-i0)^{-n-1-\delta_1}=(-1-i0)^{-n-1}(-1-i0)^{-\delta_1}\tag{3.8.2}$$

The first factor can be evaluated smoothly by introducing the limit value $(-1)^{-n-1}$. However, the second factor is ambiguous because of the non-integer exponent δ_1. The negative sign in front of $i0$ suggests that we may make the replacement

$$-1-i0=e^{-i\pi},\tag{3.8.3}$$

therefore, we expanded in ϵ, we have

$$(-1-i0)^{-\delta_1}=e^{i\pi\delta_1}.\tag{3.8.4}$$

Similarly for the other case

$$-1+i0=e^{i\pi},\tag{3.8.5}$$

and hence

$$(-1+i0)^{\delta_2}=e^{i\pi\delta_2}.\tag{3.8.6}$$

This procedure helps us to obtain the correct imaginary and real terms in the loop integrals.

3.9 Conclusion

This chapter starts from some basic techniques of Feynman loop diagram calculation. We first went through the calculation of photon self-energy. Then, we calculated the scalar triangular loop diagram at the heavy mass limit $M \gg m$; the real and imaginary parts of the amplitude were obtained separately. Then, we introduced the expansion by regions method, and used it to calculate the scalar triangular loop. The results obtained from expansion by regions agree well with the result from the direct calculation. This fact is another support to our previous discussion of the necessity of introducing a proper regularization procedure in the loop diagram calculation.

Chapter 4

Calculation of the Higgs boson decay with dispersion relation

4.1 Introduction

The decay of Higgs boson to two photons is a crucial process in the discovery and studies of the Higgs boson at CERN. It is also a very important process in the physics of Standard Model. The Higgs boson was first discovered through this decay channel [64]. This process has been well studied since 1970s [65, 66, 67]. We have mentioned in Chapter 2 that Gastmans et al. [3, 4] have recently cast doubt over the rate of the Higgs boson decay into two photons. They claimed that the old results [68, 65, 69, 70] were wrong, and the reason is adopting dimensional regularization in the calculation. We [5], and many other people [48, 49, 50, 51, 52] have discussed the necessity of using regularization in the calculation of Higgs decay. In this chapter, we want to use another approach called dispersion relation (DR), to calculate the decay of Higgs boson to two photons. In this method, one starts from the imaginary part of the decay amplitude, which can be obtained by Cutkosky rules. Then, by substituting the imaginary part into the dispersion relations, one can calculate the whole amplitude. In this procedure, one will not encounter any divergence, so there is no need for introducing the regularization. By comparing the result obtained in this method with the standard expression of the Higgs decay amplitude, we can tell if the regularization does cause some error, as Gastmans et al. stated. The standard expression of the amplitude of the decay of Higgs to two photons [68, 65, 69, 70] can be obtained by introducing the W boson and top quark loop corrections. The amplitude is

$$\mathcal{M} = \frac{e^2 g}{(4\pi)^2 M_W} F \left(k_1 \cdot k_2 g^{\mu\nu} - k_2^\mu k_1^\nu\right) \epsilon_\mu \left(k_1\right) \epsilon_\nu \left(k_2\right) \tag{4.1.1}$$

where the function F is composed of the contributions from W and fermion loops,

$$F = F_W \left(\beta_W\right) + \sum_f N_c Q_f^2 F_f \left(\beta_f\right), \tag{4.1.2}$$

and $N_c = 3$ is the color factor for the top quark; lighter quarks are negligible. The function F_W and F_f are the W boson and fermion loop form factors correspondingly. The variables in the brackets of F_f are defined as $\beta_W = \frac{4M_W^2}{M_H^2}$, and $\beta_f = \frac{4M_f^2}{M_H^2}$. The W boson and fermion loop form factors have the following expressions

$$F_W \left(\beta\right) = 2 + 3\beta + 3\beta \left(2 - \beta\right) f \left(\beta\right) \tag{4.1.3}$$

$$F_f \left(\beta\right) = -2\beta \left[1 + \left(1 - \beta\right) f \left(\beta\right)\right], \tag{4.1.4}$$

where the function $f(\beta)$ is defined by

$$f(\beta) = \begin{cases} \arcsin^2\left(\beta^{-\frac{1}{2}}\right) & \text{for } \beta \geq 1 \\ -\frac{1}{4}\left[\ln\frac{1+\sqrt{1-\beta}}{1-\sqrt{1-\beta}} - i\pi\right]^2 & \text{for } \beta \leq 1 \end{cases}$$

Since we are interested in the case of heavy Higgs decay, we will focus on the second expression of $f(\beta)$ in this chapter. In the high mass limit, the Higgs decay rate can be obtained by directly calculating the loop diagrams [68].

The method using the Cutkosky rules and the dispersion relations for the calculation of the decay of Higgs into photons was discussed in the paper of Horejsi and Stohr [71]. In that paper, they pointed out that the standard form factor of Higgs decay is composed of an unsubtracted form factor $F_W^{(\mathrm{un})}$ plus 2. $F_W^{(\mathrm{un})}$ is obtained by using the unsubtracted dispersion relation $F_W^{(\mathrm{un})}(q^2; m^2) = \frac{1}{\pi}\int_{4m^2}^{\infty} \mathrm{ImF_W}(\mathrm{s};\mathrm{m}^2)\frac{\mathrm{ds}}{\mathrm{s-q}^2}$, where m is the mass in the loop. From now on, for the sake of simplicity, we adopt the notations M_W, $M_f \to m$, and $M_H \to M$. By comparing the low energy limit $q^2 \to 0$ of $F_W^{(\mathrm{un})}(q^2; m^2)$ and the result from the low energy theorem, the authors in [71] conclude that a subtraction of -2 is needed for the general expression obtained from the calculation with dispersion relation. The subtraction was extended to the high energy limit $q^2 \to \infty$, or $m \to 0$ equivalently. The term they subtracted $\lim_{m\to 0} F_W\left(\frac{m^2}{M^2}\right) = 2$ agrees with the high energy limit of the form factor recovered by the Goldstone boson "equivalence theorem" [72].

In section II of this chapter, we apply the method of DR to the calculation of decay of Higgs to photons through top quark loops. We notice the form factor obtained in this way agrees with the standard result. In section III, we apply DR to the decay of Higgs to photons through W boson loops. The standard result is once again confirmed. In section IV, we look into the questions brought up by Horejsi and Stohr [71], to can have a better understanding of the calculations with DR. We put the details of the derivation of DR and the calculation of the W boson loop form factor into section V, which is the appendix of this chapter.

4.2 Applying DR to Higgs decay through top quarks

Now, let us start by applying the dispersion relations in the calculation of the decay of Higgs boson to photons through fermion loop. There is no debate in this calculation, since the contribution from the decay through top loop satisfies the decoupling theorem [3, 4]. The decay channel considered here is the decay through the top quark triangular loop. This process can be represented by the following diagram

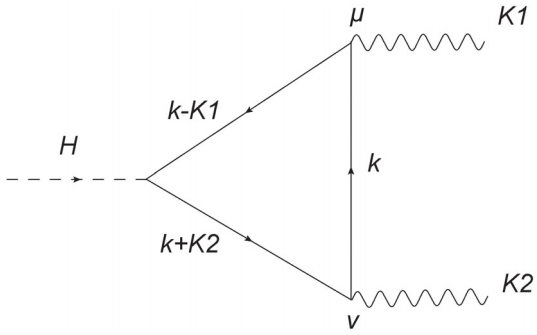


Figure 4.1: Higgs decay through top quark loop

The corresponding amplitude of this process can be written as

$$iM\left(K_1,K_2\right)=\int\frac{d^4k}{\left(2\pi\right)^4}\mathrm{Tr}\Bigg[\left(-i\frac{m}{v}\right)\frac{\left(\not{k}-\not{K}_1+m\right)}{\left(k-K_1\right)^2-m^2}i\frac{2e}{3}\gamma^\mu\times$$
$$\times\frac{\left(\not{k}+m\right)}{k^2-m^2}i\frac{2e}{3}\gamma^\nu\frac{i\left(\not{k}+\not{K}_2+m\right)}{\left(k+K_2\right)^2-m^2}\epsilon^*_{a\mu}\epsilon^*_{b\nu}\Bigg] \tag{4.2.1}$$

We now introduce new variables,

$$P_1=k, \tag{4.2.2}$$
$$P_2=k-K_1, \tag{4.2.3}$$
$$P_3=k+K_2. \tag{4.2.4}$$

We may replace the integral with k by integrals with P_2 and P_3, together with a delta function as the constraint between the two new variables. The amplitude has the following expression

$$M^{\mu\nu}\left(H,K_1,K_2\right)=-\left(\frac{2e}{3}\right)^2\frac{m}{v}\int\frac{d^4P_2}{\left(2\pi\right)^4}\int\frac{d^4P_3}{\left(2\pi\right)^4}Tr\left[\frac{\left(\not{P}_2+m\right)}{P_2^2-m^2}\gamma^\mu\frac{\left(\not{P}_1+m\right)}{P_1^2-m^2}\gamma^\nu\frac{\left(\not{P}_3+m\right)}{P_3^2-m^2}\right]$$
$$\times\left(2\pi\right)^4\delta^4\left(P_2-P_3+M\right) \tag{4.2.5}$$

4.2.1 Cutting the top quark loop

The next step of our calculation is using the Cutkosky rules [73] to calculate the imaginary part of the decay amplitude through the cuts of the top quark loop.

According to the Cutkosky rules, the two propagators should be cut and replaced by two delta functions,

$$\tfrac{1}{P_2^2-m^2}\rightarrow-2\pi i\delta\left(P_2^2-m^2\right) \tag{4.2.6}$$
$$\tfrac{1}{P_3^2-m^2}\rightarrow-2\pi i\delta\left(P_3^2-m^2\right)\quad. \tag{4.2.7}$$

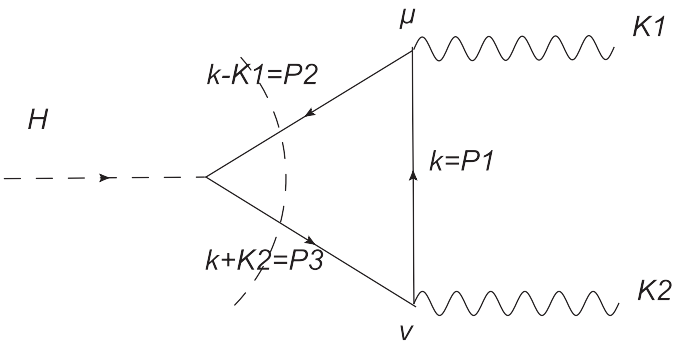


Figure 4.2: Cut on triangular loop

Then, we find the imaginary part of the amplitude to be

$$\mathrm{Im}M\left(H\right)=\frac{ge^{2}M^{2}}{64\pi m}Q_{t}^{2}\left(g^{\mu\nu}-\frac{K_{2}^{\mu}K_{1}^{\nu}}{K_{1}\cdot K_{2}}\right)e_{1\mu}e_{2\nu}\beta\left(1-\beta\right)\ln\frac{1+\sqrt{1-\beta}}{1-\sqrt{1-\beta}}, \tag{4.2.8}$$

where $\beta=\frac{4m^{2}}{M^{2}}$. In the decay of Higgs to photon through top quark loop, there is another diagram contributing to this process. In its diagram, the polarization vectors are interchanged, as shown bellow. This diagram gives the same contribution to the total imaginary part as the previous one.

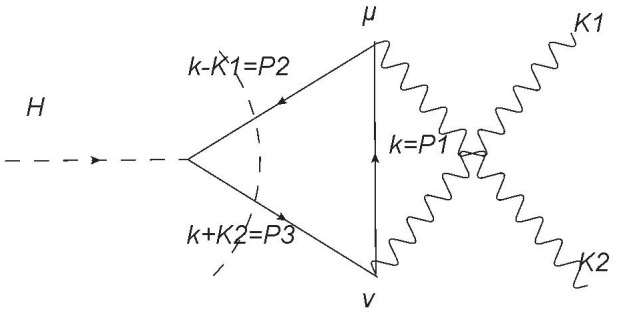


Figure 4.3: Top quark loop with interchanged photons

Hence the total imaginary part of the whole amplitude is

$$\mathrm{Im}M\left(H\right)=-\frac{ge^{2}}{16\pi m}Q_{t}^{2}\left(K_{1}\cdot K_{2}g^{\mu\nu}-K_{2}^{\mu}K_{1}^{\nu}\right)e_{1\mu}e_{2\nu}\beta\left(1-\beta\right)\ln\frac{1+\sqrt{1-\beta}}{1-\sqrt{1-\beta}} \tag{4.2.9}$$

which agrees well with the standard result [68, 65, 69, 70].

4.2.2 The whole amplitude

Using the imaginary part obtained in the last subsection (4.2.9), we can calculate the whole amplitude with DR. To achieve this goal, we first need to introduce the DR working properly in this problem. The unsubtracted dispersion relation is used in this case

$$F\left(x\right)=\frac{1}{\pi}\int_{bc}^{\infty}\frac{\mathrm{Im}F\left(y\right)}{\left(y-x\right)}dy \tag{4.2.10}$$

where bc is the beginning of the branch cut. In our calculation, the whole amplitude can be written as

$$M\left(q^{2}\right)=\frac{1}{\pi}\int_{4m^{2}}^{\infty}\frac{\mathrm{Im}M\left(p^{2}\right)}{\left(p^{2}-q^{2}\right)}dp^{2} \tag{4.2.11}$$

Substituting (4.2.9) into above equation, we obtain the final expression of the whole amplitude

$$M(H) = \frac{ge^2}{16\pi^2 m} Q_t^2 F \left(K_1 \cdot K_2 g^{\mu\nu} - K_2^\mu K_1^\nu\right) e_{1\mu} e_{2\nu} \tag{4.2.12}$$

where the F function is defined by (4.1.4). We can see that this result is identical to the standard result (4.1.1).

4.3 The W boson loop

Now, we look at the decay of Higgs through the W boson loop. This is where the debate happened. Gastmans et al. argued that the standard result of the one-loop W contribution to the decay is wrong, since it does not satisfy the decoupling theorem [3, 4]. They believe it is the use of dimensional regularization that causes the violation of the decoupling theorem. Later it was pointed out by Shifman et al. [74] that the decoupling is supposed to be absent for the decay through W boson loop in the $m_W \to 0$ limit, and the standard result is correct. In this section, we use the Cutkosky rules and DR to calculate the decay through W boson, so we can avoid the divergences that have to be encountered in the direct calculation. By comparing our result with the standard result and the result given by Gastmans et al., we can tell whose argument is correct.

In the case of the Higgs decay through W boson loop, we have two types of diagrams. The first type includes two triangular loop diagrams with the photons interchanged like in the case of the top loop. Its Feynman diagram with the standard expression of the loop momenta is shown bellow. In order to calculate the amplitude with the optical theorem, we may denote the loop momenta separately as presented in the following diagram.

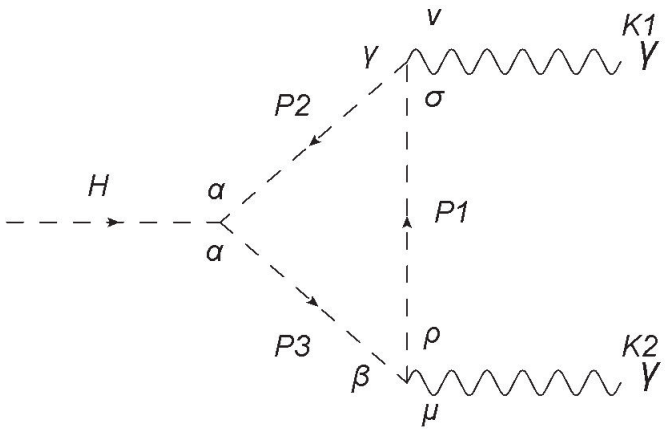


Figure 4.4: W boson triangular loop

In the second type of diagram, instead of a triangular loop, we have a W boson bubble loop.

In the calculation of this decay process, instead of using the unsubtracted dispersion relation as the authors of [71] did, we adopt the once subtracted dispersion relation (10.3.4).

$$F(q^2) = F(0) + \frac{q^2}{\pi} \int_{4m^2}^{\Lambda^2} dy \frac{\mathrm{Im} F(y)}{y(y - q^2)} + \frac{q^2}{2\pi i} \oint_{|y|=\Lambda^2} dy \frac{F(y)}{y(y - q^2)} \tag{4.3.1}$$

where the second integral vanishes in this case

$$\frac{q^2}{2\pi i} \oint_{|y|=\Lambda^2} dy \frac{F(y)}{y(y - q^2)} = 0, \tag{4.3.2}$$

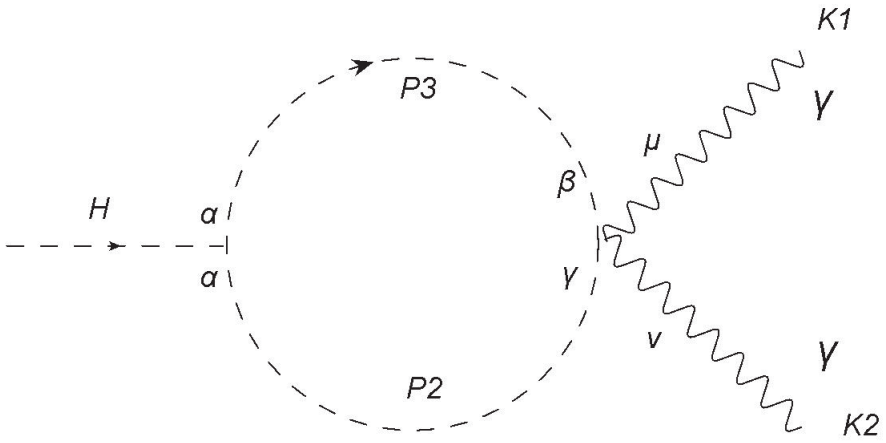


Figure 4.5: W boson bubble loop

so we can calculate $F(q^2)$ knowing the expression of $\mathrm{Im}F(y)$ and the value of $F(0)$. Under the condition $q^2 = H \equiv M^2$, the form factor we obtained is

$$F(H) = \frac{e^2 g}{16\pi^2 m}\left[2 + 3\beta + 3\beta(2-\beta) f\right] \tag{4.3.3}$$

where $f(\beta) = -\frac{1}{4}\left[\ln\frac{1+\sqrt{1-\beta}}{1-\sqrt{1-\beta}} - i\pi\right]^2$. This result agrees with the standard result of the Higgs decay through W loop.

4.4 More discussion on DR

As we mentioned in the introduction, the calculation of decay of Higgs to photons through W boson loop was discussed by Horejsi and Stohr [71]. In that paper, instead of a once subtracted DR, they use an unsubtracted DR, and introduced a term 2 to compensate the difference of their result with the standard result in the low Higgs mass limit. That is to say, their form factor of Higgs decay is composed of an unsubtracted form factor $F_W^{(un)}$ plus 2. In this section, we will first briefly discuss their approach. Then we will present a discussion of the properties of DR, in order to better understand this method. In their paper, the form factor $F_W^{(un)}$ is obtained by using the unsubtracted dispersion relation

$$F_W^{(\mathrm{un})}\left(q^2; m^2\right) = \frac{1}{\pi}\int_{4m^2}^{\infty} \mathrm{ImF_W}\left(s;\, m^2\right)\frac{ds}{s-q^2} \tag{4.4.1}$$

The expression of form factors at the low Higgs energy and soft W boson limits are

$$\lim_{q^2\to 0} F_W^{(un)}\left(q^2; m^2\right) = 5 \tag{4.4.2}$$

$$\lim_{m^2\to 0} F_W^{(un)}\left(q^2; m^2\right) = 0 \tag{4.4.3}$$

However, according to the low-energy theorem [66, 75, 76, 77], the form factor has the following limit

$$\lim_{q^2\to 0} F_W\left(q^2; m^2\right) = 7 \tag{4.4.4}$$

By comparing (4.4.2) and (4.4.4), Horejsi and Stohr concluded that the true expression of the form factor should be

$$F_W\left(q^2; m^2\right) = F_W^{(un)}\left(q^2; m^2\right) + 2 \tag{4.4.5}$$

Horejsi and Stohr further noticed that the 2 is the limit within the Goldstone-boson (GB) approximation

$$\lim_{m^2\to 0} F_W\left(m^2/q^2\right) = 2 \tag{4.4.6}$$

Indeed, we know that the longitudinal W boson contributes the leading term at the $M_H^2 \to \infty$ limit [74].

Their observations are very insightful. However, we notice some open questions in their argument.

1. First, why is the subtraction of the differences of the form factors at the low energy limit applicable for the whole range of the value of q^2. Why this subtraction can be extended even to the high energy limit?

2. Second, why we need a finite subtraction in some cases (the Higgs decay through W boson loop for example), but not for the other cases (the Higgs decay through fermion loop for example)?

3. Last but not least, is the calculation of a Feynman diagram with dispersion relation sufficient to give the exact result, or do we have to compare its result with an exact result obtained by some other method?

Let us look into the above questions, and try to have a better understanding of the calculations based on the dispersion relations.

4.4.1 When can one use the unsubtracted DR in the calculation

In order to answer the first question, let us start by comparing the unsubtracted and the once subtracted dispersion relation,

$$F(q^2) = F(0) + \frac{q^2}{\pi}\int_{4m^2}^{\Lambda^2} dy \frac{\mathrm{Im}F(y)}{y(y-q^2)} + \frac{q^2}{2\pi i}\oint_{|y|=\Lambda^2} dy \frac{F(y)}{y(y-q^2)} \tag{4.4.7}$$

$$F(q^2) = \frac{1}{\pi}\int_{4m^2}^{\Lambda^2} dy \frac{\mathrm{Im}F(y)}{(y-q^2)} + \frac{1}{2\pi i}\oint_{|y|=\Lambda^2} dy \frac{F(y)}{(y-q^2)}, \tag{4.4.8}$$

Applying (4.4.8) in the $q^2 \to 0$ limit, the low-energy limit of the form factor can be written as

$$F(0) = \frac{1}{\pi}\int_{4m^2}^{\Lambda^2} dy \frac{\mathrm{Im}F(y)}{y} + \frac{1}{2\pi i}\oint_{|y|=\Lambda^2} dy \frac{F(y)}{y} \tag{4.4.9}$$

In the decay of Higgs through W boson loop, the reason that an unsubtracted DR $F(q^2) = \frac{1}{\pi}\int_{4m^2}^{\infty} dy \frac{\mathrm{Im}F(y)}{(y-q^2)}$ does not work is that the second term in (4.4.8) does not vanish. This term generates a finite contribution. This contribution at the $q^2 \to 0$ limit can be calculated by substituting the integral $\frac{1}{\pi}\int_{4m^2}^{\Lambda^2} dy \frac{\mathrm{Im}F(y)}{y} = 5$, and the known result $F(0) = 7$ into the equation (4.4.9). The circular integral at the low-energy limit henceforth can be obtained

$$\frac{1}{2\pi i}\oint_{|y|=\Lambda^2} dy \frac{F(y)}{y} = 2. \tag{4.4.10}$$

It is exactly the term 2 that has been introduced in (4.4.5).

4.4.1.1 Deformation of the contour

In order to understand the meaning of the term (4.4.10), let us carefully examine it again. If we rewrite the variable $y = \Lambda^2 e^{i\theta}$, we will transform the integration variable $dy = i\Lambda^2 e^{i\theta} d\theta$. We notice that the integral is along a circle at infinity. Now, we may introduce a new variable z by letting

$$z = \frac{1}{y},\ dy = \frac{-1}{z^2} dz \tag{4.4.11}$$

Henceforth, the circular integral turns out to be

$$\frac{1}{2\pi i} \oint_{|y|=\Lambda^2} dy \frac{F(y)}{y} = \frac{-1}{2\pi i} \oint_{|z|\to 0} dz \frac{F(z)}{z}, \tag{4.4.12}$$

Noticing that by introducing the new variable z, we deform the contour at infinity to a circle around zero, and the contour direction is also flipped. Therefore, the following relation is obtained

$$\frac{1}{2\pi i} \oint_{|y|=\Lambda^2} dy \frac{F(y)}{y} = \frac{1}{2\pi i} \oint_{|z|\to 0} dz \frac{F(z)}{z} \tag{4.4.13}$$

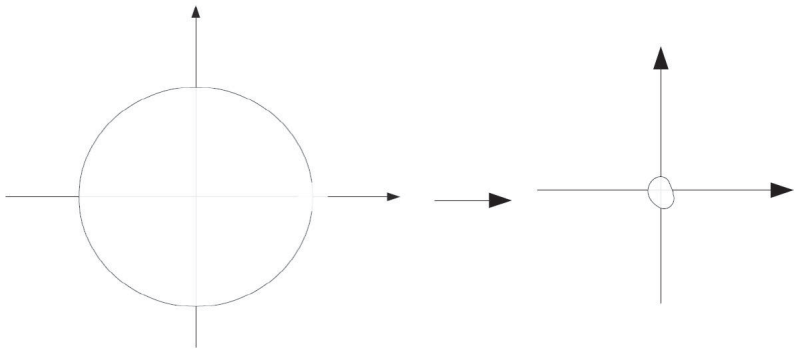


Figure 4.6: Deformation of the contour

Since $\frac{F(z)}{z}$ is bounded as $z \to 0$ along the positive real axis, we can join the disconnected ends of the contour, and have a close circle around zero. Due to Cauchy's residue theorem, the integral is nothing but $F(z=0)$, which is equivalent to $F(y \to \infty)$. It is the form factor as the incoming momentum approaches infinity. This explains why 2 has to be added to the result of unsubtracted DR relation. This fact also explains why the contribution from the Goldstone boson diagram equals 2: because it corresponds to the high energy contribution, due to the equivalence theorem.

4.4.1.2 Subtraction dependence on q^2

To answer the first question that we asked in the beginning of this section, let us examine how the subtraction depends upon the squared incident momentum q^2. Since $\frac{1}{y-q^2} = \frac{1}{y} + \frac{q^2}{y(y-q^2)}$, we may rewrite the integral into a summation of two separate circular integrals

$$\begin{aligned} &\frac{1}{2\pi i} \oint_{|y|=\Lambda^2} dy \frac{F(y)}{(y-q^2)} = \frac{1}{2\pi i} \oint_{|y|=\Lambda^2} dy \frac{F(y)}{y} \\ &+ \frac{q^2}{2\pi i} \oint_{|y|=\Lambda^2} dy \frac{F(y)}{y(y-q^2)}. \end{aligned}$$

By substituting the exact result of the form factor (4.1.3) into above integral, we find that in the case of W boson and fermion loop, the second term in the above expression is 0. Hence, the integral can be written as

$$\frac{1}{2\pi i}\oint_{|y|=\Lambda^2} dy \frac{F(y)}{(y-q^2)} = \frac{1}{2\pi i}\oint_{|y|=\Lambda^2} dy \frac{F(y)}{y} = F(y\to\infty), \tag{4.4.14}$$

This result is independent of q^2. This is why the term 2 employed in [71] is always the same for different values of q^2.

4.4.2 The reason that the unsubtracted DR works with the fermion loop

Our second question is also mentioned by the authors of [71]. Let us look at what happens in the calculation of the top quark loop. From the discussion of previous sections, we can see that if and only if the last term in (4.4.9)

$$\frac{1}{2\pi i}\oint_{|y|=\Lambda^2} dy \frac{F(y)}{y} \tag{4.4.15}$$

vanishes, an unsubtracted DR works. We have argued that this integral is precisely $F(p^2=\infty)$. Thus, whether the form factor vanishes at infinity decides the applicability of the unsubtracted DR. Now, let us take the calculation of the top quark loop that we did before for example. We know that for the top quark loop, the form factor

$$F(p^2) = -2\beta\left[1+(1-\beta)f(\beta)\right], \tag{4.4.16}$$

where $f(\beta) = -\frac{1}{4}\left[\ln\frac{1+\sqrt{1-\beta}}{1-\sqrt{1-\beta}} - i\pi\right]^2$, and $\beta = \frac{4m^2}{p^2}$. The circular integral (4.4.15) can be written into

$$\frac{1}{2\pi i}\oint_{|y|=\Lambda^2} dy \frac{F(y)}{y} = \frac{1}{2\pi i}\oint_{|y|=\Lambda^2} dy \frac{-2\frac{4m^2}{y}\left[1-\frac{\left(1-\frac{4m^2}{y}\right)}{4}\left[\ln\frac{1+\sqrt{1-\frac{4m^2}{y}}}{1-\sqrt{1-\frac{4m^2}{y}}}-i\pi\right]^2\right]}{y} \tag{4.4.17}$$

Now, like what we did for the W boson loop, we introduce a new variable z

$$z=\frac{1}{y},\ dy=\frac{-1}{z^2}dz \tag{4.4.18}$$

Then, the integral turns out to be

$$\begin{aligned}\frac{1}{2\pi i}\oint_{|y|=\Lambda^2} dy \frac{F(y)}{y} &= \frac{1}{2\pi i}\oint_{|z|\to 0} dz \frac{F(z)}{z} \\ &= \frac{1}{2\pi i}\oint_{|z|\to 0} dz \frac{-2\cdot 4m^2 z\left[1-\frac{\left(1-4m^2z\right)}{4}\left[\ln\frac{1+\sqrt{1-4m^2z}}{1-\sqrt{1-4m^2z}}-i\pi\right]^2\right]}{z}\end{aligned}$$

By expanding the integrand, it is easy to see that the residue at 0 is 0. Hence, we have proved $\frac{1}{2\pi i}\oint_{|y|=\Lambda^2} dy\frac{F(y)}{y} = 0$. This is equivalent to the condition $F(p^2=\infty)=0$. Therefore, the last term in (4.4.9) can be omitted in this fermion loop calculation, and the unsubtracted DR is sufficient.

4.4.3 Is DR a self-sufficient method?

Our last question was noticed as a flaw of the unsubtracted DR in [71]. Can we calculate the exact result simply from DR, or DR can only give us some "educated guess"? First of all, according to our previous discussion, the unsubtracted DR does not determine the form factor completely all by itself. Instead, we have to know the soft W boson $m^2 \to 0$ limit of the form factor, so we can subtract this value from the result calculated with the unsubtracted DR, and obtain the correct answer. Alternatively, if we know the form factor at low energy limit $q^2 \to 0$, we can take this limit on both sides of (4.4.8), as the authors of [71] did, and obtain value of the circular integral, which is the term to be subtracted. This method is equivalent to employing the once subtracted DR that we adopted in our calculation in section 4.3. The calculation based on the once subtracted DR gives us the exact result if the last integral in (4.4.7) vanishes. Now, it is worth noticing there might be another potential problem in our argument. The validity of equation (4.4.14) also depends on the fact that the last integral of (4.4.7) $\frac{q^2}{2\pi i}\oint_{|y|=\Lambda^2} dy \frac{F(y)}{y(y-q^2)}$ is 0. In the Higgs decay process, we know this is true, since we know the exact expression of $F(y)$. What shall we do if we do not know what the exact result is? We now prove here, at least for the circumstances with finite high energy limits, the condition

$$\frac{q^2}{2\pi i}\oint_{|y|=\Lambda^2} dy \frac{F(y)}{y(y-q^2)} = 0 \tag{4.4.19}$$

is satisfied. In fact, as long as we know that $F(y \to \infty)$ is bounded, we can always do the trick of deforming the contour (4.4.13). First, we may introduce a new function $F'(y) \equiv \frac{F(y)}{y-q^2}$. Then the integral can be written as

$$\frac{q^2}{2\pi i}\oint_{|y|=\Lambda^2} dy \frac{F'(y)}{y}. \tag{4.4.20}$$

Then, by introducing a new variable $z = \frac{1}{y}$, and deforming the contour to a infinitely small circle around the origin, we obtain

$$\frac{q^2}{2\pi i}\oint_{|y|=\Lambda^2} dy \frac{F'(y)}{y} = \frac{q^2}{2\pi i}\oint_{|z|\to 0} dz \frac{F'(z)}{z} = q^2 \lim_{y\to\infty} \frac{F(y)}{y-q^2} = 0 \tag{4.4.21}$$

Therefore we can see, as long as the high energy limit of the form factor is bounded, the integral $\frac{q^2}{2\pi i}\oint_{|y|=\Lambda^2} dy \frac{F(y)}{y(y-q^2)}$ is zero. Henceforth the subtraction term $\frac{1}{2\pi i}\oint_{|y|=\Lambda^2} dy \frac{F(y)}{(y-q^2)}$ is independent of q^2. This observation justifies our calculation using the once subtracted DR.

4.5 Conclusion

We have presented the calculations for the $H \to \gamma + \gamma$ process with the Cutkosky rules and DR. We found the unsubtracted DR gives a correct result for the fermion loop, and the once subtracted DR generates a correct result for the W loop. By comparing the unsubtracted DR and the once subtracted DR, we figure out why a subtraction is needed for the calculation of W loop using unsubtracted DR. The subtraction is proved to be the high energy limit of the result. We have shown that the procedure employed in [71] is equivalent to using the once subtracted DR. The reason that the circular integral in the once subtracted DR (4.4.14) is a constant has been discussed. If the high (or low) energy limit of the form factor is known, an exact result can be calculated by the unsubtracted DR plus a constant term, which is 2 in our case. This result can equivalently be calculated using the once subtracted DR, if we know the high energy limit of the form factor is bounded. In this case, we do not have to know the

exact value of the form factor at the high (or low) energy limit. The amplitude of Higgs boson decay to two photons calculated with DR agrees with the standard result. The necessity of the regularization in the direct calculation is confirmed once again.

Chapter 5

Magnetic moment of Positronium Ion system

5.1 Introduction

The positronium ion Ps^- is a bound state of two electrons and one positron. Discovered in 1981 [9], it is now being precisely studied with the goal of determining its lifetime [78, 79], the binding energy, and the photodetachment cross section [80]. These observables have been precisely predicted [81, 82, 83, 84, 85, 86, 87]. The recent progress has occurred thanks to the prospect of intense positron sources on the experimental side [88, 89, 90] and by improved variational calculations of the three-body wave function and incorporation of relativistic and some radiative effects on the theory side. In this chapter, we focus on the magnetic moment of this three-body system. In its ground state the two electrons are in a spatially symmetric wave function, thus form a spin singlet to make their total wave function antisymmetric. Thus, the whole magnetic moment of this system is due to the positron. If the bound-state effects were neglected, the magnetic moment is given by $g\frac{\hbar}{2}\frac{e}{2m}$, where g is the gyromagnetic ratio of a free positron (or electron)

$$g = 2 + \frac{\alpha}{\pi} + \dots \tag{5.1.1}$$

This free-particle g factor is known due to the recent calculation of the astonishing five-loop order, $\mathcal{O}\left(\left(\frac{\alpha}{\pi}\right)^5\right)$ [91].

The purpose of this chapter is to determine to what extent the interaction of the positron with the two electrons modifies the magnetic moment of the ion. This effect is expected to be analogous to that in hydrogen-like atoms and ions, where the nuclear electric field modifies the g of an electron [92], and thus be a correction of order α^2, enhanced relative to the free-particle effects in this order in the coupling constant. Effects of this origin have been studied with high precision in hydrogen-like ions [93, 94, 95]. Combined with measurements with a five-fold ionized carbon [96, 97, 98] they are the basis of the most precise determination of the electron mass.

Present theory of the binding effects on the g factor in hydrogen-like ions includes up to two-loop self-interaction of the electron, and binding effects of order up to $(Z\alpha)^4$ where Z is the atomic number. Even some $(Z\alpha)^5$ effects have recently been evaluated [99, 100]. Without the electron self interactions, the binding effects are known to all orders in $Z\alpha$ [92]. For a three-body system like Ps^-, theoretical calculations are more difficult because the wave function is not known analytically, in any approximation. Thus, even without self interactions, the binding effect has not been evaluated yet. In this paper we neglect self interactions and focus on the

dynamics of a charged particle, bound with two antiparticles.

The challenge in determining the magnetic interaction of the positronium ion is that the all the components have equal masses, thus their motions have to be taken into account. This is harder than in hydrogen, where the nuclear recoil can be considered a small perturbation. On the other hand, this problem has been overcome in the relatively simple scenario of the positronium atom (Ps).

The magnetic moment of the electron bound in Ps was calculated in 1972 by Faustov [101] with the so called quasipotential method, and by Grotch and Kashuba [102] who transformed the Breit Hamiltonian to separate the motion of the whole system from its internal dynamics. They further expanded the Hamiltonian around the non-relativistic limit using the Chraplyvy transformation [103, 104, 105], an extension of the Foldy-Wouthuysen (FW) transformation. Later [106] Sebastian proposed a new way of constructing the Hamiltonian by combining the Breit potential describing the interaction between the particles, and the FW transformed Hamiltonian describing the interaction of the particles with the external magnetic field. The Hamiltonian obtained in this way is a function of the LAB coordinate and momentum of each particle. It is expressed in terms of the center of mass (CM) variables [107] using the Krajcik-Foldy (KF) relation [108].

The calculation of Zeeman effect of the positronium system was done using first-order perturbation calculation. The nonrelativistic wave function of the system in the CM frame was used to do the calculation [102, 107]. In our calculation of the magnetic moment of the positronium ion system that will be discussed in the following sections, we will also use first-order perturbation method. We will explain that the motion of a charged system is still separable from its internal motion, hence the nonrelativistic wave function of the ion can be used in the first-order perturbation calculation. The Hamiltonian can be derived either by the Chraplyvy transformation to the Breit interaction, or by Sebastian's method. The next step is crucial, the LAB variables in the Hamiltonian need to be changed into the CM variables, so that the internal motion of the system can be separated from its external motion. We cannot use the unitary transformation adopted by Grotch and Hegstrom, since their method works only for a neutral system [105]. We choose to use the KF relation relation as Anthony and Sebastian did in their calculation [107]. We will explain that the KF relation is still applicable for a three-body charged system in the following discussion.

5.2 Hamiltonian of a polyelectron system

One way to construct the Hamiltonian is following Sebastian's procedure [106]. The total Hamiltonian of a system composed of N particles in free space can be straightforwardly written down to the first order of $1/c^2$ as

$$H = \sum_{i=1}^{N} \tilde{H}_i^{(0)} + \sum_{i>j} U_{ij} \tag{5.2.1}$$

where $\tilde{H}_i^{(0)} = \frac{\mathbf{p}_i^2}{2m_i} - \frac{\mathbf{p}_i^4}{8m_i^3c^2}$ is the free particle Hamiltonian for the ith particle, $\mathbf{p}_i$ is the LAB momentum of the ith particle. U_{ij} is the interaction between particles i and j. It is composed of two terms:

$$U_{ij} = U_{ij}^{(0)} + U_{ij}^{(1)} \tag{5.2.2}$$

where the first term

$$U_{ij}^{(0)} = \frac{e_i e_j}{r_{ij}} \tag{5.2.3}$$

is the Coulomb interaction between particles i and j. The second term can be written as

$$\begin{aligned} U_{ij}^{(1)} \equiv\ & U\left(\mathbf{p}_i, \mathbf{p}_j, \mathbf{r}_{ij}\right) = -\frac{e_i e_j}{2m_i m_j c^2}\left\{ \frac{\mathbf{p}_i \cdot \mathbf{p}_j}{r_{ij}} + \frac{\mathbf{r}_{ij} \cdot \left(\mathbf{r}_{ij} \cdot \mathbf{p}_i\right)\mathbf{p}_j}{r_{ij}^3} \right. \\ & -\frac{2}{r_{ij}^3}\left(\mathbf{r}_{ij} \times \mathbf{p}_i\right) \cdot \mathbf{s}_i + \frac{2}{r_{ij}^3}\left(\mathbf{r}_{ij} \times \mathbf{p}_i\right) \cdot \mathbf{s}_j \\ & -\frac{m_i}{m_j r_{ij}^3}\left(\mathbf{r}_{ij} \times \mathbf{p}_j\right) \cdot \mathbf{s}_j + \frac{m_j}{m_i r_{ij}^3}\left(\mathbf{r}_{ij} \times \mathbf{p}_i\right) \cdot \mathbf{s}_i \\ & +\pi\left(\frac{m_i}{m_j} + \frac{m_j}{m_i}\right)\delta^3\left(\mathbf{r}_{ij}\right) \\ & \left. -\frac{2}{r_{ij}^3}\left[\mathbf{s}_i \cdot \mathbf{s}_j - \frac{3\left(\mathbf{s}_i \cdot \mathbf{r}_{ij}\right) \cdot \left(\mathbf{s}_j \cdot \mathbf{r}_{ij}\right)}{r_{ij}^2}\right] + \frac{16\pi}{3}\mathbf{s}_i \cdot \mathbf{s}_j \delta^3\left(\mathbf{r}_{ij}\right) \right\} \end{aligned} \tag{5.2.4}$$

$U^{(1)}$ together with the Coulomb term $U^{(0)}$ is the Fermi-Breit interaction.

The Hamiltonian including an interaction with an external electromagnetic field has to fulfill two conditions. The Schrï¿œdinger equation in the presence of a vector potential $\mathbf{A}$ should be gauge invariant. Second, when the internal interaction between the particles goes to zero, the Hamiltonian of a composite system should be a simple sum of the FW transformed Hamiltonians of single spin-$\frac{1}{2}$ particles in the presence of an external vector potential. The correct Hamiltonian satisfying both of these requirements can be found by the FW transformation [106]; for the ith particle, the Hamiltonian without interactions between each pair of particles in the system can be written as

$$\tilde{H}_i^{(0)} \to \tilde{H}_i \equiv \tilde{H}_i^{(0)}\left(\mathbf{p}_i - \frac{e_i}{c}\mathbf{A}_i\right) - \frac{e_i}{m_i c}\mathbf{s}_i \cdot \mathbf{B} + \frac{e\mathbf{p}_i^2\left(\mathbf{s}_i \cdot \mathbf{B}\right)}{2m_i^3 c^3} \tag{5.2.5}$$

In the case of three particles with identical mass for Ps^-, we label the electrons with 1 and 2, and the positron with 3, and put $m_1 = m_2 = m_3 \equiv m$ in the expression of the total Hamiltonian [107]:

$$H = \sum_{i<j=1}^{3} U_{ij}^{(0)} + \sum_{i<j=1}^{3} U^{(1)}\left(\mathbf{\Pi}_i, \mathbf{\Pi}_j, \mathbf{r}_{ij}\right) + \sum_{i=1}^{3} \tilde{H}_i\left(\mathbf{\Pi}_i\right) \tag{5.2.6}$$

where $\mathbf{\Pi}_i = \mathbf{p}_i - \frac{e_i}{c}\mathbf{A}_i$ is the minimally subtracted momentum. The same Hamiltonian can be obtained by the extended FW transformation to the Breit Hamiltonian [103, 104, 105]. We

notice that the Hamiltonian of the three body system is a simple extension of the two-body Hamiltonian, because no three-body term is involved in our calculation. The vector potential $\mathbf{A}_i$ can be chosen as $\frac{1}{2}\mathbf{B}\times\mathbf{r}_i$, therefore, the minimal subtracted momentum turns out to be

$$\mathbf{\Pi}_i = \mathbf{p}_i - \frac{e_i}{c}\mathbf{A}_i = \mathbf{p}_i - \frac{e_i}{2c}\mathbf{B}\times\mathbf{r}_i \tag{5.2.7}$$

We write the Hamiltonian in a form consistent with previously published expressions [105, 107],

$$H = \sum_{n=0}^{7} H_n \tag{5.2.8}$$

According to (5.2.6, 5.2.5, 5.2.4), the terms in the Hamiltonian can be written separately as

$$H_0 = \frac{\mathbf{\Pi}_1^2}{2m} + \frac{\mathbf{\Pi}_2^2}{2m} + \frac{\mathbf{\Pi}_3^2}{2m} + \frac{e^2}{r_{12}} - \frac{e^2}{r_{13}} - \frac{e^2}{r_{23}} \tag{5.2.9}$$

$$H_1 = -\frac{\mathbf{\Pi}_1^4}{8m^3c^2} - \frac{\mathbf{\Pi}_2^4}{8m^3c^2} - \frac{\mathbf{\Pi}_3^4}{8m^3c^2} \tag{5.2.10}$$

$$H_3 = -\frac{e^2}{2m^2c^2}\mathbf{s}_3\cdot\frac{\mathbf{r}_{23}\times\mathbf{\Pi}_3}{r_{23}^3} - \frac{e^2}{2m^2c^2}\mathbf{s}_3\cdot\frac{\mathbf{r}_{13}\times\mathbf{\Pi}_3}{r_{13}^3} \tag{5.2.11}$$

$$H_4 = \frac{e^2}{m^2c^2}\mathbf{s}_3\cdot\frac{\mathbf{r}_{13}\times\mathbf{\Pi}_1}{r_{13}^3} + \frac{e^2}{m^2c^2}\mathbf{s}_3\cdot\frac{\mathbf{r}_{23}\times\mathbf{\Pi}_2}{r_{23}^3} \tag{5.2.12}$$

$$H_5 = -\frac{e}{mc}\mathbf{s}_3\cdot\mathbf{B}\left(1 - \frac{\mathbf{\Pi}_3^2}{2m^2c^2}\right) \tag{5.2.13}$$

$$\begin{aligned} H_6 = {} & \frac{e^2}{2m^2c^2}\left[\frac{\mathbf{\Pi}_1\cdot\mathbf{\Pi}_3}{r_{13}} + \frac{\mathbf{r}_{13}\cdot(\mathbf{r}_{13}\cdot\mathbf{\Pi}_1)\,\mathbf{\Pi}_3}{r_{13}^3}\right] \\ & -\frac{e^2}{2m^2c^2}\left[\frac{\mathbf{\Pi}_1\cdot\mathbf{\Pi}_2}{r_{12}} + \frac{\mathbf{r}_{12}\cdot(\mathbf{r}_{12}\cdot\mathbf{\Pi}_1)\,\mathbf{\Pi}_2}{r_{12}^3}\right] \\ & +\frac{e^2}{2m^2c^2}\left[\frac{\mathbf{\Pi}_2\cdot\mathbf{\Pi}_3}{r_{23}} + \frac{\mathbf{r}_{23}\cdot(\mathbf{r}_{23}\cdot\mathbf{\Pi}_2)\,\mathbf{\Pi}_3}{r_{23}^3}\right] \end{aligned} \tag{5.2.14}$$

where $r_{ij}\equiv|\mathbf{r}_{ij}| = |\mathbf{r}_i - \mathbf{r}_j|$. Here we only retain the terms that can contribute to the magnetic moment in the desired order of α. The H_2 does not depend on the spin operators, and the H_7 is quadratic in the spin operators. Thus, both of them are omitted in our calculation. The terms proportional to $\mathbf{s}_1$ and $\mathbf{s}_2$ are symmetric in the particle indices 1 and 2. However, the Ps^- wave function is antisymmetric in 1 and 2. Therefore the expectation values of these terms are zero, and they have been omitted in the above expressions.

5.3 CM coordinates

The Zeeman effect describes the splitting of the energy spectral line of an atomic system within a static magnetic field. It represents the intrinsic magnetic property of the system. The term of the Hamiltonian representing the Zeeman effect is

$$\begin{aligned} H_M &= -\boldsymbol{\mu}\cdot\mathbf{B} = -\mu_B\left(g_l\mathbf{l} + g_s\mathbf{s}\right)\cdot\mathbf{B} \\ &= -\mu_B g_s\mathbf{s}\cdot\mathbf{B} \qquad\qquad \text{for } (l=0)\,, \end{aligned} \tag{5.3.1}$$

where $\boldsymbol{\mu}$ is the magnetic moment of the atom, μ_B is the Bohr magneton, and $g_s \equiv g$ is the g factor that we are looking for. Hence, the internal dynamics needs to be separated from the motion of the whole system. The whole system behaves like a particle with some intrinsic

features. That is to say, we would like to write the wave function of the Ps^- as a product of the external wave function and the internal wave function.

$$\Psi = \psi\left(\mathbf{P}, \mathbf{R}, \mathbf{S}\right) \phi\left(\boldsymbol{\pi}_i, \boldsymbol{\rho}_i, \boldsymbol{\sigma}_i\right) \quad i = 1, 2 \ldots N \tag{5.3.2}$$

We call the variables $\{\mathbf{R}, \mathbf{P}, \boldsymbol{\pi}_i, \boldsymbol{\rho}_i, \boldsymbol{\sigma}_i, | i = 1, 2 \ldots N\}$ the "Center of mass variables" (CM), where $\mathbf{R}$ and $\mathbf{P}$ are the position and momentum of the center of mass of the system and $\boldsymbol{\pi}_i$ and $\boldsymbol{\rho}_i$ are the position and momentum of the ith particle in the center of mass frame. On the other hand, the set of coordinates of each particle in the lab frame $\{\mathbf{r}_i, \mathbf{p}_i | i = 1, 2 \ldots N\}$ are the "LAB variables" (LAB).

5.3.1 Independence of the total momentum P

In order to write down the wave function (5.3.2), one has to know that the external and the internal wavefunction of the system is separable. The Hamiltonian of a system can always be written in the single-particle form

$$\begin{aligned} H &= \sqrt{\left(\mathbf{P} - Q\mathbf{A}/c\right)^2 c^2 + h^2} - \frac{Q\mathbf{S}\cdot\mathbf{B}c}{h} \\ &= \sqrt{\left(P^2 - Q\mathbf{P}\cdot\mathbf{A}/c - Q\mathbf{A}\cdot\mathbf{P}/c + Q^2A^2/c^2\right)c^2 + h^2} - \frac{Q\mathbf{S}\cdot\mathbf{B}c}{h} \end{aligned}$$

where the mass term $h = Mc^2 + h^{(0)}$, $h^{(0)}$ is the internal Hamiltonian of the system. Now we can rewrite this expression into

$$\begin{aligned} H &= \sqrt{P_{\text{ext}}^2 c^2 + M^2c^4 + h^{(0)2} + 2Mh^{(0)}c^2} - \frac{Q\mathbf{S}\cdot\mathbf{B}}{Mc}\left(1 + \frac{h^{(0)}}{Mc^2} + \cdots\right) \\ &= Mc^2\left[1 + \frac{P_{\text{ext}}^2c^2 + h^{(0)2}}{2M^2c^4} + \frac{h^{(0)}}{Mc^2} - \frac{1}{8M^2c^4}\left(\frac{P_{\text{ext}}^2c^2 + h^{(0)2}}{Mc^2} + 2h^{(0)}\right)^2 + \cdots\right] \end{aligned}$$

where $P_{\text{ext}}^2 = P^2 - Q\mathbf{P}\cdot\mathbf{A}/c - Q\mathbf{A}\cdot\mathbf{P}/c + Q^2A^2/c^2$ only contains external variables. We can see from above expression, that there is no term containing both external and internal variables (we call it mixed term) until the first power of $1/c^2$. In this way we realize that the external and internal wave functions are separable in the first order perturbation calculation, where nonrelativistic wave functions are taken as the basis functions.

5.3.2 KF relations with an external magnetic field

In order to calculate the magnetic moment, we need the Hamiltonian expressed in the CM variables. This can be achieved by using the KF relations between the CM and LAB variables [108],

$$\begin{aligned} \mathbf{r}_i &= \boldsymbol{\rho}_i + \mathbf{R} - \frac{1}{2c^2}\left[\frac{\boldsymbol{\rho}_i\cdot\mathbf{P}}{M}\left[\frac{\boldsymbol{\pi}_i}{m} + \frac{\mathbf{P}}{2M}\right] + H.c.\right] - \frac{1}{2c^2}\sum_j\left[\frac{\pi_j^2\boldsymbol{\rho}_j}{2mM} + H.c.\right] + \sum_j\frac{\left(\boldsymbol{\rho}_j\times\boldsymbol{\pi}_j\right)}{2M^2c^2}\times\mathbf{P} \\ &- \frac{\boldsymbol{\sigma}_i\times\mathbf{P}}{2mMc^2} + \sum_j\frac{\boldsymbol{\sigma}_j\times\boldsymbol{\pi}_j}{2mMc^2} + \sum_j\frac{\boldsymbol{\sigma}_j\times\mathbf{P}}{2M^2c^2} - \frac{1}{M}\mathrm{W}^{(1)} - \frac{i}{M}\left[\int_0^P d\mathbf{p}\cdot\mathrm{W}^{(1)}, \boldsymbol{\rho}_i\right], \\ \mathbf{p}_i &= \boldsymbol{\pi}_i + \frac{m}{M}\mathbf{P} + \left[\frac{\pi_i^2}{2m} - \frac{m}{M}\sum_j\frac{\pi_j^2}{2m} + \frac{\boldsymbol{\pi}_i\cdot\mathbf{P}}{2M}\right]\frac{\mathbf{P}}{Mc^2} - \frac{i}{M}\left[\int_0^P d\mathbf{p}\cdot\mathrm{W}^{(1)}, \boldsymbol{\pi}_i\right], \\ \mathbf{s}_i &= \boldsymbol{\sigma}_i - \frac{\boldsymbol{\sigma}_i\times\left(\boldsymbol{\pi}_i\times\mathbf{P}\right)}{2mMc^2} - \frac{i}{M}\left[\int_0^P d\mathbf{p}\cdot\mathrm{W}^{(1)}, \boldsymbol{\sigma}_i\right], \end{aligned} \tag{5.3.3}$$

where $\mathbf{r}_i$, $\mathbf{p}_i$, and $\mathbf{s}_i$ are the LAB particle variables of the ith particle in the system, $\boldsymbol{\rho}_i$, $\boldsymbol{\pi}_i$, and $\boldsymbol{\sigma}_i$ are the corresponding CM variables. M is the total mass of the system. $\mathrm{W}^{(1)}$ is one term of the Poincaré boost generator whose definition will be briefly discussed later.

Now let us think about the KF relations for a system within an external magnetic field. If we turn off the external field, the generators should change back into their original forms in the field free case. This fact tells us that the expressions of the field-free generators, written in both the LAB and the CM forms, are the leading order terms of the generators of a system within an external electromagnetic field. We notice that the definition of the position of a certain particle should not involve the external field. The transformation of the LAB variables to the CM variables should only involve the intrinsic variables like momentum, position, and spin, but not the external parameter like the magnetic field. Otherwise, if one switches on/off the external magnetic field, the dynamic variables like the momentum, position, and the spin cannot suddenly change, the equivalence of coordinates expressed by the KF relations will be broken. Thus in our calculation of the magnetic moment of the positronium ion system, the external magnetic field does not affect the KF transformation.

V operator

Now let us look at the operator $\mathbf{V}$ in the LAB Poincaré representation in equations (2.3) of [108]. The Lie algebra of the Poincaré group given in equations (2.2) of the same paper, requires the following conditions to be satisfied

$$\begin{aligned}
&[U, \mathbf{P}] = [U, \mathbf{J}] = 0 \\
&[J_i, V_j] = i\epsilon_{ijk} V_k \\
&[V_i, P_j] = i\delta_{ij} U/c^2 \\
&\left[V_i, \sum_\mu K_\mu^j\right] - (i \longleftrightarrow j) + [V_i, V_j] = 0
\end{aligned} \tag{5.3.4}$$

The first relation can be verified by noticing that U is a scalar function of the CM coordinates. We can further verify that the following definition of V satisfies above restrictions conveniently

$$\begin{aligned}
U^{(0)} &= \frac{1}{2c^2} \sum_{i,j=1}^{N} u^{ij(0)} \\
V &= \frac{1}{2c^2} \sum_{i,j=1}^{N} \mathbf{R}_{ij} u^{ij(0)} = \frac{V^{(1)}}{c^2}
\end{aligned} \tag{5.3.5}$$

where $\mathbf{R}_{ij} = (m_i \mathbf{r}_i + m_j \mathbf{r}_j)/(m_i + m_j) = (\mathbf{r}_i + \mathbf{r}_j)/2$ in system composed of particles with equal masses, and $u^{ij(0)} = u^{(0)}(|\mathbf{r}_i - \mathbf{r}_j|)$. The second relation in (5.3.4) can be verified by noticing $\mathbf{V}$ is a vector. The third relation can be verified by substituting the definition (5.3.5) into the commutator, and using the definition $\mathbf{P} = \sum_{i=1}^{N} \mathbf{p}_i$. The forth relation can be proved by noticing the fact $[r_i, p_j] = [r_j, p_i]$, and $[V_i, V_j] = 0$. In the derivation of the KF transformation, an operator $W^{(1)}$ is introduced in the following way

$$V^{(1)} = \frac{1}{2}\left(\mathbf{R}U^{(0)} + U^{(0)}\mathbf{R}\right) + W^{(1)} \tag{5.3.6}$$

Thus under the current choice of the $V^{(1)}$, one can easily derive its expression [108]

$$W^{(1)} = V^{(1)} - \frac{1}{2}\left(\mathbf{R}U^{(0)} + U^{(0)}\mathbf{R}\right) = \frac{1}{2}\sum_{i,j=1}^{N} \boldsymbol{\rho}_{ij}^{+} u^{ij(0)} \tag{5.3.7}$$

where $\boldsymbol{\rho}_{ij}^{+} = \left(\boldsymbol{\rho}_i + \boldsymbol{\rho}_j\right)/2$. We can see that for a system of two particles, $W^{(1)} = 0$, while for a three particle system, it generally is nonzero.

Counting the power of 1/c

When we use the KF relations to transform the Hamiltonian into the function of the CM plus internal variables, we only keep terms up to $1/c^3$, which leads to contributions to α^3. Here we have used a general trick that we normally use in the calculation of a poly-electron system. The terms with higher power of $1/c$ can be omitted because the power of $1/c$ equals to the power of α. This relation can be clearly seen if we introduce the Hartree atomic units

$$e = m_e = \hbar = 1$$
$$c = \frac{1}{\alpha}$$

into the Hamiltonian.

5.4 g factor in a two-body atoms

Before we consider the three-body ion, we show how the known corrections for simple one-electron atoms can be reproduced.

5.4.1 Positronium

Positronium is a two-body system with the symmetry due to equal masses, so the Hamiltonian simplifies. Among the parts of the Hamiltonian shown in eqs. (5.2.9-5.2.13), only $H_{0,3,4,5}$ contribute to the order α^2. The Ps atom contains only the electron $i = 1$ and the positron $i = 3$, so all terms where the label $i = 2$ appears can be neglected. On the other hand, in $H_{3,4,5}$, we have to account for the spin of the electron (not included in (5.2.11-5.2.13) in anticipation of cancellations in Ps^-, due to the symmetry of its wave function). This is achieved by replacing $\mathbf{s}_3 \to \mathbf{s}_3 - \mathbf{s}_1$.

We set $e_3 = -e_1 = e$ and $\boldsymbol{\pi}_3 = -\boldsymbol{\pi}_1 = \boldsymbol{\pi}$. Neglecting terms containing R and P, we find that in the transformation LAB→CM, eq. (5.3.3), the only term relevant for the Ps atom is

$$\mathbf{r}_i \to \boldsymbol{\rho}_i + \sum_j \frac{\boldsymbol{\sigma}_j \times \boldsymbol{\pi}_j}{2mMc^2} = \boldsymbol{\rho}_i + \frac{(\boldsymbol{\sigma}_3 - \boldsymbol{\sigma}_1) \times \boldsymbol{\pi}}{4m^2c^2}, \tag{5.4.1}$$

while the momentum and spin transform trivially, $\mathbf{p}_i \to \boldsymbol{\pi}_i$ and $\mathbf{s}_i \to \boldsymbol{\sigma}_i$.

Since the transformation (5.4.1) adds a term suppressed by $1/c^2$, we only need to apply it to the lowest order term H_0, where it affects the vector potential in the kinetic term. The resulting contribution to the magnetic moment is (here and below we average over the directions of position and momentum, since we are interested in the S-wave ground state),

$$\Pi_1^2 = \left(p_1 - \frac{e_1}{c}A_1\right)^2 \to -\left\{\boldsymbol{\pi}, \frac{e}{2c}\mathbf{B} \times \frac{(\boldsymbol{\sigma}_3 - \boldsymbol{\sigma}_1) \times \boldsymbol{\pi}}{4m^2c^2}\right\} \to \frac{e}{6m^2c^3}(\boldsymbol{\sigma}_3 - \boldsymbol{\sigma}_1) \cdot \boldsymbol{B}\pi^2. \tag{5.4.2}$$

The same effect arises from the kinetic energy of the positron. In total,

$$\frac{\Pi_1^2 + \Pi_3^2}{2m} \to \frac{e}{6m^3c^3}(\boldsymbol{\sigma}_3 - \boldsymbol{\sigma}_1) \cdot \boldsymbol{B}\pi^2. \tag{5.4.3}$$

The next corrections are expressed by position operators of $e^{\pm}$. We have, after the transformation to CM, $\boldsymbol{r}_1 \to \boldsymbol{\rho}_1 \equiv -\frac{\boldsymbol{r}}{2}$, $\boldsymbol{r}_3 \to \boldsymbol{\rho}_3 \equiv +\frac{\boldsymbol{r}}{2}$, and $\boldsymbol{r}_{13} \to -\boldsymbol{r}$. The sum of terms 3 and 4 in the Hamiltonian, eqs. (5.2.11-5.2.12), gives the magnetic interaction

$$H_3 + H_4 \to \frac{e^2}{2m^2c^2}\left(\boldsymbol{\sigma}_3 - \boldsymbol{\sigma}_1\right) \cdot \frac{\boldsymbol{r} \times \left(\frac{e}{4}\boldsymbol{B} \times \boldsymbol{r}\right)}{r^3} \to \frac{e^3}{12m^2c^2r}\left(\boldsymbol{\sigma}_3 - \boldsymbol{\sigma}_1\right) \cdot \boldsymbol{B}. \tag{5.4.4}$$

Finally, H_5 gives

$$H_5 \to -\frac{e}{mc}\left(\boldsymbol{\sigma}_3 - \boldsymbol{\sigma}_1\right) \cdot \boldsymbol{B}\left(1 - \frac{\pi^2}{2m^2c^2}\right). \tag{5.4.5}$$

The total magnetic moment interaction is the sum of (5.4.3-5.4.5). Its expectation value with the ground state spatial part of the wave function gives

$$-\frac{e}{mc}\left(\boldsymbol{\sigma}_3 - \boldsymbol{\sigma}_1\right) \cdot \boldsymbol{B}\left\langle 1 - \frac{\pi^2}{6m^2c^2} - \frac{\pi^2}{2m^2c^2} - \frac{e^2}{12mcr}\right\rangle = -\frac{e}{mc}\left(\boldsymbol{\sigma}_3 - \boldsymbol{\sigma}_1\right) \cdot \boldsymbol{B}\left(1 - \frac{5\alpha^2}{24}\right), \tag{5.4.6}$$

confirming the well known result [105, 109, 110]. The resulting interaction does not have diagonal elements neither in spin singlet nor triplet states of Ps. However, it mixes the $m = 0$ state of the triplet with the singlet. Measurements of the resulting splitting among the oPs states determine the hyperfine splitting of positronium.

5.4.2 Hydrogen

In hydrogen there are further simplifications, since the spin-other orbit term H_4 does not contribute in the leading order, due to the suppression by the proton mass. Also, there is no difference between the LAB and the CM frames, in the leading order in $1/M$. Thus only H_5 and the spin-orbit term H_3 contribute (we replace $\mathbf{s}_3 \to \mathbf{s}$ and $\boldsymbol{r}_{13} \to \boldsymbol{r}$),

$$H_3 \to \frac{e^2}{2m^2c^2}\mathbf{s} \cdot \frac{\boldsymbol{r} \times \left(\frac{e}{2c}\boldsymbol{B} \times \boldsymbol{r}\right)}{r^3} \to \frac{e^3}{6m^2c^3r}\mathbf{s} \cdot \boldsymbol{B}$$
$$H_5 \to \frac{e}{mc}\mathbf{s} \cdot \boldsymbol{B}\left(1 - \frac{\pi^2}{2m^2c^2}\right)$$

and the total magnetic moment interaction in the ground state of H becomes

$$\frac{e}{mc}\mathbf{s} \cdot \boldsymbol{B}\left\langle 1 - \frac{\pi^2}{2m^2c^2} + \frac{e^2}{6mc^2r}\right\rangle = \frac{e}{mc}\mathbf{s} \cdot \boldsymbol{B}\left(1 - \frac{\alpha^2}{3}\right), \tag{5.4.7}$$

in agreement with the classic result by Breit [92].

5.4.3 Hydrogen-like ions, including recoil effects

Now we consider an ion consisting of a nucleus with charge Ze and a single electron with $-e$. Among the systems, for which binding effects on the g factors have been evaluated, this is the closest one to the positronium ion, which is also charged and in which recoil effects are not suppressed, since there is no heavy nucleus.

Since we have already established which terms are relevant to the order we need, we set $c = 1$ from now on. The relevant terms of the KF transformation become, using $\boldsymbol{r} \equiv \boldsymbol{r}_e - \boldsymbol{r}_p$, m for the mass of the electron and, only in this section, M for the mass of the nucleus, for easier

comparison with ref. [105]

$$\begin{aligned}\boldsymbol{r}_e &\to \boldsymbol{R} + \frac{M}{M+m}\boldsymbol{r} + \frac{\mathbf{s}_e \times \boldsymbol{p}_e}{2m(M+m)},\\ \boldsymbol{r}_p &\to \boldsymbol{R} - \frac{m}{M+m}\boldsymbol{r} + \frac{\mathbf{s}_e \times \boldsymbol{p}_e}{2m(M+m)}.\end{aligned} \tag{5.4.8}$$

This introduces the spin interaction into the kinetic energy term H_0,

$$H_0 = \frac{\mathbf{\Pi}_e^2}{2m} + \frac{\mathbf{\Pi}_p^2}{2M} \to -\frac{e\mathbf{s}\cdot\boldsymbol{B}}{6(M+m)}\left(\frac{1}{m^2} + \frac{Z}{mM}\right)\left\langle \pi^2 \right\rangle, \tag{5.4.9}$$

and in the ground state $\langle \pi^2 \rangle = Z^2\alpha^2\mu^2$ where $\mu = \frac{Mm}{M+m}$ is the reduced mass.

If the nuclear mass is taken as finite, the spin-orbit and spin-other orbit terms become

$$H_3 + H_4 \to \frac{\alpha}{2m^2r^3}\mathbf{s}\cdot\boldsymbol{r}\times\mathbf{\Pi}_e - \frac{\alpha}{mMr^3}\mathbf{s}\cdot\boldsymbol{r}\times\mathbf{\Pi}_p \to \frac{eZ^2\alpha^2\mu}{6m^2M(M+m)}\mathbf{s}\cdot\boldsymbol{B}\left(M^2 - 2Zm^2\right). \tag{5.4.10}$$

Finally, the last correction comes from H_5,

$$H_5 \to \frac{e\mathbf{s}\cdot\boldsymbol{B}}{m}\left(1 - \frac{Z^2\alpha^2\mu^2}{2m^2}\right). \tag{5.4.11}$$

The sum of (5.4.9, 5.4.10, 5.4.11) gives the total magnetic moment interaction in the ion,

$$\frac{e\mathbf{s}\cdot\boldsymbol{B}}{m}\left(1 - Z^2\alpha^2\frac{M^2(3m+2M) + Zm^2(3M+2m)}{6(M+m)^3}\right), \tag{5.4.12}$$

in agreement with Eq. (43) in [105]. We note that the correction is symmetric with respect to the exchange of the electron and nucleus mass and charge, $M \leftrightarrow m$, $Z \leftrightarrow 1$; in the limit $M \gg m$ reproduces our non-recoil result (5.4.7); and in the limit $Z \to 1$, $M \to m$ agrees with the correction in the positronium atom (5.4.6).

5.5 Positronium Ion

5.5.1 The contributions to the magnetic moment from the Hamiltonian

Let us look into the details of minimal subtracted momentum written in the center of mass coordinates. The expression of $\mathbf{R}_{ij} - \mathbf{R}$ can be further written to the zero order of $1/c$ as

$$\begin{aligned}\mathbf{R}_{ij} - \mathbf{R} &= \frac{\mathbf{r}_i^{(0)} + \mathbf{r}_j^{(0)}}{2} - \mathbf{R}\\ &= \frac{\left(\mathbf{r}_i^{(0)} - \mathbf{R}\right) + \left(\mathbf{r}_j^{(0)} - \mathbf{R}\right)}{2}\\ &= \frac{\boldsymbol{\rho}_i + \boldsymbol{\rho}_j}{2} = \boldsymbol{\rho}_{ij}^{+}\end{aligned} \tag{5.5.1}$$

since in our system $m_i \equiv m$ $(i = 1, 2, 3)$. Thus we have obtained an expression for $W^{(1)}$,

$$W^{(1)} = \frac{1}{2}\sum_{ij}\boldsymbol{\rho}_{ij}^{+}u_{ij}^{(0)} \tag{5.5.2}$$

Substituting these relations into our definition of $\mathbf{\Pi}_i$, one has

$$\begin{aligned}\mathbf{\Pi}_i &= \boldsymbol{\pi}_i - \frac{e_i}{2c}\mathbf{B}\times\mathbf{r}_i \\ &= \boldsymbol{\pi}_i - \frac{e_i}{2c}\mathbf{B}\times\left\{\boldsymbol{\rho}_i - \frac{1}{2c^2}\sum_{j=1}^{3}\left[\frac{\pi_j^2\boldsymbol{\rho}_j}{2mM} + H.c.\right] + \sum_{j=1}^{3}\frac{\boldsymbol{\sigma}_j\times\boldsymbol{\pi}_j}{2mMc^2} - \frac{1}{M}W^{(1)}\right\} \\ &= \boldsymbol{\pi}_i + \mathbf{F}_i + \mathbf{G}_i \end{aligned} \tag{5.5.3}$$

where

$$\mathbf{F}_i = -\frac{e_i}{2c}\mathbf{B}\times\left[\boldsymbol{\rho}_i - \frac{1}{12m^2c^2}\sum_{j=1}^{N}\left[\pi_j^2\boldsymbol{\rho}_j + H.c.\right] - \frac{1}{6mc^2}\sum_{jk}\boldsymbol{\rho}_{jk}^{+}u_{jk}^{(0)}\right] \tag{5.5.4}$$

$$\mathbf{G}_i = -\frac{e_i}{2c}\mathbf{B}\times\sum_j\frac{\boldsymbol{\sigma}_j\times\boldsymbol{\pi}_j}{6m^2c^2} \tag{5.5.5}$$

Keeping the term linear in the magnetic field strength $\mathbf{B}$, one would get the terms contributing to Zeeman effect. The terms that are linear in spin operator can be divided into three groups, according to the spin they are proportional to. Keeping only the term linear in B, the summation of H_3 and H_4 generates a simpler expression

$$\begin{aligned}H_3 + H_4 \Longrightarrow\ & \frac{e^3}{4m^2c^3\rho_{13}^3}\left[\sigma_{3z}B\left(\boldsymbol{\rho}_{13}\cdot\boldsymbol{\rho}_{12}\right) - \left(\boldsymbol{\sigma}_3\cdot\boldsymbol{\rho}_{12}\right)\rho_{13z}B\right] \\ &+ \frac{e^3}{4m^2c^3\rho_{23}^3}\left[\sigma_{3z}B\left(\boldsymbol{\rho}_{23}\cdot\boldsymbol{\rho}_{21}\right) - \left(\boldsymbol{\sigma}_3\cdot\boldsymbol{\rho}_{21}\right)\rho_{23z}B\right]\end{aligned} \tag{5.5.6}$$

The contribution from H_5 is

$$H_5 \Rightarrow -\frac{e}{mc}\sigma_{3z}B\left(1 - \frac{\pi_3^2}{2m^2c^2}\right) \tag{5.5.7}$$

Next contribution to the Zeeman effect comes from H_0. According to (5.2.9) we know that only the first three terms contribute

$$\begin{aligned}H_0 \Longrightarrow & \sum_i\frac{\mathbf{\Pi}_i^2}{2m} \to \sum_i\frac{\boldsymbol{\pi}_i\cdot\mathbf{G}_i + \mathbf{G}_i\cdot\boldsymbol{\pi}_i}{2m} \\ &= -\frac{1}{12m^3c^3}\sum_{i=1,2}e_i\left[\left(\boldsymbol{\pi}_i\cdot\boldsymbol{\sigma}_3\right)\pi_{3z}B - \left(\boldsymbol{\pi}_i\cdot\boldsymbol{\pi}_3\right)\sigma_{3z}B\right]\end{aligned} \tag{5.5.8}$$

Now we will prove that there is no contribution from H_1. According to (5.2.10)

$$H_1 = -\tfrac{1}{8m^3c^2}\textstyle\sum_i\mathbf{\Pi}_i^4 \tag{5.5.9}$$

Retaining terms to the first order of $1/c$ and $\mathbf{B}$, and with $\mathrm{O}\left(\frac{1}{m}\right) \le 3$ we have

$$\begin{aligned}&\mathbf{\Pi}_i^4 = \left(\boldsymbol{\pi}_i + \mathbf{F}_i + \mathbf{G}_i\right)^2\left(\boldsymbol{\pi}_i + \mathbf{F}_i + \mathbf{G}_i\right)^2 \\ &\to -\frac{e_i}{c}\pi_i^2\left[\boldsymbol{\pi}_i\cdot\left(\mathbf{B}\times\boldsymbol{\rho}_i\right) + \left(\mathbf{B}\times\boldsymbol{\rho}_i\right)\cdot\boldsymbol{\pi}_i\right] \propto \mathbf{B}\cdot\left(\boldsymbol{\rho}_i\times\boldsymbol{\pi}_i - \boldsymbol{\pi}_i\times\boldsymbol{\rho}_i\right) \\ &\Rightarrow 0\end{aligned} \tag{5.5.10}$$

where we have used the fact that the expectation value of $\left(\boldsymbol{\rho}_i\times\boldsymbol{\pi}_i - \boldsymbol{\pi}_i\times\boldsymbol{\rho}_i\right)$ between ground states is zero. Thus H_1 does not contribute. Now transform the CM position operators into relative distances, we have

$$\begin{aligned}\mathbf{R} &= \frac{1}{3}\left(\mathbf{r}_1 + \mathbf{r}_2 + \mathbf{r}_3\right) \\ \mathbf{r}_{12} &= \mathbf{r}_2 - \mathbf{r}_1 \\ \mathbf{r}_{13} &= \mathbf{r}_3 - \mathbf{r}_1\end{aligned} \tag{5.5.11}$$

Correspondingly, the relations between the gradients of the two coordinate systems are

$$\begin{aligned}\nabla_1 &= \frac{1}{3}\nabla_{\mathbf{R}} - \nabla_{12} - \nabla_{13} \\ \nabla_2 &= \frac{1}{3}\nabla_{\mathbf{R}} + \nabla_{12} \\ \nabla_3 &= \frac{1}{3}\nabla_{\mathbf{R}} + \nabla_{13}\end{aligned} \tag{5.5.12}$$

Thus π_3^2 is transformed into $-\nabla_{13}^2$. A straightforward observation tells us, there is no contribution to the magnetic moment to the order of $1/c^3$ from the last Hamiltonian component H_6 under the KF transformation. Finally, by summing the contributions from H_0 to H_5, we obtain the components in the Hamiltonian, that is linear in $\boldsymbol{\sigma}_3$ and $\mathbf{B}$.

$$H_Z = \sigma_{3z}\mathbf{B}\left[-\frac{e}{m} - \frac{11e}{18m^3}\boldsymbol{\nabla}_{13}^2\right] + \sigma_{3z}\mathbf{B}\frac{e^3}{6m^2}\left[\frac{\boldsymbol{\rho}_{13}\cdot\boldsymbol{\rho}_{12}}{\rho_{13}^3} + \frac{\boldsymbol{\rho}_{23}\cdot\boldsymbol{\rho}_{21}}{\rho_{23}^3}\right] \tag{5.5.13}$$

Here since we do not have to count the power of $1/c$ anymore, powers of $1/c$ have been omitted by setting $c = 1$. The Zeeman effect is calculated by taking the expectation of H_Z in the ground state $|n = 1, \mathbf{J} = \mathbf{L} + \mathbf{S} = \mathbf{S} = \boldsymbol{\sigma}_3, S_{3z} = \sigma_{3z} = \frac{1}{2}\rangle$ of the positronium ion system

$$\begin{aligned}&\left\langle 1, {}^2S_{\frac{1}{2}},\, S_{3z} = \frac{1}{2}\right| H_Z \left| 1, {}^2S_{\frac{1}{2}},\, S_{3z} = \frac{1}{2}\right\rangle \\ &= \mu_B g \left\langle 1, {}^2S_{\frac{1}{2}},\, S_{3z} = \frac{1}{2}\right| \mathbf{S}_3\cdot\mathbf{B} \left| 1, {}^2S_{\frac{1}{2}},\, S_{3z} = \frac{1}{2}\right\rangle\end{aligned} \tag{5.5.14}$$

Correspondingly, the g factor becomes

$$g = 2\left[1 - \frac{11\alpha^2}{18}\left\langle\pi_{13}^2\right\rangle - \frac{\alpha^2}{6}\left(\left\langle\frac{\boldsymbol{\rho}_{13}\cdot\boldsymbol{\rho}_{12}}{\rho_{13}^3}\right\rangle + \left\langle\frac{\boldsymbol{\rho}_{23}\cdot\boldsymbol{\rho}_{21}}{\rho_{23}^3}\right\rangle\right)\right]. \tag{5.5.15}$$

What we are looking for is the coefficient of the α^2 term; this can be obtained by calculating the expectation with trial function.

5.5.2 Optimization procedure

We are using the same trial wave function as used in the study of the di-positronium molecule [111]. In particular

$$\phi = \sum_{i=1}^{N} c_i \exp\left[-\sum_{a<b} w_{ab}^i \rho_{ab}^2\right] \tag{5.5.16}$$

where ρ_{jk} are the three inter-particle separations. Also, we use H_C to denote the non-relativistic Coulomb Hamiltonian

$$H_C = \sum_{i=1}^{3}\frac{\mathbf{p}_i^2}{2m} + \sum_{i<j}\frac{e_i e_j}{\rho_{ij}} \tag{5.5.17}$$

The optimization procedure used to determine the three parameters w_{ab}^i in each of the N functions in (5.5.16) is based on that used in [111]. This process begins by using QR decomposition and inverse iteration to find the eigenvalue of H_C corresponding to a variational upper limit on the bound state energy of the system. Thereafter parameters minimizing the energy are found by using Powell's method. In particular, three parameters of a basis wave function are changed, the initial QR decomposition is updated accordingly, and inverse iteration then gives the change in energy. Powell's method finds the parameters that give the largest decrease in

energy for each set of three parameters. The basis elements are cycled through in this manner until convergence is reached for a particular value of N. At this point more basis elements can be added and the above procedure repeated. Using the wave function obtained in this procedure, one determines the expectation value of (5.5.13) and finds

$$\begin{aligned} g_{\mathrm{Ps}^-} &= g_{\mathrm{free}} + \Delta g_{\mathrm{bound}}, \\ \Delta g_{\mathrm{bound}} &= -0.51(1)\alpha^2. \end{aligned} \tag{5.5.18}$$

Here $g_{\mathrm{free}} = 2\left[1 + \frac{\alpha}{2\pi} - 0.328\left(\frac{\alpha}{\pi}\right)^2 + \dots\right]$ is the g-factor of a free electron [91]. The error in (5.5.18) arises primarily from higher-order binding corrections, beyond the scope of this paper. Note that the binding correction (5.5.18) exceeds the same order effect, $\mathcal{O}(\alpha^2)$, in g_{free}, about 15 times. Our final prediction for the gyromagnetic factor of the positronium ion is

$$g_{\mathrm{Ps}^-} = 2.00461(1). \tag{5.5.19}$$

We see that the correction (5.5.18) is smaller in magnitude than in hydrogen, Eq. (5.4.7), where it is $-0.67\alpha^2$, but larger than in the positronium atom, Eq. (5.4.7), $-0.42\alpha^2$. Indeed, this confirms the naive expectation that the value should be in between these two and closer to positronium. The entire magnetic moment of the three-body ion can be thought of as being due to the magnetic moment of the positron, whose gyromagnetic ratio g is modified by the binding to the two electrons. If the two electrons are considered as a kind of a nucleus in whose field the g factor of the positron is modified, it is heavier than in the positronium atom, but much lighter than in hydrogen.

5.6 Conclusion

We determine the gyromagnetic factor of the positronium ion, a three-body system consisting of two electrons and a positron, including first relativistic corrections. We find that the g-factor is modified by a term $-0.51(1)\alpha^2$, exceeding 15 times the α^2 correction for a free electron. We compare this effect with analogous results found previously in atomic positronium and in hydrogen-like ions. Can this quantity be measured? The main challenge is the very short lifetime of the ion, only four times longer than that of the atomic parapositronium, or about half a nanosecond. With an intense beam and a strong external magnetic field, a possible scenario of a measurement could be as follows. An ion with a known initial polarization could be subjected to the magnetic field, where its polarization (the direction of the positron spin) would precess. The annihilation process occurs predominantly within a spin-singlet electron-positron pair, so that the total spin direction of the ion is preserved by the surviving electron, and can be detected. Such a measurement, if precise enough to detect the binding effects obtained in this study, would provide a valuable insight into the inner structure of this exotic system.

Chapter 6

Muon decay asymmetry

6.1 Introduction

The muon decay is a paradigm for all charged current flavor transformations. It is a purely leptonic process, $\mu \to e\bar{\nu}_e\nu_\mu$, whose properties can be theoretically predicted with very high precision. Measurements of its lifetime [13] and distributions of the daughter electron [14, 15, 16] determine fundamental parameters of the Standard Model and probe its extensions.

Since muons produced in decays of pions are polarized, the angle θ between the muon spin direction and the daughter electron momentum can be observed. The electron distribution in space is

$$\frac{\mathrm{d}\Gamma\left(\mu^- \to e^-\bar{\nu}_e\nu_\mu\right)}{\mathrm{d}\cos\theta} = \frac{\Gamma + \Gamma_0 A\cos\theta}{2}, \tag{6.1.1}$$

where A is the asymmetry and $\Gamma_0 = G_F^2 m_\mu^5/(192\pi^3)$ is the muon decay rate in the massless electron limit, and without radiative corrections. G_F is the Fermi constant.

The decay rate of an unpolarized muon decay, given by the Γ-term in Eq. (6.1.1), has been extensively studied both theoretically and experimentally. It was the first decay process of a charged particle to which one-loop [112] and, four decades later, two-loop [113] corrections were computed. Together with the recent measurement [114], these results give the best value of the Fermi constant G_F, one of the pillars of precise electroweak studies. Corrections to more differential quantities such as the energy spectrum of electrons, were considered in Refs. [115, 116, 117, 118].

The A-term in Eq.(6.1.1) is less well studied, and is the subject of the present paper. Since $\cos\theta \sim \vec{s}\cdot\vec{p}_e$, it violates parity and, as such, it was central in establishing the structure of the electroweak interaction. Indeed, the two experiments [119, 120] that confirmed Madame Wu's discovery of the parity non-conservation [121], observed the angular asymmetry of the positron distribution in the antimuon decay.

Before we describe our calculation in detail, we briefly discuss the origin of the simplicity of Eq. (6.1.1), neglecting the electron mass and radiative corrections. This simple decay pattern is due to the spin 1/2 of the muon. If we do not observe neutrinos nor the polarization of the daughter electron, two functions of the electron energy fully describe the decay distribution. They are the probability amplitudes $\mathcal{M}_\pm$ of the electron emission along the muon spin, and in the opposite direction.

Indeed, the probability amplitude for the emission of the electron in another direction, described by spherical coordinates θ and ϕ with respect to the muon spin, follows from the spin 1/2

rotation,

$$\mathcal{M}(\theta,\phi) = \cos\frac{\theta}{2}\mathcal{M}_+ + i\sin\frac{\theta}{2}e^{i\phi}\mathcal{M}_-. \tag{6.1.2}$$

Since the electron is produced left-handed, the amplitude $\mathcal{M}_+$ describes the situation when the electron spin points against the muon spin; thus, the projection of the angular momentum carried by neutrinos on the electron momentum should be minus one, cf. Fig. 6.1. This is easy to arrange when the neutrinos are flying back-to-back, since the helicities of ν_μ and $\bar{\nu}_e$ are opposite, as happens when the neutrinos carry most of the energy and the the electron little. For the electrons of the highest energy, $\mathcal{M}_+$ vanishes. Conversely, $\mathcal{M}_-$ describes the configuration when the electron has the same spin projection as the muon, and the projection of the neutrinos' angular momentum on the electron direction of motion vanishes. This favours configurations with both neutrinos going in the same direction. Relative to $\mathcal{M}_-$, the amplitude $\mathcal{M}_+$ contains a factor $\sqrt{2(1-x)}$ (from the Lorentz boost of the polarization vector of the $\nu\bar{\nu}$ pair, treated as a spin-one particle of mass $m_{\nu\nu} = \sqrt{1-x}m_\mu$ where $x = 2E_e/m_\mu$). $\mathcal{M}_+$ therefore vanishes for $x = 1$. As a result, there is a parity violating asymmetry of the electron distribution with respect to the muon spin, favouring the production of high energy electrons in the direction counter to the muon spin. Since the muon decay is suppressed at small electron energies, the asymmetry averaged over electron energies is negative.

Precise studies of angular effects in the muon decay turned out to be challenging for both experiment and theory. Measurements of angular distributions have been performed ever since the pioneering study [122] following the discovery of parity violation. The results are usually presented in terms of the product of the degree of the muon polarization P and ξ, one of the so-called Michel-Kinoshita-Sirlin parameters [123], related to the decay asymmetry by $A = P\xi/3$, up to tiny electron mass effects. The current best value is

$$|P\xi| = 1.00084^{+0.00029+0.00165}_{-0.00029-0.00063}, \tag{6.1.3}$$

the first error is statistical and the second systematic.

Since $\alpha/\pi \sim 2\cdot 10^{-3}$, where α is the fine structure constant, the theoretical prediction for the asymmetry should at the very least include one-loop QED corrections. Interestingly, progress with evaluation such corrections was slow. Although the one-loop asymmetry was computed in 1958 [124], its dependence on the electron mass was determined only in 2001 [125], *five years after the two-loop effects were obtained for the lifetime*.

As we will see, the one-loop corrections to the asymmetry are substantial, warranting an estimate of the next-to-next-to-leading order (NNLO) effects, the ultimate goal of this paper. We note that there is an intrinsic ambiguity in defining the polarization asymmetry in events with additional electron-positron pairs that appear at NNLO for the first time. This ambiguity leads to the infra-red enhancement of the NNLO QED corrections by $(\alpha/\pi)^2 \ln m_\mu^2/m_e^2$, so they might be larger than the naive counting suggests. Careful definition of the asymmetry is needed if we use the massless electron approximation. We discuss this in detail in Section 6.3.

The remainder of the paper is organized as follows. In the next Section we discuss technical details of the computation. In Section 6.3 we discuss multi-electron final states and describe the infra-red safe definition of the asymmetry. In Section 6.4 we provide numerical results for the asymmetry and discuss their significance for the interpretation of measurements.

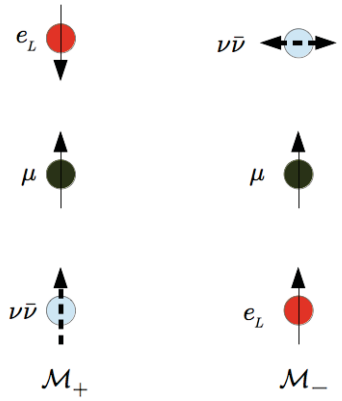


Figure 6.1: Amplitudes describing the polarized muon decay. The electron spin is opposite to its momentum. If e is emitted along the muon spin, the projection of the total neutrino spin (dotted line) on the z axis must be $+1$; if e is emitted in the opposite direction, the $\nu\bar{\nu}$ spin projection vanishes.

6.2 Details of the calculation

Using the simplicity of the differential spectrum, Eq. (6.1.1), we obtain the asymmetry A by choosing the degree of polarization $P = 1$,

$$A = \left.\frac{\mathrm{d}\Gamma}{\mathrm{d}\cos\theta}\right|_{\cos\theta=+1} - \left.\frac{\mathrm{d}\Gamma}{\mathrm{d}\cos\theta}\right|_{\cos\theta=-1}. \tag{6.2.1}$$

Hence, we need to compute the difference of the muon decay rates for the cases when the muon spin points in the direction of the outgoing electron and when the muon spin points in the opposite direction.

Calculation of the differential decay rate for the polarized muon $\mathrm{d}\Gamma$ is performed using the numerical code developed for the computation of NNLO QCD corrections to semileptonic top and bottom quark decays [126, 127]. In turn, that calculation was made possible by novel methods developed for computations of higher-order perturbative corrections in QCD [128, 129, 130], employing a combination of sector-decomposition and phase-space partitioning to extract and cancel soft and collinear divergences in a systematic way.

The code developed for the studies of unpolarized quark decays [126, 127] averages over their spins. It has to be modified to deliver the spin asymmetry. We did so in two ways, obtaining identical results (a useful check).

First, we recalculated all NNLO amplitudes, keeping the muon spin quantization axis arbitrary. Second, the original amplitudes [126, 127], also determine amplitudes for an arbitrary quantization axis. Indeed, denote by $A_\lambda(\vec{n})$ the decay amplitude with the muon spin quantization axis $\vec{n}$ and helicity λ. The amplitudes with a different quantization axis are related by a linear transformation

$$A_{\lambda_2,\vec{n}_2} = \sum_{\lambda_1=\pm} A_{\lambda_1,\vec{n}_1}\ \rho_{\lambda_2,\vec{n}_2;\lambda_1,\vec{n}_1}, \tag{6.2.2}$$

where the complex numbers $\rho_{\lambda_2,\vec{n}_2;\lambda_1,\vec{n}_1}$ describe a rotation between spinor bases. Assuming that $\vec{n}_i = (\sin\theta_i\cos\varphi_i, \sin\theta_i\sin\varphi_i, \cos\theta_i)$, we find

$$\begin{aligned}
\rho_{+,\vec{n}_2,+,\vec{n}_1} &= c_2c_1 + s_2s_1e^{i\varphi_{21}},\\
\rho_{+,\vec{n}_2,-,\vec{n}_1} &= -c_2s_1 + s_2s_1e^{i\varphi_{21}},\\
\rho_{-,\vec{n}_2,+,\vec{n}_1} &= -\rho^*_{+,\vec{n}_2,-,\vec{n}_1}e^{i\varphi_{21}},\\
\rho_{-,\vec{n}_2,-,\vec{n}_1} &= \rho^*_{+,\vec{n}_2,+,\vec{n}_1}e^{i\varphi_{21}},
\end{aligned}$$

where $c_i \equiv \cos\theta_i/2$, $s_i \equiv \sin\theta_i/2$, and $\varphi_{21} \equiv \varphi_2 - \varphi_1$. We use Eq. (6.2.2) to translate between the original amplitudes and those where the muon spin quantization axis is suitable for the calculation of the asymmetry.

6.3 Multi-electron final states

At both the leading and the next-to-leading order in α, muon always decays to a final state with a single electron. But at NNLO, the final state can have an additional electron-positron pair $\mu^- \to e^- e^- e^+ \bar{\nu}_e \nu_\mu$. In the approximation when electron mass is neglected, this process is not separately collinear-safe since a collinear e^+e^- pair is indistinguishable from a photon.

Moreover, multi-electron final states pose a problem for the computation of the asymmetry: which of the electrons should define the muon quantization axis? The algorithm should be infra-red and collinear safe to ensure the cancellation of singularities in the final result.

Suppose we decide to choose the direction of the hardest electron in the computation of the asymmetry. This choice creates no problem if this electron is produced in the hard $\mu \to e\bar{\nu}\nu$ transition. However, if the hardest electron originates from the photon splitting into a collinear e^+e^- pair, and if its momentum is picked up as the direction to compute the asymmetry, the counter-term for this amplitude will have the *photon* momentum as the reference direction for the asymmetry. This counter-term will therefore not cancel with the divergence of the virtual correction where there is just one electron in the final state so that its direction is automatically taken as the quantization axis for the muon spin.

Hence, the issue of the definition of the spin asymmetry is subtle. However, it is similar to infra-red problems encountered in the context of the quark jets forward-backward asymmetry in perturbative QCD [131]. A full solution depends on experimental details, including how electrons and photons are operationally defined. Unfortunately, such details, and especially a discussion of multi-electron final states, are absent in Ref. [123].

To address this issue in a way that is theoretically sound and has a potential to make a contact with experiment, we decided to define the spin asymmetry in terms of infra-red and collinear-safe objects, echoing similar studies of the forward-backward asymmetry in perturbative QCD [132]. To this end, for each muon decay event with an arbitrary final state, we will define a set of electron and photon jets, and then use the *hardest* among the reconstructed *electron jets* as the direction to calculate the asymmetry. This is legitimate because Eq. (6.1.1) remains valid if we interpret the angle θ there as the direction of the electron jet rather than the direction of the electron proper.

The theory of an infra-red safe definition of jet algorithms is a well developed in QCD (see e.g. Ref. [133] for a review). However, traditional jet algorithms are flavor-blind which is unacceptable for us since we need well-defined "electron" jets. The required modification was worked out in [134] and we borrow a suitable jet algorithm from that work. The Durham jet algorithm, that allows tracking the jet "flavor", is defined by its distance measure that we take to be

$$y_{ij}^{(F)} = \frac{2(1-\cos\theta_{ij})}{m_\mu^2} \times \begin{cases} \max(E_i^2, E_j^2), \text{softer of } i,\ j \text{ is flavoured}, \\ \min(E_i^2, E_j^2), \text{softer of } i,\ j \text{ is flavourless}, \end{cases} \tag{6.3.1}$$

and by the clustering procedure that we take to be a simple addition of the four-momenta of partons that are re-combined to a jet. When the measure in Eq. (6.3.1) is applied to an event

in the muon decay, the flavor of a parton is equated to its electric charge and the flavor of a jet is given by the sum of flavors of its LABs. The procedure is iterative: partons are re-combined into a pre-jet if a distance $y_{ij}^{(F)}$ between them is smaller than some chosen value y and the algorithm continues until no further re-combinations are possible.

With this modification, the asymmetry is calculated with respect to the direction of the hardest of the electron jets, if more than one are reconstructed by the jet algorithm, or with respect to the direction of the double-electron jet if both electrons end up in a single jet. In the limit, when the jet resolution parameter vanishes, $y \to 0$, the ill-defined no-jet computation of the asymmetry should be recovered. This means that, at order α^2, the asymmetry contains $\alpha^2 \ln y$ terms.

To choose the jet resolution parameter y in a sensible way, we note that a high-energy electron predominantly emits photons in a cone of the size $\theta \sim m_e/E_e$ around its direction. We imagine that those photons should be treated as part of the electron jet, while photons emitted at larger angles should be distinguishable experimentally. Hence, a physics-motivated choice of the jet resolution parameter is

$$y \sim \frac{\theta^2 E^2}{m_\mu^2} \sim \frac{m_e^2}{m_\mu^2} \sim 2 \times 10^{-5} \tag{6.3.2}$$

Note that, for this choice of the resolution parameter, the magnitude of $\alpha^2 \ln y$ is similar to that of $\alpha^2 \ln(m_\mu^2/m_e^2)$ which would have appeared, had the mass of the electron been retained. Although $\ln(10^{-5}) \sim 12 \gg 1$, a resummation of $\alpha^2 \ln y$ corrections is not needed because the QED coupling constant is small, so $\alpha^2 \ln y \ll 1$, and also because the contribution of multi-electron states (the only place where such enhanced corrections appear) to the asymmetry is relatively small.

6.4 Results and discussion

Choosing the jet resolution parameter $y = 10^{-5}$, we find the asymmetry

$$A(y = 10^{-5}) = A_0 \left[1 - 2.95\, a + 11.2(1)\, a^2\right], \tag{6.4.1}$$

where $A_0 = -1/3$, $a = \bar{\alpha}/\pi$ and $\bar{\alpha}$ is the $\overline{\text{MS}}$ QED coupling renormalized at the scale $\mu = m_\mu$. It is slightly larger than the canonical fine structure constant, $\bar{\alpha} = 1/135.90$. The second order correction to the asymmetry evaluates to 0.6×10^{-4}. This is much smaller than the current experimental precision of $2.9 \cdot 10^{-4}$ (statistical) and $\sim 10^{-3}$ (systematic).

We note that the dependence of the asymmetry on the jet resolution parameter is peculiar. The leading order asymmetry A_0 is independent of y. The NLO coefficient exhibits a linear dependence on y for small y. The dependence of the NNLO correction to the asymmetry on the jet resolution parameter for small y can be approximated by $9.5(1) \ln y - 0.14(1)$, as shown in Fig. 6.2. That Figure shows that a change in the jet resolution parameter from 10^{-5} to 10^{-2}, changes the second order correction to the asymmetry by 10 percent. As we already noticed, a choice of y is, in some sense, equivalent to understanding a correspondence between the measurement setup [123] and the theoretical calculation reported here. It follows from Fig. 6.2 that this issue becomes relevant when the precision of the asymmetry measurement becomes comparable to 0.6×10^{-5}, far from the current level.

We note that the acceptance of the TWIST experiment is fairly complicated; electrons are accepted in particular angular and energy regions. It is therefore interesting to understand what extent the asymmetry depends on the electron energy range selected in the experimental analysis. To find out, we computed four values of the asymmetry that differ by the cut on

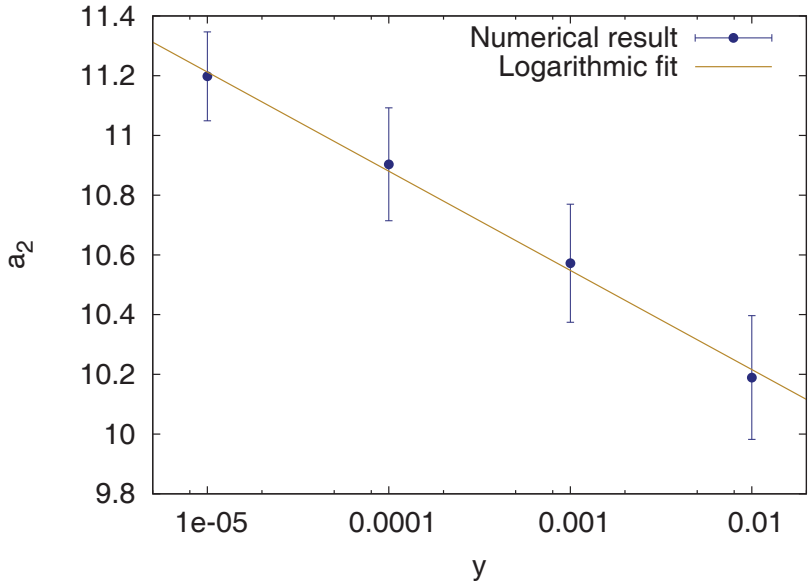


Figure 6.2: Dependence of the second order relative correction to the asymmetry on the jet resolution parameter y. The solid line is the fit to the function $c_1 + c_2 \ln y$, with $c_1 = 9.5(1)$ and $c_2 = -0.14(1)$.

the minimal energy of the electron jet $E_{\rm min} < E_{\rm jet}$. We consider four values of the minimal jet energy cut, $E_{\rm min} = 10,\ 20,\ 30,\ 40$ MeV. The results are shown in Table 6.1 for two values of the jet resolution parameter. It is apparent from that Table that corrections strongly depend on the value of y and on the jet energy interval. This is the consequence of the fact that electron energy is not a collinear-safe observable in $m_e \to 0$ limit, so that NNLO corrections to electron energy spectrum containt $\ln^2 y$-enhanced terms. Analogous logarithmic corrections to the asymmetry at NNLO $\alpha^2 \ln^{2,1} m_\mu/m_e$ were computed in Refs. [115, 117]. As follows from Table 6.1, QED corrections are particularly large in case of $y = 10^{-5}$, especially in the limit when the cut on the minimal electron jet energy approaches the kinematic boundary $m_\mu/2$. These results strongly suggest that the asymmetry is a strong function of the electron (or electron jet) energy. This feature will hamper the interpretation of results if improved asymmetry measurements become available, unless the asymmetry can be theoretically computed including the experimental cuts. Since muon decay experiments do not use the concept of lepton jets, fully differential computations with massive electrons may be needed. This remains an interesting challenge for the future.

It is interesting to compare corrections to the asymmetry and the corrections to the total rate. Corrections to the rate, computed in Ref. [113], read

$$\Gamma = \Gamma_0 \left[1 - 1.81\ a + 6.74\ a^2\right]. \tag{6.4.2}$$

Since the decay rate Γ is infra-red finite, Eq. (6.4.2) is independent of y. Comparing Eq. (6.4.2) and Eq. (6.4.1), we find that corrections to the asymmetry are larger. However, the relative size of subsequent coefficients in the perturbative series is comparable in both cases.

Another source of corrections to the asymmetry and to the total rate are the electron mass effects $\mathcal{O}(m_e/m_\mu)$ and it is interesting to compare them with the size of NNLO QED corrections, for both the decay rate and the asymmetry. The correction of order $\mathcal{O}(\alpha^2)$ to the total decay width is less important than the effect of the electron mass in the lowest order decay rate. In case of

	$a^{(0)}$		$a^{(1)}$		$a^{(2)}$		$\delta_{\rm NLO}, \%$		$\delta_{\rm NNLO}, \%$	
$E_{\rm min}$	10^{-5}	10^{-2}	10^{-5}	10^{-2}	10^{-5}	10^{-2}	10^{-5}	10^{-2}	10^{-5}	10^{-2}
10 MeV	1.01	1.01	-4.01	-3.25	12.6	11.7	-0.9	-0.8	$6.9 \cdot 10^{-3}$	$6.4 \cdot 10^{-3}$
20 MeV	1.05	1.05	-5.96	-3.73	21.1	13.8	-1.3	-0.8	$1.1 \cdot 10^{-2}$	$7.2 \cdot 10^{-3}$
30 MeV	1.05	1.05	-9.24	-4.19	49.3	15.9	-2.1	-0.9	$2.6 \cdot 10^{-2}$	$8.3 \cdot 10^{-3}$
40 MeV	0.87	0.87	-11.78	-3.79	98.4	14.1	-3.2	-1.0	$6.2 \cdot 10^{-2}$	$8.9 \cdot 10^{-3}$

Table 6.1: Spin asymmetry as a function of the minimal jet energy cut. The asymmetry is written as $A = -1/3\,(a_0 + a_1\bar{a} + a_2\bar{a}^2)$. The coefficients $a_{0,1,2}$ are given above for two values of the jet cut parameter $y = 10^{-5}$ and $y = 10^{-2}$. The relative corrections to the leading order asymmetry due to NLO and NNLO contributions are shown in the last two columns, in percent.

the asymmetry, the electron mass effect is suppressed by additional two powers of m_e/m_μ and thus is practically negligible [125]. Thus, for the asymmetry, the radiative corrections are more important than the electron mass effects.

Should future tests of the $V-A$ structure of the muon decay interaction be undertaken, they will not be encumbered with potentially large radiative corrections. However, if the experimental precision reaches the size of the two-loop effects, one will have to carefully match the details of theoretical computations with the experimental setup.

Chapter 7

Appendix 1: Transformation from LAB to CM coordinates

In the first section of this Appendix, we discuss in more detail the construction of the Poincaré generators of a particle system in an external electromagnetic field. We will see that a Lorentz transformation which is equivalent to a gauge transformation can transform a spinor of a free particle into a spinor of a particle within an external electromagnetic field. Under this transformation, the Poincaré generators are transformed from their original forms without the electromagnetic field, to the Poincaré generators for system within an external electromagnetic field. In the second section of this Appendix, we look into a statement made by Sebastian and Yun that the boost operator given by Krajcik and Foldy need to be altered. We prove that there is no need to do so.

7.1 Poincaré generators of a composite particle system within an external field

In the presence of an external electromagnetic (EM) field, the KF transformation [108] might need to be altered. The most straightforward way that may come into our mind is to introduce the external EM potential to the momentum of a CM by "Minimal Subtraction"

$$\mathbf{p} \to \mathbf{p}^{'} = \mathbf{p} - \frac{q}{c}\mathbf{A}\left(\mathbf{r}\right). \tag{7.1.1}$$

where q is the charge of the particle. Accordingly, the total momentum of a system composed of N particles is the summation of the transformed momenta

$$\mathbf{P} \to \mathbf{P}^{'} \equiv \sum_{a=1}^{N} \mathbf{p}_{a}^{'} = \mathbf{P} - \sum_{a=1}^{N} \frac{q_a}{c}\mathbf{A}\left(\mathbf{r}_a\right), \tag{7.1.2}$$

The internal relative momentum turns out to be

$$\pi_a \to \pi_a^{'} \equiv \mathbf{p}_a - \frac{m_a}{M}\mathbf{P}^{'} = \pi_a - \frac{q_a}{c}\mathbf{A}\left(\mathbf{r}_a\right) + \frac{m_a}{M}\sum_{b=1}^{N}\frac{q_b}{c}\mathbf{A}\left(\mathbf{r}_b\right) \tag{7.1.3}$$

Now, we have the Poincaré group generators $\{\mathbf{p}, \mathbf{P}, \pi\}$ replaced by $\left\{\mathbf{p}^{'}, \mathbf{P}^{'}, \pi^{'}\right\}$. The problem comes when we verify the Lie algebra of the Poincaré group with the new set of generators. For

example, we notice that the momentum of a particle does not commute with itself anymore

$$\begin{aligned}\left[p_a^{'i}, p_b^{'j}\right] &= \left[p_a^i - \frac{q_a}{c}A^i\left(\mathbf{r}_a\right), p_b^j - \frac{q_b}{c}A^j\left(\mathbf{r}_b\right)\right] \\ &= -\delta_{ab}\frac{q_a}{c}\left\{\left[p_a^i, A^j\left(\mathbf{r}_b\right)\right] + \left[A^i\left(\mathbf{r}_a\right), p_b^j\right]\right\} \end{aligned} \tag{7.1.4}$$

Generally, the above expression does not equal to zero. This conclusion can be supported by two examples. In the first example, we assume $A = \{0, \mathbf{A}\}$, where $\mathbf{A} = \frac{1}{2}\mathbf{B}\times\mathbf{r}$. Thus, we have the terms in the brackets of (7.1.4)

$$\begin{aligned}&\left[p^i, A^j(\mathbf{r})\right] + \left[A^i(\mathbf{r}), p^j\right] = \frac{1}{2}\left\{\left[p^i, (\mathbf{B}\times\mathbf{r})^j\right] + \left[(\mathbf{B}\times\mathbf{r})^i, p^j\right]\right\} \\ &= \frac{1}{2}\left\{\left[p^i, \epsilon_{klj}B^k r^l\right] + \left[\epsilon_{mni}B^m r^n, p^j\right]\right\} = \frac{1}{2}\left[-i\epsilon_{klj}B^k\delta_{li} + i\epsilon_{mni}B^m\delta_{nj}\right] \\ &= -i\epsilon_{ijk}B^k \neq 0 \end{aligned} \tag{7.1.5}$$

The second example is a plane wave electromagnetic 4-potential $A^\mu = \varepsilon^\mu f\left(n\cdot r\right)$, where $f\left(n\cdot r\right) = -\frac{B}{\sqrt{2}}\left(n\cdot r\right)$. ε^μ is the polarization vector of the potential, n is the propagation vector. In this case the following relations are satisfied

$$\varepsilon\cdot\mathrm{n}=0 \tag{7.1.6}$$

$$n\cdot n = 0 \tag{7.1.7}$$

$$\varepsilon\cdot\varepsilon = -1 \tag{7.1.8}$$

The sum of the commutators turns out to be

$$\begin{aligned}&\left[p^i, A^j(\mathbf{r})\right] + \left[A^i(\mathbf{r}), p^j\right] = -\frac{B}{\sqrt{2}}\left\{\left[p^i, \varepsilon^j n^k r_k\right] + \left[\varepsilon^i n^k r_k, p^j\right]\right\} \\ &= -\frac{B}{\sqrt{2}}\left\{\varepsilon^j n^k\left(-i\delta_{ik}\right) + \varepsilon^i n^k\left(-i\delta_{kj}\right)\right\} = \frac{iB}{\sqrt{2}}\left(\varepsilon^j n^i - \varepsilon^i n^j\right) \neq 0 \end{aligned} \tag{7.1.9}$$

Therefore one cannot say that the components of a transformed momentum commute with each other. Since the transformed generator $\mathbf{P}'$ corresponds to the total momentum of the system, we may further construct it in the same way as Krajcik and Foldy did in their paper

$$\mathbf{P}' \equiv \sum_{a=1}^{N}\mathbf{p}_a' \tag{7.1.10}$$

the components of $\mathbf{P}'$ do not commute with each other either. Henceforth the Lie algebra of the Poincaré group is broken. The above observation is not unexpected after all, since by introducing an external electromagnetic field, we have broken the original symmetries of the system. Here we intend to derive the relations between the LAB coordinates and the CM coordinates in the same way as Krajcik and Foldy did in their paper [108]. We need to find a way to restore the Lie algebra of the Poincaré group. One way of solving this problem is introducing the external field to the generators, by using a non-singular evolution operator $V\left(A\right)$ [135]

$$\begin{aligned}&G \rightarrow V\left(A\right)GV^{-1}\left(A\right) \\ &= G + \left[V\left(A\right), G\right]V^{-1}\left(A\right) \end{aligned} \tag{7.1.11}$$

The transformed generators satisfy the commutation relations of the Poincaré algebra. The problem is how to find this operator. Fortunately, there always exists such kind of evolution operator in the case of the external electromagnetic field is a plane wave. From now on, we call this transformation "Dynamic Transformation" (**DT**). With the new set of generators, we may follow a similar procedure as the one Krajcik and Foldy used, and obtain the KF relations in the present of a plane wave external field. We will not go into all the details of this procedure in this section; further discussion will be given in the next few sections.

7.1.1 Relativistic gauge invariance

In this subsection we would like to find the Lorentz transformation that is equivalent to a gauge transformation of electromagnetic plane waves. We will first derive general expression of such kind of transformation. Then, using this general expression, we will look for a specific form of the transformation, that transforms a particle moving in a electromagnetic field to its rest frame.

First, we know that the general Lorentz transformation of a four-vector can be expressed as

$$\begin{bmatrix} ct' \\ \mathbf{r}' \end{bmatrix} = \begin{bmatrix} \gamma & -\gamma\beta^{\top} \\ -\gamma\beta & I + (\gamma - 1)\,\beta\beta^{\top}/\beta^2 \end{bmatrix} \begin{bmatrix} ct \\ \mathbf{r} \end{bmatrix}, \tag{7.1.12}$$

where $\beta = v/c$, $\gamma = \frac{1}{\sqrt{1-\beta^2}} = (1-\beta^2)^{-\frac{1}{2}}$. Suppose we have an electromagnetic plane wave which travels along the x-axis of the laboratory frame L. Then, the relativistic invariant $\tau = n \cdot r = ct - x$, where $n = (1, \mathbf{n})$, and $x = (ct, \mathbf{r})$. n is called the propagation direction. In this case, the fields of the plane wave are functions of τ. It can be proved that one can always find a Lorentz transformation $\mathcal{M}$, which leaves the electromagnetic fields unaltered

$$\begin{pmatrix} \varphi' \\ \mathbf{A}' \end{pmatrix} \equiv \mathcal{M} \begin{pmatrix} \varphi \\ \mathbf{A} \end{pmatrix} = \begin{pmatrix} \varphi - \frac{\partial \lambda}{\partial t} \\ \mathbf{A} + \frac{\partial \lambda}{\partial \mathbf{r}} \end{pmatrix} \tag{7.1.13}$$

where λ is a function of space and time. In order to find the transformation $\mathcal{M}$, we construct it with a special Lorentz rotation $\mathcal{L}$ [136] with an arbitrary transformation velocity $\boldsymbol{\beta}$, followed by a pure rotation $\mathcal{R}$ in space. This transformation has to preserve the direction of the space coordinate axes. Thus, we obtain

$$\mathcal{M} \begin{pmatrix} \varphi \\ \mathbf{A} \end{pmatrix} = \mathcal{R}\mathcal{L} \begin{pmatrix} \varphi \\ \mathbf{A} \end{pmatrix} = \mathcal{R} \begin{pmatrix} \gamma\,(\varphi - \boldsymbol{\beta} \cdot \mathbf{A}) \\ \mathbf{A} + (\gamma - 1)\,(\boldsymbol{\beta} \cdot \mathbf{A})\,\beta^{-2}\boldsymbol{\beta} - \gamma\varphi\boldsymbol{\beta} \end{pmatrix} \tag{7.1.14}$$

We may choose $\boldsymbol{\beta}$ in the (x, y) plane, and let α be the angle between $\mathbf{n}$ and β. Since the Lorentz transformation $\mathcal{M}$ that we are looking for should also be a gauge transformation, the propagation direction $\mathbf{n}$ of the plane wave field will not be modified by the Lorentz transformation. Henceforth the rotation $\mathcal{R}$ should be in the $(\mathbf{n}, \beta)$ plane, which is around the z axis. So $\mathcal{M}$ can be written as

$$\begin{aligned} \mathcal{M} = \mathcal{R}(\psi)\mathcal{L}(\beta, \alpha) = &\begin{pmatrix} 1 & & & \\ & \cos\psi & -\sin\psi & \\ & \sin\psi & \cos\psi & \\ & & & 1 \end{pmatrix} \\ \times &\begin{pmatrix} \gamma & -\gamma\beta\cos\alpha & -\gamma\beta\sin\alpha & 0 \\ -\gamma\beta\cos\alpha & 1 + (\gamma-1)\cos^2\alpha & (\gamma-1)\sin\alpha\cos\alpha & 0 \\ -\gamma\beta\sin\alpha & (\gamma-1)\sin\alpha\cos\alpha & 1 + (\gamma-1)\sin^2\alpha & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} \end{aligned} \tag{7.1.15}$$

The $\mathcal{M}$ that we are looking for does not alter the electromagnetic fields. Thus, we require the potentials φ, $\mathbf{A}$, φ', $\mathbf{A}'$ and the gauge function λ are functions of τ. This requirement gives us the following relations

$$\begin{aligned} \frac{\partial \lambda}{\partial t} + \frac{\partial \lambda}{\partial x} &= 0 \\ \frac{\partial \lambda}{\partial y} = \frac{\partial \lambda}{\partial z} &= 0 \end{aligned} \tag{7.1.16}$$

Since the plane wave is propagating along the x axis, the electric field along x should be zero, we obtain $\varphi = A_x$. Using above relations and the expressions in (7.1.13) and (7.1.15), we derive the following equations

$$\begin{aligned}
&[\sin\psi + (\gamma-1)\cos\alpha\sin(\alpha+\psi) - \gamma\beta\sin(\alpha+\psi)]\,\varphi + \\
&\qquad + [\cos\psi - 1 + (\gamma-1)\sin\alpha\sin(\alpha+\psi)]\,A_y = 0, \qquad (7.1.17)\\
&[\cos\psi + (\gamma-1)\cos\alpha\cos(\alpha+\psi) + \gamma\beta\cos\alpha - \gamma\beta\cos(\alpha+\psi) - \gamma]\,\varphi + \\
&\qquad + [-\sin\psi + (\gamma-1)\sin\alpha\cos(\alpha+\psi) + \gamma\beta\sin\alpha]\,A_y = 0 \qquad (7.1.18)
\end{aligned}$$

Solving these equations, we obtain the angles

$$\begin{aligned}
&\alpha = \arccos\frac{\gamma-1}{\gamma\beta} = \arccos\frac{\gamma\beta}{\gamma+1} \Leftrightarrow 1 - \beta\cos\alpha = \frac{1}{\gamma}\\
&\psi = \pi - 2\alpha \qquad (7.1.19)
\end{aligned}$$

This result leads to the general expression of the Lorentz transformation, which is also a gauge transformation of a given electromagnetic plane wave.

$$\mathcal{M}(\gamma) = \begin{pmatrix} \gamma & -(\gamma-1) & -[2(\gamma-1)]^{\frac{1}{2}} & 0 \\ (\gamma-1) & (2-\gamma) & -[2(\gamma-1)]^{\frac{1}{2}} & 0 \\ [2(\gamma-1)]^{\frac{1}{2}} & [2(\gamma-1)]^{\frac{1}{2}} & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} \qquad (7.1.20)$$

Next, we want to look for a specific form of the Lorentz transformation that transforms a particle moving in a electromagnetic field to its rest frame. The corresponding pure spacial rotation and Lorentz rotation should also be obtained. It is known that if in the laboratory frame L, a particle was at rest before the electromagnetic field was turn on. Then, this particle's four momentum satisfies

$$E(\tau) = m\left(1-\nu^2(\tau)\right)^{-\frac{1}{2}} \approx m\left(1+\frac{\nu^2(\tau)}{2}\right) \qquad (7.1.21)$$

$$\mathbf{P}(\tau) = m\nu(\tau)\,\mathbf{j} + \frac{1}{2}m\nu^2(\tau)\,\mathbf{n} \qquad (7.1.22)$$

where $\nu(\tau) = \frac{e}{m}\left(-A^\mu A_\mu\right)^{\frac{1}{2}}$ is a dimensionless parameter. Now, we will show that the momentum of this particle can always be transformed to its rest frame by a Lorentz transformation $\mathcal{M}(\gamma)$ that is equivalent to a gauge transformation

$$\mathcal{M}(\gamma)\begin{pmatrix} E(\tau) \\ \mathbf{P}(\tau) \end{pmatrix} = \begin{pmatrix} m \\ \mathbf{0} \end{pmatrix} \qquad (7.1.23)$$

In order to find a $\mathcal{M}(\gamma)$ satisfying this equation, we need to calculate the corresponding expression of γ. Using (7.1.20) and above equation, we obtain its expression as

$$\gamma(\tau) = 1 + \frac{\nu^2(\tau)}{2}, \qquad (7.1.24)$$

Henceforth the Lorentz transformation can be written as

$$\mathcal{M}(\gamma) = \begin{pmatrix} 1+\frac{\nu^2}{2} & -\frac{\nu^2}{2} & -\nu & 0 \\ \frac{\nu^2}{2} & 1-\frac{\nu^2}{2} & -\nu & 0 \\ \nu & \nu & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} \qquad (7.1.25)$$

The equation (7.1.23) can be viewed in another way

$$\begin{pmatrix} E(\tau) \\ \mathbf{P}(\tau) \end{pmatrix} = \mathcal{M}^{-1}(\nu) \begin{pmatrix} m \\ \mathbf{0} \end{pmatrix} = \mathcal{M}(-\nu) \begin{pmatrix} m \\ \mathbf{0} \end{pmatrix} \tag{7.1.26}$$

One can assert that the electromagnetic fields in the rest frame R is the same as it is in the laboratory frame L, where the field was switched on a particle at rest initially. The operator $\mathcal{M}(-\nu)$ can also be interpreted as an evolution operator which evolves the particle from its initial state at rest to its current moving state.

Substituting (7.1.19) and (7.1.24) into (7.1.15), we obtain the rotation and Lorentz transform operators as functions of ν

$$\mathcal{R}(\nu(\tau)) = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & \frac{1-\nu^2/4}{1+\nu^2/4} & -\frac{\nu}{1+\nu^2/4} & 0 \\ 0 & \frac{\nu}{1+\nu^2/4} & \frac{1-\nu^2/4}{1+\nu^2/4} & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} \tag{7.1.27}$$

$$\mathcal{L}(\nu(\tau)) = \begin{pmatrix} 1+\frac{\nu^2}{2} & -\frac{\nu^2}{2} & -\nu & 0 \\ -\frac{\nu^2}{2} & 1+\frac{\nu^4}{8(1+\nu^2/4)} & \frac{\nu^3}{4(1+\nu^2/4)} & 0 \\ -\nu & \frac{\nu^3}{4(1+\nu^2/4)} & 1+\frac{\nu^2}{2(1+\nu^2/4)} & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} \tag{7.1.28}$$

We should keep in mind that all the transformations that we are talking about are operation in the four-vector space. The boost velocity $\boldsymbol{\beta}$ is chosen to be in the (x, y) plane. In the next subsection, we will derive the Lorentz transformation with $\boldsymbol{\beta}$ in an arbitrary direction. Moreover, we will see that the elements of the transformation tensors can be written into more compact forms.

7.1.2 Lorentz transformation along an arbitrary direction

The boost velocity $\boldsymbol{\beta}$ may be chosen in an arbitrary direction. We notify the angle between $\boldsymbol{\beta}_\perp$and the y axis as θ, where $\boldsymbol{\beta}_\perp$is the projection of $\boldsymbol{\beta}$ on the (y, z) plane. Then, the Lorentz transformation $\mathcal{L}$ and the rotation $\mathcal{R}$ can be obtained in the following way [137]

$$\mathcal{L}(\nu, \theta) = \mathcal{P}(\theta)\mathcal{L}(\nu, \theta = 0)\mathcal{P}^{-1}(\theta), \qquad \mathcal{R}(\nu, \theta) = \mathcal{P}(\theta)\mathcal{R}(\nu, \theta = 0)\mathcal{P}^{-1}(\theta), \tag{7.1.29}$$

where $\mathcal{P}(\theta)$ is a rotation matrix of angle θ around the x axis. The rotation $\mathcal{R}$ is around the unit vector

$$\mathbf{u} = \frac{\mathbf{n} \times \boldsymbol{\beta}}{\sqrt{(\mathbf{n} \times \boldsymbol{\beta})^2}} \tag{7.1.30}$$

with an angle

$$\alpha = \pi - 2\cos^{-1}\left\{\beta^{-1}\left[1 - \left(1-\beta^2\right)^{1/2}\right]\right\}, \tag{7.1.31}$$

where $\mathbf{n}$ is the propagation unit vector of the plane wave. When $\mathbf{n}$ is chosen to be along the x axis as we did before, we have [137]

$$\mathcal{L}(\nu, \theta) = \begin{pmatrix} 1+\frac{\nu^2}{2} & -\frac{\nu^2}{2} & -\nu\cos\theta & -\nu\sin\theta \\ -\frac{\nu^2}{2} & 1+\frac{\nu^4}{8(1+\nu^2/4)} & \frac{\nu^3\cos\theta}{4(1+\nu^2/4)} & \frac{\nu^3\sin\theta}{4(1+\nu^2/4)} \\ -\nu\cos\theta & \frac{\nu^3\cos\theta}{4(1+\nu^2/4)} & 1+\frac{\nu^2\cos^2\theta}{2(1+\nu^2/4)} & \frac{\nu^2\sin 2\theta}{4(1+\nu^2/4)} \\ -\nu\sin\theta & \frac{\nu^3\sin\theta}{4(1+\nu^2/4)} & \frac{\nu^2\sin 2\theta}{4(1+\nu^2/4)} & 1+\frac{\nu^2\sin^2\theta}{2(1+\nu^2/4)} \end{pmatrix} \tag{7.1.32}$$

$$\mathcal{R}(\nu,\theta)=\begin{pmatrix}1+\frac{\nu^2}{4} & 0 & 0 & 0\\ 0 & 1-\frac{\nu^2}{4} & -\nu\cos\theta & -\nu\sin\theta\\ 0 & \nu\cos\theta & 1-\frac{\nu^2}{4}\cos 2\theta & -\frac{\nu^2}{4}\sin 2\theta\\ 0 & \nu\sin\theta & -\frac{\nu^2}{4}\sin 2\theta & 1+\frac{\nu^2}{4}\cos 2\theta\end{pmatrix}\left(1+\frac{\nu^2}{4}\right)^{-1} \tag{7.1.33}$$

Consequently, the total Lorentz transformation can be written in the following form

$$\mathcal{M}(\nu,\theta)=\mathcal{R}(\nu,\theta)\mathcal{L}(\nu,\theta)=\begin{pmatrix}1+\frac{\nu^2}{2} & -\frac{\nu^2}{2} & -\nu\cos\theta & -\nu\sin\theta\\ \frac{\nu^2}{2} & 1-\frac{\nu^2}{2} & -\nu\cos\theta & -\nu\sin\theta\\ -\nu\cos\theta & \nu\cos\theta & 1 & 0\\ -\nu\sin\theta & \nu\sin\theta & 0 & 1\end{pmatrix}$$

We may simplify the above expressions by introducing a set of unit four-vectors

$$f=\left(1+\frac{\nu^2}{4}\right)^{-\frac{1}{2}}\begin{pmatrix}0\\ \frac{1}{2}\nu\\ \cos\theta\\ \sin\theta\end{pmatrix},\qquad h=\left(1+\frac{\nu^2}{4}\right)^{-\frac{1}{2}}\begin{pmatrix}0\\ -1\\ \frac{1}{2}\nu\cos\theta\\ \frac{1}{2}\nu\sin\theta\end{pmatrix} \tag{7.1.34}$$

$$k=\begin{pmatrix}1\\0\\0\\0\end{pmatrix},\qquad l=\begin{pmatrix}0\\-1\\-\sin\theta\\\cos\theta\end{pmatrix} \tag{7.1.35}$$

One can be easily verify that $k^2=-f^2=-h^2=-l^2=1$, and $f\cdot h=k\cdot f=f\cdot l=h\cdot k=h\cdot l=k\cdot l=0$. The other two four-vectors that we will need are

$$a=\begin{pmatrix}0\\ \mathbf{a}\end{pmatrix}=\begin{pmatrix}0\\0\\\cos\theta\\\sin\theta\end{pmatrix};\qquad j=n+a=\begin{pmatrix}1\\1\\\cos\theta\\\sin\theta\end{pmatrix} \tag{7.1.36}$$

Here we notice that $j^2=a^2=-1$ and $j\cdot n=a\cdot n=0$. Now, the components of the transformation matrices can be written as functions of these vectors

$$\begin{aligned}\mathcal{L}^{\sigma}_{\rho}(\nu,\theta)&=\left(1+\frac{1}{2}\nu^2\right)\delta^{\sigma}_{\rho}+\frac{1}{2}\nu^2h^{\sigma}h_{\rho}+\frac{1}{2}\nu^2l^{\sigma}l_{\rho}\\&+\left(1+\frac{\nu^2}{4}\right)^{1/2}\nu g^{\sigma\omega}\epsilon_{\omega\rho\alpha\beta}h^{\alpha}l^{\beta}\end{aligned}$$

$$\mathcal{R}^{\mu}_{\sigma}(\nu,\theta)=\left(1+\frac{\nu^2}{4}\right)^{-1}\left[\left(1-\frac{\nu^2}{4}\right)\delta^{\mu}_{\sigma}+\frac{1}{2}\nu^2k^{\mu}k_{\sigma}-\frac{1}{2}\nu^2l^{\mu}l_{\sigma}-\nu g^{\mu\omega}\epsilon_{\omega\sigma\alpha\beta}k^{\alpha}l^{\beta}\right] \tag{7.1.37}$$

$$\begin{aligned}\mathcal{M}^{\mu}_{\rho}(\nu,j)&=\mathcal{R}^{\mu}_{\sigma}\mathcal{L}^{\sigma}_{\rho}\\&=\delta^{\mu}_{\rho}+\nu\left(n^{\mu}j_{\rho}-j^{\mu}n_{\rho}\right)+\frac{1}{2}\nu^2n^{\mu}n_{\rho}\end{aligned} \tag{7.1.38}$$

7.1.3 Lorentz operator in spinor space

Our above discussion is all about finding the Lorentz operator in the four-vector space-time space. The operator is supposed to be equivalent to a gauge transformation on a electromagnetic field four-potential. In the case of quantum mechanics, we wonder if there is such kind of Lorentz operator acting on a spinor. Actually, this goal indeed can be achieved. One can find

an evolution operator $\mathcal{V}$ of a spin $\frac{1}{2}$ particle, that transforms a given solution φ of the field-free Dirac equation into $\psi = \mathcal{V}\varphi$, which is the solution of the corresponding minimal-subtracted Dirac equation. That is to say, φ and ψ are solutions of the following equations correspondingly

$$\begin{aligned} &[i\gamma_\mu \partial^\mu - m]\,\varphi = 0 \\ &[\gamma_\mu\,(i\partial^\mu - qA^\mu\,(\tau)) - m]\,\psi = 0 \end{aligned} \tag{7.1.39}$$

The solution of equation (7.1.39) is called Volkov solution [138, 55]

$$\psi_p = T_p\,(\tau)\,exp\,[-ie\lambda_p\,(\tau)]\,\varphi_p \tag{7.1.40}$$

where

$$\begin{aligned} T_p\,(\tau) &= exp\left[-\frac{q}{2\,(n\cdot p)}\gamma\cdot A\gamma\cdot n\right] = 1 - \frac{q}{2\,(n\cdot p)}\gamma\cdot A\gamma\cdot n \\ \lambda_p\,(\tau) &= -\frac{1}{(n\cdot p)}\int_{-\infty}^{\tau}\left[p\cdot A\left(\tau'\right) - \frac{q}{2}A^2\left(\tau'\right)\right]d\tau' \end{aligned} \tag{7.1.41}$$

Since

$$\not{a}\not{b} = a\cdot b - 2ia_\mu b_\nu s^{\mu\nu}, \tag{7.1.42}$$

noticing the factor $n\cdot\epsilon$ that leads to $n\cdot A = 0$, we can write the operator $T_p\,(\tau)$ as

$$T_p\,(\tau) = exp\left[-\frac{q}{2\,(n\cdot p)}\gamma\cdot A\gamma\cdot n\right] = exp\left[-i\frac{q}{2\,(n\cdot p)}G_{\mu\nu}s^{\mu\nu}\right] \tag{7.1.43}$$

where $s^{\mu\nu} = \frac{i}{4}\left[\gamma^\mu,\gamma^\nu\right]$, and $G_{\mu\nu} = k_\mu A_\nu - k_\nu A_\mu$. From now on, we will notify $(n\cdot p)$ as n_p. Therefore $T_p\,(\tau) = exp\left[-i\frac{q}{2n_p}G_{\mu\nu}s^{\mu\nu}\right]$.

Now, let us derive the evolution operator $\mathcal{V}$. We assume that the operator $\mathcal{M}$ that we are looking for depends on the momentum of the particle. The particle is not generally in a pure state of the given momentum p. The Lorentz operator $\mathcal{M}$ may depend on t, $\mathbf{r}$, and the four-momentum p, and henceforth in general it does not commute with p and A. In order to use the relativistic invariance of the Dirac equation, we introduce additional conditions

$$\begin{aligned} \left[\partial^\rho, \mathcal{M}^\mu_\rho\right] &= 0 \\ \left[A^\rho, \mathcal{M}^\mu_\rho\right] &= 0 \end{aligned}$$

We also introduce the generalized gauge transformations

$$A^\mu \to A^\mu + \left[\partial^\mu, \lambda\right], \qquad \psi \to exp\,(ie\lambda)\,\psi \tag{7.1.44}$$

where λ satisfies

$$\begin{aligned} &[\lambda, A^\mu] = 0 \\ &[\lambda, [\partial^\mu, \lambda]] = 0 \end{aligned}$$

One can verify that $\mathcal{M}$, λ, and $[\partial^\mu,\lambda] = n^\mu\,[\partial/\partial\tau,\lambda]$ commute with each other. Using the relativistic invariance of the Dirac equation, and the fact that $\mathcal{M}$ should be of the Lorentz type. One may rewrite the field-free Dirac equation as [137]

$$\left(\gamma_\rho \mathcal{M}^\rho_\mu \mathcal{M}^\mu_\alpha i\partial^\alpha - m\right)\varphi = 0 \tag{7.1.45}$$

Suppose T is the spinor operator corresponding to the Lorentz operator $\mathcal{M}$, we thus have the following relations

$$\mathcal{M}_{\mu}^{\rho}\gamma_{\rho} = T^{-1}\gamma_{\mu}T$$
$$T^{-1} = \gamma^{0}T^{\dagger}\gamma^{0}$$

Then, the equation (7.1.45) can be rewritten into

$$\left(\gamma_{\mu}\mathcal{M}_{\alpha}^{\mu}i\partial^{\alpha} - m\right)T\varphi = i\gamma_{\mu}\left[M_{\rho}^{\mu}\partial^{\rho}, T\right]\varphi \tag{7.1.46}$$

Starting from the equation (7.1.39), by using the generalized gauge transformation, we have the equation

$$\left[\gamma_{\mu}\left(i\partial^{\mu} - qA^{\mu}\left(\tau\right) - qn^{\mu}\left[\frac{\partial}{\partial\tau}, \lambda\right]\right) - m\right] exp\left[ie\lambda\right]\psi = 0 \tag{7.1.47}$$

The above two equations are supposed to be identical, therefore we must have the following relations

$$\mathcal{M}_{\alpha}^{\mu}i\partial^{\alpha} = i\partial^{\mu} - qA^{\mu}\left(\tau\right) - qn^{\mu}\left[\frac{\partial}{\partial\tau}, \lambda\right]$$
$$\gamma_{\mu}\left[i\partial^{\mu} - qA^{\mu}\left(\tau\right) - qn^{\mu}\left[\frac{\partial}{\partial\tau}, \lambda\right], T\right] = 0 \tag{7.1.48}$$

By solving these equations, we obtain the λ

$$\lambda = -\left(n\cdot\partial\right)^{-1}\left[Z\left(\tau\right)\cdot\partial + \frac{i}{2}qB\left(\tau\right)\right], \tag{7.1.49}$$

where

$$Z^{\mu}\left(\tau\right) = \int_{-\infty}^{\tau} A^{\mu}\left(\tau^{'}\right)d\tau^{'}$$
$$B\left(\tau\right) = \int_{-\infty}^{\tau} A^{2}\left(\tau^{'}\right)d\tau^{'}.$$

The other relation obtained from (7.1.48) is

$$\mathcal{M}_{\alpha}^{\mu}i\partial^{\alpha} = i\partial^{\mu} - qA^{\mu}\left(\tau\right) + n^{\mu}\left[qA\left(\tau\right)\cdot\partial + \frac{i}{2}q^{2}A^{2}\left(\tau\right)\right]\left(n\cdot\partial\right)^{-1} \tag{7.1.50}$$

The operator $\left(n\cdot\partial\right)^{-1}$ is well defined on a plane wave solution φ^{p}. We have $\left(n\cdot\partial\right)^{-1} \rightarrow i\left(n\cdot p\right)^{-1} = in_{p}^{-1}$. $n_{p} \neq 0$ for a massive particle. Using (7.1.50) we find how the operator $\mathcal{M}$ transform the electromagnetic potential

$$\mathcal{M}_{\rho}^{\sigma}A^{\rho}\left(\tau\right) = A^{\sigma}\left(\tau\right) + \left[\partial^{\sigma}, \chi\right], \tag{7.1.51}$$

where

$$\chi = -i\left(n\cdot\partial\right)^{-1}qB\left(\tau\right) \tag{7.1.52}$$

Hence the Lorentz operator $\mathcal{M}$ is indeed a generalized gauge transformation. By combining equations (7.1.38) and (7.1.50), one obtains

$$\nu = -iq\left(n\cdot\partial\right)^{-1}\left[-A^{2}\left(\tau\right)\right]^{1/2}$$
$$j^{\mu}\left(\tau\right) = \left[-A^{2}\left(\tau\right)\right]^{-1/2}A^{\mu}\left(\tau\right)$$

Now, we want to know how the Lorentz operator $\mathcal{M}$ transform a quantum state. Since $\mathcal{M}$ is composed of operator $\mathcal{L}$ and $\mathcal{R}$, the spinor operator corresponding to $\mathcal{M}$ can be found by combing the spinor operator corresponding to $\mathcal{L}$ and $\mathcal{R}$ respectively. On one hand, it is know that the following spinor operator [55]

$$S(\mathcal{L}) = \cosh\left(\frac{1}{2}\tanh^{-1}\beta\right) - \gamma^0(\boldsymbol{\gamma}\cdot\boldsymbol{\beta})\beta^{-1}\sinh\left(\frac{1}{2}\tanh^{-1}\beta\right) \tag{7.1.53}$$

corresponds to a Lorentz transformation with velocity $\boldsymbol{\beta}$. On the other hand, the spinor operator corresponding to a rotation of angle α around a unit vector $\mathbf{u}$ is

$$S(\mathcal{R}) = \cos\left(\frac{1}{2}\alpha\right) + i\boldsymbol{\Sigma}\cdot\mathbf{u}\sin\left(\frac{1}{2}\alpha\right), \tag{7.1.54}$$

where $\boldsymbol{\Sigma} = \frac{i}{2}\boldsymbol{\gamma}\times\boldsymbol{\gamma}$. The associated velocity $\boldsymbol{\beta}$ can be obtained through the relation

$$\mathcal{L}\begin{pmatrix}1\\ \mathbf{0}\end{pmatrix} = \left(1-\beta^2\right)^{-1/2}\begin{pmatrix}1\\ -\boldsymbol{\beta}\end{pmatrix} \tag{7.1.55}$$

Using above equation and (7.1.19), we have $\boldsymbol{\beta} = \left(1+\frac{1}{2}\nu^2\right)^{-1}\left(\nu\mathbf{a}+\frac{1}{2}\nu^2\mathbf{n}\right)$. The expressions of α and $\mathbf{u}$ are given by (7.1.30) and (7.1.31). We finally obtain the spinor operator T corresponding to the transformation $\mathcal{M} = \mathcal{R}\mathcal{L}$

$$T = S(\mathcal{R})S(\mathcal{L}) = 1 + \frac{1}{2}\nu\gamma\cdot n\gamma\cdot j \tag{7.1.56}$$

This expression agrees with Volkov's result if φ is an eigenstate of $i\partial$, saying, if $\varphi = \varphi_p$.

By comparing the equations (7.1.46) and (7.1.47) we find that $\psi_p = T_p(\tau)\,exp\left[-ie\lambda_p(\tau)\right]\varphi_p$. Thus,

$$V = T_p(\tau)\,exp\left[-ie\lambda_p(\tau)\right] \tag{7.1.57}$$

is the evolution operator that we have been looking for. It transforms the solution of the field-free Dirac equation into the solution of the Dirac equation with the momentum operator minimum subtracted by a plane wave electromagnetic field. Under this transformation, the generators of the Poincaré group transform to [135]

$$p_\mu \to p_\mu'(A) = p_\mu + k_\mu\frac{q}{2n_p}\left(qA^2 - 2AP - \not{F}\right), \tag{7.1.58}$$

$$r_\mu \to r_\mu'(A) = r_\mu - \frac{q}{2n_p}\left[r_\mu, \int d\tau'\left(qA^2\left(\tau'\right) - 2A\left(\tau'\right)\cdot p\right) - \not{G}\right], \tag{7.1.59}$$

where $\not{F} \equiv F_{\mu\nu}s^{\mu\nu}$ and $\not{G} \equiv G_{\mu\nu}s^{\mu\nu}$.

Transformation on the Schrï¿œdinger eigenstates

Here we must remind ourselves that the transformation is acting on the 4-components spinor $\begin{pmatrix}\varphi\\ \chi\end{pmatrix}$, but our calculations of the polyelectron systems are based on the eigenstates φ_{Sch} of the Schrï¿œdinger equation. Now, let us first look at how the transformation V act on the upper component φ of a spinor. We know that

$$\begin{pmatrix}\varphi'\\ \chi'\end{pmatrix} = exp\left[-\frac{iq}{2n_p}G_{\mu\nu}s^{\mu\nu}\right]exp\left[\frac{-i}{2n_p}\int_{-\infty}^{\tau}\left[2qp\cdot A\left(\tau'\right) - q^2A^2\left(\tau'\right)\right]d\tau'\right]\begin{pmatrix}\varphi\\ \chi\end{pmatrix}, \tag{7.1.60}$$

where $\begin{pmatrix} \varphi \\ \chi \end{pmatrix}$ is a solution of the field-free Dirac equation. The matrices $s^{\mu\nu}$ in Weyl representation have the following expressions

$$s^{0i} = \frac{i}{4}\left[\gamma^0, \gamma^i\right] = \frac{-i}{2}\begin{pmatrix} \sigma^i & 0 \\ 0 & -\sigma^i \end{pmatrix} \tag{7.1.61}$$

$$s^{ij} = \frac{i}{4}\left[\gamma^i, \gamma^j\right] = \frac{1}{2}\epsilon^{ijk}\begin{pmatrix} \sigma^k & 0 \\ 0 & \sigma^k \end{pmatrix} \tag{7.1.62}$$

Hence for the upper component φ of a spinor, the transformation can be written in the following way

$$\varphi^{'} = exp\left[-\frac{iq}{2n_p}G_{\mu\nu}\alpha^{\mu\nu}\right] exp\left[\frac{-i}{2n_p}\int_{-\infty}^{\tau}\left[2qp\cdot A\left(\tau^{'}\right) - q^2A^2\left(\tau^{'}\right)\right]d\tau^{'}\right]\varphi, \tag{7.1.63}$$

where

$$\alpha^{0i} = \frac{-i}{2}\sigma^i = -iS^i$$
$$\alpha^{ij} = \frac{1}{2}\epsilon^{ijk}\sigma^k = \epsilon^{ijk}S^k$$

S^i is the spin operator for spin-$\frac{1}{2}$ particle. Using the relation that we presented in (9.1.20) of the Appendix 9

$$\varphi_{Sch} = \left(1 + \frac{p^2}{8m^2c^2}\right)\varphi$$
$$\varphi = \left(1 - \frac{p^2}{8m^2c^2}\right)\varphi_{Sch} \tag{7.1.64}$$

the equation (7.1.63) can be rewritten into

$$\left[\left(1 - \frac{p^2}{8m^2c^2}\right)\varphi_{Sch}\right]^{'} = \varphi_{Sch}^{'} - \left(\frac{p^2}{8m^2c^2}\varphi_{Sch}\right)^{'}$$
$$= exp\left[-\frac{iq}{2n_p}G_{\mu\nu}\alpha^{\mu\nu}\right] exp\left[\frac{-i}{2n_p}\int_{-\infty}^{\tau}\left[2qp\cdot A\left(\tau^{'}\right) - q^2A^2\left(\tau^{'}\right)\right]d\tau^{'}\right]\left(1 - \frac{p^2}{8m^2c^2}\right)\varphi_{Sch}$$

Keeping terms to the first order of $1/c^2$, we find the transformation of φ_{Sch} can be written as

$$\varphi_{Sch}^{'} = exp\left[-\frac{iq}{2n_p}G_{\mu\nu}\alpha^{\mu\nu}\right] exp\left[\frac{-i}{2n_p}\int_{-\infty}^{\tau}\left[2qp\cdot A\left(\tau^{'}\right) - q^2A^2\left(\tau^{'}\right)\right]d\tau^{'}\right]\varphi_{Sch} \tag{7.1.65}$$

Therefore the transformation on a eigenstate of the Schrï¿œdinger equation looks identical to the transformation on a spinor to the first order of $(1/c^2)$.

7.1.4 Effect of external magnetic field on Poincaré generators of a composite particle system

We have explained in Chapter 5 that the external magnetic field has no effect on the KF relations. In this subsection, we will explain the reason of that argument in more details. First of all, we would like to point out that if we turn off the external field, the generators should change back to their original forms in the field free case. This fact tells us that the expressions of the field free generators, written in both the LAB and the CM forms, are the leading order

terms of the generators within an external electromagnetic field. The reason is, according to (7.1.59), the expressions of the generators can be expanded with powers of A/c. As we have explained in our calculation of the magnetic moment of the positronium ion system, the external EM field does not affect the transformation relations between the LAB LAB coordinates and the CM coordinates. To see it more specifically, let us see what happens to the equation of boost generators after the external field was introduced. Analogy to the field-free situation, we may still expand the generators and the transform operators as equation (2.17) in Krajcik and Foldy's paper [108]. However, here instead of expanding them with $1/c^2$, we expand them with $1/c$, since the terms introduced by DT are in odd powers of $1/c$

$$\begin{aligned}
\xi &= I + \sum_{n=0} \frac{\xi^{(2n+1)}}{c^{2n+1}} + \sum_{n=1} \frac{\xi^{(2n)}}{c^{2n}} \\
\vec{k} &= \vec{k}^{(0)} + \sum_{n=0} \frac{\vec{k}^{(2n+1)}}{c^{2n+1}} + \sum_{n=1} \frac{\vec{k}^{(2n)}}{c^{2n}} \\
\vec{\mathrm{k}} &= \vec{\mathrm{k}}^{(0)} + \sum_{n=1} \frac{\vec{\mathrm{k}}^{(n)}}{c^{2n}}
\end{aligned} \tag{7.1.66}$$

Starting from the equation

$$\xi \vec{k} = \vec{\mathrm{k}} \xi \tag{7.1.67}$$

By matching the terms with the same power of $1/c$, we derive

$$\begin{aligned}
&\vec{k}^{(0)} = \vec{\mathrm{k}}^{(0)} \\
&\left(1 + \frac{\xi^{(1)}}{c}\right)\left(k^{(0)} + \frac{\vec{k}^{(1)}}{c}\right) = \left(\vec{\mathrm{k}}^{(0)} + \frac{\vec{\mathrm{k}}^{(1)}}{c}\right)\left(1 + \frac{\xi^{(1)}}{c}\right) \\
&\left(1 + \frac{\xi^{(1)}}{c} + \frac{\xi^{(2)}}{c^2}\right)\left(k^{(0)} + \frac{\vec{k}^{(1)}}{c} + \frac{\vec{k}^{(2)}}{c^2}\right) = \left(\vec{\mathrm{k}}^{(0)} + \frac{\vec{\mathrm{k}}^{(1)}}{c} + \frac{\vec{\mathrm{k}}^{(2)}}{c^2}\right)\left(1 + \frac{\xi^{(1)}}{c} + \frac{\xi^{(2)}}{c^2}\right)
\end{aligned} \tag{7.1.68}$$

These equations lead to the following relations

$$\begin{aligned}
&\xi^{(1)} k^{(0)} + \vec{k}^{(1)} = \vec{\mathrm{k}}^{(0)} \xi^{(1)} + \vec{\mathrm{k}}^{(1)} \\
&\vec{k}^{(2)} + \xi^{(2)} k^{(0)} + \xi^{(1)} \vec{k}^{(1)} = \vec{\mathrm{k}}^{(2)} + \vec{\mathrm{k}}^{(1)} \xi^{(1)} + \vec{\mathrm{k}}^{(0)} \xi^{(2)}
\end{aligned}$$

Henceforth

$$\begin{aligned}
\vec{k}^{(1)} &= \vec{\mathrm{k}}^{(1)} + \left[k^{(0)}, \xi^{(1)}\right] \\
\vec{k}^{(2)} &= \vec{\mathrm{k}}^{(2)} + \left[\vec{\mathrm{k}}^{(0)}, \xi^{(2)}\right] + \left[\vec{\mathrm{k}}^{(1)}, \xi^{(1)}\right] - \xi^{(1)}\left[k^{(0)}, \xi^{(1)}\right]
\end{aligned}$$

All the terms in the first order of $1/c$ come from the correction of the external field. They should be canceled between two sides of the equations. Part of the terms to the second order of $1/c$ are from the original definition, and the rest of them come from the external field correction. They can be separated into two equations. Since according to (7.1.59), all the terms come from the external field correction contain the same power of A/c, they must be equal on both sides of the equations. Therefore the introducing of the external field would not affect the validity of the original field-free equations, and henceforth the KF relations will not be altered.

7.1.5 Constructing the Poincaré generators for system within an external field

A more straightforward way of looking at the problem of the external field effect is constructing the Poincaré group generators directly, and derive the coordinates transformation relations with

Krajcik and Foldy's method. We have explained in previous subsections that the external field can be introduced to the generators through the relation (7.1.11) for a set of generators of a single particle. Now, we would like to work out the generators of a system composed of multiple particles. In the case of a LAB coordinates system, the generators can be constructed in the same way as it is in the field-free case. That is

$$\vec{\mathcal{P}} = \sum_a \mathbf{p}_a^{'} \tag{7.1.69}$$

$$\vec{\mathcal{J}} = \sum_a \left(\mathbf{r}_a^{'} \times \mathbf{p}_a^{'} + \mathbf{s}_a^{'}\right) \tag{7.1.70}$$

$$\vec{\mathcal{K}} = \sum_a \vec{K}_a^{'} + \beta \mathbf{V}^{'} \tag{7.1.71}$$

$$\vec{K}_a = \frac{1}{2c^2}\left(\mathbf{r}_a^{'} H_a^{'} + H_a^{'} \mathbf{r}_a^{'}\right) - \frac{\mathbf{s}_a^{'} \times \mathbf{p}_a^{'}}{H_a^{'} + m_a c^2} - t\mathbf{p}_a^{'} \tag{7.1.72}$$

$$\mathcal{H} = \sum_a H_a^{'} + \beta U^{'}, \quad H_a^{'} = \left(p_a^{'2} c^2 + m_a^2 c^4\right)^{1/2} \tag{7.1.73}$$

where the prime indicates the operator has been dynamically transformed. We notice that all the commutation relations for the free-particle are preserved

$$\begin{aligned}
&\left[r_a^{'i}, r_b^{'j}\right] = \left[p_a^{'i}, p_b^{'j}\right] = \left[s_a^{'i}, r_b^{'j}\right] = \left[s_a^{'i}, p_b^{'j}\right] = 0 \\
&\left[r_a^{'i}, p_b^{'j}\right] = i\delta_{ab}\delta_{ij}, \\
&\left[s_a^{'i}, s_b^{'j}\right] = i\delta_{ab}\epsilon_{ijk} s_b^{'k}
\end{aligned} \tag{7.1.74}$$

after introducing the external field by DT. Henceforth the Lie algebra of the Poincaré group is preserved with these transformed generators.

To define V more specifically, let us look at the transformation of U. Being the interaction between the particles, it is of particular interest. In order to guarantee that the commutation relations between U, $\vec{\mathcal{P}}$ and $\vec{\mathcal{J}}$ are preserved, so that the Lie algebra of the Poincaré group is preserved after DT, we expect U transforms in the following way

$$U \to VUV^{-1} \tag{7.1.75}$$

In our system, the interactions between the particles are Coulomb potential, hence we have

$$U \propto \sum_{a>b} \frac{1}{|\mathbf{r}_a - \mathbf{r}_b|} \tag{7.1.76}$$

It is easy to verify that $V(\mathbf{r})\frac{1}{r}V^{-1}(\mathbf{r}) = \left(V(\mathbf{r})\, rV^{-1}(\mathbf{r})\right)^{-1}$. Using the fact that $V(\mathbf{r}_a)$ commutes with $\mathbf{r}_b$ if $a \neq b$, we obtain

$$\frac{1}{|\mathbf{r}_a - \mathbf{r}_b|} \to V(\mathbf{r}_a) V(\mathbf{r}_b) \frac{1}{|\mathbf{r}_a - \mathbf{r}_b|} V^{-1}(\mathbf{r}_b) V^{-1}(\mathbf{r}_a) \tag{7.1.77}$$

Therefore we may define the evolution operator of the system of N particles as

$$V = \prod_{a=1}^{N} V(\mathbf{r}_a) \tag{7.1.78}$$

Here we should keep in mind that the transformed generators, such as $\mathbf{p}_a^{'}$ and $\mathbf{r}_a^{'}$, have lost their initial physical meaning. They are just conjugate operators satisfying the Lie algebra of

the Poincaré group. Through them, we may derive the transformation relations of the physical operators of different coordinate systems.

The next step is constructing the generators in the so called "CM" form, which means the generators are written as functions of the CM coordinates. To accomplish this goal, let us expand the equations (2.2) of [108] in orders of $1/c$. We know that the leading order relations are identical to the field-free case. Now let us look at how the first order relations look like

$$\begin{aligned}
&\left[\mathcal{P}_i^{(1)},\mathcal{H}^{(0)}\right]+\left[\mathcal{P}_i^{(0)},\mathcal{H}^{(1)}\right]=0\\
&\left[\mathcal{J}_i^{(1)},\mathcal{H}^{(0)}\right]+\left[\mathcal{J}_i^{(0)},\mathcal{H}^{(1)}\right]=0\\
&\left[\mathcal{P}_i^{(1)},\mathcal{P}_j^{(0)}\right]+\left[\mathcal{P}_i^{(0)},\mathcal{P}_j^{(1)}\right]=0\\
&\left[\mathcal{J}_i^{(1)},\mathcal{J}_j^{(0)}\right]+\left[\mathcal{J}_i^{(0)},\mathcal{J}_j^{(1)}\right]=i\epsilon_{ijk}\mathcal{J}_k^{(1)}\\
&\left[\mathcal{J}_i^{(1)},\mathcal{P}_j^{(0)}\right]+\left[\mathcal{J}_i^{(0)},\mathcal{P}_j^{(1)}\right]=i\epsilon_{ijk}\mathcal{P}_k^{(1)}\\
&\left[\mathcal{J}_i^{(1)},\mathcal{K}_j^{(0)}\right]+\left[\mathcal{J}_i^{(0)},\mathcal{K}_j^{(1)}\right]=i\epsilon_{ijk}\mathcal{K}_k^{(1)}\\
&\left[\mathcal{H}^{(0)},\mathcal{K}_j^{(1)}\right]+\left[\mathcal{H}^{(1)},\mathcal{K}_j^{(0)}\right]=i\mathcal{P}_j^{(1)}\\
&\left[\mathcal{K}_i^{(0)},\mathcal{K}_j^{(1)}\right]+\left[\mathcal{K}_i^{(1)},\mathcal{K}_j^{(0)}\right]=0\\
&\left[\mathcal{P}_i^{(0)},\mathcal{K}_j^{(1)}\right]+\left[\mathcal{P}_i^{(1)},\mathcal{K}_j^{(0)}\right]=0
\end{aligned}\tag{7.1.79}$$

We know that

$$\begin{aligned}
\mathcal{K}_j^{(0)}&=MR_j^{(0)}-tP_j^{(0)}\\
\mathcal{P}_i^{(0)}&=\sum_a p_{i,a}^{(0)}\\
\mathcal{P}_i^{(1)}&=\sum_a p_{i,a}^{(1)}
\end{aligned}\tag{7.1.80}$$

where $\mathbf{p}_a^{(1)}=-\frac{\mathbf{n}q}{2cn_p}\left(2\mathbf{A}_a\cdot\mathbf{p}_a^{(0)}-\not{F}_a\right)=-\frac{\mathbf{n}q}{2cn_p}\left\{2\left[\mathbf{A}\left(\mathbf{R}\right)+\mathbf{A}\left(\rho_a\right)\right]\cdot\mathbf{p}_a^{(0)}-\not{F}_a\right\}$. In this expression, we have used the fact that the external potential is linear in position, and the leading order of the coordinate transformation is the Galilean transformation. Similarly, the position operators in $\not{F}_a$ can also be Galilean transformed to the CM frame. Using the last equation of (7.1.79), we can obtain the formula of the boost operator $\mathcal{K}_j^{(1)}$ in the first order of $1/c$, with a term as a function of π_a, ρ_a, σ_a undetermined. From the third last equation in (7.1.79), that term can be determined. Similarly, we can obtain all the other generators to the first order of $1/c$ in the CM form. Then, one can use these definitions of generators to the first order of $1/c$ to derive the transformation of coordinates to the first order of $1/c$. Using that transformation relations and the commutation relations to the second order of $1/c$, one can obtain the definition of the generators to the second order of $1/c$ in the CM form. In the end, by using these generators, one can derive the transformation relations of the coordinate systems to the second order of $1/c$.

7.1.6 Definition of Poincaré generators of spinors

In this subsection, we would like to show how the In the spinor space, the expression of the generators $\mathcal{J}$ and $\mathcal{K}$ may be given in a simpler way

$$\begin{aligned} M_{\mu\nu} &= r_\mu p_\nu - r_\nu p_\mu + s_{\mu\nu} \\ \mathcal{J}_{ij} &\equiv M_{ij} = r_i p_j - r_j p_i + s_{ij} = \epsilon_{ijk}\mathcal{J}^k \\ \mathcal{K}_i &= \frac{M_{0i}}{c} = \frac{1}{c}\left(r_0 p_i - r_i p_0 + s_{0i}\right) \equiv \frac{1}{c}\left(l_{0i} + s_{0i}\right) \end{aligned} \tag{7.1.81}$$

where

$$l_{0i} = r_0 p_i - r_i p_0 \tag{7.1.82}$$

$$s_{\mu\nu} = \tfrac{i}{4}\left[\gamma_\mu, \gamma_\nu\right] \tag{7.1.83}$$

and henceforth

$$s_{ij} = \frac{i}{4}\left[\gamma_i, \gamma_j\right] = \frac{1}{2}\epsilon_{ijk}\begin{pmatrix} \sigma^k & \\ & \sigma^k \end{pmatrix} \tag{7.1.84}$$

$$s_{0i} = \frac{i}{4}\left[\gamma_0, \gamma_0\right] = -\frac{i}{2}\begin{pmatrix} \sigma^i & \\ & -\sigma^i \end{pmatrix} \tag{7.1.85}$$

It is easy to verify that the Lie algebra of thePoincaré group is satisfied by these definitions. For example, we may check the commutation

$$\left[\mathcal{K}_i, \mathcal{K}_j\right] = -i\epsilon_{ijk}\mathcal{J}^k/c^2 \tag{7.1.86}$$

According to our definition (7.1.81), the commutator can be written into

$$\begin{aligned} \left[\mathcal{K}_i, \mathcal{K}_j\right] &= \frac{1}{c^2}\left[l_{0i} + s_{0i},\ l_{0j} + s_{0j}\right] \\ &= \frac{1}{c^2}\left(\left[l_{0i}, l_{0j}\right] + \left[s_{0i}, s_{0j}\right]\right) \end{aligned} \tag{7.1.87}$$

where

$$\begin{aligned} &\left[l_{0i}, l_{0j}\right] = \left[r_0 p_i - r_i p_0,\ r_0 p_j - r_j p_0\right] \\ &= -\left[r_0 p_i,\ r_j p_0\right] - \left[r_i p_0,\ r_0 p_j\right] \\ &= i\left(\delta_{ij} E t + r_j p_i\right) - i\left(\delta_{ji} E t + r_i p_j\right) \\ &= -i\left(r_i p_j - r_j p_i\right) = -i l_{ij} \end{aligned} \tag{7.1.88}$$

and

$$\begin{aligned} \left[s_{0i}, s_{0j}\right] &= -\frac{1}{4}\left[\begin{pmatrix} \sigma^i & \\ & -\sigma^i \end{pmatrix}, \begin{pmatrix} \sigma^j & \\ & -\sigma^j \end{pmatrix}\right] \\ &= -\frac{i}{2}\epsilon_{ijk}\begin{pmatrix} \sigma^k & \\ & \sigma^k \end{pmatrix} = -i s_{ij} \end{aligned} \tag{7.1.89}$$

Thus, we have proved that

$$\left[\mathcal{K}_i, \mathcal{K}_j\right] = -\frac{i}{c^2}\left(l_{ij} + s_{ij}\right) = -\frac{i}{c^2}\mathcal{J}_{ij} = -\frac{i}{c^2}\epsilon_{ijk}\mathcal{J}^k \tag{7.1.90}$$

where we have used the definition: $\mathcal{J}_{ij} = \epsilon_{ijk}\mathcal{J}^k$.

7.2 Independence of commutators

The validity of the definition of the V operator in Krajcik and Foldy's paper [108] was questioned by Sebastian and Yun in their paper [139]. They argued that some of the conditions Krajcik and Foldy used to construct V is actually independent and cannot be omitted in the derivation, as Krajcik and Foldy did. In this subsection, we will look into this argument. We find, the relations that Sebastian and Yun claimed to be independent actually can be derived from other conditions that Krajcik and Foldy used to construct V.

According to the Lie algebra of the Poincaré group, the following commutation relations,

$$[\mathcal{P}_i, \mathcal{P}_j] = 0, \tag{7.2.1}$$
$$[\mathcal{J}_i, \mathcal{J}_j] = i\epsilon_{ijk}\mathcal{J}_k, \qquad [\mathcal{J}_i, \mathcal{P}_j] = i\epsilon_{ijk}\mathcal{P}_k, \tag{7.2.2}$$
$$[\mathcal{J}_i, \mathcal{K}_j] = i\epsilon_{ijk}\mathcal{K}_k, \tag{7.2.3}$$
$$[\mathcal{K}_i, \mathcal{P}_j] = i\delta_{ij}\frac{H}{c^2}, \quad [\mathcal{K}_i, \mathcal{K}_j] = -i\epsilon_{ijk}\frac{J_k}{c^2}, \tag{7.2.4}$$

and

$$\begin{aligned}[\mathcal{P}_i, \mathcal{H}] &= [\mathcal{J}_i, \mathcal{H}] = 0 \\ [\mathcal{K}_i, \mathcal{H}] &= i\mathcal{P}_i\end{aligned} \tag{7.2.5}$$

have to be satisfied. The generators may be expressed as functions of the composite variables as

$$\begin{aligned}\vec{\mathcal{P}} &= \sum_a \mathbf{p}_a \\ \vec{\mathcal{J}} &= \sum_a (\mathbf{r}_a \times \mathbf{p}_a + \mathbf{s}_a) \\ \vec{\mathcal{K}} &= \sum_a \vec{K}_a + \beta V \\ \vec{K}_a &= \frac{1}{2c^2}(\mathbf{r}_a H_a + H_a \mathbf{r}_a) - \frac{\mathbf{s}_a \times \mathbf{p}_a}{H_a + m_a c^2} - t\mathbf{p}_a \\ \mathcal{H} &= \sum_a H_a + \beta U, \quad H_a = \left(p_a^2 c^2 + m_a^2 c^4\right)^{1/2}\end{aligned} \tag{7.2.6}$$

where $U^{(0)}$ is the total internal interaction, and $V = \frac{V^{(1)}}{c^2}$ is the corresponding interaction boost as we stated before in Chapter 5. Krajcik and Foldy [108] pointed out that the last three commutators in (7.2.5) are not independent, they can be derived from the relations in (7.2.2). The interaction dependent boost operator $V^{(1)}$, according to the equations in (7.2.2), has to satisfy the relations

$$\begin{aligned}\left[\mathcal{J}_i, V_j^{(1)}\right] &= i\epsilon_{ijk}V_k^{(1)} \\ \left[V_i^{(1)}, \mathcal{P}_j\right] &= i\delta_{ij}\frac{U}{c^2} \\ \left[V_i^{(1)}, \sum_a K_a^j\right] &- (i \longleftrightarrow j) + \beta\left[V_i^{(1)}, V_j^{(1)}\right] = 0\end{aligned}$$

Sebastian and Yun [139] argued that the commutation relations in (7.2.5) is independent of the relations in (7.2.2), except to the leading order of $1/c^2$. They pointed out that to the higher order of $1/c^2$, in order to obtain the proper interaction boost operators, all commutation

relations including the relations in (7.2.5) have to be considered to the same order of $1/c^2$. Thus, further restriction coming out of the relations in (7.2.5) was introduced, which makes the determination of the function $W^{(1)}$ even more troublesome. We would like to point out here that this is unnecessary. The commutation relations given by Sebastian and Yun to the zeroth and the first order in $1/c^2$ are

$$\begin{aligned}
&\left[\mathcal{J}_i, \mathcal{K}_j^{(0)}\right] = i\epsilon_{ijk}\mathcal{K}_k^{(0)}, \\
&[\mathcal{K}_i, \mathcal{P}_j] = i\delta_{ij}M \\
&\left[\mathcal{K}_i^{(0)}, \mathcal{K}_j^{(0)}\right] = 0 \\
&\left[\mathcal{J}_i, \mathcal{K}_j^{(1)}\right] = i\epsilon_{ijk}\mathcal{K}_k^{(1)} \\
&[\mathcal{K}_i, \mathcal{P}_j] = i\delta_{ij}\frac{\mathcal{H}^{(0)}}{c^2} \\
&\left[\mathcal{K}_i^{(1)}, \mathcal{K}_j^{(0)}\right] + \left[\mathcal{K}_i^{(0)}, \mathcal{K}_j^{(1)}\right] = -i\epsilon_{ijk}J_k/c^2
\end{aligned} \tag{7.2.7}$$

and

$$\begin{aligned}
&\left[\mathcal{P}_i, \mathcal{H}^{(1)}\right] = \left[\mathcal{J}_i, \mathcal{H}^{(1)}\right] = 0 \\
&\left[\mathcal{K}_i^{(1)}, \mathcal{H}^{(0)}\right] + \left[\mathcal{K}_i^{(0)}, \mathcal{H}^{(1)}\right] = 0
\end{aligned} \tag{7.2.8}$$

Sebastian and Yun argue that (7.2.8) cannot be derived from (7.2.7). Here we would like to point out that the equations (7.2.7) and (7.2.8) that they used in their argument are not well defined, and some of them are wrong. The correct expressions of commutation relations within (7.2.5) can be derived from the correct expressions of commutation relations in (7.2.2) to the first order of $1/c^2$. To achieve this, we should first notice that not only the generators $\mathcal{K}$, and $\mathcal{H}$ can be expanded with $1/c^2$, but also the generators $\mathcal{P}$ and $\mathcal{J}$ should also be expanded with $1/c^2$

$$\mathcal{P} = \mathcal{P}^{(0)} + \textstyle\sum_{i=1}^{\infty} \frac{\mathcal{P}^{(i)}}{c^{2i}} \tag{7.2.9}$$

$$\mathcal{J} = \mathcal{J}^{(0)} + \textstyle\sum_{i=1}^{\infty} \frac{\mathcal{J}^{(i)}}{c^{2i}} \tag{7.2.10}$$

The other thing that is worth to be noticed is: unlike the other generators, the power of $1/c^2$ for a certain term in the expansion of $\mathcal{H}$ is different from its upper index. For example, when we write

$$\mathcal{H} = \mathcal{H}^{(0)} + \sum_{i=1}^{\infty} \frac{\mathcal{H}^{(i)}}{c^{2i}} \tag{7.2.11}$$

the first term $\mathcal{H}^{(0)} = Mc^2 \propto (1/c^2)^{-1}$, the second term $\mathcal{H}^{(1)} \propto (1/c^2)^0$ etc.. Now, let us look at the commutation relations being concerned.

$[\mathcal{J}_i, \mathcal{H}] = 0$ to the order of $1/c^2$

We start with the commutator $[\mathcal{J}_i, \mathcal{H}] = 0$ to the first order of $1/c^2$. From the Jacobi identities, we know that

$$\begin{aligned}
&\left[\mathcal{P}_l^{(1)}, \left[\mathcal{J}_i^{(0)}, \mathcal{K}_j^{(0)}\right]\right] + \left[\mathcal{J}_i^{(0)}, \left[\mathcal{K}_j^{(0)}, \mathcal{P}_l^{(1)}\right]\right] + \left[\mathcal{K}_j^{(0)}, \left[\mathcal{P}_l^{(1)}, \mathcal{J}_i^{(0)}\right]\right] = 0 \\
&\left[\mathcal{P}_l^{(0)}, \left[\mathcal{J}_i^{(0)}, \mathcal{K}_j^{(1)}\right]\right] + \left[\mathcal{J}_i^{(0)}, \left[\mathcal{K}_j^{(1)}, \mathcal{P}_l^{(0)}\right]\right] + \left[\mathcal{K}_j^{(1)}, \left[\mathcal{P}_l^{(0)}, \mathcal{J}_i^{(0)}\right]\right] = 0 \\
&\left[\mathcal{P}_l^{(0)}, \left[\mathcal{J}_i^{(1)}, \mathcal{K}_j^{(0)}\right]\right] + \left[\mathcal{J}_i^{(1)}, \left[\mathcal{K}_j^{(0)}, \mathcal{P}_l^{(0)}\right]\right] + \left[\mathcal{K}_j^{(0)}, \left[\mathcal{P}_l^{(0)}, \mathcal{J}_i^{(1)}\right]\right] = 0
\end{aligned} \tag{7.2.12}$$

On the other hand, we can easily obtain the following relations from (7.2.2)

$$\left[\mathcal{J}_i^{(0)}, \mathcal{K}_j^{(0)}\right] = i\epsilon_{ijk}\mathcal{K}_k^{(0)}; \left[\mathcal{J}_i^{(0)}, \mathcal{K}_j^{(1)}\right] + \left[\mathcal{J}_i^{(1)}, \mathcal{K}_j^{(0)}\right] = i\epsilon_{ijk}\mathcal{K}_k^{(1)}, \tag{7.2.13}$$

$$\left[\mathcal{P}_l^{(0)}, \mathcal{J}_i^{(0)}\right] = -i\epsilon_{ilk}\mathcal{P}_k^{(0)}; \left[\mathcal{K}_j^{(0)}, \mathcal{P}_l^{(1)}\right] + \left[\mathcal{K}_j^{(1)}, \mathcal{P}_l^{(0)}\right] = i\delta_{jl}\frac{\mathcal{H}^{(1)}}{c^2}, \tag{7.2.14}$$

$$\left[\mathcal{K}_j^{(0)}, \mathcal{P}_l^{(0)}\right] = i\delta_{jl}\frac{\mathcal{H}^{(0)}}{c^2}. \tag{7.2.15}$$

By using above relations and combining the equations in (7.2.12), we obtain

$$0 = \left[\mathcal{P}_l^{(0)}, i\epsilon_{ijk}\mathcal{K}_k^{(1)}\right] + \left[\mathcal{P}_l^{(1)}, i\epsilon_{ijk}\mathcal{K}_k^{(0)}\right] \tag{7.2.16}$$

$$+ \left[\mathcal{J}_i^{(0)}, i\delta_{jl}\mathcal{H}^{(1)}/c^2\right] + \left[\mathcal{J}_i^{(1)}, i\delta_{jl}\mathcal{H}^{(0)}/c^2\right] \tag{7.2.17}$$

$$+ \left[\mathcal{K}_j^{(0)}, -i\epsilon_{ilk}\mathcal{P}_k^{(1)}\right] + \left[\mathcal{K}_j^{(1)}, -i\epsilon_{ilk}\mathcal{P}_k^{(0)}\right] \tag{7.2.18}$$

the first line and the last line cancel each other, leaving us the second line

$$\left[\mathcal{J}_i^{(0)}, i\delta_{jl}\mathcal{H}^{(1)}/c^2\right] + \left[\mathcal{J}_i^{(1)}, i\delta_{jl}\mathcal{H}^{(0)}/c^2\right] = 0 \tag{7.2.19}$$

Since this equation is valid for any set of i, j, and l, we thus derive

$$\left[\mathcal{J}_i^{(0)}, \mathcal{H}^{(1)}\right] + \left[\mathcal{J}_i^{(1)}, \mathcal{H}^{(0)}\right] = 0 \tag{7.2.20}$$

Therefore the commutation relation $[\mathcal{J}_i, \mathcal{H}] = 0$ is correct to the first order of $1/c^2$. Similarly, one can prove $[\mathcal{K}_i, \mathcal{H}] = i\mathcal{P}_i$ and $[\mathcal{P}_i, \mathcal{H}] = 0$ to the first order of $1/c^2$. We have proved that these commutators indeed can be derived from (7.2.7), and henceforth are not independent.

Chapter 8

Appendix 2: Polyelectron systems

This Appendix is supplementary to our discussion of the polyelectron systems in previous chapters. In the first section of this Appendix, we present the definition of the g factor of Positron, and its leading order value. The second section of this Appendix gives more details of the numerical calculation of the positronium ion system. In subsection 8.2.1 to 8.2.5, detail of the numerical evaluation of the eigenstate of the positronium ion system is given. We introduce some useful matrix expressions in the calculation of the magnetic moment of positronium ion in 8.2.6. We have set the total momentum and position of the positronium ion system to be zero in 5.3.1. Here in subsection 8.2.7, we will justify this treatment.

8.1 Positron spin g factor

The linear relation between a magnetic moment and the corresponding angular momentum can be written as

$$\mu = \frac{qg}{2m}\mathbf{j} = \gamma\,\mathbf{j} \tag{8.1.1}$$

in atomic units. γ is called gyromagnetic ratio, and g is called g factor. The well known g factor (or gyromagnetic ratio) for an isolated positron is 2, to the first order of $1/c$ approximation. We will show how to calculate this value in this Appendix. The derivation here is borrowed from Landau & Lifshitz's text book [55]. In the non-relativistic limit, the two components χ of the bispinor $\psi = \begin{pmatrix} \phi \\ \chi \end{pmatrix}$ is much smaller than the upper component ϕ. We aim to obtain an equation only for the component ϕ, by a formal expansion of the wave function in powers of $1/c$. The Dirac equation of an positron in an external field can be written as

$$i\hbar\frac{\partial\psi}{\partial t} = \left\{c\boldsymbol{\alpha}\cdot\left(\mathbf{p} - \frac{e}{c}\mathbf{A}\right) + \beta mc^2 + e\Phi\right\}\psi. \tag{8.1.2}$$

In order to exclude the rest energy mc^2, we introduce a new wave function ψ'

$$\psi = \psi' e^{-imc^2 t/\hbar}. \tag{8.1.3}$$

The corresponding equation for the new function ψ' is

$$\left(i\hbar\frac{\partial}{\partial t} + mc^2\right)\psi' = \left\{c\boldsymbol{\alpha}\cdot\left(\mathbf{p} - \frac{e}{c}\mathbf{A}\right) + \beta mc^2 + e\Phi\right\}\psi'. \tag{8.1.4}$$

The new function that we are considering is still a bispinor, $\psi' = \begin{pmatrix} \phi' \\ \chi' \end{pmatrix}$. By substituting this expression into the above equation, we then obtain the equations for each components of the

spinor

$$\begin{cases} \left(i\hbar\frac{\partial}{\partial t} - e\Phi\right)\phi' = c\boldsymbol{\sigma}\cdot\left(\mathbf{p} - \frac{e}{c}\mathbf{A}\right)\chi' \\ \left(i\hbar\frac{\partial}{\partial t} - e\Phi + 2mc^2\right)\chi' = c\boldsymbol{\sigma}\cdot\left(\mathbf{p} - \frac{e}{c}\mathbf{A}\right)\phi' \end{cases} \tag{8.1.5}$$

In the leading order approximation, only the term $2mc^2\chi'$ is retained on the left-hand side of the second equation. Without confusion, we may neglect the primes and write it into

$$\chi = \frac{1}{2mc}\boldsymbol{\sigma}\cdot\left(\mathbf{p} - \frac{e}{c}\mathbf{A}\right)\phi. \tag{8.1.6}$$

Substituting this expression into the first equation of (8.1.5), we have

$$\left(i\hbar\frac{\partial}{\partial t} - e\Phi\right)\phi = \frac{1}{2m}\left(\boldsymbol{\sigma}\cdot\left(\mathbf{p} - \frac{e}{c}\mathbf{A}\right)\right)^2\phi \tag{8.1.7}$$

Since for the Pauli matrices, there the following relations

$$(\boldsymbol{\sigma}\cdot\mathbf{a})(\boldsymbol{\sigma}\cdot\mathbf{b}) = \mathbf{a}\cdot\mathbf{b} + i\boldsymbol{\sigma}\cdot(\mathbf{a}\times\mathbf{b}) \tag{8.1.8}$$

and

$$\begin{aligned} &\left[\left(\mathbf{p} - \frac{e}{c}\mathbf{A}\right)\times\left(\mathbf{p} - \frac{e}{c}\mathbf{A}\right)\right]\phi = \frac{ie\hbar}{c}\left\{\mathbf{A}\times\boldsymbol{\nabla} + \boldsymbol{\nabla}\times\mathbf{A}\right\}\phi \\ &= \frac{ie\hbar}{c}\left(\boldsymbol{\nabla}\times\mathbf{A}\right)\phi \end{aligned} \tag{8.1.9}$$

are satisfied, we obtain the expression of the term

$$\left(\boldsymbol{\sigma}\cdot\left(\mathbf{p} - \frac{e}{c}\mathbf{A}\right)\right)^2 = \left(\mathbf{p} - \frac{e}{c}\mathbf{A}\right)^2 - \frac{e\hbar}{c}\boldsymbol{\sigma}\cdot\mathbf{H}, \tag{8.1.10}$$

where $\mathbf{H} = curl\ \mathbf{A}$ is the magnetic field. Therefore, we obtain the equation of ϕ

$$i\hbar\frac{\partial\phi}{\partial t} = H\phi = \left[\frac{1}{2m}\left(\mathbf{p} - \frac{e}{c}\mathbf{A}\right)^2 + e\Phi - \frac{e\hbar}{2mc}\boldsymbol{\sigma}\cdot\mathbf{H}\right]\phi \tag{8.1.11}$$

This equation is called Pauli's equation. Its Hamiltonian differs from the non-relativistic Hamiltonian by the last term on the right hand side of the equation. This last term is from the magnetic dipole energy in the external field. Thus, the magnetic moment for the isolated positron is

$$\boldsymbol{\mu} = \frac{e\hbar}{mc}\mathbf{s} = \frac{e}{m}\mathbf{s} \qquad \text{(in natural units)} \tag{8.1.12}$$

The g factor of an isolated positron is 2, twice as its value of a magnetic moment due to orbital motion. This result was first derived by Dirac in 1928 [6].

8.1.1 Another interpretation

The nonrelativistic limit value of the g factor can also be obtained by considering the amplitude for positron scattering from an external electromagnetic field

$$\Delta H_{int} = \int d^3x\, eA^{cl}_{\mu} j^{\mu}, \tag{8.1.13}$$

where $j^\mu(x) = \bar{\psi}(x)\gamma^\mu\psi(x)$ is the electromagnetic current, and A^{cl}_μ is a fixed classical potential. In the leading order, the S-matrix element is

$$iM(2\pi)\delta(p^{0'} - p^0) = -ie\bar{u}(p')\gamma^\mu u(p) \cdot A^{cl}_\mu(p' - p), \tag{8.1.14}$$

where $A^{cl}_\mu(p' - p)$ is the Fourier transformation of $A^{cl}_\mu(x)$. Let us set $A^{cl}_\mu(x) = \big(0, \mathbf{A}^{cl}(x)\big)$, henceforth the amplitude for scattering from this field is

$$M = e\left[\bar{u}(p')\gamma^i u(p)\right] A^{cl}_\mu(\mathbf{q}). \tag{8.1.15}$$

Now, what we want to do is extracting a contribution linear in q^i from this amplitude. In order to accomplish this goal, we take a nonrelativistic expansion of the spinors $u(p)$. Keeping terms to the first order in momenta, we have

$$u(p) = \begin{pmatrix} \sqrt{p\cdot\sigma}\xi \\ \sqrt{p\cdot\bar{\sigma}}\xi \end{pmatrix} \approx \sqrt{m}\begin{pmatrix} (1 - \mathbf{p}\cdot\boldsymbol{\sigma}/2m)\,\xi \\ (1 + \mathbf{p}\cdot\boldsymbol{\sigma}/2m)\,\xi \end{pmatrix}. \tag{8.1.16}$$

Hence the term within the brackets can be written as

$$\bar{u}(p')\gamma^i u(p) = 2m\xi'^\dagger\left(\frac{\mathbf{p}'\cdot\boldsymbol{\sigma}}{2m}\sigma^i + \sigma^i\frac{\mathbf{p}\cdot\boldsymbol{\sigma}}{2m}\right)\xi. \tag{8.1.17}$$

Using the identity of Pauli matrix $\sigma^i\sigma^j = \delta^{ij} + i\epsilon^{ijk}\sigma^k$, the above equation turns out to be

$$\bar{u}(p')\gamma^i u(p) = 2m\xi'^\dagger\left(\frac{\left(p^{i'} + p^i\right)}{2m} + \frac{i\epsilon^{ijk}\left(p^j - p'^j\right)\sigma^k}{2m}\right)\xi, \tag{8.1.18}$$

where the first term in brackets is spin independent. It comes from the standard kinetic energy term of nonrelativistic quantum mechanics. The second term is the magnetic moment interaction, that we are looking for. Hence we may keep only the second term of the expression, and obtain

$$\bar{u}(p')\gamma^i u(p) = 2m\xi'^\dagger\left(\frac{-i\epsilon^{ijk}q^j\sigma^k}{2m}\right)\xi. \tag{8.1.19}$$

Thus, the amplitude has the expression of

$$M = -(2m)\cdot e\xi'^\dagger\left(\frac{-1}{2m}\sigma^k\right)\xi B^k(\mathbf{q}), \tag{8.1.20}$$

where $B^k(\mathbf{q}) = -i\epsilon^{ijk}q^i A^j_{cl}(\mathbf{q})$. It is easy to prove that $B^k(\mathbf{q})$ is the kth component of the Fourier transform of the magnetic field produced by $A^{cl}(x)$. Using the following relation

$$M = -(2m)\cdot\xi'^\dagger V(\mathbf{q})\xi, \tag{8.1.21}$$

we have

$$V(\mathbf{q}) = -\frac{e}{2m}\sigma^k B^k(\mathbf{q}). \tag{8.1.22}$$

Its Fourier transformation is

$$V(\mathbf{x}) = -\boldsymbol{\mu}\cdot\mathbf{B}(\mathbf{x}), \tag{8.1.23}$$

where the magnetic moment is

$$\boldsymbol{\mu} = \frac{e}{m}\frac{\boldsymbol{\sigma}}{2}. \tag{8.1.24}$$

Hence we obtain the value of the g factor $g = 2$. Above derivation can be found in Peskin's book [73].

8.1.2 Fourier transform of the magnetic field

Since the magnetic field can is the curl of the magnetic potential

$$\mathbf{B}(\mathbf{x}) = \boldsymbol{\nabla} \times \mathbf{A}(\mathbf{x}) \tag{8.1.25}$$

we have the following expression

$$\begin{aligned}\mathbf{B}(\mathbf{q}) &= \int e^{-i\mathbf{q}\cdot\mathbf{r}}\mathbf{B}(\mathbf{x})\, d^3r \\ &= \int e^{iq^s r_s}\boldsymbol{\nabla} \times \mathbf{A}(\mathbf{x}) d^3r = \int e^{iq^s r_s}\epsilon_{ijk}\partial_i A_j d^3r \\ &= -iq^i\epsilon_{ijk}\mathbf{e}_k A_j(\mathbf{q})\end{aligned} \tag{8.1.26}$$

8.2 Positronium ion system

We present more details of the numerical calculation of the positronium ion system in this section. The derivation presented here is largely borrowed from Paul's thesis[140]. The three-body system consisting of two electrons and a positron is called positronium ion. Suppose, particle 1 and 2 are electrons, particle 3 is a positron, the Hamiltonian for this system is

$$H = -\frac{1}{2}\left[\nabla^2\mathbf{A}_1 + \nabla^2\mathbf{A}_2 + \nabla^2\mathbf{A}_3\right] + \left[\frac{1}{r_{12}} - \frac{1}{r_{13}} - \frac{1}{r_{23}}\right] \tag{8.2.1}$$

It will be more convenient for us to deal with the inter-particle distances rather than the absolute displacements in above formula. We hence introduce the relative coordinates in the center of mass frame

$$\mathbf{R} = \frac{1}{3}(\mathbf{A}_1 + \mathbf{A}_2 + \mathbf{A}_3), \tag{8.2.2}$$

$$\mathbf{r}_{12} = \mathbf{A}_1 - \mathbf{A}_2, \qquad \mathbf{r}_{13} = \mathbf{A}_1 - \mathbf{A}_3. \tag{8.2.3}$$

Therefore the gradients of the two coordinate systems have relations as

$$\begin{aligned}\boldsymbol{\nabla}\mathbf{A}_1 &= \frac{1}{3}\boldsymbol{\nabla}_{\mathbf{R}} + \boldsymbol{\nabla}_{\mathbf{r_{12}}} + \boldsymbol{\nabla}_{\mathbf{r_{13}}} \\ \boldsymbol{\nabla}\mathbf{A}_2 &= \frac{1}{3}\boldsymbol{\nabla}_{\mathbf{R}} - \boldsymbol{\nabla}_{\mathbf{r_{12}}} \\ \boldsymbol{\nabla}\mathbf{A}_3 &= \frac{1}{3}\boldsymbol{\nabla}_{\mathbf{R}} - \boldsymbol{\nabla}_{\mathbf{r_{13}}}.\end{aligned}$$

The kinetic energy operator then turns out to be

$$T = -\left[\nabla^2_{\mathbf{r_{12}}} + \nabla^2_{\mathbf{r_{13}}} + \nabla_{\mathbf{r_{12}}}\cdot\nabla_{\mathbf{r_{13}}}\right], \tag{8.2.4}$$

here we have omitted the term containing $\nabla^2_{\mathbf{R}}$ corresponding to the kinetic energy of the center-of mass of the system, which has no effect on the internal dynamics that we are interested in. The whole Hamiltonian in this inter-particle coordinate system can be written as

$$H = -\left[\nabla^2_{\mathbf{r_{12}}} + \nabla^2_{\mathbf{r_{13}}} + \nabla_{\mathbf{r_{12}}}\cdot\nabla_{\mathbf{r_{13}}}\right] + \left[\frac{1}{r_{12}} - \frac{1}{r_{13}} - \frac{1}{r_{23}}\right] \tag{8.2.5}$$

8.2.1 The trial function

We choose Gaussian like functions as the spatial part of our trial function

$$\phi_i^{12} = exp\left\{-a_i r_{12}^2 - b_i r_{13}^2 - d_i r_{23}^2\right\} \tag{8.2.6}$$

The electron pair is in spin-singlet state, hence we have the spin function

$$\chi = \frac{1}{\sqrt{2}}\left(\uparrow_1\downarrow_2 - \downarrow_1\uparrow_2\right). \tag{8.2.7}$$

By combining these functions, we obtain our basic building block for our trial functions

$$f_i = \chi\phi_i^{12} \tag{8.2.8}$$

Since the electron pair has to be anti-symmetrized, we introduce the following permutation operator

$$A = (1 - P_{12}) \tag{8.2.9}$$

By acting this operator on the basis function, we obtain the whole function

$$|\psi_i\rangle = Af_i = \chi\left(\phi_i^{12} + \phi_i^{21}\right) \tag{8.2.10}$$

8.2.2 Coordinate shift approach for Gaussian Integrals

First, let us consider the overlap integral

$$\langle\psi_i^{12}|\psi_j^{12}\rangle = \int d^3\mathbf{A}_1 d^3\mathbf{A}_2 d^3\mathbf{A}_3\, e^{-ar_{12}^2 - br_{13}^2 - dr_{23}^2} = I\left(a,b,d\right), \tag{8.2.11}$$

where $a = a_i + a_j$, $b = b_i + b_j$, and $d = d_i + d_j$. Let us move to center-of-mass coordinates $\mathbf{R}_i$, defined by

$$\mathbf{A}_i = \mathbf{R} + \mathbf{R}_i \qquad\qquad (i = 1,2), \tag{8.2.12}$$

where $\mathbf{R} = \frac{1}{3}\left(\mathbf{A}_1 + \mathbf{A}_2 + \mathbf{A}_3\right)$. The Jacobian for this transformation is easy to compute

$$\frac{\partial\left(\mathbf{A}_1, \mathbf{A}_2, \mathbf{A}_3\right)}{\partial\left(\mathbf{R}_1, \mathbf{R}_2, \mathbf{R}\right)} = 3^3. \tag{8.2.13}$$

The volume element in center-of-mass coordinates then turns out to be $3^3 d^3\mathbf{R}_1 d^3\mathbf{R}_2$. Since the trial function is independent of $\mathbf{R}$, and the resulting divergent integral can be canceled by normalization, we have omitted integration over $d^3\mathbf{R}$. The next step is to move from the direct coordinates to relative coordinates by introducing new variables $\mathbf{r}_{12} = \mathbf{R}_1 - \mathbf{R}_2$and $\mathbf{r}_{13} = \mathbf{R}_1 - \mathbf{R}_3$, the corresponding Jacobian of this transformation is

$$\frac{\partial\left(\mathbf{R}_1, \mathbf{R}_2\right)}{\partial\left(\mathbf{r}_{12}, \mathbf{r}_{13}\right)} = 3^{-3}. \tag{8.2.14}$$

Thus, the overlap integral can be written as

$$I\left(a,b,d\right) = \int d^3\mathbf{r}_{12} d^3\mathbf{r}_{13}\, e^{-ar_{12}^2 - br_{13}^2 - dr_{23}^2}. \tag{8.2.15}$$

To compute this integral, we want diagonalize the argument of the exponential. This can be achieved by shifting the coordinates as

$$\begin{aligned}\mathbf{r}_{12} &= \mathbf{x} + m\mathbf{y},\\ \mathbf{r}_{13} &= \mathbf{y},\\ \mathbf{r}_{23} &= \mathbf{r}_{13} - \mathbf{r}_{12} = -\mathbf{x} + (1-m)\,\mathbf{y},\end{aligned}$$

The corresponding Jacobian is 1. Then, the argument can be transformed into a simpler form as

$$-ar_{12}^2 - br_{13}^2 - dr_{23}^2 \equiv -\alpha_x x^2 - \alpha_y y^2, \tag{8.2.16}$$

where

$$\begin{aligned}\alpha_x &= a + d,\\ \alpha_y &= \frac{ab + ad + bd}{a + d}.\end{aligned}$$

Thus, the overlap integral is easy to calculate

$$\begin{aligned}I\left(a,b,d\right) &= \frac{\pi^3}{\left(\alpha_x\alpha_y\right)^{3/2}}\\ &= \frac{\pi^3}{\left(ab + ad + bd\right)^{3/2}}.\end{aligned}$$

8.2.3 Matrix elements

We may first work out the specific form of the kinetic term. First compute the gradients of the trial function $|\psi_i^{12}\rangle$ with respect to $\mathbf{r}_{12}$ and $\mathbf{r}_{13}$

$$\begin{aligned}\boldsymbol{\nabla}_{\mathbf{r_{12}}}|\psi\rangle &= \left[-2\left(a+d\right)\mathbf{r}_{12} + 2d\mathbf{r}_{13}\right]|\psi\rangle,\\ \boldsymbol{\nabla}_{\mathbf{r_{13}}}|\psi\rangle &= \left[2d\mathbf{r}_{12} - 2\left(b+d\right)\mathbf{r}_{13}\right]|\psi\rangle.\end{aligned}$$

Further calculation gives us the second gradient terms as

$$\begin{aligned}\nabla_{\mathbf{r}_{12}}^2|\psi\rangle &= \left[-6\left(a+d\right) + 4\left[\left(a+d\right)^2 r_{12}^2 + d^2 r_{13}^2 - 2d\left(a+d\right)\mathbf{r}_{12}\cdot\mathbf{r}_{13}\right]\right]|\psi\rangle\\ \nabla_{\mathbf{r}_{13}}^2|\psi\rangle &= \left[-6\left(b+d\right) + 4\left[d^2 r_{12}^2 + \left(b+d\right)^2 r_{13}^2 - 2d\left(b+d\right)\mathbf{r}_{12}\cdot\mathbf{r}_{13}\right]\right]|\psi\rangle\\ \boldsymbol{\nabla}_{\mathbf{r_{12}}}\cdot\boldsymbol{\nabla}_{\mathbf{r_{13}}}|\psi\rangle &= \left[6d + 4\left[-d\left(a+d\right)r_{12}^2 - d\left(b+d\right)r_{13}^2 + \left(d^2 + \left(a+d\right)\left(b+d\right)\right)\mathbf{r}_{12}\cdot\mathbf{r}_{13}\right]\right]|\psi\rangle,\end{aligned}$$

where we have temporarily omitted all the wave function and parameter indices. Hence we obtain the whole expression for the kinetic operator T acting on a trial state

$$\begin{aligned}T|\psi\rangle = \Big[&6\left(a+b+d\right) - 2\left(2a^2 + ab + ad - bd\right)r_{12}^2\\ &- 2\left(2b^2 + ab + bd - ad\right)r_{13}^2\\ &- 2\left(2d^2 + ad + bd - ab\right)r_{23}^2\Big]|\psi\rangle.\end{aligned} \tag{8.2.17}$$

By shifting the coordinates and solving the integrals, it is not hard to find out the matrix elements that we need for the variational calculation. As what we have discussed in last subsection, the overlap term is

$$\langle\phi_i|\phi_j\rangle = \frac{\pi^3}{\left[\left(a_i+a_j\right)\left(b_i+b_j\right)+\left(a_i+a_j\right)\left(d_i+d_j\right)+\left(b_i+b_j\right)\left(d_i+d_j\right)\right]^{3/2}}. \tag{8.2.18}$$

Here ϕ_i can be the state with any order of particle 1 and 2, since the only difference between ϕ_i^{12} and ϕ_i^{21} is the order of the coefficients in front of each variables. We can work out all the other matrix elements by adopting the same coordinates system as in above derivation. Hence we get the potential term

$$\left\langle \phi_i \left| \frac{1}{r_{12}} - \frac{1}{r_{13}} - \frac{1}{r_{23}} \right| \phi_j \right\rangle = \frac{2\pi^{5/2}}{(ab+ad+bd)} \times \left[\frac{1}{\sqrt{b+d}} - \frac{1}{\sqrt{a+b}} - \frac{1}{\sqrt{a+d}} \right], \tag{8.2.19}$$

where $a = a_i + a_j$, $b = b_i + b_j$, and $d = d_i + d_j$. A certain term within the kinetic terms, T_{13} for example, is

$$\begin{aligned} T_{13}(a,b,d) &\equiv \int d^3\mathbf{r}_{12} d^3\mathbf{r}_{13} \left(r_{13}^2\right) e^{-ar_{12}^2 - br_{13}^2 - dr_{23}^2} \\ &= \int d^3\mathbf{x} d^3\mathbf{y} \left(y^2\right) e^{-\alpha_x x^2 - \alpha_y y^2} \\ &= \frac{3\pi^3}{2\alpha_y \left(\alpha_x \alpha_y\right)^{3/2}} = \frac{3\pi^3 (a+d)}{2\left(ab+ad+bd\right)^{5/2}}. \end{aligned} \tag{8.2.20}$$

According to (8.2.17), we know that the general form of the kinetic term is

$$\begin{aligned} \langle\phi_i|T|\phi_j\rangle &= 6\left(a_j+b_j+d_j\right)\langle\phi_i|\phi_j\rangle \\ &-2\left(2a_j^2+a_jb_j+a_jd_j-b_jd_j\right)\langle\phi_i|r_{12}^2|\phi_j\rangle \\ &-2\left(2b_j^2+a_jb_j+b_jd_j-a_jd_j\right)\langle\phi_i|r_{13}^2|\phi_j\rangle \\ &-2\left(2d_j^2+a_jd_j+b_jd_j-a_jb_j\right)\langle\phi_i|r_{23}^2|\phi_j\rangle. \end{aligned} \tag{8.2.21}$$

where the terms other than T_{13} can be found from (8.2.20) by permuting the parameters. Using these expressions and by permuting the parameters, we can get the expression for the whole Overlap and Hamiltonian matrix elements.

8.2.4 Symmetrization of wave functions

The matrix element for any spin-independent operator O, which is symmetrical under the permutation of identical particle coordinates can be written as

$$\langle A\chi f_i\,|O|\,A\chi f_j\rangle = \langle\chi f_i\left|A^\dagger O A\right|\chi f_j\rangle. \tag{8.2.22}$$

Since $[A,O]=0$, *and* $A^\dagger = A$, for any projector A, we have $AA = A$. Hence we obtain

$$\langle\chi f_i\,|O|\,A\chi f_j\rangle = \langle\phi_i^{12}\,|O|\,\phi_j^{12}\rangle + \langle\phi_i^{12}\,|O|\,\phi_j^{21}\rangle. \tag{8.2.23}$$

8.2.5 Results

Table 8.1 shows the results of our calculations of the ground state energy of the positronium ion. We see the gradual decrease of the energy showing the covergence of the variational approach.

Basis size	Basis growth step	Ground state energy
100	10	-0.2620043
320	20	-0.262005062
370	50	-0.262005059

Table 8.1: Numerical results for the positronium ion energy.

8.2.6 Determination of the matrix elements

Here we briefly describe how the operators in Eq. (5.5.13) are evaluated using the variational method. We expand the trial wave function in an explicitly correlated Gaussian basis, following the steps described in a study of the di-positronium molecule [111] (5.5.16), where ρ_{ab} are the three inter-particle separations and N is the size of the basis; we use $N = 200$. The parameters w_{ab}^i are optimized using the the non-relativistic Coulomb Hamiltonian

$$H_C = \sum_{a=1}^{3} \frac{\mathbf{p}_a^2}{2m_a} + \sum_{a<b} \frac{e_a e_b}{\rho_{ab}}. \tag{8.2.24}$$

The inter-particle vectors are related ($\boldsymbol{\rho}_{12} + \boldsymbol{\rho}_{23} - \boldsymbol{\rho}_{13} = 0$) so one of them can be eliminated in the evaluation of expectation values. The resulting integrands have an exponential whose argument is of second order in two of the inter-particle distances.

The new operator that has to be evaluated is the second term in (5.5.13). We rewrite it as

$$\frac{\boldsymbol{\rho}_{13} \cdot \boldsymbol{\rho}_{12}}{\rho_{13}^3} = \frac{1}{2}\left(\frac{1}{\rho_{13}} - \frac{\rho_{23}^2 - \rho_{12}^2}{\rho_{13}^3}\right), \tag{8.2.25}$$

and find, using $w_{ab}^{ij} \equiv w_{ab}^i + w_{ab}^j$,

$$\begin{aligned}
\left\langle \phi_i \left| \frac{1}{\rho_{13}} \right| \phi_j \right\rangle &= \frac{2\pi^{5/2}}{\left[\sum_{a\neq b<c} w_{ab}^{ij} w_{ac}^{ij}\right] \sqrt{w_{12}^{ij} + w_{23}^{ij}}} \\
\left\langle \phi_i \left| \frac{\rho_{23}^2 - \rho_{12}^2}{\rho_{13}^3} \right| \phi_j \right\rangle &= \left[\frac{\mathrm{d}}{\mathrm{d}w_{12}^{ij}} - \frac{\mathrm{d}}{\mathrm{d}w_{23}^{ij}}\right] \left\langle \phi_i \left| \frac{1}{\rho_{13}^3} \right| \phi_j \right\rangle \\
&= \int \mathrm{d}^3x\, \mathrm{d}^3y\, \frac{1}{y^3} \left[\frac{\mathrm{d}}{\mathrm{d}w_{12}^{ij}} - \frac{\mathrm{d}}{\mathrm{d}w_{23}^{ij}}\right] \exp\left\{-\alpha_x x^2 - \alpha_y y^2\right\} \qquad (8.2.26) \\
&= -\left\langle \phi_i \left| \frac{1}{\rho_{13}} \right| \phi_j \right\rangle \left[\frac{\mathrm{d}}{\mathrm{d}w_{12}^{ij}} - \frac{\mathrm{d}}{\mathrm{d}w_{23}^{ij}}\right] \alpha_y \qquad (8.2.27) \\
&= \frac{2\pi^{5/2}\left(w_{12}^{ij} - w_{23}^{ij}\right)}{\left[\sum_{a\neq b<c} w_{ab}^{ij} w_{ac}^{ij}\right] \left(w_{12}^{ij} + w_{23}^{ij}\right)^{3/2}} \qquad (8.2.28)
\end{aligned}$$

where $\alpha_x \equiv w_{12}^{ij} + w_{23}^{ij}$ and $\alpha_x \alpha_y \equiv \sum_{a\neq b<c} w_{ab}^{ij} w_{ac}^{ij}$. In going from line (8.2.26) to (8.2.27) we use $\left[\frac{\mathrm{d}}{\mathrm{d}w_{12}^{ij}} - \frac{\mathrm{d}}{\mathrm{d}w_{23}^{ij}}\right] \exp\left\{-\alpha_x x^2\right\} = 0$.

8.2.7 Independence of the external variables

In our calculation above, we have set the total momentum $\mathbf{P}$ and the position $\mathbf{R}$ of the system to be zero. In order to justify this simplification, let us write down the exact formula of the external

wave function, and calculate the expectation value of the terms concerned with the external wave function. Assuming the external magnetic field $\mathbf{B}$ is along the z direction, therefore the electromagnetic potential $\mathbf{A} = \frac{1}{2}\mathbf{B} \times \mathbf{r} = \frac{1}{2}(-By, Bx, 0)$. Starting with the Hamiltonian with the minimal coupling to the external electromagnetic field, the Hamiltonian of a system with charge e, and spin $\mathbf{S}$ can be written as

$$H = \frac{1}{2M}\left(P_x + eBy/c\right)^2 + \frac{1}{2M}\left(P_y - eBx/c\right)^2 + \frac{1}{2M}P_z^2 - 2\mu_B S_z B \tag{8.2.29}$$

where M is the total mass of the system. This Hamiltonian can be further written into

$$H = \frac{P_z^2}{2M} + H_{xy} - 2\mu_B S_z B \tag{8.2.30}$$

where $H_{xy} = \frac{1}{2M}\left(P_x^2 + P_y^2\right) + \frac{M\omega_L^2}{2}\left(x^2 + y^2\right) - \omega_L l_z$, $l_z = xP_y - yP_x = -i\frac{\partial}{\partial\varphi}$, and $\omega_L = \frac{eB}{2Mc}$. Therefore

$$H = \frac{P_z^2}{2M} + \frac{1}{2M}P_{xy}^2 + \frac{M\omega_L^2}{2}\rho^2 + i\omega_L\frac{\partial}{\partial\varphi} - 2\mu_B S_z B \tag{8.2.31}$$

Hence the variables can be separated into three groups $\{x, y\}$, $\{z\}$, and $\{\varphi\}$. The external wave function can be written accordingly into

$$\psi(\mathbf{P}, \mathbf{R}) = R(\rho)\, e^{im_l\varphi} f(z)\, \chi(\mathbf{S}, m_s)\ , m_l = l, l-1, \ldots, -l.\ m_s = S, \ldots - S \tag{8.2.32}$$

where $\rho = x^2 + y^2$. $\chi(\mathbf{S}, m_s)$ is the spin component of the wave function. $f(z)$ is a function of z that has been normalized. It can be chosen as $e^{-iP_z z}$ for a plane wave, or $\frac{1}{(2\pi\lambda)^{1/4}}e^{-\frac{z^2}{4\lambda}}$ for a wave packet of a static system. m_l is the eigenvalue of l_z. Now let us solve the equation of $R(\rho)$

$$\begin{aligned}&\left[-\frac{1}{2M}\left(\frac{\partial^2}{\partial\rho^2} + \frac{1}{\rho}\frac{\partial}{\partial\rho}\right) + \frac{M\omega_L^2}{2}\rho\right] R(\rho) = \left[E + (m_l + 2m_s)\,\omega_L\right] R(\rho)\\ &= \left[E + m\omega_L\right] R(\rho) \qquad\qquad (m \equiv m_l + 2m_s = l + 2S, l + 2S - 1, \ldots, -l - 2S)\end{aligned}$$

This is a two dimensional harmonic oscillator potential equation. The solution of this equation is

$$\begin{aligned}&E = (N+1)\,\omega_L\\ &N = (2n_\rho + |m| + m) = 0, 2, 4, \ldots,\ n_\rho = 0, 1, 2, \ldots\end{aligned}$$

and the corresponding wave function

$$R_{n_\rho|m|}(\rho) = \rho^{|m|} F\left(-n_\rho, |m|+1, \alpha_M^2\rho^2\right) e^{-\alpha_M^2\rho^2/2} \tag{8.2.33}$$

where F is confluent hypergeometric function, and $\alpha_M = \sqrt{M\omega_L} = \sqrt{eB/2c}$. The ground state is $R_{n_\rho 0}(\rho) = e^{-eB\rho^2/4c} = e^{-eB\left(x^2+y^2\right)/4c}$. Let us look at the terms containing powers of the total momentum $\mathbf{P}$, and having the potential to contribute to the magnetic moment. The expectation values of the terms with odd power of P_i is zero, because the wave function is even in P_i, and the integral of odd power of P_i gives zero. It is the terms with even power of P_i concern us. We first calculate the expectation of P_x^2 and P_y^2 with the ground state wave function $\psi_{ground}(\mathbf{P}, \mathbf{R})$, and obtain

$$\langle P_x^2\rangle = N_0^2\int e^{-eBx^2/4c}\left(-\overleftarrow{\partial_x}\cdot\overrightarrow{\partial_x}\right)e^{-eBx^2/4c} = \frac{eB}{4c} \tag{8.2.34}$$

and

$$\langle P_y^2 \rangle = N_0^2 \int e^{-eBy^2/4c} \left(-\overleftarrow{\partial_y} \cdot \overrightarrow{\partial_y} \right) e^{-eBy^2/4c} = \frac{eB}{4c} \tag{8.2.35}$$

where N_0 is the normalization factor. The coefficients of the Hamiltonian elements containing P_i^2 are proportional to $1/c^3$, and the expectation we calculate above contributes another power of $1/c$, from this point of view, they are negligible. Next step is to calculate the expectation value of P_z^2, in order to do this, we first choose the z component wave function to be

$$f(z) = \frac{1}{(2\pi\lambda)^{1/4}} e^{-\frac{z^2}{4\lambda}} \tag{8.2.36}$$

and the expectation value

$$\langle P_z^2 \rangle = \frac{1}{(2\pi\lambda)^{1/2}} \int e^{-\frac{z^2}{4\lambda}} \left(-\partial_z^2 \right) e^{-\frac{z^2}{4\lambda}} = \frac{1}{4\lambda^2} \overset{\lambda \to \infty}{\longrightarrow} 0 \tag{8.2.37}$$

The wave function is infinitely degenerate along z direction, and the momentum P_z can be from $-\infty$ to ∞. This means since there is no constraint on the Hamiltonian along z direction, one is free to choose the system to be spreading to infinity along z direction, by letting $\lambda \to \infty$. Correspondingly, the expectation $\langle P_z^2 \rangle \to 0$, this is exactly what Sebastian did in his calculation. On the other hand, if λ is comparable to the average value of the internal distance $\langle \rho \rangle$, due to the uncertainty principle, we obtain

$$\langle P_z^2 \rangle \sim \frac{1}{4} \left\langle \frac{1}{\rho} \right\rangle^2 = \frac{\langle \pi \rangle^2}{4}$$
$$\hookrightarrow |V_z| \sim \frac{|v|}{2N}$$

where N is the number of particles in the system. Hence the speed of the whole system must be also comparable to the average speed of the LAB particle within the system. This normally is not the case in an experiment, thus we can safely adopt Sebastian's treatment to a poly-electron system with or without an overall charge.

8.2.7.1 Finding the magnetic moment

When we try to locate the contributions from the external variable $\mathbf{P}$ and $\mathbf{R}$, there are several principles that we want to keep in mind.

1. If the power of $1/c$ is larger than 3, this term can be omitted.
2. The expectation value of a term in the Hamiltonian should be linear in the magnetic filed B.
3. The term should be linear in the spin operator hence the Pauli matrices σ.
4. Generally, a term is proportional to $R_i^a P_j^b$. Since the external wave function is even in R_i and P_j, $a + b$ must be an even number for a non-vanishing expectation value.

After examining the terms of the Hamiltonian components (5.2.9 — 5.2.14) one by one, we find no contribution from the external motion of the system to its magnetic moment.

Chapter 9

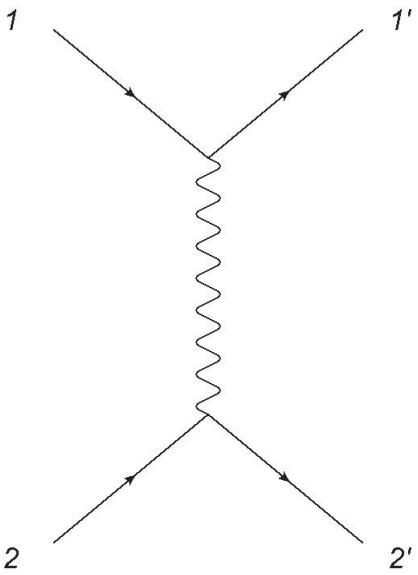
Appendix 3: Derivation of the polyelectron Hamiltonian

In Chapter 5 we have mentioned that the Hamiltonian of a polyelectron system can be obtained in Sebastian's way [141]. In his method, the Hamiltonian is composed of two parts. The first part is the Breit potential describing the interactions between the particles. The derivation of the Breit potential is given in the first section of this Appendix. The second part of the Hamiltonian represents the interaction of the particles with the external field. It is obtained from the Foldy-Wouthuysen reduction. This technique will be discussed in the second section of this Appendix.

9.1 Breit potential

Breit potential formally describes the interaction of two or more massive spin 1/2 particles to the first order in perturbation theory. Breit derived his equation in 1929 [142] based on the Dirac equation. In order to present this derivation in this Appendix, we will start with the relativistic expression of the scattering amplitude of two particles. In the nonrelativistic approximation, this amplitude becomes the Born amplitude. Taking account of the terms to the first order of $1/c^2$ to calculate the second-order terms of the amplitude, we can obtain the expression of the corresponding potential.

In this derivation we are considering the scattering of two different particles, which is represented by the diagram bellow,



the corresponding amplitude can be written as

$$M_{fi} = e^2 \left(\bar{u}_1 \gamma^\mu u_1\right) D_{\mu\nu}(q) \left(\bar{u}_2^{'} \gamma^\nu u_2\right) \tag{9.1.1}$$

$$\mathbf{q} = \mathbf{p}_1' - \mathbf{p}_1 = \mathbf{p}_2 - \mathbf{p}_2' \tag{9.1.2}$$

where we are assuming the particles have the identical charge e.

9.1.1 The first approximation

In order to simplify the calculation, we choose to work with the Coulomb gauge. In the Coulomb gauge, the photon propagators are

$$D_{00} = -\frac{4\pi}{\mathbf{q}^2}, \qquad D_{0i} = 0, \qquad D_{ik} = \frac{4\pi}{\mathbf{q}^2 - \omega^2/c^2 - i0} \left(\delta_{ik} - \frac{q_i q_k}{\mathbf{q}^2}\right). \tag{9.1.3}$$

Hence the amplitude can be written into

$$M_{fi} = e^2 \left\{ \left(\bar{u}_1' \gamma^0 u_1\right) \left(\bar{u}_2' \gamma^0 u_2\right) D_{00} + \left(\bar{u}_1' \gamma^i u_1\right) \left(\bar{u}_2' \gamma^k u_2\right) D_{ik} \right\} \tag{9.1.4}$$

neglecting the $1/c$ terms. The second term in this formula is in a higher order of $1/c^2$ relative to the first one. Therefore the second term can be neglected in this derivation.

Proof:

The amplitudes have the following forms

$$u_p = \begin{pmatrix} \sqrt{(E+m)}\omega \\ \sqrt{E-m}\,(\mathbf{n}\cdot\boldsymbol{\sigma})\,\omega \end{pmatrix}, \qquad u_{-p} = \begin{pmatrix} \sqrt{E-m}\,(\mathbf{n}\cdot\boldsymbol{\sigma})\,\omega' \\ \sqrt{(E+m)}\omega' \end{pmatrix}. \tag{9.1.5}$$

The gamma matrices that we are using can be chosen as

$$\gamma^0 \equiv \beta = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \boldsymbol{\gamma} = \begin{pmatrix} 0 & \boldsymbol{\sigma} \\ -\boldsymbol{\sigma} & 0 \end{pmatrix};$$

$$\boldsymbol{\alpha} = \begin{pmatrix} 0 & \boldsymbol{\sigma} \\ \boldsymbol{\sigma} & 0 \end{pmatrix}, \gamma^0\gamma^i = \alpha^i,\ \gamma^0\gamma^0 = I$$

On one hand, the first term can be written into

$$\bar{u}_1'\gamma^0 u_1 \bar{u}_2'\gamma^0 u_2 = \left[\left(E+mc^2\right)\omega_1'^{\dagger}\omega_1 + \left(E-mc^2\right)\omega_1'^{\dagger}\omega_1\right]\left[\left(E+mc^2\right)\omega_2'^{\dagger}\omega_2 + \left(E-mc^2\right)\omega_2'^{\dagger}\omega_2\right]$$
$$= \left(2E\omega_1'^{\dagger}\omega_1\right)\left(2E\omega_2'^{\dagger}\omega_2\right) \propto E^2 \propto c^4 \tag{9.1.6}$$

On the other hand, the second term satisfies the following relations

$$\bar{u}_1'\gamma^i u_1 \bar{u}_2'\gamma^k u_2 = 2\sqrt{E^2-m^2C^4}\,\omega_1'^{\dagger}\sigma_i\left(\mathbf{n}\cdot\boldsymbol{\sigma}\right)\omega_1$$
$$\times\, 2\sqrt{E^2-m^2C^4}\,\omega_2'^{\dagger}\sigma_k\left(\mathbf{n}\cdot\boldsymbol{\sigma}\right)\omega_2 \propto \left(E^2-m^2C^4\right) = q^2c^2 \propto c^2 \tag{9.1.7}$$

Thus, the second term is an order higher in $1/c^2$ compared to the first term. **End of proof**.

Substituting the expressions of photon propagators into (9.1.4), and working under the first-order approximation, we have the scattering amplitude written as

$$M_{fi} = -2m_1\cdot 2m_2\left(w_1'^{\dagger}w_1\right)\left(w_2'^{\dagger}w_2\right)U\left(\mathbf{q}\right), \tag{9.1.8}$$

where the function

$$U\left(\mathbf{q}\right) = 4\pi e^2/\mathbf{q}^2. \tag{9.1.9}$$

$w_1^{(0)}$, $w_2^{(0)}$ represent the spinor amplitudes of the non-relativistic plane waves. The function $U\left(\mathbf{q}\right)$ is the Fourier transformation of the Coulomb potential $U\left(r\right) = e^2/r$.

9.1.2 Approximation with respect to 1/c

We denote the Schrï¿œdinger wave function of the free particle as ϕ_{Sch}. It obeys the following equation

$$H^{(0)}\phi_{Sch} = \left(E-mc^2\right)\phi_{Sch}, \tag{9.1.10}$$

where the energy

$$E = \sqrt{m^2c^4+q^2c^2} = mc^2\left(1+\frac{q^2}{m^2c^2}\right)^{1/2}$$
$$= mc^2 + \frac{q^2}{2m} - \frac{q^4}{8m^3c^2} \tag{9.1.11}$$

To the first order of $1/c^2$, the Hamiltonian can be written as

$$H^{(0)} = \frac{\mathbf{p}^2}{2m} - \frac{\mathbf{p}^4}{8m^3c^2}, \qquad \mathbf{p} = -i\boldsymbol{\nabla}, \tag{9.1.12}$$

In order to derive the none-relativistic approximation, one may exclude the rest energy mc^2 by introducing a new wave function

$$\psi = \psi' e^{-imc^2t/\hbar} \tag{9.1.13}$$

Then, the Dirac equation of this new wave function turns out to be

$$\left(\left(i\hbar\frac{\partial}{\partial t}+mc^2\right)\right)\psi' = \left\{c\boldsymbol{\alpha}\cdot\left(\mathbf{p}-\frac{e}{c}\mathbf{A}\right)+\beta mc^2+e\Phi\right\}\psi' \tag{9.1.14}$$

Substituting $\psi' = \begin{pmatrix}\phi\\ \chi\end{pmatrix}$ into this equation, we have a group of equations

$$\left(i\hbar\frac{\partial}{\partial t}-e\Phi\right)\phi = c\boldsymbol{\sigma}\cdot\left(\mathbf{p}-\frac{e}{c}\mathbf{A}\right)\chi \tag{9.1.15}$$

$$\left(i\hbar\frac{\partial}{\partial t}-e\Phi+2mc^2\right)\chi = c\boldsymbol{\sigma}\cdot\left(\mathbf{p}-\frac{e}{c}\mathbf{A}\right)\phi \tag{9.1.16}$$

In the first order of $1/c$ approximation, the second equation gives us

$$\chi = \frac{1}{2mc}\boldsymbol{\sigma}\cdot\left(\mathbf{p}-\frac{e}{c}\mathbf{A}\right)\phi. \tag{9.1.17}$$

On one hand, the density of the spinor can be written as

$$\rho = |\phi|^2 + |\chi|^2 = |\phi|^2 + \frac{\hbar^2}{4m^2c^2}\left|\boldsymbol{\sigma}\cdot\boldsymbol{\nabla}\phi\right|^2 \tag{9.1.18}$$

On the other hand, we may write the density in terms of the wave function corresponding to a Schrï¿œdinger equation $\rho = \phi^*_{Sch}\phi_{Sch}$. Henceforth we have

$$\begin{aligned}\int \phi^*_{Sch}\phi_{Sch}d^3\mathbf{r} &= \int\left[\phi^*\phi + \frac{\hbar^2}{4m^2c^2}\left(\boldsymbol{\nabla}\phi^*\cdot\boldsymbol{\sigma}\right)\left(\boldsymbol{\sigma}\cdot\boldsymbol{\nabla}\phi\right)\right]d^3\mathbf{r}\\ &= \int\left[\phi^*\phi - \frac{\hbar^2}{8m^2c^2}\left(\phi^*\Delta\phi + \phi\Delta\phi^*\right)\right]d^3\mathbf{r}\end{aligned} \tag{9.1.19}$$

Comparing the two expressions of the density (9.1.18) and (9.1.19), we obtain the relations

$$\phi_{Sch} = \left(1+\frac{\mathbf{p}^2}{8m^2c^2}\right)\phi \tag{9.1.20}$$

$$\phi = \left(1-\frac{\mathbf{p}^2}{8m^2c^2}\right)\phi_{Sch} \tag{9.1.21}$$

to the first order if $1/c^2$.

In the next step, we want to write the scattering amplitude in terms of the Schrï¿œdinger spinor amplitude ω. Using equations (9.1.17) and (9.1.20), we introduce the bispinor amplitude u of the free particle

$$u = \sqrt{2m}\begin{pmatrix}\left(1-\mathbf{p}^2/8m^2c^2\right)\omega\\ \left(\boldsymbol{\sigma}\cdot\mathbf{p}/2mc\right)\omega\end{pmatrix}. \tag{9.1.22}$$

9.1.3 Terms in the Hamiltonian

In the discussion of this subsection, we will need to work with the Pauli matrices, so here we first present some useful relations

$$\left(\boldsymbol{\sigma}\cdot\mathbf{a}\right)\boldsymbol{\sigma} = \mathbf{a} + i\boldsymbol{\sigma}\times\mathbf{a} \tag{9.1.23}$$

$$\boldsymbol{\sigma}\left(\boldsymbol{\sigma}\cdot\mathbf{a}\right) = \mathbf{a} + i\mathbf{a}\times\boldsymbol{\sigma} \tag{9.1.24}$$

$$\sigma_i\sigma_k + \sigma_k\sigma_i = 2\delta_{ik} \tag{9.1.25}$$

$$\sigma_i\sigma_k = i\epsilon_{ikl}\sigma_l + \delta_{ik} \tag{9.1.26}$$

Let us look at the following term

$$\begin{aligned}&\bar{u}'_1\gamma^0 u_1 = u'^{\dagger}_1 u_1\\ &= (2m_1)\left[\left(1-\mathbf{p}'^2_1/8m^2c^2\right)\left(1-\mathbf{p}^2/8m^2c^2\right)\omega'^{\dagger}_1\omega_1\right.\\ &\left.+\frac{1}{4m_1^2c^2}\omega'^{\dagger}_1\boldsymbol{\sigma}^{\dagger}\cdot\mathbf{p}'_1\boldsymbol{\sigma}\cdot\mathbf{p}_1\omega_1\right]\\ &= 2m_1\left(1-\frac{\mathbf{p}'^2_1+\mathbf{p}^2_1}{8m_1^2c^2}\right)\omega'^{\dagger}_1\omega_1\\ &+\frac{1}{2m_1c^2}\omega'^{\dagger}_1\left(\boldsymbol{\sigma}\cdot\mathbf{p}'_1\right)\left(\boldsymbol{\sigma}\cdot\mathbf{p}_1\right)\omega_1\end{aligned} \tag{9.1.27}$$

where the product

$$\begin{aligned}
&(\boldsymbol{\sigma}\cdot\mathbf{p}_1')\,(\boldsymbol{\sigma}\cdot\mathbf{p}_1) = (\sigma_i p_{1i}')\,(\sigma_k p_{1k}) \\
&= (\delta_{ik} + i\varepsilon_{ikl}\sigma_l)\, p_{1i}' p_{1k} \\
&= p_{1i}' p_{1i} + i\varepsilon_{ikl} p_{1i}' p_{1k}\sigma_l \\
&= \mathbf{p}_1'\cdot\mathbf{p}_1 + i\boldsymbol{\sigma}\cdot\mathbf{p}_1'\times\mathbf{p}_1
\end{aligned} \tag{9.1.28}$$

The product of the spinor and its conjugate is

$$\begin{aligned}
&u_1^{'\dagger}u_1 = 2m_1\omega_1^{'\dagger}\Bigg[1 - \frac{\mathbf{p}_1^{'2}+\mathbf{p}_1^2}{8m_1^2c^2} \\
&+ \frac{1}{4m_1^2c^2}\left(\mathbf{p}_1'\cdot\mathbf{p}_1 + i\boldsymbol{\sigma}\cdot\mathbf{p}_1'\times\mathbf{p}_1\right)\Bigg]\omega_1 \\
&= 2m_1\omega_1^{'\dagger}\left[1 - \frac{\mathbf{q}^2}{8m_1^2c^2} + \frac{i\boldsymbol{\sigma}\cdot\mathbf{p}_1'\times\mathbf{p}_1}{4m_1^2c^2}\right]\omega_1
\end{aligned} \tag{9.1.29}$$

The expectation of the gamma matrices have the following expression

$$\begin{aligned}
&u_1^{'}\boldsymbol{\gamma}u_1 = u_1^{'\dagger}\boldsymbol{\alpha}u_1 \\
&= 2m_1\left(\left(1 - \frac{\mathbf{p}_1^{'2}}{8m_1^2c^2}\right)\omega_1^{'\dagger}, \omega_1^{'\dagger}\boldsymbol{\sigma}^\dagger\cdot\frac{\mathbf{p}_1^{'}}{2m_1c}\right) \\
&\begin{pmatrix} 0 & \boldsymbol{\sigma} \\ \boldsymbol{\sigma} & 0 \end{pmatrix}\begin{pmatrix} \left(1-\mathbf{p}_1^2/8m_1^2c^2\right)\omega_1 \\ \left(\boldsymbol{\sigma}\cdot\mathbf{p}_1/2m_1c\right)\omega_1 \end{pmatrix} \\
&= 2m_1\left(\left(\omega_1^{'\dagger}\boldsymbol{\sigma}\cdot\mathbf{p}_1'/2m_1c\right)\boldsymbol{\sigma}, \left(1-\mathbf{p}_1^{'2}/8m_1^2c^2\right)\omega_1^{'\dagger}\boldsymbol{\sigma}\right) \\
&\begin{pmatrix} \left(1-\mathbf{p}_1^2/8m_1^2c^2\right)\omega_1 \\ \left(\boldsymbol{\sigma}\cdot\mathbf{p}_1/2m_1c\right)\omega_1 \end{pmatrix} \\
&= \frac{1}{c}\Bigg[\omega_1^{'\dagger}\boldsymbol{\sigma}\cdot\mathbf{p}_1'\boldsymbol{\sigma}\left(1-\mathbf{p}_1^2/8m_1^2c^2\right)\omega_1 \\
&+ \left(1-\mathbf{p}_1^{'2}/8m_1^2c^2\right)\omega_1^{'\dagger}\boldsymbol{\sigma}\boldsymbol{\sigma}\cdot\mathbf{p}_1\omega_1\Bigg] \\
&= \frac{1}{c}\omega_1^{'\dagger}\left[\boldsymbol{\sigma}\left(\boldsymbol{\sigma}\cdot\mathbf{p}_1\right) + \left(\boldsymbol{\sigma}\cdot\mathbf{p}_1'\right)\boldsymbol{\sigma}\right]\omega_1 \\
&= \frac{1}{c}\omega_1^{'\dagger}\left[p_{1k}\mathbf{e_i}\left(\delta_{ik} + i\varepsilon_{ikl}\sigma_l\right) + p_{1k}^{'}\mathbf{e_i}\left(\delta_{ik} + i\varepsilon_{kil}\sigma_l\right)\right]\omega_1 \\
&= \frac{1}{c}\omega_1^{'\dagger}\left[\mathbf{p_1} + i\left(\mathbf{p_1}\times\boldsymbol{\sigma}\right) + \mathbf{p_1'} + i\left(\boldsymbol{\sigma}\times\mathbf{p_1'}\right)\right]\omega_1 \\
&= \frac{1}{c}\omega_1^{'\dagger}\left[i\left(\boldsymbol{\sigma}\times\mathbf{q}\right) + 2\mathbf{p_1} + \mathbf{q}\right]\omega_1
\end{aligned} \tag{9.1.30}$$

It is easy to write down one element of this product

$$\begin{aligned}
&u_1^{'}\gamma_\mathbf{i}u_1 = u_1^{'\dagger}\alpha_\mathbf{i}u_1 \\
&= \frac{1}{c}\omega_1^{'\dagger}\left[i\left(\boldsymbol{\sigma}\times\mathbf{q}\right)_i + 2\mathbf{p}_{1i} + \mathbf{q}_i\right]\omega_1
\end{aligned} \tag{9.1.31}$$

We have stated in last subsection that the amplitude of our scattering process can be written as

$$M_{fi} = e^2\left\{\left(\bar{u}_1'\gamma^0u_1\right)\left(\bar{u}_2'\gamma^0u_2\right)D_{00} + \left(\bar{u}_1'\gamma^iu_1\right)\left(\bar{u}_2'\gamma^ku_2\right)D_{ik}\right\} \tag{9.1.32}$$

The first term in the right hand side of above equation is

$$
\begin{aligned}
& e^2\left[\left(\bar{u}_1'\gamma^0 u_1\right)\left(\bar{u}_2'\gamma^0 u_2\right) D_{00}\right] \\
& = e^2 2m_1\omega_1^{'\dagger}\left[1-\frac{\mathbf{q}^2}{8m_1^2c^2}+\frac{i\boldsymbol{\sigma}\cdot\mathbf{q}\times\mathbf{p}_1}{4m_1^2c^2}\right]\omega_1 \\
& \times 2m_2\omega_2^{'\dagger}\left[1-\frac{\mathbf{q}^2}{8m_2^2c^2}-\frac{i\boldsymbol{\sigma}\cdot\mathbf{q}\times\mathbf{p}_2}{4m_2^2c^2}\right]\omega_2\cdot\left(-\frac{4\pi}{\mathbf{q}^2}\right) \\
& = -2m_1 2m_2\frac{4\pi e^2}{\mathbf{q}^2}\omega_1^{'\dagger}\omega_2^{'\dagger}\left[1-\frac{\mathbf{q}^2}{8m_1^2c^2}+\frac{i\boldsymbol{\sigma}_1\cdot\mathbf{q}\times\mathbf{p}_1}{4m_1^2c^2}]\right] \\
& \left[1-\frac{\mathbf{q}^2}{8m_2^2c^2}-\frac{i\boldsymbol{\sigma}_2\cdot\mathbf{q}\times\mathbf{p}_2}{4m_2^2c^2}]\right]\omega_1\omega_2 \\
& = -2m_1 2m_2\frac{4\pi e^2}{\mathbf{q}^2}\omega_1^{'\dagger}\omega_2^{'\dagger}\left[1-\frac{\mathbf{q}^2}{8m_1^2c^2}-\frac{\mathbf{q}^2}{8m_2^2c^2}+\frac{i\boldsymbol{\sigma}_1\cdot\mathbf{q}\times\mathbf{p}_1}{4m_1^2c^2}-\frac{i\boldsymbol{\sigma}_2\cdot\mathbf{q}\times\mathbf{p}_2}{4m_2^2c^2}\right]\omega_1\omega_2, \qquad (9.1.33)
\end{aligned}
$$

where the indices 1 and 2 of the Pauli matrices represent the spinors that they are acting to. The second term of the amplitude is

$$
\begin{aligned}
& e^2\left[\left(\bar{u}_1'\gamma^i u_1\right)\left(\bar{u}_2'\gamma^k u_2\right) D_{ik}\right] \\
& = \frac{e^2}{c^2}\omega_1^{'\dagger}\left[i\left(\boldsymbol{\sigma}_1\times\mathbf{q}\right)_i+2p_{1i}+q_i\right]\omega_1 \\
& \times\omega_2^{'\dagger}\left[-i\left(\boldsymbol{\sigma}_2\times\mathbf{q}\right)_k+2p_{1k}-q_k\right]\omega_2\cdot\frac{4\pi}{\mathbf{q}^2}\left(\delta_{ik}-\frac{q_iq_k}{\mathbf{q}^2}\right) \\
& = \frac{4\pi e^2}{\mathbf{q}^2c^2}\omega_1^{'\dagger}\omega_2^{'\dagger}\left[i\left(\boldsymbol{\sigma}_1\times\mathbf{q}\right)_i+2p_{1i}+q_i\right]\cdot\left[-i\left(\boldsymbol{\sigma}_2\times\mathbf{q}\right)_k+2p_{1k}-q_k\right] \\
& \times\left(\delta_{ik}-\frac{q_iq_k}{\mathbf{q}^2}\right)\omega_1\omega_2, \qquad (9.1.34)
\end{aligned}
$$

where the product

$$
\begin{aligned}
& \left[i\left(\boldsymbol{\sigma}_1\times\mathbf{q}\right)_i+2p_{1i}+q_i\right]\cdot\left[-i\left(\boldsymbol{\sigma}_2\times\mathbf{q}\right)_k+2p_{1k}-q_k\right] \\
& = \left[\left(\boldsymbol{\sigma}_1\times\mathbf{q}\right)_i\left(\boldsymbol{\sigma}_2\times\mathbf{q}\right)_k+2ip_{2k}\left(\boldsymbol{\sigma}_1\times\mathbf{q}\right)_i-2ip_{1i}\left(\boldsymbol{\sigma}_2\times\mathbf{q}\right)_k\right. \\
& -i\left(\boldsymbol{\sigma}_1\times\mathbf{q}\right)_i q_k-i\left(\boldsymbol{\sigma}_2\times\mathbf{q}\right)_k q_i+4p_{1i}p_{2k} \\
& \left.-2p_{1i}q_k+2p_{2k}q_i-q_iq_k\right]\cdot\left(\delta_{ik}-\frac{q_iq_k}{\mathbf{q}^2}\right), \qquad (9.1.35)
\end{aligned}
$$

The first term δ_{ik} in the last brace of above equation gives us the following expression

$$
\begin{aligned}
& \left(\boldsymbol{\sigma}_1\times\mathbf{q}\right)\cdot\left(\boldsymbol{\sigma}_2\times\mathbf{q}\right)+2i\mathbf{p}_2\cdot\left(\boldsymbol{\sigma}_1\times\mathbf{q}\right)-2i\mathbf{p}_1\cdot\left(\boldsymbol{\sigma}_2\times\mathbf{q}\right) \\
& +4\mathbf{p}_1\cdot\mathbf{p}_2-2\mathbf{p}_1\cdot\mathbf{q}+2\mathbf{p}_2\cdot\mathbf{q}-\mathbf{q}^2, \qquad (9.1.36)
\end{aligned}
$$

The second term $-\frac{q_iq_k}{\mathbf{q}^2}$ contributes

$$
-\frac{1}{\mathbf{q}^2}\left[4\left(\mathbf{p}_1\cdot\mathbf{q}\right)\left(\mathbf{p}_2\cdot\mathbf{q}\right)-2\mathbf{p}_1\cdot\mathbf{q}\mathbf{q}^2+2\mathbf{p}_2\cdot\mathbf{q}\mathbf{q}^2-\mathbf{q}^4\right]. \qquad (9.1.37)
$$

Combining these two expressions, we obtain

$$
\begin{aligned}
& \left(\boldsymbol{\sigma}_1\times\mathbf{q}\right)\cdot\left(\boldsymbol{\sigma}_2\times\mathbf{q}\right)+2i\mathbf{p}_2\cdot\left(\boldsymbol{\sigma}_1\times\mathbf{q}\right)-2i\mathbf{p}_1\cdot\left(\boldsymbol{\sigma}_2\times\mathbf{q}\right) \\
& \qquad +4\mathbf{p}_1\cdot\mathbf{p}_2-4\left(\mathbf{p}_1\cdot\mathbf{q}\right)\left(\mathbf{p}_2\cdot\mathbf{q}\right)/\mathbf{q}^2, \qquad (9.1.38)
\end{aligned}
$$

where

$$
\begin{aligned}
&(\boldsymbol{\sigma}_1 \times \mathbf{q}) \cdot (\boldsymbol{\sigma}_2 \times \mathbf{q}) = \sigma_{1i} q_j \varepsilon_{ijk} \mathbf{e}_k \cdot \sigma_{2l} q_s \varepsilon_{lsm} \mathbf{e}_m \\
&= \sigma_{1i} q_j \varepsilon_{ijk} \varepsilon_{lsk} \sigma_{2l} q_s \\
&= \sigma_{1i} q_j \sigma_{2l} q_s \left[\delta_{il}\delta_{js} - \delta_{is}\delta_{jl}\right] \\
&= \left(\boldsymbol{\sigma}_1 \cdot \boldsymbol{\sigma}_2\right) \mathbf{q}^2 - \left(\boldsymbol{\sigma}_1 \cdot \mathbf{q}\right) \cdot \left(\boldsymbol{\sigma}_2 \cdot \mathbf{q}\right), \qquad (9.1.39)
\end{aligned}
$$

and

$$
\begin{aligned}
&2i\mathbf{p}_2 \cdot (\boldsymbol{\sigma}_1 \times \mathbf{q}) \\
&= 2ip_{2i}\mathbf{e}_i \cdot \mathbf{e}_s \sigma_{1j} q_k \varepsilon_{jks} = 2ip_{2i}\sigma_{1j} q_k \varepsilon_{jki} \\
&= 2i\boldsymbol{\sigma}_1 \cdot (\mathbf{q} \times \mathbf{p}_2), \qquad (9.1.40)
\end{aligned}
$$

Similarly,

$$
2i\mathbf{p}_1 \cdot (\boldsymbol{\sigma}_2 \times \mathbf{q}) = 2i\boldsymbol{\sigma}_2 \cdot (\mathbf{q} \times \mathbf{p}_1). \qquad (9.1.41)
$$

Substituting these formulas into (9.1.34) and combining with (9.1.33), we obtain the amplitude

$$
M_{fi} = -2m_1 \cdot 2m_2 \left(\omega_1^{'\dagger} \omega_2^{'\dagger} U\left(\mathbf{p}_1, \mathbf{p}_2, \mathbf{q}\right) \omega_1 \omega_2\right), \qquad (9.1.42)
$$

where the potential function can be written as

$$
\begin{aligned}
U\left(\mathbf{p}_1, \mathbf{p}_2, \mathbf{q}\right) = 4\pi e^2 \Bigg\{ &\frac{1}{\mathbf{q}^2} - \frac{1}{8m_1^2 c^2} - \frac{1}{8m_2^2 c^2} + \frac{\left(\mathbf{p}_1 \cdot \mathbf{q}\right)\left(\mathbf{p}_2 \cdot \mathbf{q}\right)}{m_1 m_2 \mathbf{q}^4 c^2} \\
&- \frac{\mathbf{p}_1 \cdot \mathbf{p}_2}{m_1 m_2 \mathbf{q}^2 c^2} + \frac{i\boldsymbol{\sigma}_1 \cdot \mathbf{q} \times \mathbf{p}_1}{4m_1^2 c^2 \mathbf{q}^2} - \frac{i\boldsymbol{\sigma}_1 \cdot \mathbf{q} \times \mathbf{p}_2}{2m_1 m_2 c^2 \mathbf{q}^2} - \frac{i\boldsymbol{\sigma}_2 \cdot \mathbf{q} \times \mathbf{p}_2}{4m_2^2 c^2 \mathbf{q}^2} \\
&+ \frac{i\boldsymbol{\sigma}_2 \cdot \mathbf{q} \times \mathbf{p}_1}{2m_1 m_2 c^2 \mathbf{q}^2} + \frac{\left(\boldsymbol{\sigma}_1 \cdot \mathbf{q}\right) \cdot \left(\boldsymbol{\sigma}_2 \cdot \mathbf{q}\right)}{4m_1 m_2 c^2 \mathbf{q}^2} - \frac{\boldsymbol{\sigma}_1 \cdot \boldsymbol{\sigma}_2}{4m_1 m_2 c^2} \Bigg\}. \qquad (9.1.43)
\end{aligned}
$$

This potential function is in the momentum space. We may need the potential function in the coordinate space as well. They can be related by the Fourier transformation

$$
\int e^{-i\mathbf{q}\cdot\mathbf{r}} U\left(\mathbf{r}\right) d^3x = U\left(\mathbf{q}\right), \qquad (9.1.44)
$$

where $\mathbf{r} = \mathbf{r}_1 - \mathbf{r}_2$. It is easy to notice, that we may get the $U\left(\mathbf{p}_1, \mathbf{p}_2, \mathbf{r}\right)$ by calculating the integral

$$
\int e^{i\mathbf{q}\cdot\mathbf{r}} U\left(\mathbf{p}_1, \mathbf{p}_2, \mathbf{q}\right) d^3q / \left(2\pi\right)^3, \qquad (9.1.45)
$$

and replacing $\mathbf{p}$ by their corresponding operators $\mathbf{p}_i = -i\nabla_i \quad i = 1, 2$. Before doing the integral, we want to take a note of a basic Fourier transform

$$
\int e^{i\mathbf{q}\cdot\mathbf{r}} \frac{4\pi}{\mathbf{q}^2} \frac{d^3q}{\left(2\pi\right)^3} = \frac{1}{r}. \qquad (9.1.46)
$$

Taking the gradient of this formula gives us

$$
\int e^{i\mathbf{q}\cdot\mathbf{r}} \frac{4\pi\mathbf{q}}{\mathbf{q}^2} \frac{d^3q}{\left(2\pi\right)^3} = -i\nabla\frac{1}{r} = \frac{i\mathbf{r}}{r^3}. \qquad (9.1.47)
$$

Generally, one has the Fourier transform as

$$
\hat{f}\left(\nu\right) = \int_{-\infty}^{\infty} f\left(x\right) e^{-i\nu x} dx, \qquad (9.1.48)
$$

More generally, we can deduce the following relation

$$x^n f(x) \longrightarrow i^n \frac{d^n \hat{f}(\nu)}{d\nu^n}. \tag{9.1.49}$$

Therefore we have

$$\begin{aligned}
&\int e^{i\mathbf{q}\cdot\mathbf{r}} \frac{4\pi (\mathbf{a}\cdot\mathbf{q})\cdot(\mathbf{b}\cdot\mathbf{q})}{\mathbf{q}^4} \frac{d^3q}{(2\pi)^3} \\
&= -4\pi i \left(\mathbf{a}\cdot\frac{\partial}{\partial\mathbf{r}}\right) \int e^{i\mathbf{q}\cdot\mathbf{r}} \frac{\mathbf{b}\cdot\mathbf{q}}{\mathbf{q}^4} \frac{d^3q}{(2\pi)^3} \\
&= \frac{4\pi i}{2} \left(\mathbf{a}\cdot\frac{\partial}{\partial\mathbf{r}}\right) \int e^{i\mathbf{q}\cdot\mathbf{r}} \left(\mathbf{b}\cdot\frac{\partial}{\partial\mathbf{q}}\right) \frac{1}{\mathbf{q}^2} \frac{d^3q}{(2\pi)^3},
\end{aligned} \tag{9.1.50}$$

where the integral can be calculated

$$\begin{aligned}
&4\pi i \int e^{i\mathbf{q}\cdot\mathbf{r}} \left(\mathbf{b}\cdot\frac{\partial}{\partial\mathbf{q}}\right) \frac{1}{\mathbf{q}^2} \frac{d^3q}{(2\pi)^3} \\
&= 4\pi i \int e^{iq_i r^i} b_j \partial_q^j \frac{1}{q^2} \frac{dq^j}{(2\pi)^3} \\
&= \frac{4\pi i}{(2\pi)^3} \left(\frac{b_j}{q^2} e^{iq_i r^i}|_{q_j=0}^{\infty} - \int \frac{1}{\mathbf{q}^2} b_j \partial_j e^{i\mathbf{q}\cdot\mathbf{r}} d^3q \right) \\
&= \frac{-4\pi i}{(2\pi)^3} \int \frac{1}{\mathbf{q}^2} \left(\mathbf{b}\cdot\frac{\partial}{\partial\mathbf{q}}\right) e^{i\mathbf{q}\cdot\mathbf{r}} d^3q \\
&= \frac{1}{(2\pi)^3} \int \frac{4\pi}{\mathbf{q}^2} (\mathbf{b}\cdot\mathbf{r}) e^{i\mathbf{q}\cdot\mathbf{r}} d^3q = \frac{\mathbf{b}\cdot\mathbf{r}}{r}.
\end{aligned} \tag{9.1.51}$$

Thus, equation (9.1.50) turns out to be

$$\begin{aligned}
&\int e^{i\mathbf{q}\cdot\mathbf{r}} \frac{4\pi (\mathbf{a}\cdot\mathbf{q})\cdot(\mathbf{b}\cdot\mathbf{q})}{\mathbf{q}^4} \frac{d^3q}{(2\pi)^3} = \frac{1}{2} (\mathbf{a}\cdot\nabla) \frac{\mathbf{b}\cdot\mathbf{r}}{r} \\
&= \frac{1}{2} a_i \partial^i \frac{b_j r^j}{(r^k r_k)^{1/2}} = \frac{1}{2} \left[\frac{\delta_{ij}}{(r^k r_k)^{1/2}} - r^j \frac{r_k \delta_k^i}{(r^k r_k)^{3/2}} \right] \\
&= \frac{1}{2r} \left[\mathbf{a}\cdot\mathbf{b} - \frac{(\mathbf{a}\cdot\mathbf{r})\cdot(\mathbf{b}\cdot\mathbf{r})}{r^2} \right].
\end{aligned} \tag{9.1.52}$$

The last type of Fourier transform that we may be interested in is

$$\begin{aligned}
&\int e^{i\mathbf{q}\cdot\mathbf{r}} \frac{4\pi (\mathbf{a}\cdot\mathbf{q})\cdot(\mathbf{b}\cdot\mathbf{q})}{\mathbf{q}^2} \frac{d^3q}{(2\pi)^3} \\
&= -\left(\mathbf{a}\cdot\frac{\partial}{\partial\mathbf{r}}\right) \left(b\cdot\frac{\partial}{\partial\mathbf{r}}\right) \int \frac{4\pi e^{i\mathbf{q}\cdot\mathbf{r}}}{\mathbf{q}^2} \frac{d^3q}{(2\pi)^3} \\
&= -(\mathbf{a}\cdot\boldsymbol{\nabla})(\mathbf{b}\cdot\boldsymbol{\nabla}) \frac{1}{r}.
\end{aligned} \tag{9.1.53}$$

In this case, we must remember that there is a $\delta(\mathbf{r})$ in this expression. In order to obtain this term, let us average the expression over the direction of $\mathbf{r}$. First, let us look at the integrand

$$-(\mathbf{a}\cdot\boldsymbol{\nabla})(\mathbf{b}\cdot\boldsymbol{\nabla}) \frac{1}{r} = -a_k \partial^k b_i \partial^i \frac{1}{r} = -a_k b_i \partial^k \partial^i \frac{1}{r} \tag{9.1.54}$$

The average of the expression over the direction of $\mathbf{r}$ for the non-diagonal terms are

$$\int \partial_i \partial_j \frac{1}{r} d\Omega = 0 \qquad\qquad (for \quad i \neq j)\,. \tag{9.1.55}$$

Henceforth the average over the spacial angle can be written as

$$\begin{aligned}
&\int -\left(\mathbf{a}\cdot\boldsymbol{\nabla}\right)\left(\mathbf{b}\cdot\boldsymbol{\nabla}\right)\frac{1}{r}d\Omega = -\int\left(\partial_1^2\frac{b_1a_1}{r}+\partial_2^2\frac{b_2a_2}{r}+\partial_3^2\frac{b_3a_3}{r}\right)d\Omega \\
&= -\int\left(a_ib^i\right)\partial_j^2\frac{\delta_{ij}}{r}
\end{aligned} \tag{9.1.56}$$

Using the formulas

$$\int \partial_i^2 \frac{1}{r} d\Omega = \int \left(\frac{1}{r^3} - \frac{3r_i^2}{r^5}\right) d\Omega \tag{9.1.57}$$

and

$$\int \frac{x^2}{r^5} d\Omega = \int \frac{y^2}{r^5} d\Omega = \int \frac{z^2}{r^5} d\Omega = \frac{2\pi}{3}; \tag{9.1.58}$$

$$\int \partial_1^2 \frac{1}{r} d\Omega = \int \partial_2^2 \frac{1}{r} d\Omega = \int \partial_3^2 \frac{1}{r} d\Omega. \tag{9.1.59}$$

It is easy to find that

$$\overline{-\left(\mathbf{a}\cdot\boldsymbol{\nabla}\right)\left(\mathbf{b}\cdot\boldsymbol{\nabla}\right)\frac{1}{r}} = \overline{-\frac{1}{3}\left(\mathbf{a}\cdot\mathbf{b}\right)\Delta\frac{1}{r}} = \frac{4\pi}{3}\left(\mathbf{a}\cdot\mathbf{b}\right)\delta\left(\mathbf{r}\right). \tag{9.1.60}$$

Thus, we have the $\delta\left(\mathbf{r}\right)$ term. Now, the entire Fourier transform can be written as

$$\begin{aligned}
&\int e^{i\mathbf{q}\cdot\mathbf{r}}\frac{4\pi\left(\mathbf{a}\cdot\mathbf{q}\right)\cdot\left(\mathbf{b}\cdot\mathbf{q}\right)}{\mathbf{q}^2}\frac{d^3q}{\left(2\pi\right)^3} = -\left(\mathbf{a}\cdot\boldsymbol{\nabla}\right)\left(\mathbf{b}\cdot\boldsymbol{\nabla}\right)\frac{1}{r}+\frac{4\pi}{3}\left(\mathbf{a}\cdot\mathbf{b}\right)\delta\left(\mathbf{r}\right) \\
&= -\left(a_i\partial^i\right)\left(b_j\partial^j\right)\frac{1}{\left(x_kx^k\right)^{1/2}}+\frac{4\pi}{3}\left(\mathbf{a}\cdot\mathbf{b}\right)\delta\left(\mathbf{r}\right) \\
&= \frac{\mathbf{a}\cdot\mathbf{b}}{r^3}-3\frac{\left(\mathbf{a}\cdot\mathbf{r}\right)\left(\mathbf{b}\cdot\mathbf{r}\right)}{r^5}+\frac{4\pi}{3}\left(\mathbf{a}\cdot\mathbf{b}\right)\delta\left(\mathbf{r}\right) \\
&= \frac{1}{r^3}\left\{\mathbf{a}\cdot\mathbf{b}-3\frac{\left(\mathbf{a}\cdot\mathbf{r}\right)\left(\mathbf{b}\cdot\mathbf{r}\right)}{r^2}\right\}+\frac{4\pi}{3}\left(\mathbf{a}\cdot\mathbf{b}\right)\delta\left(\mathbf{r}\right).
\end{aligned} \tag{9.1.61}$$

Using these formulas, we obtain all types of Fourier transform corresponding to each term of $U(\mathbf{p}_1, \mathbf{p}_2, \mathbf{q})$

$$\frac{4\pi e^2}{q^2} \longrightarrow \frac{e^2}{r}, \tag{9.1.62}$$

$$-\frac{4\pi e^2}{8m_i^2c^2} \longrightarrow -\frac{\pi e\hbar^2}{2c^2m_i^2}\delta(\mathbf{r}) \qquad (i=1,2) \tag{9.1.63}$$

$$\frac{4\pi e^2}{m_1m_2c^2}\frac{(\mathbf{q}\cdot\mathbf{p}_1)\cdot(\mathbf{q}\cdot\mathbf{p}_2)}{\mathbf{q}^4} \longrightarrow \frac{e^2}{2m_1m_2c^2r}\left[\mathbf{p}_1\cdot\mathbf{p}_2 - \frac{(\mathbf{p}_1\cdot\mathbf{r})\cdot(\mathbf{p}_2\cdot\mathbf{r})}{r^2}\right] \tag{9.1.64}$$

$$-\frac{4\pi e^2}{m_1m_2c^2}\frac{\mathbf{p}_1\cdot\mathbf{p}_2}{\mathbf{q}^2} \longrightarrow -\frac{\mathbf{p}_1\cdot\mathbf{p}_2e^2}{m_1m_2c^2r} \tag{9.1.65}$$

$$\frac{i4\pi e^2}{4m_1^2c^2}\frac{\boldsymbol{\sigma}_1\cdot(\mathbf{q}\times\mathbf{p}_1)}{\mathbf{q}^2} \longrightarrow -\frac{e^2\hbar^2}{4m_1^2c^2r^3}\boldsymbol{\sigma}_1\cdot(\mathbf{r}\times\mathbf{p}_1) \tag{9.1.66}$$

$$\frac{4\pi e^2}{4m_1m_2c^2}\frac{(\boldsymbol{\sigma}_1\cdot\mathbf{q})\cdot(\boldsymbol{\sigma}_2\cdot\mathbf{q})}{\mathbf{q}^2} \longrightarrow \frac{e^2\hbar^2}{4m_1m_2c^2}\left\{\frac{1}{r^3}\left[\boldsymbol{\sigma}_1\cdot\boldsymbol{\sigma}_2 - \frac{3(\boldsymbol{\sigma}_1\cdot\mathbf{r})\cdot(\boldsymbol{\sigma}_2\cdot\mathbf{r})}{r^2}\right]\right. \tag{9.1.67}$$

$$\left. + \frac{4\pi}{3}\boldsymbol{\sigma}_1\cdot\boldsymbol{\sigma}_2\delta(\mathbf{r})\right\} \tag{9.1.68}$$

$$-\frac{4\pi e^2\boldsymbol{\sigma}_1\cdot\boldsymbol{\sigma}_2}{4m_1m_2c^2} \longrightarrow -\frac{\pi e^2\hbar^2\boldsymbol{\sigma}_1\cdot\boldsymbol{\sigma}_2}{m_1m_2c^2}\delta(\mathbf{r}) \tag{9.1.69}$$

Using these formulas, we can finally write down the interaction operator in the coordinate space

$$\begin{aligned} U(\mathbf{p}_1,\mathbf{p}_2,\mathbf{r}) &= \frac{e^2}{r} - \frac{\pi e^2\hbar^2}{2c^2}\left(\frac{1}{m_1^2}+\frac{1}{m_2^2}\right)\delta(\mathbf{r}) \\ &- \frac{e^2}{2m_1m_2c^2\mathbf{r}}\left[\mathbf{p}_1\cdot\mathbf{p}_2 + \frac{\mathbf{r}\cdot(\mathbf{r}\cdot\mathbf{p}_1)\,\mathbf{p}_2}{r^2}\right] - \frac{e^2\hbar}{4m_1^2c^2r^3}\mathbf{r}\times\mathbf{p}_1\cdot\boldsymbol{\sigma}_1 \\ &+ \frac{e^2\hbar}{4m_2^2c^2r^3}\mathbf{r}\times\mathbf{p}_2\cdot\boldsymbol{\sigma}_2 - \frac{e^2\hbar}{2m_1m_2c^2r^3}\left[\boldsymbol{\sigma_2}\cdot(\mathbf{r}\times\mathbf{p_1}) - \boldsymbol{\sigma}_1\cdot(\mathbf{r}\times\mathbf{p}_2)\right] \\ &+ \frac{e^2\hbar^2}{4m_1m_2c^2}\left\{\frac{1}{r^3}\left[\boldsymbol{\sigma}_1\cdot\boldsymbol{\sigma}_2 - \frac{3(\boldsymbol{\sigma}_1\cdot\mathbf{r})\cdot(\boldsymbol{\sigma}_2\cdot\mathbf{r})}{r^2}\right] - \frac{8\pi}{3}\boldsymbol{\sigma}_1\cdot\boldsymbol{\sigma}_2\delta(\mathbf{r})\right\}. \end{aligned} \tag{9.1.70}$$

The total Hamiltonian of the two-particle system is

$$H = H_1^{(0)} + H_2^{(0)} + U, \tag{9.1.71}$$

where $H_i^{(0)}$ is the free particle Hamiltonian. For positronium, we have $m_1 = m_2 = m$, $e_1 = -e_2 = e$, and henceforth $e^2 \to -e^2$. The potential turns out to be

$$\begin{aligned} U_{Breit}(\mathbf{p}_1,\mathbf{p}_2,\mathbf{r}) &= -\frac{e^2}{r} + \frac{\pi e^2\hbar^2}{m^2c^2}\delta^3(\mathbf{r}) \\ &+ \frac{e^2}{2m^2c^2r}\left[\mathbf{p}_1\cdot\mathbf{p}_2 + \frac{\mathbf{r}\cdot(\mathbf{r}\cdot\mathbf{p}_1)\,\mathbf{p}_2}{r^2}\right] + \frac{e^2\hbar}{4m^2c^2r^3}(\mathbf{r}\times\mathbf{p}_1)\cdot\boldsymbol{\sigma}_1 \\ &- \frac{e^2\hbar}{4m^2c^2r^3}(\mathbf{r}\times\mathbf{p}_2)\cdot\boldsymbol{\sigma}_2 + \frac{e^2\hbar}{2m^2c^2r^3}\left[\boldsymbol{\sigma_2}\cdot(\mathbf{r}\times\mathbf{p_1}) - \boldsymbol{\sigma}_1\cdot(\mathbf{r}\times\mathbf{p}_2)\right] \\ &- \frac{e^2\hbar^2}{4m^2c^2}\left\{\frac{1}{r^3}\left[\boldsymbol{\sigma}_1\cdot\boldsymbol{\sigma}_2 - \frac{3(\boldsymbol{\sigma}_1\cdot\mathbf{r})\cdot(\boldsymbol{\sigma}_2\cdot\mathbf{r})}{r^2}\right] - \frac{8\pi}{3}\boldsymbol{\sigma}_1\cdot\boldsymbol{\sigma}_2\delta(\mathbf{r})\right\}. \end{aligned} \tag{9.1.72}$$

9.2 Foldy-Wouthuysen reduction

In this section, we will present the derivation of the Foldy-Wouthuysen reduction. The upper and lower components of a spinor is mixed by the Hamiltonian of the Dirac equation. The terms

in the Hamiltonian that mix the upper and lower components are called odd operators. The terms do not mix the upper and lower terms are called even operators. Foldy and Wouthuysen developed a method to decouple these components. Henceforth the Driac equation can be reduced to a Schrï¿œdinger equation with relativistic corrections. Starting from the Dirac equation of a positron

$$\begin{aligned} i\hbar\frac{\partial\psi}{\partial t} &= H\psi = \left\{\boldsymbol{\alpha}\cdot\left(\mathbf{p}-\frac{e}{c}\mathbf{A}\right)+\beta m+e\Phi\right\}\psi \\ &= (\beta m+\theta+\mathcal{E}) \end{aligned}$$

where the odd operator $\theta = \boldsymbol{\alpha}\cdot(\mathbf{p}-e\mathbf{A})$, and the even operator $\mathcal{E} = e\Phi$. Let us first introduce the transformation $\psi^{'} = e^{iS}\psi$. Under this transformation, the eigenvalue equation is rewritten into

$$i\frac{\partial\psi^{'}}{\partial t} = e^{iS}He^{-iS}\psi^{'} = H^{'}\psi^{'}. \tag{9.2.1}$$

On the other hand, we know that the Hamiltonian transforms as

$$e^{iS}He^{-iS} = H + i\left[S,H\right] + \frac{(i)^2}{2!}\left[S,[S,H]\right] + \cdots \tag{9.2.2}$$

The operator S can be chosen as $S = -i\beta\theta/2m$. Henceforth, the odd operator in the first order of the transformed Hamiltonian vanishes

$$H^{'} = H + i\left[S,H\right] = \beta m + \mathcal{E} \tag{9.2.3}$$

In this case , we can derive that the commutator

$$i\left[S,H\right] = -\theta + \frac{\beta}{2m}\left[\theta,\mathcal{E}\right] + \frac{1}{m}\beta\theta^2 \tag{9.2.4}$$

$$\frac{i^2}{2}\left[S,[S,H]\right] = -\frac{\beta\theta^2}{2m} - \frac{1}{8m^2}\left[\theta,[\theta,\mathcal{E}]\right] - \frac{1}{2m^2}\theta^3 \tag{9.2.5}$$

$$\frac{i^3}{3!}\left[S,[S,[S,H]]\right] = \frac{\theta^3}{6m^2} - \frac{1}{6m^3}\beta\theta^4 \tag{9.2.6}$$

$$\frac{i^4}{4!}\left[S,[S,[S,[S,H]]]\right] = \frac{1}{24m^3}\beta\theta^4 \tag{9.2.7}$$

Noticing that

$$-\dot{S} = \frac{i\beta\dot{\theta}}{2m} \tag{9.2.8}$$

and

$$-\frac{i}{2}\left[S,\dot{S}\right] = -\frac{i}{8m^2}\left[\theta,\dot{\theta}\right] \tag{9.2.9}$$

The transformed Hamiltonian can be written into

$$\begin{aligned} H^{'} &= \beta\left(m+\frac{\theta^2}{2m}-\frac{\theta^4}{8m^3}\right)+\mathcal{E}-\frac{1}{8m^2}\left[\theta,[\theta,\mathcal{E}]\right]-\frac{i}{8m^2}\left[\theta,\dot{\theta}\right] \\ &+\frac{\beta}{2m}\left[\theta,\mathcal{E}\right]-\frac{\theta^3}{3m^2}+\frac{i\beta\dot{\theta}}{2m} = \beta m+\mathcal{E}^{'}+\theta^{'} \end{aligned} \tag{9.2.10}$$

where the new odd operator

$$\theta^{'} = \frac{\beta}{2m}\left[\theta,\mathcal{E}\right]-\frac{\theta^3}{3m^2}+\frac{i\beta\dot{\theta}}{2m}, \tag{9.2.11}$$

and the new even operator

$$\mathcal{E}^{'} = \beta\left(\frac{\theta^2}{2m}-\frac{\theta^4}{8m^3}\right)+\mathcal{E}-\frac{1}{8m^2}\left[\theta,[\theta,\mathcal{E}]\right]-\frac{i}{8m^2}\left[\theta,\dot{\theta}\right]. \tag{9.2.12}$$

We can see that the odd operators are now in $1/m$ order. In order to further reduce them, we do the F-W transformation again by introducing a new transformation operator

$$S' = \frac{-i\beta}{2m}\theta' \tag{9.2.13}$$

Transforming the Hamiltonian with the new operator, we now have

$$\begin{aligned} H' &= \beta m + \mathcal{E}' + \frac{\beta}{2m}\left[\theta', \mathcal{E}'\right] + \frac{i\beta\dot{\theta'}}{2m} \\ &= \beta m + \mathcal{E}' + \theta'', \end{aligned} \tag{9.2.14}$$

where $\theta'' = \frac{\beta}{2m}\left[\theta', \mathcal{E}'\right] + \frac{i\beta\dot{\theta'}}{2m}$ is in $1/m^2$ order. Since we want to eliminate the odd operators in higher order, so let us do the F-W transformation once more. Now, we introduce $S'' = \frac{-i\beta\theta''}{2m}$ and henceforth obtain

$$\begin{aligned} H''' &= \beta m + \mathcal{E}' \\ &= \beta\left(m + \frac{\theta^2}{2m} - \frac{\theta^4}{8m^3}\right) + \mathcal{E} - \frac{1}{8m^2}\left[\theta, [\theta, \mathcal{E}]\right] - \frac{i}{8m^2}\left[\theta, \dot{\theta}\right] \end{aligned} \tag{9.2.15}$$

which is correct to $1/m^3$order. By substituting the specific expression of θ into above expression, we will have the specific form of the transformed Hamiltonian. Now, let us look at the quadratic term in θ first

$$\boldsymbol{\alpha} = \begin{pmatrix} 0 & \boldsymbol{\alpha} \\ \boldsymbol{\alpha} & 0 \end{pmatrix} \qquad \beta = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \tag{9.2.16}$$

$$\begin{aligned} \theta^2 = \left[\boldsymbol{\alpha}\cdot(\mathbf{p} - e\mathbf{A})\right]^2 &= \begin{pmatrix} 0 & \boldsymbol{\sigma}\cdot(\mathbf{p}-e\mathbf{A}) \\ \boldsymbol{\sigma}\cdot(\mathbf{p}-e\mathbf{A}) & 0 \end{pmatrix}\begin{pmatrix} 0 & \boldsymbol{\sigma}\cdot(\mathbf{p}-e\mathbf{A}) \\ \boldsymbol{\sigma}\cdot(\mathbf{p}-e\mathbf{A}) & 0 \end{pmatrix} \\ = \begin{pmatrix} \pi^2 - \frac{e\hbar}{c}\boldsymbol{\sigma}\cdot\mathbf{B} & 0 \\ 0 & \pi^2 - \frac{e\hbar}{c}\boldsymbol{\sigma}\cdot\mathbf{B} \end{pmatrix} &= \begin{pmatrix} \pi^2 - \frac{e}{c}\boldsymbol{\sigma}\cdot\mathbf{B} & 0 \\ 0 & \pi^2 - \frac{e}{c}\boldsymbol{\sigma}\cdot\mathbf{B} \end{pmatrix} \text{ in natural units} \end{aligned} \tag{9.2.17}$$

Henceforth

$$\begin{aligned} \theta^4 &= \begin{pmatrix} \left(\pi^2 - \frac{e}{c}\boldsymbol{\sigma}\cdot\mathbf{B}\right)^2 & 0 \\ 0 & \left(\pi^2 - \frac{e}{c}\boldsymbol{\sigma}\cdot\mathbf{B}\right)^2 \end{pmatrix} \\ &= \begin{pmatrix} \pi^4 - \frac{e}{c}\left[\pi^2, \boldsymbol{\sigma}\cdot\mathbf{B}\right]_+ + \frac{e^2}{c^2}\left(\boldsymbol{\sigma}\cdot\mathbf{B}\right)^2 & 0 \\ 0 & \pi^4 - \frac{e}{c}\left[\pi^2, \boldsymbol{\sigma}\cdot\mathbf{B}\right]_+ + \frac{e^2}{c^2}\left(\boldsymbol{\sigma}\cdot\mathbf{B}\right)^2 \end{pmatrix} \end{aligned} \tag{9.2.18}$$

$$\begin{aligned} H''' &= \beta m + \mathcal{E}' \\ &= \beta\left(m + \frac{\pi^2}{2m} - \frac{\pi^4}{8m^3c^2}\right) - \frac{e\boldsymbol{\sigma}\cdot\mathbf{B}}{2mc} + \frac{e\left[\pi^2, \boldsymbol{\sigma}\cdot\mathbf{B}\right]_+}{8m^3c^3} - \frac{e^2\left(\boldsymbol{\sigma}\cdot\mathbf{B}\right)^2}{8m^3c^4} \\ &+ \mathcal{E} - \frac{1}{8m^2}\left[\theta, [\theta, \mathcal{E}]\right] - \frac{i}{8m^2}\left[\theta, \dot{\theta}\right] \end{aligned} \tag{9.2.19}$$

Now, let us look at the last two terms in (9.2.19). On one hand, we have

$$\begin{aligned} \left[\theta, \mathcal{E}\right] &= \boldsymbol{\alpha}\cdot(\mathbf{p} - e\mathbf{A})\, e\Phi - e\Phi\boldsymbol{\alpha}\cdot(\mathbf{p} - e\mathbf{A}) \\ &= e\boldsymbol{\alpha}\cdot(\mathbf{p}\Phi) \end{aligned} \tag{9.2.20}$$

On the other hand, in the last term of (9.2.19) we have

$$i\dot{\theta} = i\frac{\partial}{\partial t}\boldsymbol{\alpha}\cdot(\mathbf{p}-e\mathbf{A}) \tag{9.2.21}$$

Combining these two terms, we obtain

$$\frac{1}{8m^2}\left([\theta,\mathcal{E}]+i\dot{\theta}\right) = \frac{e}{8m^2}\left(-i\boldsymbol{\alpha}\cdot\boldsymbol{\nabla}\Phi - i\boldsymbol{\alpha}\cdot\mathbf{A}\right) = \frac{ie}{8m^2}\boldsymbol{\alpha}\cdot\mathbf{E}$$

In the derivation of the last equivalence, we have used the relation $\mathbf{E} = -\boldsymbol{\nabla}\Phi - \mathbf{A}$. Thus, the contribution from the third and forth terms can be written as

$$\begin{aligned}
&\left[\theta, \frac{ie}{8m^2}\boldsymbol{\alpha}\cdot\mathbf{E}\right] = \frac{ie}{8m^2}\left[\boldsymbol{\alpha}\cdot\mathbf{p} - \frac{e}{c}\boldsymbol{\alpha}\cdot\mathbf{A}, \boldsymbol{\alpha}\cdot\mathbf{E}\right] \\
&= \frac{ie}{8m^2}\left[\boldsymbol{\alpha}\cdot\mathbf{p}, \boldsymbol{\alpha}\cdot\mathbf{E}\right] = \frac{e}{8m^2}\boldsymbol{\nabla}\cdot\mathbf{E} + \frac{ie}{8m^2}\boldsymbol{\sigma}\cdot(\boldsymbol{\nabla}\times\mathbf{E}) + \frac{e}{4m^2}\boldsymbol{\sigma}\cdot(\mathbf{E}\times\mathbf{p})
\end{aligned}$$

Henceforth, the FW transformed Hamiltonian (5.2.5) used in Chapter 5 can finally be obtained

$$\begin{aligned}
H''' &= \beta\left(m + \frac{\pi^2}{2m} - \frac{\pi^4}{8m^3c^2}\right) - \frac{e\boldsymbol{\sigma}\cdot\mathbf{B}}{2mc} + \frac{e\left[\pi^2, \boldsymbol{\sigma}\cdot\mathbf{B}\right]_+}{8m^3c^3} - \frac{e^2\left(\boldsymbol{\sigma}\cdot\mathbf{B}\right)^2}{8m^3c^4} + \mathcal{E} \\
&- \frac{e}{8m^2}\boldsymbol{\nabla}\cdot\mathbf{E} - \frac{ie}{8m^2}\boldsymbol{\sigma}\cdot(\boldsymbol{\nabla}\times\mathbf{E}) - \frac{e}{4m^2}\boldsymbol{\sigma}\cdot(\mathbf{E}\times\mathbf{p}) \\
&= H\left(\mathbf{p} - \frac{e}{c}\mathbf{A}\right) - \frac{e}{mc}\mathbf{s}\cdot\mathbf{B} + \frac{ie}{4m^2}\mathbf{s}\cdot(\mathbf{p}\times\mathbf{E} - 2\mathbf{E}\times\mathbf{p}) + \frac{e}{4m^3c^3}\left[p^2, \mathbf{s}\cdot\mathbf{B}\right]_+ \\
&- \frac{e^2\left(\mathbf{s}\cdot\mathbf{B}\right)^2}{2m^3c^4} - \frac{e^2}{4m^3c^4}\left(\left[\mathbf{p},\mathbf{A}\right]_+\mathbf{s}\cdot\mathbf{B} + H.c.\right)
\end{aligned}$$

where we have used the relations

$$\begin{aligned}
\left[\pi^2, \boldsymbol{\sigma}\cdot\mathbf{B}\right]_+ &= \left[p^2, \boldsymbol{\sigma}\cdot\mathbf{B}\right]_+ - \frac{e}{c}\left[\left[\mathbf{p},\mathbf{A}\right]_+, \boldsymbol{\sigma}\cdot\mathbf{B}\right]_+ \\
&+ \frac{e^2}{c^2}\left[\mathbf{A}^2, \boldsymbol{\sigma}\cdot\mathbf{B}\right]_+
\end{aligned}$$

and kept only the terms linear in the electromagnetic field. The Foldy-Wouthuysen reduction has been done.

Chapter 10

Appendix 4: Calculation techniques

Details of various techniques in loop calculation will be given in this Appendix. The fist section is about how to do the general integrals encountered in the calculation of triangular loop. In the second section, we include our FORM code used in the calculation of the photon-photon scattering. In section 3 we briefly discuss the derivation of the dispersion relations. In the last section, a detailed calculation of the form factor of the W boson loop is given.

10.1 The general integrals in triangular loop calculation

Convention 1

The factors in the denominator of the general integrand of a triangular loop can be combined through Feynman parametrization

$$\begin{aligned}
D_T &= \frac{1}{k^{2a_1}\left(k-q\right)^{2a_2}\left(k+p^{'}\right)^{2a_3}} \\
&= \frac{1}{B\left(a_2,a_3\right)k^{2a_1}}\int_0^1 dx\,\frac{x^{a_2-1}\left(1-x\right)^{a_3-1}}{\left[x\left(k+p^{'}\right)^2+\left(1-x\right)\left(k-q\right)^2\right]^{a_2+a_3}} \\
&= \frac{1}{B\left(a_2,a_3\right)}\int_0^1 dx\,\frac{x^{a_2-1}\left(1-x\right)^{a_3-1}}{k^{2a_1}\left[k^2+2xk\cdot p^{'}-2\left(1-x\right)k\cdot q\right]^{a_2+a_3}} \\
&= \frac{1}{B\left(a_2,a_3\right)B\left(a_2+a_3,a_1\right)}\int_0^1 dx\,x^{a_2-1}\left(1-x\right)^{a_3-1}\int_0^1 dy\,y^{a_2+a_3-1}\left(1-y\right)^{a_1-1} \\
&\times\frac{1}{\left[k^2+2k\cdot\left(xyp^{'}-y\left(1-x\right)q\right)\right]^{a_1+a_2+a_3}} \\
&= \frac{1}{B\left(a_2,a_3\right)B\left(a_2+a_3,a_1\right)}\int_0^1 dx\,x^{a_2-1}\left(1-x\right)^{a_3-1}\int_0^1 dy\,y^{a_2+a_3-1}\left(1-y\right)^{a_1-1} \\
&\times\frac{1}{\left[K^2-Q^2\right]^{a_1+a_2+a_3}},
\end{aligned} \tag{10.1.1}$$

where we have introduced

$$K = k+Q = k+xyp^{'}-y\left(1-x\right)q \tag{10.1.2}$$

$$Q^2 = -y^2x\left(1-x\right)M^2 \tag{10.1.3}$$

Now, let us define a new function

$$f(a_1,a_2,a_3,a_4) \equiv \frac{1}{B(a_2,a_3)\,B(a_2+a_3,a_1)} \int_0^1 dx\, x^{a_2-1}(1-x)^{a_3-1} \int_0^1 dy\, y^{a_2+a_3-1}(1-y)^{a_1-1} \times \frac{1}{[K^2-Q^2]^{a_4}}, \tag{10.1.4}$$

Then a reduction of this function can be done

$$\begin{aligned} K^2 f(a_1,a_2,a_3,a_4) &\to f(a_1,a_2,a_3,a_4-1) \\ &- y^2 x(1-x) M^2 f(a_1,a_2,a_3,a_4). \end{aligned} \tag{10.1.5}$$

A general form of the integral can be obtained

$$\begin{aligned} & x^a y^b f(a_1,a_2,a_3,a_4) \\ &= \frac{1}{B(a_2,a_3)\,B(a_2+a_3,a_1)} \int \frac{d^D K}{(2\pi)^D} \int_0^1 dx\, x^{a+a_2-1}(1-x)^{a_3-1} \\ &\times \int_0^1 dy\, y^{b+a_2+a_3-1}(1-y)^{a_1-1} \frac{1}{[K^2-Q^2]^{a_4}} \\ &= i(-1)^{a_4} \frac{1}{B(a_2,a_3)\,B(a_2+a_3,a_1)} \int \frac{d^D K}{(2\pi)^D} \int_0^1 dx\, x^{a+a_2-1}(1-x)^{a_3-1} \\ &\times \int_0^1 dy\, y^{b+a_2+a_3-1}(1-y)^{a_1-1} \frac{1}{[K^2+Q^2]^{a_4}} \\ &= \frac{i(-1)^{a_4}}{(4\pi)^{D/2}} \frac{1}{B(a_2,a_3)\,B(a_2+a_3,a_1)} \int_0^1 dx\, x^{a+a_2-1}(1-x)^{a_3-1} \\ &\times \int_0^1 dy\, y^{b+a_2+a_3-1}(1-y)^{a_1-1} \left(\frac{1}{Q^2}\right)^{a_4-D/2} \\ &= \frac{i(-1)^{-\frac{D}{2}}}{(4\pi)^{D/2}} \frac{1}{B(a_2,a_3)\,B(a_2+a_3,a_1)} \times \\ &\times \int_0^1 dx\, x^{a+a_2-1}(1-x)^{a_3-1} \int_0^1 dy\, y^{b+a_2+a_3-1}(1-y)^{a_1-1} \left(\frac{-1}{Q^2}\right)^{a_4-D/2} \end{aligned} \tag{10.1.6}$$

We did the last step because $Q^2 \leq 0$. Using the integral formula

$$\int_0^1 x^{\mu-1}(1-x)^{\nu-1}\,dx = B(\mu,\nu), \tag{10.1.7}$$

we may write the integral as

$$\begin{aligned} x^a y^b f(a_1,a_2,a_3,a_4) &= \frac{i(-1)^{\epsilon}}{(4\pi)^{D/2}} \left(\frac{1}{M^2}\right)^{a_4-2} \left(\frac{1}{M^2}\right)^{\epsilon} \frac{\Gamma(a_1+a_2+a_3)\,\Gamma(a_4-2+\epsilon)}{\Gamma(a_2)\,\Gamma(a_3)\,\Gamma(a_4)} \\ & B(a+a_2-a_4+2-\epsilon,\, a_3-a_4+2-\epsilon)\, B(b+a_2+a_3-2a_4+4-2\epsilon,\, a_1) \end{aligned} \tag{10.1.8}$$

Since the Beta function

$$B(\mu,\nu) = \frac{\Gamma(\mu)\,\Gamma(\nu)}{\Gamma(\mu+\nu)}, \tag{10.1.9}$$

the whole expression can be written as a combination of Gamma functions.

Convention 2

The denominator term can also be written into the following form

$$
\begin{aligned}
D_T &= \frac{1}{k^{2a_1}\left(k-q\right)^{2a_2}\left(k+p^{'}\right)^{2a_3}} \\
&= \frac{1}{B\left(a_2,a_3\right)k^{2a_1}}\int_0^1 dx\,\frac{x^{a_2-1}\left(1-x\right)^{a_3-1}}{\left[x\left(k+p^{'}\right)^2+\left(1-x\right)\left(k-q\right)^2\right]^{a_2+a_3}} \\
&= \frac{1}{B\left(a_2,a_3\right)}\int_0^1 dx\,\frac{x^{a_2-1}\left(1-x\right)^{a_3-1}}{k^{2a_1}\left[k^2+2xk\cdot p^{'}-2\left(1-x\right)k\cdot q\right]^{a_2+a_3}} \\
&= \frac{1}{B\left(a_2,a_3\right)B\left(a_2+a_3,a_1\right)}\int_0^1 dx\,x^{a_2-1}\left(1-x\right)^{a_3-1}\int_0^1 dy\,y^{a_2+a_3-1}\left(1-y\right)^{a_1-1} \\
&\times\frac{1}{\left[k^2+2k\cdot\left(xyp^{'}-y\left(1-x\right)q\right)\right]^{a_1+a_2+a_3}} \\
&= \frac{1}{B\left(a_2,a_3\right)B\left(a_2+a_3,a_1\right)}\int_0^1 dx\,x^{a_2-1}\left(1-x\right)^{a_3-1}\int_0^1 dy\,y^{a_2+a_3-1}\left(1-y\right)^{a_1-1} \\
&\times\frac{1}{\left[K^2-Q^2\right]^{a_1+a_2+a_3}},
\end{aligned}
\tag{10.1.10}
$$

where

$$
K = k+Q = k+xyp^{'}-y\left(1-x\right)q \tag{10.1.11}
$$

$$
Q^2 = -y^2x\left(1-x\right)M^2 \tag{10.1.12}
$$

Now define a new function

$$
\begin{aligned}
f\left(a_1,a_2,a_3,a_4\right) &\equiv \frac{1}{B\left(a_2,a_3\right)B\left(a_2+a_3,a_1\right)}\int_0^1 dx\,x^{a_2-1}\left(1-x\right)^{a_3-1}\int_0^1 dy\,y^{a_2+a_3-1}\left(1-y\right)^{a_1-1} \\
&\times\frac{1}{\left[K^2-Q^2\right]^{a_4}},
\end{aligned}
\tag{10.1.13}
$$

and do the reduction

$$
\begin{aligned}
&K^2 f\left(a_1,a_2,a_3,a_4\right)\rightarrow f\left(a_1,a_2,a_3,a_4-1\right) \\
&-y^2x\left(1-x\right)M^2 f\left(a_1,a_2,a_3,a_4\right).
\end{aligned}
\tag{10.1.14}
$$

A general form of the integral can be obtained

$$
\begin{aligned}
& x^a y^b f\left(a_1, a_2, a_3, a_4\right) \\
& = \frac{1}{B\left(a_2, a_3\right) B\left(a_2+a_3, a_1\right)} \int \frac{d^D K}{(2\pi)^D} \int_0^1 dx\, x^{a+a_2-1} (1-x)^{a_3-1} \\
& \times \int_0^1 dy\, y^{b+a_2+a_3-1} (1-y)^{a_1-1} \frac{1}{\left[K^2-Q^2\right]^{a_4}} \\
& = i(-1)^{a_4} \frac{1}{B\left(a_2, a_3\right) B\left(a_2+a_3, a_1\right)} \int \frac{d^D K}{(2\pi)^D} \int_0^1 dx\, x^{a+a_2-1} (1-x)^{a_3-1} \\
& \times \int_0^1 dy\, y^{b+a_2+a_3-1} (1-y)^{a_1-1} \frac{1}{\left[K^2+Q^2\right]^{a_4}} \\
& = \frac{i(-1)^{a_4}}{(4\pi)^{D/2}} \frac{1}{B\left(a_2, a_3\right) B\left(a_2+a_3, a_1\right)} \int_0^1 dx\, x^{a+a_2-1} (1-x)^{a_3-1} \\
& \times \int_0^1 dy\, y^{b+a_2+a_3-1} (1-y)^{a_1-1} \left(\frac{1}{Q^2}\right)^{a_4-D/2} \\
& = \frac{i(-1)^{-\frac{D}{2}}}{(4\pi)^{D/2}} \frac{1}{B\left(a_2, a_3\right) B\left(a_2+a_3, a_1\right)} \int_0^1 dx\, x^{a+a_2-1} (1-x)^{a_3-1} \\
& \times \int_0^1 dy\, y^{b+a_2+a_3-1} (1-y)^{a_1-1} \left(\frac{-1}{Q^2}\right)^{a_4-D/2}
\end{aligned}
\tag{10.1.15}
$$

The last step is done because $Q^2 \leq 0$. Using the integral formula

$$
\int_0^1 x^{\mu-1} (1-x)^{\nu-1} dx = B(\mu, \nu), \tag{10.1.16}
$$

the integral can be calculated

$$
\begin{aligned}
& x^a y^b f\left(a_1, a_2, a_3, a_4\right) = \frac{i(-1)^\epsilon}{(4\pi)^{D/2}} \left(\frac{1}{M^2}\right)^{a_4-2} \left(\frac{1}{M^2}\right)^\epsilon \frac{\Gamma\left(a_1+a_2+a_3\right) \Gamma\left(a_4-2+\epsilon\right)}{\Gamma\left(a_2\right) \Gamma\left(a_3\right) \Gamma\left(a_4\right)} \\
& B\left(a+a_2-a_4+2-\epsilon,\, a_3-a_4+2-\epsilon\right) B\left(b+a_2+a_3-2a_4+4-2\epsilon,\, a_1\right)
\end{aligned}
\tag{10.1.17}
$$

Using the Beta function

$$
B(\mu, \nu) = \frac{\Gamma(\mu) \Gamma(\nu)}{\Gamma(\mu+\nu)}, \tag{10.1.18}
$$

we can write the whole expression as a combination of Gamma functions.

10.2 FORM code for the photon-photon scattering

The FORM code for calculation of the scattering amplitude M_{++++} of the Photon-photon scattering process, with a particular circularly polarized radiation is given here as an example. The result corresponds to small values of the Mandelstam variables s, t, and u.

```
\#-
off statistics; \#procedure averac(P) if (count('P',1) != multipleof(2)
) discard; id 'P'.'P' = {[]p.p{[]}; id 'P' = {[]sqrt(x){[]}{*}'P'; ToTensor
dd,'P'; id n = acc(4-2{*}ep); id {[]p.p{[]} = 'P'.'P'; .sort {*} replace
powers of {[]sqrt(x){[]} by a combinatorial factor and powers of P.P
```

```
if ( count({[}sqrt(x){]},1) ) id {[}sqrt(x){]}s? = acc((1-ep){*}POINV(s/2+2,-1)){*}
'P'.'P'(s/2)/2(s/2); .sort \#endprocedure\par s {[}z exp{]}; \#procedure
exps(di,df,diff,order,small,smallorder) id 1/'di' = 1/('df') + 'diff';
id 'di' = 'df' {*} {[}z exp{]}; \#do n = 1,'order' id {[}z exp{]}
= 1 - 'df' {*} 'diff' {*} {[}z exp{]}; if(count('small') > 'smallorder')
discard; .sort \#enddo id {[}z exp{]} = 1; \#endprocedure V ki, k1,
k2, k3, k4; v q,e1,e2,e3,e4; s k,m,{[}p.p{]},{[}sqrt(x){]},ep,n,s,t,u,cosp,sinp;
Symbols{[}1/(q2-m2){]},{[}1/((q+k1)2-m2){]},{[}1/((q-k3)2-m2){]};
Symbols{[}1/((q-k4)2-m2){]},{[}1/((q+k1+k2)2-m2){]},{[}1/((q+k1+k3)2-m2){]};
cf acc,POINV; \#define EXPORD \textquotedbl{}6\textquotedbl{} \#define
SMALLORDER \textquotedbl{}5\textquotedbl{}\par g diag1 = g(1,e1){*}
(g(1,q) + m){*}{[}1/(q2-m2){]}{*} g(1,e4){*} (g(1,q) - g(1,k4) + m){*}{[}1/((q-k4)2-m2
g(1,e3){*} (g(1,q) + g(1,k1) + g(1,k2) + m){*}{[}1/((q+k1+k2)2-m2){]}{*}
g(1,e2){*} (g(1,q) + g(1,k1) + m){*}{[}1/((q+k1)2-m2){]};\par g diag2
= g(1,e1) {*} (g(1,q) + m) {*} {[}1/(q2-m2){]} {*} g(1,e3) {*} (g(1,q)
- g(1,k3) + m) {*} {[}1/((q-k3)2-m2){]}{*} g(1,e4) {*} (g(1,q) + g(1,k1)
+ g(1,k2) + m) {*} {[}1/((q+k1+k2)2-m2){]}{*} g(1,e2) {*} (g(1,q)
+ g(1,k1) + m){*}{[}1/((q+k1)2-m2){]};\par g diag3 = g(1,e1) {*}
(g(1,q) + m) {*} {[}1/(q2-m2){]}{*} g(1,e4) {*} (g(1,q) - g(1,k4)
+ m) {*} {[}1/((q-k4)2-m2){]}{*} g(1,e2) {*} (g(1,q) + g(1,k1) + g(1,k3)
+ m) {*} {[}1/((q+k1+k3)2-m2){]}{*} g(1,e3) {*} (g(1,q) + g(1,k1)
+ m){*}{[}1/((q+k1)2-m2){]};\par g total = diag1 + diag2 + diag3;
trace4,1;\par \#call exps({[}1/((q+k1)2-m2){]},{[}1/(q2-m2){]},(k1.k1
+ 2 {*} q.k1), 'EXPORD',k1\,1\,k2\,1\,k3\,1\,k4\,1,'SMALLORDER')\par \#call
exps({[}1/((q-k3)2-m2){]},{[}1/(q2-m2){]},(k3.k3 - 2 {*} q.k3), 'EXPORD',k1\,1\,k2\,1\
exps({[}1/((q-k4)2-m2){]},{[}1/(q2-m2){]},(k4.k4 - 2 {*} q.k4), 'EXPORD',k1\,1\,k2\,1\
exps({[}1/((q+k1+k2)2-m2){]},{[}1/(q2-m2){]}, (k1.k1 + k2.k2 + 2{*}q.k1
+ 2{*}q.k2 + 2{*}k1.k2), 'EXPORD',k1\,1\,k2\,1\,k3\,1\,k4\,1,'SMALLORDER')\par \#call
exps({[}1/((q+k1+k3)2-m2){]},{[}1/(q2-m2){]}, (k1.k1 + k3.k3 + 2{*}q.k1
+ 2{*}q.k3 + 2{*}k1.k3), 'EXPORD',k1\,1\,k2\,1\,k3\,1\,k4\,1,'SMALLORDER')\par \#call
averac(q) .sort \#call pochtablenew id acc(x?) = x; .sort s {[}q2-m2{]};
id q.q = 1/{[}1/(q2-m2){]} + m2; .sort {*} Wick rotation s {[}Q2+m2{]},f4,f3,f5,f6,f7,
id {[}1/(q2-m2){]} = -{[}1/(Q2+m2){]};\par if(count({[}1/(Q2+m2){]},1)>8)
discard;\par id {[}1/(Q2+m2){]}8 = 1/42/m12; id {[}1/(Q2+m2){]}7
= 1/30/m10; id {[}1/(Q2+m2){]}6 = 1/20/m8; id {[}1/(Q2+m2){]}5 = 1/12/m6;
id {[}1/(Q2+m2){]}4 = 1/6/m4; id {[}1/(Q2+m2){]}3 = 1/2/m2; id {[}1/(Q2+m2){]}2
= 1/ep; if (count(ep,1) > 0) discard; .sort\par repeat; id k1.k1
= 0; id k2.k2 = 0; id k3.k3 = 0; id k4.k4 = 0; id k1.k2 = s/2; id
k1.k3 = t/2; id k1.k4 = u/2; id k2.k3 = u/2; id k2.k4 = t/2; id k3.k4
= s/2; id k1.e1 = 0; id k1.e2 = 0; id k2.e1 = 0; id k2.e2 = 0; id
k3.e3 = 0; id k3.e4 = 0; id k4.e3 = 0; id k4.e4 = 0;\par {*} e1 up
id e1.k3 = -i{*}k{*}sinp; id e1.k4 = i{*}k{*}sinp; {*} e2 up id e2.k3
= i{*}k{*}sinp; id e2.k4 = -i{*}k{*}sinp; {*} e3 up id e3.k1 = i{*}k{*}sinp;
id e3.k2 = -i{*}k{*}sinp; {*} e4 up id e4.k1 = -i{*}k{*}sinp; id e4.k2
= i{*}k{*}sinp; {*}for UUUU id e1.e2 = -2; id e3.e4 = -2; id e1.e3
= 2{*}u/s; id e2.e4 = 2{*}u/s; id e1.e4 = 2{*}t/s; id e2.e3 = 2{*}t/s;\par id
e1.e1 = 0; id e2.e2 = 0; id e3.e3 = 0; id e4.e4 = 0; endrepeat;\par repeat;
id k2{*}sinp2 = u{*}t/s; endrepeat;\par repeat; id u = - s - t; endrepeat;\par print
+s total; .end
```

10.3 Dispersion relations

In this section, we briefly discuss the unsubtracted and once subtracted DR. A summary of how DR works in loop calculation can be found in [143].

Due to Cauchy's Residue Theorem, a function $F(q^2)$ that is analytic of q^2 can be viewed as an integral along a contour around q^2. So generally speaking, we have

$$\begin{aligned} F(q^2) &= \frac{1}{2\pi i}\oint_C dy \frac{F(y)}{y-q^2} \\ &= \frac{1}{2\pi i}\left(\int_{4m^2}^{\Lambda^2} dy \frac{F(y+i\epsilon)-F(y-i\epsilon)}{y-q^2} + \oint_{|y|=\Lambda^2} dy \frac{F(y)}{y-q^2}\right) \end{aligned}$$

By calculating the integral along the contour shown in the graph below, one obtains the full expression of the unsubtracted dispersion relation

$$F(q^2) = \frac{1}{\pi}\int_{4m^2}^{\Lambda^2} dy \frac{\mathrm{Im}F(y)}{y-q^2} + \frac{1}{2\pi i}\oint_{|y|=\Lambda^2} dy \frac{F(y)}{y-q^2}, \tag{10.3.1}$$

where the circular integral is along the outer circle in the following graph. On one hand, if the integrand within the second integral decreases fast enough as the variable approaching the infinity, we can omit the second term and obtain the usual unsubtracted DR

$$F(q^2) = \frac{1}{\pi}\int_{4m^2}^{\infty} dy \frac{\mathrm{Im}F(y)}{y-q^2} \tag{10.3.2}$$

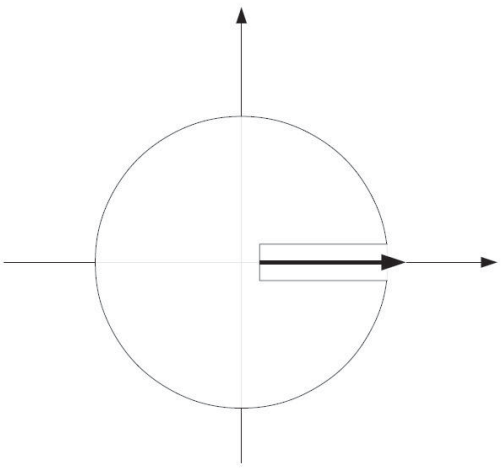


Figure 10.1: Contour of the integration

On the other hand, if the second term in (10.3.1) does not vanish, we need to subtract the value of F at some real point $q_0^2 < 4m^2$ and obtain

$$F(q^2) = F\left(q_0^2\right) + \frac{q^2-q_0^2}{\pi}\int_{4m^2}^{\Lambda^2} dy \frac{\mathrm{Im}F(y)}{(y-q_0^2)(y-q^2)} + \frac{q^2-q_0^2}{2\pi i}\oint_{|y|=\Lambda^2} dy \frac{F(y)}{(y-q_0^2)(y-q^2)}. \tag{10.3.3}$$

Particularly, by setting $q_0^2 = 0$ we obtain the once subtracted DR

$$F(q^2) = F(0) + \frac{q^2}{\pi}\int_{4m^2}^{\Lambda^2} dy \frac{\mathrm{Im}F(y)}{y(y-q^2)} + \frac{q^2}{2\pi i}\oint_{|y|=\Lambda^2} dy \frac{F(y)}{y(y-q^2)} \tag{10.3.4}$$

10.4 Form factor of the W boson loop

The amplitude corresponding to the triangular W boson loop 4.4 can be written as

$$\begin{aligned}
M_1 = & -ie^2 g M_w \int \frac{d^4P_2}{(2\pi)^4} \int \frac{d^4P_3}{(2\pi)^4} (2\pi)^4 \delta^4 (P_2 - P_3 + H) \\
& \times \left[g_\alpha^\beta - P_{3\alpha} P_3^\beta / M_W^2 \right] \\
& \times \left[g^{\rho\sigma} - P_1^\rho P_1^\sigma / M_W^2 \right] \\
& \times \left[g^{\alpha\gamma} - P_2^\alpha P_2^\gamma / M_W^2 \right] \\
& \times \left[(P_3 + K_2)_\rho g_{\beta\mu} + (P_1 - K_2)_\beta g_{\mu\rho} - (P_3 + P_1)_\mu g_{\rho\beta} \right] \\
& \times \frac{\left[(P_2 - K_1)_\sigma g_{\gamma\nu} + (P_1 + K_1)_\gamma g_{\nu\sigma} - (P_2 + P_1)_\nu g_{\sigma\gamma} \right]}{\left[P_1^2 - M_W^2 + i\epsilon \right] \left[P_2^2 - M_W^2 + i\epsilon \right] \left[P_3^2 - M_W^2 + i\epsilon \right]} \varepsilon_{1\nu} \varepsilon_{2\mu}
\end{aligned} \tag{10.4.1}$$

According to the Cutkosky rules, the imaginary part of this amplitude can be deduced

$$2\mathrm{Im} M_1 = e^2 g M_w \int \frac{d^3P_3}{(2\pi)^3} \frac{1}{4|E_2 E_3|} \mathrm{T}_1 \frac{1}{2P_3 \cdot K_2} 2\pi\delta (E_2 - E_3 + M) \tag{10.4.2}$$

where the symbol T_1 is defined by

$$\begin{aligned}
\mathrm{T}_1 = & \left[g_\alpha^\beta - P_{3\alpha} P_3^\beta / M_W^2 \right] \\
& \times \left[g^{\rho\sigma} - P_1^\rho P_1^\sigma / M_W^2 \right] \\
& \times \left[g^{\alpha\gamma} - P_2^\alpha P_2^\gamma / M_W^2 \right] \\
& \times \left[(P_3 + K_2)_\rho g_{\beta\mu} + (P_1 - K_2)_\beta g_{\mu\rho} - (P_3 + P_1)_\mu g_{\rho\beta} \right] \\
& \times \left[(P_2 - K_1)_\sigma g_{\gamma\nu} + (P_1 + K_1)_\gamma g_{\nu\sigma} - (P_2 + P_1)_\nu g_{\sigma\gamma} \right] \varepsilon_{1\nu} \varepsilon_{2\mu}.
\end{aligned} \tag{10.4.3}$$

We may write the amplitude of the bubble loop 4.5 as

$$\begin{aligned}
M_2 = & -ie^2 g M_w \int \frac{d^4P_2}{(2\pi)^4} \int \frac{d^4P_3}{(2\pi)^4} (2\pi)^4 \delta^4 (P_2 - P_3 + H) \\
& \times \left[g_\alpha^\beta - P_{3\alpha} P_3^\beta / M_W^2 \right] \\
& \times \left[g^{\alpha\gamma} - P_2^\alpha P_2^\gamma / M_W^2 \right] \\
& \times \frac{\left[2g_{\mu\nu} g_{\beta\gamma} - g_{\mu\beta} g_{\nu\gamma} - g_{\mu\gamma} g_{\nu\beta} \right]}{\left[P_2^2 - M_W^2 + i\epsilon \right] \left[P_3^2 - M_W^2 + i\epsilon \right]} \varepsilon_{1\mu} \varepsilon_{2\nu}
\end{aligned} \tag{10.4.4}$$

Using the Cutkosky rules, the imaginary part of this amplitude can be deduced

$$2\mathrm{Im} M_2 = e^2 g M_w \int \frac{d^3P_3}{(2\pi)^3} \frac{1}{4\,|E_2 E_3|} \mathrm{T}_2 2\pi\delta (E_2 - E_3 + M) \tag{10.4.5}$$

where the symbol T_2 is defined by

$$\begin{aligned}
\mathrm{T}_2 = & \left[g_\alpha^\beta - P_{3\alpha} P_3^\beta / M_W^2 \right] \\
& \times \left[g^{\alpha\gamma} - P_2^\alpha P_2^\gamma / M_W^2 \right] \\
& \times \left[2g_{\mu\nu} g_{\beta\gamma} - g_{\mu\beta} g_{\nu\gamma} - g_{\mu\gamma} g_{\nu\beta} \right] \varepsilon_{1\mu} \varepsilon_{2\nu}.
\end{aligned} \tag{10.4.6}$$

Following a similar procedure as the one used for the fermion loop discussed in section 4.2, we write down the imaginary part of the decay amplitude for a diagram with W loop as

$$\begin{aligned}\mathrm{Im}M\left(p^2\right) &= \frac{2A}{p^2}\left(1-\frac{2m^2}{p^2}\right)\ln\frac{1+\sqrt{1-\frac{4m^2}{p^2}}}{1-\sqrt{1-\frac{4m^2}{p^2}}}\left(K_1\cdot K_2 g^{\mu\nu}-K_2^{\mu}K_1^{\nu}\right)\varepsilon_{1\mu}\varepsilon_{2\nu}\\ &= \mathrm{Im}F\left(p^2\right)\left(K_1\cdot K_2 g^{\mu\nu}-K_2^{\mu}K_1^{\nu}\right)\varepsilon_{1\mu}\varepsilon_{2\nu}\end{aligned}$$

where the imaginary part of the form factor

$$\mathrm{Im}F\left(p^2\right) = 2A\frac{\left(1-\frac{2m^2}{p^2}\right)}{p^2}\ln\frac{1+\sqrt{1-\frac{4m^2}{p^2}}}{1-\sqrt{1-\frac{4m^2}{p^2}}}, \tag{10.4.7}$$

Let us calculate the whole form factor $F(q^2)$ with DR, using only its imaginary part $\mathrm{Im}F$. As we stated before, instead of using the unsubtracted dispersion relation used by authors of [71], we adopt the once subtracted dispersion relation (10.3.4)

$$F(q^2) = F\left(0\right)+\frac{q^2}{\pi}\int_{4m^2}^{\Lambda^2}dy\frac{\mathrm{Im}F\left(y\right)}{y\left(y-q^2\right)}+\frac{q^2}{2\pi i}\oint_{|y|=\Lambda^2}dy\frac{F\left(y\right)}{y\left(y-q^2\right)} \tag{10.4.8}$$

Since the second integral vanishes $\frac{q^2}{2\pi i}\oint_{|y|=\Lambda^2}dy\frac{F(y)}{y(y-q^2)}=0$, we can calculate $F(q^2)$ if we know the expression of $\mathrm{Im}F\left(y\right)$ and the value of $F\left(0\right)$. Let us focus on the first integral of (10.4.8). Substituting (10.4.7) into (10.4.8) we have

$$F(q^2) = F\left(0\right)+\frac{q^2}{\pi}\lim_{\Lambda^2\to\infty}\int_{4m^2}^{\Lambda^2}dy\frac{\mathrm{Im}F(y)}{y(y-q^2)} = F\left(0\right)+\frac{2Aq^2}{\pi}\int_{4m^2}^{\infty}\frac{\left(1-\frac{2m^2}{y}\right)}{y^2(y-q^2)}\ln\frac{1+\sqrt{1-\frac{4m^2}{y}}}{1-\sqrt{1-\frac{4m^2}{y}}}dy$$

Doing the integral, the whole amplitude appears to be a function of q^2

$$F\left(q^2\right) = F\left(0\right)+\frac{A}{2\pi m^2}\left(-\frac{5}{3}+\tau+\left(1-\frac{\tau}{2}\right)\tau\left(\frac{\pi^2}{2}-\frac{1}{2}\ln^2\frac{1+\sqrt{1-\tau}}{1-\sqrt{1-\tau}}+i\pi\ln\frac{1+\sqrt{1-\tau}}{1-\sqrt{1-\tau}}\right)\right),$$

In our system, the condition $q^2=H\equiv M^2$ is satisfied. Thus, the form factor can be further written into

$$\begin{aligned}F\left(H\right) &= F\left(0\right)+\frac{A}{2\pi m^2}\left(-\frac{5}{3}+\beta+\left(1-\frac{\tau}{2}\right)\beta\left(\frac{\pi^2}{2}-\frac{1}{2}\ln^2\frac{1+\sqrt{1-\beta}}{1-\sqrt{1-\beta}}+i\pi\ln\frac{1+\sqrt{1-\beta}}{1-\sqrt{1-\beta}}\right)\right)\\ &\times\left(K_1\cdot K_2 g^{\mu\nu}-K_2^{\mu}K_1^{\nu}\right)e_{1\mu}e_{2\nu} \qquad (10.4.9)\\ &= F\left(0\right)+\frac{e^2g}{16\pi^2m}\left[-5+3\beta+3\beta\left(2-\beta\right)f\left(\beta\right)\right] \qquad (10.4.10)\end{aligned}$$

where the function $f\left(\beta\right)=-\frac{1}{4}\left[\ln\frac{1+\sqrt{1-\beta}}{1-\sqrt{1-\beta}}-i\pi\right]^2$. Since the value of $F\left(q^2,m\right)$ at the limit of $q^2\to 0$ is known to be $\frac{e^2g}{16\pi^2m}\times 7$ [66], we may substitute this result into (10.4.10), and obtain the form factor

$$F\left(H\right) = \frac{e^2g}{16\pi^2m}\left[2+3\beta+3\beta\left(2-\beta\right)f\right] \tag{10.4.11}$$

Thus, the standard result of the Higgs decay through W loop has been restored. There is no need to put a subtraction by hand.

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