"I was born not knowing and have had only a little time to change that here and there."

Richard P. Feynman

University of Alberta

Hyperfine Splitting in Heavy Quarkonium: Matching the Perturbative and Lattice Approach.

by

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Abstract

We study the mass difference between the spin singlet and spin triplet states of heavy quarkonium. The quarkonium meson is a non-relativistic quark-antiquark bound-state of quantum chromodynamics (QCD). We set up a matching procedure between the perturbative analysis of the short-distance interactions, and the nonperturbative lattice analysis of the long-distance effects. To this end, we calculate the part of the corresponding Wilson coefficient in the continuum QCD region, to first order in the strong coupling constant. We then improve upon the first order result by all-order resummation of the large logarithms of the lattice spacing.

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Contents

List of Figures

List of Abbreviations

List of commonly used abbreviations

QED	Quantum Electrodynamics
QCD	Quantum Chromodynamics
QFT	Quantum Field Theory
EFT	Effective Field Theory
NR	Non Relativistic
QM	Quantum mechanics
LO	Leading Order
NLO	Next to Leading Order
LL	Leading Log
HFS	Hyperfine Splitting
UV	Ultra Violet
IR	Infra Red

Chapter 1

Introduction

The theoretical study of nonrelativistic heavy quark-antiquark bound states, or *quarkonium*, is among the earliest applications of perturbative quantum chromodynamics (QCD) [1]. Since the quarkonium Bohr radius is smaller than the confinement scale, where the strong interactions become nonperturbative, QCD perturbation theory can *a priori* be applied for the analysis of states with low quantum numbers. This makes heavy quark-antiquark systems an ideal laboratory for determining fundamental parameters of QCD, such as the strong coupling constant α_s and the heavy-quark masses m_Q. However, in some cases perturbative QCD fails to accurately describe the experimental data. A famous example is the so-called. "η_b-mass puzzle", which currently attracts a lot of attention from the experimental and theoretical physics communities. There is a significant discrepancy between the mass of the recently discovered η_b meson, i.e. the lowest energy spin singlet bound state of bottomonium ($b\bar{b}$), and the perturbative QCD predictions for hyperfine splitting (HFS). The resolution of this puzzle could shed new light on the dynamics of strong interactions, and may even result in the development of new methods for the quantitative analysis of heavy quarkonium systems based on first principles. This thesis is a part of the corresponding theoretical research program.

Let us introduce the problem in more detail. HFS is the energy difference between the spin triplet and spin singlet states, and is caused by the interaction of the quark spin with the magnetic field generated by the spin of the antiquark (and *vice versa*). For bottomonium $b\bar{b}$, the HFS is given by the mass difference between the spin-singlet η_b meson and the spin triplet $\Upsilon(1S)$ meson. The η_b meson has been observed by Babar and Belle collaboration in the radiative decays of the excited Υ states. Very high accuracy of Υ-spectroscopy allows for the determination of HFS with only a few MeV error. The results are given in [2] and [3], and are respectfully

$$E_{hfs}^{exp} = 71.4^{+2.3}_{-3.1}(stat) \pm 2.7(syst) MeV, \tag{1.1}$$

$$E_{hfs}^{exp} = 67.4^{+4.8}_{-4.6}(stat) \pm 2.0(syst) MeV. \tag{1.2}$$

The most accurate theoretical prediction for HFS includes the complete first-order corrections in α_s as well as the resummation of all-order next-to-leading logarithmic corrections of the form $\alpha_s^{n+1} \ln^n \alpha_s$. Numerically it gives [4]

$$E_{hfs}^{QCD} = 39 \pm 11(th)^{+9}_{-8}(\delta\alpha_s) MeV, \tag{1.3}$$

where th stands for the errors that come from higher-order perturbative corrections as well as any nonperturbative effects. The term $\delta\alpha_s$ represents the inherent uncertainty in $\alpha_s(\mathrm{M}_Z) = 0.118 \pm 0.003$. This result is about two standard deviations lower than the experimentally measured values.

One possible explanation of the above discrepancy is that perturbative QCD corrections get contributions from virtual particles with "soft" momentum $q \sim \alpha_s m_b$, which is of order of the inverse Bohr radius. The strong interaction is characterized by the corresponding running coupling at this scale, and the effective expansion parameter $\alpha_s(\alpha_s m_b) \sim 1/3$, is not very small there. It is possible therefore, that unknown higher-order perturbative corrections may be

significant. One way to get control over these higher order corrections is to use numerical lattice simulations of QCD which are not based on the expansion in α_s. However, existing lattice results do not properly take into account the contributions of the "hard" virtual momentum, on the order of heavy quark mass $q \sim m_b$, which is cut off by the lattice spacing $a >> 1/m_b$. Fortunately the hard region contribution can be more reliably calculated within perturbation theory since the corresponding expansion parameter there is almost two times smaller than in the soft region, $\alpha_s(m_b) \sim 1/5$.

The perturbative calculation of the hard region contribution has to be made consistent with the lattice simulations. This is accomplished through systematic separation of hard and soft effects. The procedure that is used is called "matching", wherein the hard contribution is given by the difference between the full QCD perturbative result, and the same order perturbative contribution from the momentum region $q < 1/a$ which is already contained in the lattice simulations. The latter can be evaluated in the standard lattice perturbation theory.

This work is the first step towards the evaluation of the hard region contribution and presents the calculation of the first order QCD corrections to the HFS in the scheme relevant for the matching procedure.

The plan of the thesis is as follows. In the next chapter we introduce the basic theory of Hydrogen-like nonrelativistic bound states in QED and QCD, where we derive the leading order approximation for HFS within the framework of non-relativistic quantum mechanics (NRQM). In Chapter 3, we set up a natural framework within relativistic quantum theory, and show that we not only recover the leading order HFS result exactly, but systematically incorporate all other effects to the effective Hamiltonian, order by order. In Chapter 4.1 we discuss the general approach to the evaluation of the perturbative corrections from higher order diagrammatic contributions [5]. In Chapter 4.2, we describe the calculation of the first order QCD corrections to the HFS with the gluon

mass as the infrared regulator relevant for the matching procedure. Finally in sections 4.3 and 4.4, we describe the renormalization group improved result for the corresponding Wilson coefficient, which resums the large logarithms of the the form $\alpha_s^n \ln^n(m_b a)$ to all orders of perturbation theory. Therein we will incorporate this piece into our calculations and present our final result for this thesis. The technical details of the calculations are given in the Appendices.

Chapter 2

Basic Properties of Hydrogen-like Systems

2.1 Hamiltonian and Quantized Energy Levels of Hydrogen

The procedure for solving the hydrogen atom can readily be applied to other systems like positronium and quarkonium. We will present a very brief overview of the subject matter and then proceed to apply it, with some minor alterations, to quarkonium in the next chapter. The unfamiliar reader may consult any introductory textbook on quantum mechanics for a more thorough treatment. [6]

The Hamiltonian for the hydrogen atom is of the standard form with a Coulomb potential

$$\hat{H} = -\frac{1}{2m_e}\nabla^2 + V_C(r) \quad : \quad V_C(r) \equiv -\frac{\alpha}{r}, \tag{2.1}$$

where $\nabla^2 = \frac{1}{r}\frac{\partial}{\partial r^2}r - \frac{1}{r^2}\hat{L}^2$, and m_e is the mass of the electron. In quantum mechanics, the structure of the orbital angular momentum is represented by the lie algebra SO(3). $\hat{L}^2$ is the operator in Hilbert space that, acting on an

eigenstate, gives the square of the total angular-momentum. Formally, $\hat{L}^2$ is the quadratic Casimir operator of SO(3) for that Hilbert space

$$\hat{L}^2 = (\hat{\mathbf{r}} \times \hat{\boldsymbol{p}}) \cdot (\hat{\mathbf{r}} \times \hat{\boldsymbol{p}}) = -(\mathbf{r} \times \boldsymbol{\nabla}) \cdot (\mathbf{r} \times \boldsymbol{\nabla}). \tag{2.2}$$

From the form of the Hamiltonian, we have made explicit that the angular momentum operator $\hat{\mathbf{L}}^2$ commutes, and can be simultaneously diagonalized. Put another way, the Hamiltonian is spherically symmetric and thus admits as its angular solutions the eigenfunctions of the angular-momentum operator. These solutions are the famous spherical harmonics $Y_m^l(\theta, \phi)$,

$$\hat{\mathbf{L}}^2 \, Y_m^l(\theta, \phi) = l(l+1) \, Y_m^l(\theta, \phi) \;\; \Rightarrow \;\; \Psi(r, \theta, \phi) \equiv \phi(r) \, Y_m^l(\theta, \phi). \tag{2.3}$$

Doing the separation of variables in (2.3) and solving, gives the hydrogen wave-functions

$$\Psi_{nlm}(r, \theta, \phi) = \sqrt{\left(\frac{2}{na_0}\right)^3 \frac{(n-l-1)!}{2n\big[(n+1)!\big]^3}} \left(\frac{2r}{na_0}\right)^l \left[L_{n-l-1}^{2l+1}\left(\frac{2r}{na_0}\right)\right] Y_m^l(\theta, \phi) \, \mathbf{e}^{-\frac{r}{na_0}}, \tag{2.4}$$

where L_{q-p}^p are the associated Laguerre polynomials. The most probable separation of the electron from the atom's center in its ground state is known as the Bohr radius, $a_0 = \frac{1}{\alpha \, m_e} \approx 53 \, pm$.

The energy levels of Hydrogen in terms of the quantum number n are

$$E_n = -\frac{\alpha^2}{2n^2} \, m_e \approx -\frac{13.6eV}{n^2}. \tag{2.5}$$

2.2 Overview of Spin Related Perturbations

2.2.1 Spin-Orbit Coupling

Any particle with spin angular-momentum acts like a magnetic dipole. If an electron (spin-$\frac{1}{2}$) is immersed in a magnetic field, it will feel a torque acting on it which tends to align its spin orientation($\hat{\boldsymbol{\mu}}$), parallel to the field. This torque can be written as $\vec{\tau} = \vec{\mu} \times \vec{B} = \vec{r} \times \vec{F}$, which has the solution $\vec{F} = \nabla_r \big(\vec{\mu} \cdot \vec{B}(r)\big)$. Integrating the expression provides us with an energy $H = -\vec{\mu} \cdot \vec{B}$.

Next, we know from classical electrodynamics that any charge moving relative to some other charged system sets up a magnetic field. In Hydrogen we tend to think about the electron as circling around the stationary nucleus. From the (non-inertial) frame of the electron, the proton appears to be circling around *it*, and thus sets up a magnetic field proportional to its apparent orbital angular-momentum[1].

The magnetic moment of the electron is proportional to its spin, thus producing the familiar term $\vec{\sigma} \cdot \vec{\mathbf{B}}$ from the Pauli-equation (a non-relativistic limit for the Dirac-equation in the presence of an electromagnetic field A^μ). This effect can and has been calculated as a perturbation to the non-relativistic Hamiltonian, the so-called spin-orbit interaction(S.O.)

$$\delta H_{s.o.} = \frac{\mu_0}{8\pi} \frac{e^2}{m_e^2 r^3} \, \mathbf{S} \cdot \mathbf{L} \ . \tag{2.6}$$

As can be seen from the above perturbation, the Hamiltonian no longer commutes individually with $\vec{L}$ and $\vec{S}$, therefore the operator eigenvalues are no longer separately conserved. Luckily L^2, S^2 and $\vec{J} = \vec{L} + \vec{S}$ *do* commute, allowing us to characterize the states of the now non-degenerate energy levels ($E_n \rightarrow E_{n,j}$), by means of their total angular momentum value and its cus-

[1] $B = \frac{\mu_0 I}{2r} = \frac{\mu_0 e v}{4\pi r^2}$. Then $L = m|\vec{r} \times \vec{v}| \sim mvr \quad \Rightarrow \quad B \sim \frac{\mu_0}{4\pi} \frac{e}{mr^3} L$.

tomarily chosen z-component J_z. This non-commutation will also necessarily appear in the Dirac Hamiltonian as well (see sec. 3.2).

2.2.2 Spin-Spin Coupling

The previous section was intended to act as a segue into the interaction of interest in this paper. Thus we will first discuss the physical concepts involved in spin-spin coupling through the viewpoint of non-relativistic quantum mechanics. We will then proceed to discuss the interaction in its natural place as an aspect of quantum field theory (QFT), in the next chapter.

The main idea, starting with hydrogen, is that the nucleus itself constitutes a magnetic dipole and so sets up another magnetic field[1] that is unrelated to the relative motion of the two particles,

$$\mathbf{B} = \frac{\mu_0}{4\pi r^3}\big[(3\boldsymbol{\mu}_p \cdot \hat{r})\hat{r} - \boldsymbol{\mu}_p\big] + \frac{2\mu_0}{3}\boldsymbol{\mu}_p\delta^3(\mathbf{r}). \tag{2.7}$$

This gives yet another magnetic field for $\boldsymbol{\mu}_e$ to couple to. The proton's gyromagnetic ratio is not simple like the electron's though, since it is a composite structure:

$$\boldsymbol{\mu}_p = \frac{g_p\, e}{2m_p}\boldsymbol{S}_p \ , \quad \boldsymbol{\mu}_e = -\frac{e}{m_e}\boldsymbol{S}_e. \tag{2.8}$$

It should be noted for later however that, for our purposes in quarkonium, both particles are elementary fermions and their gyromagnetic ratios differ only in overall sign. The perturbation then takes the form

$$\delta H_{s.s.} = \frac{g_p\, e^2}{8\pi m_e m_p c^2}\left[\frac{3(\mathbf{S_e}\cdot\hat{r})(\mathbf{S_p}\cdot\hat{r})}{r^3} - \frac{\boldsymbol{S_e}\cdot\boldsymbol{S_p}}{r^3}\right] + \frac{g_p\, e^2}{3m_e m_p c^2}\boldsymbol{S_e}\cdot\boldsymbol{S_p}\delta^3(\mathbf{r}). \tag{2.9}$$

This term gives rise to the so-called Hyperfine Splitting. In the case of hydrogen, the factor of $1/m_p$ is responsible for the HFS contribution being much less

[1] see for instance: Griffiths. *Introduction to Electrodynamics*. Pearson, 3rd edition for a derivation.

than the fine structure terms like spin-orbit coupling, owing to the proton mass being $m_p \sim 1800\, m_e$. This will not be the case in particles like quarkonium or positronium, and as such becomes a much more important effect to study. In any state where the angular momentum is zero ($l = 0$), the expectation value of the first term vanishes[2]. We are thus left with the term proportional to the delta function

$$E_{s.s.} = \langle\psi_{100}|\delta H_{s.s.}|\psi_{100}\rangle = \frac{g_p e^2}{3m_e m_p c^2}\langle \boldsymbol{S_e}\cdot\boldsymbol{S_p}\rangle|\psi_{100}(0)|^2. \tag{2.10}$$

Now at this point, we must realize that the addition of this term to the Hamiltonian makes it so that individual spins are no longer conserved. We are thus left with the problem of finding some spin related quantum numbers that *are* conserved, that can also be used to characterize the system. We can start by writing it out in terms of total angular momentum

$$\boldsymbol{S} = \boldsymbol{S_e} + \boldsymbol{S_p} \quad \Rightarrow \quad \boldsymbol{S_e}\cdot\boldsymbol{S_p} = \frac{1}{2}(\boldsymbol{S}^2 - \boldsymbol{S_e}^2 - \boldsymbol{S_p}^2). \tag{2.11}$$

Both particles are spin-1/2, thus $\boldsymbol{S}^2_{1/2} = s(s+1) = 3/4$. This still leaves the problem of finding out what the quantity S^2 is, to which we now turn.

2.3 Addition of Angular Momentum and Result for HFS

In classical physics we are capable of just adding any number of vectors together by introducing a coordinate system and projecting the vectors onto each axis, or a set of basis vectors, and then adding all the components separately. In the case of quantum mechanics, we can know *at most* the total magnitude of the angular momentum vector, and the value of one of its chosen components (typically the

[2] $\int(\boldsymbol{a}\cdot\hat{\boldsymbol{r}})(\boldsymbol{b}\cdot\hat{\boldsymbol{r}})\; dcos\theta\, d\phi = \frac{4\pi}{3}\boldsymbol{a}\cdot\boldsymbol{b}$, which when multiplied by 3 in (2.9), cancels the factor being subtracted.

z-component). The other components (say L_x and L_y) do not commute with L_z and thus we can't simultaneously diagonalize these components. This leaves us with an obvious problem: How *do* we add angular momentum vectors in quantum mechanics?

In the ground state of quarkonium, the total orbital angular momentum is zero and we are interested to know how the total spin configuration of the quark-antiquark system looks. For (anti)quarks of spin-1/2, the z-component can have only two states ($m_s = \pm 1/2$). We typically call them spin-up and spin-down, and represent them $|\uparrow\rangle$ and $|\downarrow\rangle$ respectively.

The complication arises when we wish to know not only the combined z-spin of both particles, but also the combined vector magnitude, dependant on the relative orientation of two *indeterminate* vectors. One can, similarly to the case of orbital angular momentum introduce rasing and lowering operators $S^+ = S^+_{(1)} + S^+_{(2)}$ and $S^- = S^-_{(1)} + S^-_{(2)}$ then act on all possible states :

$$|\uparrow\rangle|\uparrow\rangle, |\uparrow\rangle|\downarrow\rangle, \ ... \quad . \tag{2.12}$$

The result is that the total value of spin ranges from $-|s_1 + s_2| \rightarrow |s_1 + s_2|$ in integer steps. Specifically, we get three states with total angular momentum $|s = 1; m_s = 0, \pm 1\rangle$, called the triplet. We also get one state with total angular-momentum $|s = 0; m_s = 0\rangle$ called the singlet.

This can be written symbolically as a set of orthonormal kets:

$$\left\{ \begin{array}{l} |1,1\rangle = |\uparrow\uparrow\rangle \\ |1,0\rangle = \frac{1}{2}\big(|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle \big) \\ |1,-1\rangle = |\downarrow\downarrow\rangle \end{array} \right\} \ s = 1 \ , \tag{2.13}$$

$$\left\{ \ |0,0\rangle = \tfrac{1}{2}\big(\ |\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle \ \big) \ \right\} \ \ s=0 \ . \tag{2.14}$$

We now see how ground-state hydrogen-like atoms have their degeneracy removed. The hyperfine splitting occurs because the spin-spin perturbation takes on a different value depending on the overall spin configuration. That is to say that it depends on whether the bound system is in the triplet or singlet configuration. With this understood, we have that

$$\boldsymbol{S_e} \cdot \boldsymbol{S_p} = \frac{1}{2}(\boldsymbol{S}^2 - \boldsymbol{S_e}^2 - \boldsymbol{S_p}^2) = \frac{1}{2}\boldsymbol{S}^2 - \frac{3}{4}, \tag{2.15}$$

where $\boldsymbol{S}^2 = 0$ for the singlet, and $\boldsymbol{S}^2 = 2$ for the triplet. Therefore we get $\boldsymbol{S_e} \cdot \boldsymbol{S_p} = -3/4$ for the singlet, and $\boldsymbol{S_e} \cdot \boldsymbol{S_p} = 1/4$ for the triplet. Then if we take the difference between the two states in hydrogen, we get the famous 21cm line

$$E_{hfs} = \ \frac{4\, g_p}{3\, m_p\, m_e^2\, c^2\, a^4} = 5.88 \times 10^{-6}\text{eV}. \tag{2.16}$$

Chapter 3

Hyperfine Splitting in Quarkonium at Leading Order

It was mentioned in the last section that spin-spin coupling has its natural place in QFT, and this statement is in fact true of spin in general. The Schrodinger equation makes no mention of spin at all, being a differential operator on a scalar function. Historically, it had to be added to the theory in an ad-hoc manner. The Dirac equation is a relativistic wave equation for spin-$\frac{1}{2}$ particles, and marks the natural start for a discussion leading to the relativistic scattering expressions of interest. Of course, a thorough treatment of the subject matter is far too lengthy to fully expound in this paper. We will present it in a way that will put the necessary ideas on the table, and will assume a basic familiarity with the Dirac equation and the Feynman diagram representation of perturbation theory (whether from use in the S-matrix or in correlation functions). This will give the reader the relevant formalism required to understand the work presented throughout. We will start by introducing the largest difference between QED and QCD: colour charge.

3.1 Colour SU(3)

In studying the interactions of hadrons (baryons and mesons), experimentalists observed the Δ^{++} baryon, which has spin $S = 3/2$ and we now know consists of three up-quarks [7]. Quarks, like all fermions, carry spin 1/2. Therfore all three quarks in Δ^{++} must have their spins aligned, a state which is symmetric to particle exchange. The baryon's functional ground state is also described by a symmetric wave-function. But we know that, in order to satisfy the Pauli exclusion principle, the *overall* wave function must be anti-symmetric. It was suggested therefore that quarks carry another quantum number called colour, that was yet to be observed.

This hypothesis necessitated individual quarks to carry one of three different colour charges. The established notation is to label these by the three primary colours: Red, Green, and Blue (R,G,B) as well as their anti-colour equivalents $(\bar{R}, \bar{G}, \bar{B})$. The problem *was*, that in order to have an overall charge of $+2e$, the individual quarks must carry a charge of $+2/3e$, of which there was no evidence. It did however give an excellent phenomenological explanation of many hadrons being discovered at the time. Different sets of quark-antiquark pairs formed different mesons, and combinations of three quarks (antiquarks) formed the baryons (antibaryons), provided that they were always antisymmetric under colour SU(3) transformations. The absence of fractionally charged fermions is a problem to be explained by colour confinement in the section that follows renormalization group theory.

The details of how colour impacts the evaluation of QCD Green's functions and S-matrix elements is given in Appendix C. In this chapter we will study the tree level scattering amplitude. We compare figure 3.1 with the rule given in figure C.1, and see that we get a colour factor

$$g_s^2 \, T^a_{ij} T^a_{kl} \to C_F. \tag{3.1}$$

The equivalence follows for the singlet[1](i.e. colour invariant) configuration only. $C_F \equiv \frac{N_c^2-1}{2N_c}$, is the quadratic Casimir operator of the fundamental representation, where N_c is the dimension of the SU(N_c) colour algebra. If the quark-antiquark bound state were in the colour octet configuration, we would get $-1/2N_c = -1/6$. One consequence of colour conservation is the implication that the quark-antiquark colour singlet configuration can *exchange* a single virtual-gluon in the colour octet, but they cannot annihilate into one. If they could annihilate, there would in fact be an additional contribution to the tree level HFS potential[2].

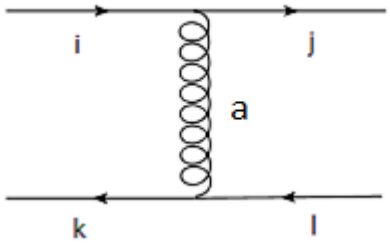

Figure 3.1: Colour Factor at Tree level

3.2 The Dirac Equation and Spin

The Schrodinger equation is non-relativistic by nature. This is immediately obvious from the fact that it is first order in time derivatives but second order in spatial derivatives. Any relativistically covariant quantum theory must treat time and space on equal footing, and reduce to the Schrodinger equation in the appropriate non-relativistic limit. The Dirac equation in momentum space, where the γ^μ are the familiar gamma matrices, and m is a fermion mass, is

[1]The details of projecting out the singlet state are presented in section A.1.2

[2]There can of course be two gluon (and higher *even* gluon number)annihilation diagrams.

$$\big(\not{p} - m\big)\psi = 0 \quad : \quad \not{p} \equiv p_\mu \gamma^\mu. \tag{3.2}$$

If we multiply this by γ^0, and go to position space, we get

$$i\frac{\partial \psi}{\partial t} = \hat{H}_D \psi \quad : \quad \hat{H}_D \equiv \gamma^0\big(i\boldsymbol{\gamma}\cdot\boldsymbol{\nabla} + m\big) = -i\boldsymbol{\alpha}\cdot\boldsymbol{\nabla} + \beta m. \tag{3.3}$$

This defines the free Dirac (or relativistic) Hamiltonian $\hat{H}_D$. The Dirac equation is a matrix equation and as such $\psi(x) = \psi^\alpha(x)$, must have four components. We know from NR quantum mechanics that fermions like the electron and the quark have only two spin degrees of freedom. The reason for a four-spinor is that relativistic quantum theory introduces antiparticles into the works. Two spin degrees of freedom are for the fermion, and two are for the antifermion. This is all consistent then, only if two degrees vanish in the fermion's rest frame.

In the classical regime where $E \gg |\vec{p}|$, so that $p \approx \langle m, \vec{0}\rangle$,

$$(\not{p} \mp m)\,\psi \;\; \Rightarrow \;\; m(\gamma^0 \mp 1)\,\psi = 0, \tag{3.4}$$

where the $-(+)$ corresponds to the fermion(anti-fermion). We choose a basis in which γ^0 is diagonal

$$\gamma^0 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \tag{3.5}$$

Then we plug this into (3.4) and get

$$\begin{pmatrix} 0 & 0 \\ 0 & \mathbb{1} \end{pmatrix}\begin{pmatrix} \phi \\ \chi \end{pmatrix} = 0 \quad \& \quad \begin{pmatrix} \mathbb{1} & 0 \\ 0 & 0 \end{pmatrix}\begin{pmatrix} \phi \\ \chi \end{pmatrix} = 0. \tag{3.6}$$

Two of the degrees of freedom vanish as predicted, and $\gamma^0 \pm 1$ acts like a projection operator that picks out the NR physics[2]. In the rest frame of the

particle, these will represent the two spin state solutions for the fermion and antifermion respectively, and we can write them in a familiar notation as

$$u_1, u_2 = \begin{pmatrix} \uparrow \\ 0 \end{pmatrix}, \begin{pmatrix} \downarrow \\ 0 \end{pmatrix} \quad v_1, v_2 = \begin{pmatrix} 0 \\ \downarrow \end{pmatrix}, \begin{pmatrix} 0 \\ \uparrow \end{pmatrix}. \tag{3.7}$$

For an unspecified four-momentum, the free Dirac equation has four linearly independent plane-wave solutions:

$$u_r(p)\, e^{-ip\cdot x}, \;\; v_s(p)\, e^{+ip\cdot x} \quad r, s = 1, 2. \tag{3.8}$$

We note that because the new four spinor representation is formed from a direct sum of two spinor representations, we get an irreducible representation of the spin operator by diagonally stacking the two dimensional representations of the spin operator (ubiquitously chosen as the pauli matrices). We then obtain the spin operator for Dirac theory: $\mathbf{\Sigma} = \boldsymbol{\sigma} \otimes \mathbb{1}_{2\times 2}$.

Let us now give precise definitions (representations) to the spinors and matrices we will be using in this paper. The presentation from here on will follow closely the section on the Breit equation given in Landau and Lifshitz [8].

A useful set of spinors for our purposes are:

$$u_s = \begin{bmatrix} \sqrt{2m}\big(1 - \frac{p^2}{8m^2c^2}\big) w_s \\ \big(\frac{\boldsymbol{\sigma}\cdot\boldsymbol{p}}{2mc}\big) w_s \end{bmatrix}, \quad v_t = \begin{bmatrix} \sqrt{2m}\big(\frac{\boldsymbol{\sigma}\cdot\boldsymbol{p}}{2mc}\big) w_t \\ \big(1 - \frac{p^2}{8m^2c^2}\big) w_t \end{bmatrix}, \tag{3.9}$$

where the w's are 2-spinors. These reduce to the rest frame spinors in the limit that momentum goes to zero, with the exception that a relativistic spinor normalization is used ($\bar{u}u = 2m$) and ($\bar{v}v = -2m$). We will also use the

[2]Indeed $(\gamma^0 - 1)^2 = -2(\gamma^0 - 1)$

following representation for the gamma matrices

$$\gamma^0 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \quad \boldsymbol{\gamma} = \begin{pmatrix} 0 & \boldsymbol{\sigma} \\ -\boldsymbol{\sigma} & 0 \end{pmatrix} \quad . \tag{3.10}$$

Now we recall from NRQM that the ad-hoc addition of spin-spin coupling fouled up commutation relations between the $\hat{H}$ and $\boldsymbol{S}$, and we can now see this explicitly. For arbitrary momentum, the spinors are energy-eigenstates, but are *not* spin-eigenstates. That is, u_r and v_s are 4-spinors that satisfy $(\not{p} - m)u_r = 0$ and $(\not{p} + m)v_s = 0$, but unless $\boldsymbol{p} = p\hat{z}$, $\Sigma_z u_r(p) \neq m_z u_r(p)$. This is because $[H, \boldsymbol{\Sigma}] \neq 0$. This should be clear since the Dirac equation introduces spin-orbit coupling explicitly in the basic spinor and gamma matrix definitions. As one would expect, the *total* angular momentum *is* conserved $[H, \boldsymbol{J}] = [H, \boldsymbol{\Sigma} + \boldsymbol{L}] = 0$. As a result of all this, it is sometimes convenient to use a particle co-moving quantization, where the spin (anti)parallel to the particle motion is chosen for diagonolization. This requires introducing a spin helicity operator $\boldsymbol{\Sigma} \cdot \hat{p}$, which ensures commutation with the Hamiltonian so that the helicity states are also simultaneously energy-eigenstates. While theoretically possible, helicity eigen-states are rarely used since the typical plane-wave spinors have definite physical energy and momentum, which is all that is usually known in experiment anyways.

3.3 Born Series of Non-Relativistic Scattering

This section will set up the last connection that we will need from NRQM, to compare with the relativistic results. Consider the time independent Schrodinger equation with a potential:

$$-\frac{1}{2m}\nabla^2\psi + V(\boldsymbol{r})\psi = E\psi \quad \Rightarrow \quad \big(\nabla^2 + \epsilon\big)\psi = \tilde{V}\psi, \tag{3.11}$$

where $\epsilon \equiv 2mE$ and $\tilde{V} \equiv 2mV$. We start by fourier transforming the equation with $V \to 0$, and replaced by a delta function source. This gives us the Green's function[1]

$$G(\boldsymbol{r}) = -\int \frac{d^3k}{(2\pi)^3} \frac{e^{i\boldsymbol{k}\cdot\boldsymbol{r}}}{k^2 - \epsilon^2} = -\frac{1}{4\pi} \frac{e^{\pm i\boldsymbol{k}\cdot\boldsymbol{r}}}{|\boldsymbol{r}|}. \tag{3.12}$$

The sign in the exponent depends on your choice of contour in the integral, which physically represents either incoming or outgoing scattering waves. From this we then know the full solution ($V \neq 0$) to this problem in terms of ψ_0 (the solution to the free equation) is just

$$\psi(\boldsymbol{r}) = \psi_0(\boldsymbol{r}) + \int d^3r' \, G(\boldsymbol{r} - \boldsymbol{r'})\tilde{V}(\boldsymbol{r'})\psi(\boldsymbol{r'}). \tag{3.13}$$

We can solve this by iteration, and it will be convenient to pull out some expansion parameter λ from the potential ($\tilde{V} \to \lambda\tilde{V}$). λ will be some (hopefully) small parameter, like a coupling constant, that is fixed by the problem

$$\psi = \psi_0 + \lambda \int G\tilde{V}\psi_0 + \lambda^2 \int\int (G\tilde{V})(G\tilde{V}\psi_0) + \mathcal{O}(\lambda^3). \tag{3.14}$$

The above series is known as a Born-series expansion, and is a very useful equation for NR quantum scattering. In a typical experiment we are interested in the probability amplitude that a particle that is initially far away from a stationary source (size r'), will scatter off the source and be in the state ψ. Let us now make the approximation of a plane wave solution ($r >> r'$) $\psi(r) \approx e^{i\boldsymbol{k}\cdot\boldsymbol{r_0}} + \frac{e^{i\boldsymbol{k}\cdot\boldsymbol{r}}}{r} f(\theta, \phi)$. Comparing this with our above expression (3.14), we can conclude:

$$f(\theta, \phi) = -\frac{\lambda}{4\pi} \int d^3r' e^{-i\boldsymbol{k}\cdot\boldsymbol{r'}} \tilde{V}\psi = -\frac{\lambda}{4\pi} \langle\psi_0|\tilde{V}|\psi\rangle. \tag{3.15}$$

[1] A thorough treatment of the method of Green's functions can be found in most textbooks on partial differential equations, e.g. Myint-U and Debnath's Linear PDE's

We see that the differential cross section for the process $|\psi_0\rangle \to |\psi\rangle$ will be proportional to the expectation value of the potential squared. We can thus, up to first order, identify the classical potential that would give rise to the relativistic scattering amplitude we are going to obtain below.

3.4 Scattering Interaction

The First order scattering amplitude for a quark and antiquark, with masses m_1 and m_2 respectively, can be written as:

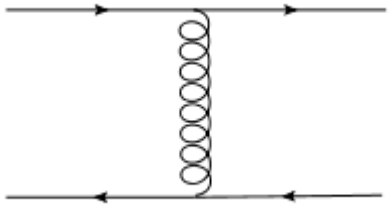

Figure 3.2: Tree Level Scattering

$$M_{scatt.} = C_F \, [\, \bar{u}_r(p_1')\gamma^\mu u_s(p_1) \,] \, D_{\mu\nu}(k^2) \, [\, \bar{v}_t(p_2)\gamma^\nu v_w(p_2') \,], \tag{3.16}$$

where $D_{\mu\nu}(k^2)$ is the gauge-propagator of the QFT. The gauge-propagator represents the propagation of photons with coupling "e" for QED, or gluons with coupling "g_s" for QCD. We will follow the custom for working in the NR limit, and use the coulomb gauge

$$D_{00} = \frac{g_s^2}{\boldsymbol{k}^2}, \quad D_{ij} = -\frac{g_s^2}{\boldsymbol{k}^2 - \omega_k^2/c^2}\Big(\delta_{ij} - \frac{k_i k_j}{\boldsymbol{k^2}}\Big). \tag{3.17}$$

Note that in all of this we are explicitly keeping factors of the speed of light ($c \neq 1$), and the reason for this is twofold. First and foremost, an expansion in $1/c$ will organize the terms, allowing us to see at which stage of the game new physics, not present in the Schrodinger equation, will appear. If we neglect all terms of order $1/c$ and higher(set $c \to \infty$), then the spinors reduce to those of NRQM and we simply get part of the D_{00} term

$$M_{scatt.} = (2m_1)(-2m_2)(w_r^\dagger w_s)\, V(k)\, (w_t^\dagger w_w) \quad : \quad V(k) = -\frac{C_F\, g_s^2}{k^2}, \tag{3.18}$$

which is just the Fourier transform of the coulomb potential generalized to

QCD, where $\boldsymbol{k} = \boldsymbol{p_1'} - \boldsymbol{p_1} = \boldsymbol{p_2} - \boldsymbol{p_2'}$[1]. Just as we suspected for the complete NR-limit, the coulomb interaction is the only term that appears in the potential.

The second reason for arranging things in terms of $1/c$ is related to the fact that radiation appears as an interactive effect in order $1/c^3$. To have any chance at describing our system via higher order contributions to the NR-Hamiltonian, we must keep only terms less than $\mathcal{O}(1/c^3)$. To be consistent with the order of the relativistic expansion, we must also include the next term in the expansion of the relativistic kinetic energy in our Hamiltonian. It is also important to ensure that we subtract off the rest mass from the energy, as the Hamiltonian operator is concerned with kinematical degrees of freedom only,

$$\hat{H}^0\,\psi = (E - m_1c^2 - m_2c^2)\psi \quad : \quad H^0 = \frac{\hat{\boldsymbol{p}}_{\boldsymbol{1}}{}^2}{2m_1} + \frac{\hat{\boldsymbol{p}}_{\boldsymbol{2}}{}^2}{2m_2} - \frac{\hat{\boldsymbol{p}}_{\boldsymbol{1}}{}^4}{8m_1^3c^2} - \frac{\hat{\boldsymbol{p}}_{\boldsymbol{1}}{}^4}{8m_1^3c^2}. \tag{3.19}$$

Let us now write out our scattering amplitude to the required accuracy. We concisely write just 1,2 and $1', 2'$ to represent both momentum and spin indices. Therefore we have for example that $u_1 \equiv u_r(p_1)$.

$$\begin{aligned} M_{scatt.} &= [\,\bar{u}_{1'}\gamma^0 u_1\,][\,\bar{v}_2\gamma^0 v_{2'}\,]D_{00} + [\,\bar{u}_{1'}\gamma^i u_1\,][\,\bar{v}_2\gamma^j v_{2'}\,]D_{ij} \\ &= [\,u^\dagger_{1'}\,u_1\,][\,v_2^\dagger\,v_{2'}\,]D_{00} + [\,\bar{u}_{1'}\gamma^i u_1\,][\,\bar{v}_2\gamma^j v_{2'}\,]D_{ij} \end{aligned} \tag{3.20}$$

We insert the expressions for the spinors and gamma matrices [eqn.'s (3.9),(3.10)], and with some massaging get

$$u^\dagger_{1'}\,u_1 = (2m_1)\,w^*_{1'}\Big[1 - \frac{k^2}{8m_1c^2} + \frac{i\boldsymbol{\sigma_1}\cdot\boldsymbol{k}\times\boldsymbol{p_1}}{4m_1c^2}\Big]w_1, \tag{3.21}$$

$$\bar{u}_{1'}\,\boldsymbol{\gamma}\,u_1 = (1/c)w^*_{1'}\big[i\boldsymbol{\sigma_1}\times\boldsymbol{k} + 2\boldsymbol{p_1} + \boldsymbol{k}\big]w_1. \tag{3.22}$$

[1]From now on in this section, we will deal only with 3-momentum, and so we can let k^2 mean $\boldsymbol{k}^2$ without possibility of confusion.

The terms arising from the anti-particle spinors are very similar($1 \to 2$ and $\mathbf{k} \to -\mathbf{k}$), thus carrying out the multiplication and simplifying gives the leading result.

$$M_{scatt.} = (2m_1)(-2m_2) w_{1'}^{\dagger} w_{2'}^{\dagger} V(\boldsymbol{p_1}, \boldsymbol{p_2}, \boldsymbol{k}) w_1 w_{2'}, \tag{3.23}$$

where the potential in momentum-space, with higher order terms in $1/c$ included, becomes:

$$\begin{aligned} V(\boldsymbol{p_1}, \boldsymbol{p_2}, \boldsymbol{k}) = -C_F g_s^2 \Bigg[& \frac{1}{k^2} - \frac{1}{8m_1c^2} - \frac{1}{8m_2c^2} + \frac{(\boldsymbol{k}\cdot\boldsymbol{p_1})(\boldsymbol{k}\cdot\boldsymbol{p_2})}{m_1 m_2 k^4} - \frac{(\boldsymbol{p_1}\cdot\boldsymbol{p_2})}{m_1 m_2 k^2} \\ & + \frac{i\boldsymbol{\sigma_1}\cdot\boldsymbol{k}\times\boldsymbol{p_1}}{4m_1^2c^2k^2} - \frac{i\boldsymbol{\sigma_2}\cdot\boldsymbol{k}\times\boldsymbol{p_2}}{4m_2^2c^2k^2} - \frac{i\boldsymbol{\sigma_1}\cdot\boldsymbol{k}\times\boldsymbol{p_2}}{2m_1m_2c^2k^2} \\ & + \frac{i\boldsymbol{\sigma_2}\cdot\boldsymbol{k}\times\boldsymbol{p_1}}{2m_1m_2c^2k^2} + \frac{(\boldsymbol{\sigma_1}\cdot\boldsymbol{k})(\boldsymbol{\sigma_2}\cdot\boldsymbol{k})}{4m_1m_2c^2k^2} - \frac{(\boldsymbol{\sigma_1}\cdot\boldsymbol{\sigma_2})}{4m_1m_2c^2} \Bigg]. \end{aligned} \tag{3.24}$$

We are of course only interested in the spin-spin interaction and thus can limit our attention to only those terms containing *both* spin operators ($\boldsymbol{\sigma}_1, \boldsymbol{\sigma}_2$), which upon examination is only the last two terms. Performing a Fourier transform on these two terms we get [8]

$$V_{spin} = -\frac{C_F g_s^2}{(16\pi)\, m_1 m_2 c^2} \left[\frac{\boldsymbol{\sigma}_1\cdot\boldsymbol{\sigma}_2}{r^3} - 3\frac{(\boldsymbol{\sigma_1}\cdot\boldsymbol{r})(\boldsymbol{\sigma_2}\cdot\boldsymbol{r})}{r^5} - \frac{2}{3}\boldsymbol{\sigma_1}\cdot\boldsymbol{\sigma_2}\delta(\boldsymbol{r}) \right]. \tag{3.25}$$

Putting in $\boldsymbol{S}_i = \frac{1}{2}\boldsymbol{\sigma}_i$, we obtain precisely the potential that we got from the perturbation theory of NRQM[1]. It is quite satisfying to see that not only have we generated the interaction of interest in the relativistic formalism, but we have systematically included all other contributions to the potential in this order.

There are several small modifications that must be made to get the equiv-

[1] if $e \to g_s$, and we include C_F, of course.

alent of hydrogen's HFS formula for quarkonium. First of all, both masses involved in the Hamiltonian are equal. As such, there can be no approximation of a stationary nucleus. We thus treat this two body problem by reducing it to a one particle problem of a reduced mass m_r, circling around the system's center of mass

$$m_r \equiv \frac{m_Q\, m_{\bar{Q}}}{m_Q + m_{\bar{Q}}} = \frac{m_Q}{2}. \tag{3.26}$$

We can use this in our already derived expression, which we repeat here for convenience

$$E_{s.s.} \;=\; \frac{2\alpha_s}{3\,(m_Q/2)^2\,c^2}\langle \boldsymbol{S_1}\cdot\boldsymbol{S_2}\rangle |\psi_{100}(0)|^2. \tag{3.27}$$

We also know that $|\psi_{100}(0)|^2 = {}^1\!/\!_{\pi\, a_0^3}$, but the analog of the Bohr radius in heavy quarkonium is $\rightarrow {}^1\!/\!_{a_0} \approx \frac{1}{2} C_F\, m_Q\, c\, \alpha_s$. Thus, the leading order result is :

$$E_{s.s.} \;=\; \frac{C_F^4 \alpha_s^4 m_Q}{3} \left\{ \begin{array}{l} -1/4 \;\; (singlet) \\ +3/4 \;\; (triplet) \end{array} \right\} \;\Rightarrow\; E_{hfs} = \frac{C_F^4 \alpha_s^4 m_Q}{3}. \tag{3.28}$$

Chapter 4

Radiative Corrections To Hyperfine splitting

4.1 Hyperfine splitting at NLO

The dynamics of nonrelativistic heavy quark-antiquark bound states is characterized by three different scales:

1. The hard scale of the heavy quark mass m_Q

2. The soft scale of the characteristic bound state three-dimensional momentum $m_Q\alpha_s$.

3. The ultrasoft scale of the bound state energy $m_Q\alpha_s^2$

In order to effectively deal with all the dynamical scales in a systematic way, the method of nonrelativistic effective theories has been developed [9]. The method creates a natural connection between the quantum field theory and its appropriate Schrödinger equation from NRQM. The hard and soft gluonic fields do not show up as real particles in quarkonium, and therefore they can be "integrated out", which induces the effective interactions of the heavy quarks. These interactions are included into the effective Hamiltonian, which

describes the evolution of the nonrelativistic quark-antiquark pair in (potential) NRQCD. These corrections are in terms of both the strong coupling constant, and heavy quark velocity, to the leading Coulomb approximation. The effective Hamiltonian valid to $\mathrm{N^3LO}$, can be written [5]

$$H = (2\pi)^3\delta(\mathbf{q})\left(\frac{\mathbf{p}^2}{m_Q} - \frac{\mathbf{p}^4}{4m_Q^3}\right) + C_c(\alpha_s)V_C(\mathbf{q}) + C_{1/m}(\alpha_s)V_{1/m}(\mathbf{q}) + \frac{\pi C_F\alpha_s}{m_Q^2} \times\left[C_\delta(\alpha_s) + C_p(\alpha_s)\frac{\mathbf{p}^2+\mathbf{p}'^2}{2\mathbf{q}^2} + C_{S^2}(\alpha_s)\mathbf{S}^2 + C_\lambda(\alpha_s)\Lambda(\mathbf{p},\mathbf{q}) + C_c(\alpha_s)T(\mathbf{q})\right]. \tag{4.1}$$

In the above expression, $\mathbf{p}$ and $\mathbf{p}'$ are the spatial momenta of the incoming and outgoing quarks respectively. The operators, in order of appearance are:

$$V_C(\mathbf{q}) = -\frac{4\pi C_F\alpha_s}{\mathbf{q}^2}, \quad V_{1/m}(\mathbf{q}) = \frac{2\pi^2 C_F\alpha_s}{m_Q\mathbf{q}}, \quad \mathbf{S} = \frac{\boldsymbol{\sigma}_1+\boldsymbol{\sigma}_2}{2},$$
$$\Lambda(\mathbf{p},\mathbf{q}) = i\,\frac{\boldsymbol{S}\cdot(\boldsymbol{p}\times\boldsymbol{q})}{\mathbf{q}^2}, \quad T(\mathbf{q}) = \boldsymbol{\sigma}_1\cdot\boldsymbol{\sigma}_2 - 3\frac{(\mathbf{q}\cdot\boldsymbol{\sigma}_1)(\mathbf{q}\cdot\boldsymbol{\sigma}_2)}{\mathbf{q^2}}\,. \tag{4.2}$$

In the above, $\boldsymbol{\sigma}_1$ and $\boldsymbol{\sigma}_2$ are the spin operators of the quark and antiquark respectively. The coefficients $C_i(\alpha_s)$, known as Wilson coefficients, incorporate the effects of the hard and soft modes that have been integrated out. They can be written as a power series in $\alpha_s(\mu)$, which is renormalized in the $\overline{MS}$ scheme. The series coefficients are functions of the mass, momentum transfer, and renormalization scale. We are interested in the coefficient of the spin-flip operator responsible for the HFS

$$C_{S^2} = \left[\frac{4}{3} + \frac{\alpha_s}{\pi}C_{S^2}^{(1)} + ...\right]. \tag{4.3}$$

The first order correction to the HFS is determined by the one-loop corrections to the Coulomb and spin-flip potential. It can be found within the standard time-independent perturbation theory for the energy levels. The result

reads [10, 11]:

$$E_{hfs}^{NLO} = \frac{C_F^4 \alpha_s^4 m_b}{3}\Bigg[1 + \frac{\alpha_s}{\pi}\Bigg(\frac{7C_A}{4}\ln\big(C_F\alpha_s\big) - \frac{C_F}{2} + \frac{2\pi^2 - 26}{9}n_l T_F + \frac{3 - 3\ln(2)}{2}T_F + \frac{122 - 11\pi^2}{18}C_A\Bigg)\Bigg]$$

$$\approx E_{hfs}^{LO}\big[1 + \alpha_s\big(1.67\ \ln(\alpha_s) + 0.61\big)\big], \tag{4.4}$$

where $C_A = N_c$ is the quadratic Casimir operator of the adjoint representation of colour SU(N_c), "n_l" is the number of massless quark flavours, and $T_F = \frac{1}{2}$ is the index of the representation. Logarithmically enhanced terms like in (4.4) are typical for the bound state perturbative series, and can be resummed to all orders by using the NR renormalization group. The details of the NLL are also presented in [11]. The numerical value is

$$E_{hfs}^{QCD} = 39 \pm 11(th)^{+9}_{-8}(\delta\alpha_s)MeV, \tag{4.5}$$

where "th" stands for the errors that come from higher-order perturbative corrections as well as any nonperturbative effects. The term $\delta\alpha_s$ represents the uncertainty in the experimental value $\alpha_s(\mathrm{M}_Z) = 0.118 \pm 0.003$.

4.2 Matching the perturbative and lattice analysis of HFS

We can now address the main calculations that are carried out in this paper. The fully perturbative NLO result quoted in (4.5), is approximately two standard deviations away from the experimentally measured values quoted in the introduction. It is very reasonable to assume that perturbation theory will give the correct result for the hard modes of the Wilson coefficient. Upon compari-

son with the experimental findings however, it must be that due to asymptotic freedom, the running coupling is too large in the softer region of the calculation for perturbation theory to obtain a convergent result.

The main idea of our approach is to use perturbation theory only for the hard contribution to the Wilson coefficient C_{S^2}, which is suppressed by powers of the reasonably small expansion parameter $\alpha_s(m_Q)$. The soft contribution is calculated in lattice NRQCD by numerically evaluating the functional integral defined on a finite lattice of spacing $a >> 1/m_Q$. This accounts for the strong interaction effects beyond the region of validity for perturbation theory. The calculation of the hard and soft regions are therefore performed in completely different ways. The results from both regions have to be *matched*, to correctly reproduce the first-order QCD result. To get the hard contribution to the Wilson coefficient consistent with the lattice result, the first-order soft corrections to the spin flip potential computed in perturbative lattice NRQCD, are subtracted from the first-order continuum QCD result for the Wilson coefficient C_{S^2}.

The perturbative calculations in the lattice NRQCD, however, are technically extremely complicated and require the use of specific unphysical infrared regulators, such as a gluon mass λ, where the momentum transfer is set to zero. For consistency therefore, we have to adopt the same regulator in the QCD calculation of C_{S^2}. This calculation is the main goal of this thesis.

The dimensionful parameters that remain are the hard scale $\nu_h \sim m_Q$, the soft cutoff $\nu_s \sim 1/a$, where a is the finite lattice spacing that is used in the calculation, and of course the ad hoc gluon mass regulator λ. It is generally true that the condition $\Lambda_{QCD} \ll 1/a \ll m_Q$ is satisfied to ensure that the calculations are both valid non-relativistically ($\ll m_Q$), and capable of being treated in perturbation theory ($\gg \Lambda_{QCD}$) for the matching region. In order to ensure that we can obtain the Wilson coefficient from the region of virtual momentum of interest $1/a < q < m_Q$, we apply a subsidiary condition on the

NRQCD lattice cutoff that says $1/a_0 < 1/a$. In other words, we arrange it so that the lattice cutoff is larger than the reciprocal of the Bohr radius a_0.

We obtain the first-order QCD correction to the Wilson coefficient by adding together the contributions of the planar box, the crossed box, and the vertex diagram. The details of calculation are presented in the appendices, and both the planar-box and crossed box have been checked by applying expansion by regions. The results for individual contributions read

$$C_{S^2}^{(1)}|_{p.b.} = C_F\Big[-2+2\ln\big(\lambda/m_Q\big)\Big], \tag{4.6}$$

$$C_{S^2}^{(1)}|_{c.b.} = -2\big(C_F-\tfrac{1}{2}C_A\big)\ln\big(\lambda/m_Q\big)\,, \tag{4.7}$$

$$C_{S^2}^{(1)}|_{F_2} = \frac{4}{3}\Big[C_F+C_A\Big(1+\ln\big(\lambda/m_Q\big)\Big)\Big]. \tag{4.8}$$

We must also include the effects of two, two-gluon annihilation box-diagrams, which contribute [12], $C_{S^2}^{(1)}|_{ann.} = 2T_f\big(1-\ln(2)\big)$. Summing all these coefficients together we get

$$C_{S^2}^{(1)} = -\frac{2}{3}C_F+\frac{1}{3}C_A\Big(4+7\ln\big(\lambda/m\big)\Big)+2T_f\big(1-\ln(2)\big). \tag{4.9}$$

The lattice NRQCD result for the first order soft contribution to the Wilson coefficient can be parameterized as follows

$$C_{S^2}^{(1s)} = A_{lat}^s+\frac{7}{3}C_A\,\ln\big(a\lambda\big), \tag{4.10}$$

where A_{lat}^s is a numerical constant. Since the singular infrared behaviour must be the same in both NRQCD and full QCD, the coefficient of the logarithm of λ is the same as in full QCD. We leave A_{lat}^s as a free parameter in this paper.

The hard contribution to the Wilson coefficient consistent with the lattice evaluation of the soft contribution is given by the difference $C_{S^2}^{(1)} - C_{S^2}^{(1s)}$ and reads

$$C_{S^2}^{(1h)} = \Big[-\frac{2}{3} C_F + \frac{4}{3} C_A + 2T_f\big(1 - \ln(2)\big) - A_{lat}^s \Big] - \frac{7}{3} C_A \ln\big(m_Q a\big). \quad (4.11)$$

The above is the main result for this thesis, and it represents a Wilson coefficient whose lower cutoff is now precisely the UV cutoff of the lattice simulations.

4.3 Renormalization Group

QCD is a non-abelian gauge theory. As was mentioned briefly in the previous section, these gauge theories are known to exhibit a property called asymptotic freedom. In order to appreciate the consequences of this, we must make a brief detour into some of the more formal complications that arise in higher order perturbative calculations in QFT.

Quantum Field theories are renowned for requiring regularization of infinities, either through a Pauli-Villars momentum cutoff, dimensional regularization, or some other means once loop diagrams are calculated. Systematic methods for absorbing these infinities into field-strength renormalizations, mass renormalizations etc. are then chosen based on the specific type of problem at hand. The basic idea can actually be very simply explained [13].

Let's say that we have calculated some loop diagram and the diagram formally diverges as we go to the infinite momentum range. This would at first be very unsettling and indeed was during the infancy of QFT. After some thought though, we begin to realise that this makes a lot of sense. This is telling us that our theory isn't valid beyond a certain range of energies. It may well be that the theory we are currently using is just an effective limit of some larger quantum field theory. In any case, let's say that we get an amplitude that looks

something like

$$M = -i\lambda + i\lambda^2 B\, ln\big(\Lambda/\mu\big), \tag{4.12}$$

where Λ is a Pauli-Villars regulator which indicates the relative momentum at which our knowledge of the theory breaks down. μ is some kinematical invariant for the diagram whose specifics are unimportant, and λ is a coupling that is used in the original perturbative expansion(for example the fine structure "constant" in QED). We are then faced with the question of what value to give to Λ and λ in this equation. In other words, we have to give some defining properties to these quantities. One useful way is to define the renormalized coupling λ_R, as the amplitude at some particular value $\mu = \mu_0$,

$$-i\lambda_R(\mu_0) = -i\lambda + i\lambda^2 B\, ln\big(\Lambda/\mu_0\big). \tag{4.13}$$

This relation is easily inverted to give $-i\lambda = -i\lambda_R - i\lambda_R^2 B\, ln\big(\Lambda/\mu_0\big)$. Then putting this into our amplitude (4.12), we now have an equation that expresses the amplitude for the process of interest at any energy we want based on measurable quantities only

$$M = -i\lambda_R(\mu_0) \;+\; i\lambda_R^2(\mu_0)\, ln(\mu_0/\mu\big). \tag{4.14}$$

Now the issue arises when we wish to measure the process at some momentum μ that is vastly different from our experimental reference point μ_0. The renormalized coupling constant may still be small, but we can't claim the same thing for the logarithm. This is where the introduction of the renormalization group becomes invaluable. We want to choose the coupling constant that is appropriate for physics at the scale μ so that the logarithm becomes small again. In other words we want it in terms of a new coupling

$$M = -i\lambda_R(\mu_0') \;+\; i\lambda_R^2(\mu_0')\, ln(\mu_0'/\mu\big). \tag{4.15}$$

We thus want to derive an equation that can tell us how the value of the coupling constant changes as we move to a new scale. A proper treatment of the subject as a whole requires an explanation of Wilsonian renormalization theory and the Callan-Symanzik equation, which is beyond the scope of this paper. For our simple example however it will be sufficient to use a little differential calculus, and some careful interpretation of the result. Take $\mu_0' \sim \mu_0 + \delta\mu_0$ for the moment and subtract eq. (4.14) from (4.15) to get:

$$\mu_0 \frac{d\lambda_R}{d\mu_0} = B\lambda_R^2. \tag{4.16}$$

This is known as a renormalization group equation and its solution, which must be supplemented with initial conditions, tells us how the renormalized coupling λ_R changes with the scale of the problem. This completely general analysis allows us to imagine several interesting situations of note. First, we can imagine that $\lambda \to e^2$, the electric charge, and that we have chanced upon the renormalization group equation. The equation tells us how the so-called "running charge" changes as we go to different energy scales. It so happens that there is a renormalization group equation for every parameter of a QFT. The electric charge, for instance, increases as we go to higher interaction energy. The strong coupling constant (g_s) decreases however, and this is precisely the asymptotic freedom we spoke of earlier.

This stage of the game is precisely where the analysis of Wilson becomes a vital part of the discourse. It studies how the importance of parameters in the Lagrangian change with scale. To re-iterate, this is precisely the case with QED being an "effective" field theory for the true electroweak theory. As we go to higher energies in QED we find that new operators, previously "irrelevant", must be included to accurately describe the phenomena. This new tool, simply put, allows us to study physics on new scales by resumming the large logs into these running parameters, and furthermore allows us to study physics at a

particular scale of interest without needing any information of the full theory by "integrating out" these degrees of freedom.

We now have the language necessary to discuss aymptotic freedom. All non-abelian gauge theories are known to exhibit this property; they are weakly interacting at high energies where their running coupling decreases, and are strongly interacting at low energies. The reason that free quarks with colour charge are never observed is then explained by the asymptotic freedom that constrains all observable particles to be colourless(i.e. colour invariant), and it means that at a certain point, usually denoted Λ_{QCD}, the perturbation theory with which QFT calculations are usually carried out, will break down.

The (solved) QCD renormalization group equation reads [7]

$$\alpha_s(q) = \frac{\alpha_s(\mu_0)}{1 + \left[\beta_0 \alpha_s(\mu_0)/2\pi\right] \ln(q/\mu_0)}, \tag{4.17}$$

where μ_0 is the reference scale that provided the initial condition. $\beta_0 \equiv \frac{11}{3} C_A - \frac{4}{3} T_F \, n_l$, is the one loop coefficient of the QCD β-function. At this point it is traditional to introduce the point Λ_{QCD} by means of the equation

$$\left(\frac{\beta_0}{2\pi}\right) \alpha_s(\mu_0) \, \ln\left(\mu_0/\Lambda_{QCD}\right) = 1, \tag{4.18}$$

which has been measured through various experiments to be approximately $\Lambda_{QCD} \sim 200 MeV$, and allows the rewriting of (4.17) as:

$$\alpha_s(q) = \frac{2\pi}{\beta_0 \, \ln(q/\Lambda_{QCD})}. \tag{4.19}$$

We can now get a more accurate estimation of our previous result (4.5), by including the effects of the leading logs. Leading log (LL) corrections come from inclusion of additional virtual gluon exchanges. As an example, there were two gluons exchanged in the box diagrams evaluated in this thesis, which resulted in a logarithmic term to a single power. If we create a ladder structure

of n-gluons, then there will be logarithmic contributions as $\ln^{n-1}\left(\frac{1}{m_Q a}\right)$ that result. We thus improve our first order result by resumming, to all-orders, the large logarithms of the lattice spacing. The leading log result is actually already known from [14]

$$C_{S^2}^{LL} = \alpha_s(\nu_h)\left[1 + \tilde{\beta}\left(z^{-2C_A+\beta_0} - 1\right)\right], \tag{4.20}$$

where $\tilde{\beta} = \frac{2\beta_0 - 7C_A}{2\beta_0 - 4C_A}$, and

$$z \equiv \left(\frac{\alpha_s(\nu_s)}{\alpha_s(\nu_h)}\right)^{1/\beta_0} = \left(\frac{\ln\left(m_Q/\Lambda_{QCD}\right)}{\ln\left(1/a\,\Lambda_{QCD}\right)}\right)^{1/\beta_0}. \tag{4.21}$$

4.4 Summary

We can add the contribution from (4.21) into our previous result, *provided* we remove the one loop log from our original result to avoid double counting

$$\begin{aligned} C_{S^2}(\alpha_s, m_Q, a) \;=\; & \left[-\frac{2}{3}\,C_F + \frac{4}{3}C_A + 2T_f\left(1 - \ln(2)\right) - A_{lat}^s\right] \\ & + \frac{4\pi}{3}\left[1 + \tilde{\beta}\left\{\left(\frac{\alpha_s(1/a)}{\alpha_s(m_Q)}\right)^{1-\frac{2C_A}{\beta_0}} - 1\right\}\right]. \end{aligned} \tag{4.22}$$

The above relation constitutes our final result for this thesis. In order to take the analysis further, we require the calculation of the matching coefficient A_{NR}, obtained from NRQCD lattice simulations. Upon determination of the matching coefficient, we can then add this contribution to the result from full lattice theory, which includes all heavy quark interaction effects up to the lattice cutoff $1/a$. The lattice results for HFS are already known, and can be found in [15], along with many details of the calculation. Their quoted result for $M(\Upsilon)$ - $M(\eta_b)$ is 61(14) MeV, however this doesn't take into account the hard

contribution, because the lattice spacing is necessarily finite. The inclusion of the one loop Wilson coefficient currently alters this value by ≈ -20 MeV. The effect of the theoretical predictions presented in this paper will depend on the NRQCD matching coefficient and hence whether the content herein will improve the agreement with experimental measurements is not *a priori* known.

Chapter 5

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Appendix A

Evaluation of Diagrams

A.1 Crossed Box

A.1.1 Setting up the problem and doing the integral

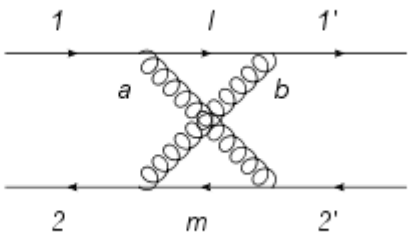

Figure A.1: Crossed Box

The above diagram can be written in the following schematic form (where the colour factor is left out, and $m = m_Q$)

$$iM \;=\; ig_s^4 \int \frac{d^4q}{(2\pi)^4} \, \frac{A + B^\mu q_\mu + C^{\mu\nu} q_\mu q_\nu}{(q^2 - \lambda^2)^2 (q^2 - 2mq_0 + i\epsilon)^2}. \tag{A.1}$$

It will be shown in Section A.3.1 that the only term important for spin is the term second order in loop momentum $C^{\mu\nu} q_\mu q_\nu$, i.e. just

$$iM_{spin} \;=\; ig_s^4 \int \frac{d^4q}{(2\pi)^4} \; \frac{C^{\mu\nu} q_\mu q_\nu}{(q^2-\lambda^2)^2 (q^2 - 2mq_0 + i\epsilon)^2}. \tag{A.2}$$

In order to solve this integral it is simplest to use a simple Feynman parametrization

$$\frac{1}{a^2 b^2} \;=\; 3! \int_0^1 \frac{x(1-x)dx}{[a + (b-a)x]^4}, \tag{A.3}$$

which can be derived by twice differentiating the standard relation

$$\frac{1}{ab} \;=\; \int_0^1 \frac{dx}{[a + (b-a)x]^2}. \tag{A.4}$$

So we now have the form

$$iM_{spin} \;=\; 3!\, ig_s^4 \int_0^1 x(1-x)dx \int \frac{d^4q}{(2\pi)^4} \; \frac{C^{\mu\nu} q_\mu q_\nu}{[(q^2-\lambda^2) + (-2mq_0 + \lambda^2 + i\epsilon)x]^4}. \tag{A.5}$$

In order to bring this into the form of a standard loop integral, we make the substitution $q_0 \rightarrow q_0' = q_0 - mx$ so that $q_0'^{\,2} - m^2x^2 \;=\; q_0^2 - 2mxq_0$. This will of course change the numerator but we note that $C^{0i} \tilde{=} O(\vec{k})$ and the term $C^{00}(2mxq_0)$ contributes an odd term which drops upon integrating over the loop momentum.

$$iM_{spin} \;=\; 3!\, ig_s^4 \int_0^1 x(1-x)dx \int \frac{d^4q}{(2\pi)^4} \; \frac{C^{\mu\nu} q_\mu q_\nu + C^{00} m^2 x^2}{[q^2 - \{m^2x^2 + \lambda^2(1-x) - i\epsilon x\}]^4}. \tag{A.6}$$

This integral is now a standard loop integral with the term in the curly brackets independent of the loop momentum. This can be evaluated by looking it up in a table (example: Peskin and Schroeder appendix B), giving:

$$iM_{spin} \;=\; -\frac{g_s^4}{(4\pi)^2}\int_0^1 x(1-x)dx\left[\frac{-\frac{1}{2}C^{\mu\nu}g_{\mu\nu}}{\Delta}+\frac{C^{00}m^2x^2}{\Delta^2}\right], \tag{A.7}$$

where $\Delta \equiv \{m^2x^2+\lambda^2(1-x)-i\epsilon x\ \}$, and we write $C^{\mu\nu}g_{\mu\nu} = C^{00}-C^{ii}$ for convenience.

$$\frac{-\frac{1}{2}C^{00}\Delta+C^{00}m^2x^2}{\Delta^2} = \frac{\frac{1}{2}C^{00}[m^2x^2-\lambda^2(1-x)+i\epsilon x)]}{\Delta^2}, \tag{A.8}$$

Thus in total the x-integral is:

$$iM_{spin} \;=\; -\frac{\alpha_s^2}{2}\int_0^1 x(1-x)dx\ \left[\frac{C^{00}[m^2x^2-\lambda^2(1-x)+i\epsilon x)]}{\Delta^2}+\frac{C^{ii}}{\Delta}\right]. \tag{A.9}$$

It will be simplest to evaluate each of these separately. Starting with the first term we have

$$iM^a_{spin} \;=\; -\frac{\alpha_s^2\ C^{00}}{2m^2}\int_0^1 dx\ \frac{[x^2-\delta^2(1-x)][1-x]x}{[x^2+\delta^2(1-x)-i\epsilon x]^2}, \tag{A.10}$$

where the m^2 terms, which lead to an overall $\frac{1}{m^2}$ multiplying the integral, have been factored out. Finally replacements with the dimensionless constant $\delta = \frac{\lambda}{m}$ have been done. the details of this integral are not very interesting and we will simply quote the result

$$iM^a_{spin} \;=\; \frac{\alpha_s^2\ C^{00}}{2m^2}\Big(2+\ln(\lambda/m)\Big). \tag{A.11}$$

The second integral is likewise evaluated

$$iM^b_{spin} \;=\; -\frac{\alpha_s^2\ C^{ii}}{2m^2}\int_0^1 dx\ \frac{(1-x)x}{x^2+\delta^2(1-x)-i\epsilon x} = \frac{\alpha_s^2\ C^{ii}}{2m^2}\Big(1+\ln(\lambda/m)\Big). \tag{A.12}$$

A.1.2 Colour Factors

The $q\bar{q}$ is necessarily in the colour singlet configuration, which in terms of standard colour spinor ket notation of red, blue,green can be written simply as

$$\frac{1}{\sqrt{3}}[\,|r\bar{r}\rangle + |b\bar{b}\rangle + |g\bar{g}\rangle]. \tag{A.13}$$

The reason for writing this expression in such a pedestrian way, is because the colour calculation will be carried out for a general SU(N) gauge group and it gives us the form of a general singlet configuration projection operator in order to carry out the calculation. From the above we see that the general singlet projector is

$$|q\bar{q}\rangle_{colour} = \frac{1}{\sqrt{N}}\sum_{i=1}^{N} |\mathbf{q_i}\rangle\,|\bar{\mathbf{q}}_\mathbf{i}\rangle = \frac{\mathbf{1}}{\sqrt{\mathbf{N}}}\sum_{\mathbf{i=1}}^{\mathbf{N}} |\mathbf{e}^\mathbf{i}_\mathbf{q}\rangle \otimes |\mathbf{e}^\mathbf{i}_{\bar{\mathbf{q}}}\rangle, \tag{A.14}$$

where the column vectors have N components, and a value of one at the position i and 0 elsewhere. An analogous expression for the post collision particles is also used $|q\bar{q}\rangle'_{colour}$. We can use the rules for an SU(N) gauge group to get the expression for the colour $\tilde{C}$

$$\tilde{C} = \frac{1}{N}\langle q_i|\, T^a_{il}T^b_{lj}\,|q'_j\rangle\,\langle\bar{q}'_j|\, T^a_{jm}T^b_{mi}\,|\bar{q}_i\rangle \;=\; \frac{1}{N}\,T^a_{il}T^b_{lj}\,T^a_{jm}T^b_{mi}. \tag{A.15}$$

We will want to commute the matrices in order to simplify, thus matrix notation will now be used. We have that

$$\tilde{C} = \frac{1}{N}(\mathbf{T^a}\cdot\mathbf{T^b})\cdot(\mathbf{T^a}\cdot\mathbf{T^b}), \tag{A.16}$$

which we can rewrite with the commutator rule: $\mathbf{T^b}\cdot\mathbf{T^a} = \mathbf{T^a}\cdot\mathbf{T^b} - if^{abc}\mathbf{T^c}$ of the lie-algebra, along with the associativity of matrix multiplication.
Plugging in and using the definition of the quadratic Casimir operator in the first term,

$$\tilde{C} = \frac{1}{N} C_F^2 \delta^{ij}\delta^{ji} - \frac{if^{abc}}{N}\mathbf{T^a}\cdot\mathbf{T^c}\cdot\mathbf{T^b} = C_F^2 + \frac{if^{abc}}{N}\mathbf{T^a}\cdot\mathbf{T^b}\cdot\mathbf{T^c}. \tag{A.17}$$

Concentrating on the second term $\tilde{C}^{(2^{nd})}$, we can use the identity

$$\begin{aligned} 2\mathbf{T^a}\cdot\mathbf{T^b} &= \frac{1}{N}\delta^{ab}\mathbb{1} + (d^{abd} + if^{abd})\mathbf{T^d} \\ \Rightarrow \tilde{C}^{(2^{nd})} &= \frac{if^{abc}}{2N}\Big(\frac{1}{N}\delta^{ab}\mathbb{1} + (d^{abd} + if^{abd})\mathbf{T^d}\Big)\cdot\mathbf{T^c}. \end{aligned} \tag{A.18}$$

Since contracting an antisymmetric tensor with a symmetric one will obviously give zero, this leaves only

$$\tilde{C}^{(2^{nd})} = -\frac{f^{abc}f^{abd}}{2N}\mathbf{T^d}\cdot\mathbf{T^c}. \tag{A.19}$$

Then using one final identity $f^{acd}f^{bcd} = N\delta^{ab}$, we get in total

$$\begin{aligned} \tilde{C} &= C_F^2 - \frac{\delta^{cd}}{2}\mathbf{T^d}\cdot\mathbf{T^c} \\ &= C_F^2 - \frac{N}{2}C_F \\ &= C_F^2 - \frac{1}{2}C_A C_F. \end{aligned} \tag{A.20}$$

We might as well just get the planar box colour factor here too. Examining Figure A.2 (p.47), it is apparent that we only need to switch the colour matrix indices on the two middle matrices of the above. This means there is no need to commute the colour matrix and we just get C_F^2.

A.1.3 Numerator Algebra

The numerator, which was written out in terms of tensors of different rank, is equivalent to the following.

$$[\bar{u_r}(p')\gamma^\mu(\not{s}+m)\gamma^\nu u_s(p)][\bar{v_t}(\bar{p})\gamma_\mu(\not{s}'+m)\gamma_\nu v_w(\bar{p}')] \tag{A.21}$$

where $s = p' - q$ and $s' = -\bar{p} + q$. We now use the identity $\gamma^\mu \not{k} = 2k^\mu - \not{k}\gamma^\mu$,

$$[\bar{u_r}(p')(2s^\mu + (-\not{s}+m)\gamma^\mu)\gamma^\nu u_s(p)][\bar{v_t}(\bar{p})(2s'_\mu + (-\not{s}'+m)\gamma_\mu)\gamma_\nu v_w(\bar{p}')]. \tag{A.22}$$

Then of course $\bar{u}_s(p')[\not{p}' - m] = 0$ and $\bar{v_t}(\bar{p})[\bar{p} + m] = 0$, leaving us with

$$[\bar{u_r}(2s^\mu + \not{q}\gamma^\mu)\gamma^\nu u_s][\bar{v_t}(2s'_\mu - \not{q}\gamma_\mu)\gamma_\nu v_w)]. \tag{A.23}$$

Now if we enumerate the terms in the first bracket as a,b and the second as c,d; we can take a closer look and save some work. Any term combined with a(c) will necessarily come with a factor s^μ (s'_μ), thus leaving only a single gamma matrix sandwiched between the spinors. So let's look at the form of the gamma matrices to see why this has no interest for us.

$$\gamma^0 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \tag{A.24}$$

$$\vec{\gamma} = \begin{pmatrix} 0 & \vec{\sigma} \\ -\vec{\sigma} & 0 \end{pmatrix} \tag{A.25}$$

The first matrix has no pauli matrices and thus contributes nothing to the spin. The second matrix contains pauli factors but they cross the two top and bottom components of the 4-spinors and in our non-relativistic approximation do not contribute. Thus only the term (b,d) will contribute to the spin structure in our approximation

$$-[\bar{u_r}\not{q}\gamma^\mu\gamma^\nu u_s][\bar{v_t}\not{q}\gamma_\mu\gamma_\nu v_w)]. \tag{A.26}$$

We can now use some gamma matrix identities to simplify the expression,

$$\gamma^\mu\gamma^\nu = \frac{1}{2}[\gamma^\mu,\gamma^\nu] + \frac{1}{2}\{\gamma^\mu,\gamma^\nu\} = g^{\mu\nu} + \sigma^{\mu\nu}, \tag{A.27}$$

$$g^{\mu\nu}g_{\mu\nu} = 4 \quad , \quad g^{\mu\nu}\sigma_{\mu\nu} = 0. \tag{A.28}$$

As before we will only be interested in terms that generate spin, so the terms where the metric has been fully contracted will leave a $\not{q}$ which is just a summation of a single gamma matrix at a time, and drops as before. Thus we are left with

$$-[\bar{u_r}\not{q}\,\sigma^{\mu\nu}\,u_s][\bar{v_t}\not{q}\,\sigma_{\mu\nu}\,v_w)]. \tag{A.29}$$

Now the form of $\sigma^{\mu\nu}$ is that of a second rank antisymmetric tensor, and as such can be represented as a two-vector $\sigma^{\mu\nu} = \langle\sigma^{0i},\sigma^{ij}\rangle = \langle\vec{\alpha}, i\vec{\Sigma}\rangle$, where its covariant equivalent is $\sigma_{\mu\nu} = \langle-\vec{\alpha}, i\vec{\Sigma}\rangle$. Here $\vec{\Sigma}$, is just the spin operator double stacked (a 4D irreducible representation), so that it also covers positron states. With a couple lines of algebra, you can convince yourself that,

$$\sigma^{\mu\nu}\sigma_{\mu\nu} = -2[\vec{\alpha_1}\cdot\vec{\alpha_2} + \vec{\Sigma_1}\cdot\vec{\Sigma_2}]\,. \tag{A.30}$$

This brings our expression into the form:

$$\begin{aligned} &2[\bar{u_r}\not{q}\,\vec{\alpha_1}\,u_s]\cdot[\bar{v_t}\not{q}\,\vec{\alpha_2}\,v_w] + 2[\bar{u_r}\not{q}\,\vec{\Sigma_1}\,u_s]\cdot[\bar{v_t}\not{q}\,\vec{\Sigma_2}\,v_w] \\ =\ &2\big([\bar{u_r}\,\gamma^\mu\,\vec{\alpha_1}\,u_s]\cdot[\bar{v_t}\,\gamma^\nu\,\vec{\alpha_2}\,v_w] + [\bar{u_r}\,\gamma^\mu\,\vec{\Sigma_1}\,u_s]\cdot[\bar{v_t}\,\gamma^\nu\,\vec{\Sigma_2}\,v_w]\big)q_\mu q_\nu. \end{aligned} \tag{A.31}$$

This is good, because it tells us right away that the only important piece for the spin is the tensor term in the integral, as stated in section A. Now again we are interested in the spin terms, which means we want the ones that have a $\mathbf{\Sigma}$ matrix sandwiched between the spinors. This means of course that in term

1 both μ and ν must **not** be zero, and in the second term they **must be** zero. Let's start by simplifying the first term, remembering $\gamma^i = \alpha^i\gamma^0$:

$$C^{ij}\, q_i q_j = \; 2\,[u_r^\dagger\, \gamma^i\, \gamma^k\, u_s][v_t^\dagger\, \gamma^j\, \gamma^k\, v_w] q_i q_j. \tag{A.32}$$

We then re-express the gamma product again, and again drop terms like $g^{ij}g_{ij}$, and replace σ^{ij} matrices by their definition

$$\sigma^{ij} = i\epsilon^{ijk}\Sigma^k, \tag{A.33}$$

$$C^{ij} \;=\; 2\,i^2\,[u_r^\dagger\, \epsilon^{ikl}\, \Sigma_1^l\, u_s][v_t^\dagger\, \epsilon^{jkm}\, \Sigma_2^m\, v_w]. \tag{A.34}$$

We simplify as follows :

$$\begin{aligned}
&\epsilon^{ikl}\epsilon^{jkm} = \delta^{ij}\delta^{lm} - \delta^{im}\delta^{lj},\\
&\big(\delta^{ij}\delta^{lm} - \delta^{im}\delta^{lj}\big)\Sigma_1^l\,\Sigma_2^m \;=\; \delta^{ij}\mathbf{\Sigma_1}\cdot\mathbf{\Sigma_2} - \Sigma_1^i\Sigma_2^j,\\
&\mathbf{\Sigma} = \sigma \otimes \mathbf{1_{2\times 2}}.
\end{aligned} \tag{A.35}$$

Now we have that

$$C^{ij} \;=\; 2\,[\xi_r^\dagger\, \zeta_t^\dagger\, (\sigma_1^i\, \sigma_2^j - \delta^{ij}\sigma_{\mathbf{1}}\cdot\sigma_{\mathbf{2}})\xi_s\zeta_w]. \tag{A.36}$$

For later convenience:

$$C^{ii} \;=\; -4\,[\xi_r^\dagger\, \zeta_t^\dagger\, (\sigma_{\mathbf{1}}\cdot\sigma_{\mathbf{2}})\xi_s\zeta_w], \tag{A.37}$$

where they are now 2-spinors. It should be clear from the above that the second term (where $\mu = \nu = 0$) leads to:

$$C^{00} \;=\; 2\,[\xi_r^\dagger\, \zeta_t^\dagger\, (\sigma_{\mathbf{1}}\cdot\sigma_{\mathbf{2}})\xi_s\zeta_w]. \tag{A.38}$$

A.1.4 Putting It Together

The first section gave us the value of the amplitude in terms of the yet undetermined numerator factors and an implied colour factor Next we determined the colour factor to be $C_F^2 - \frac{1}{2}C_A C_F$ in section A.2. Finally in Section A.3, we worked through the numerator, completing the tensor reduction analysis to get simple form factors for the appropriate spin terms. If we write the amplitude out in all its glory we get

$$iM_{spin}^{c.b.} = \frac{C_F^2 - \frac{1}{2}C_A C_F}{2m^2}\,\alpha_s^2\left[C^{00}\left(2+\ln(\lambda/m)\right) + C^{ii}\left(1+\ln(\lambda/m)\right)\right]. \quad \text{(A.39)}$$

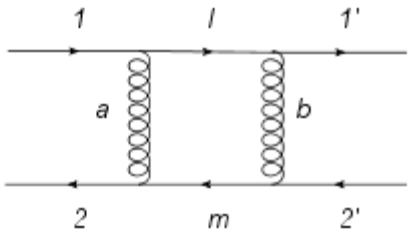

Figure A.2: Planar Box

A.2 Planar Box

In the planar box, only the denominator and the colour factor change. For the latter $\left(C_F^2 - \frac{1}{2}C_A C_F\right) \to C_F^2$, while the integral becomes the following

$$iM_{spin} = ig_s^4 \int \frac{d^4q}{(2\pi)^4} \frac{C^{\mu\nu} q_\mu q_\nu}{(q^2-\lambda^2)^2(q^2-2mq_0+i\epsilon)(q^2+2mq_0+i\epsilon)}. \quad \text{(A.40)}$$

If we're only considering the spin contribution, the form factors C^{00} and C^{ii} are identical to the ones outlined for the crossed box diagram. We can now immediately use a Feynman parametrization,

$$\begin{aligned} \frac{1}{a^2bc} &= \frac{\partial}{\partial a} \int_0^1 \int_0^x \frac{2\,dy\,dx}{[a+(b-a)x+(c-b)y]^3} \\ &= 3! \int_0^1 dx \int_0^x dy \frac{(1-x)}{[a+(b-a)x+(c-b)y]^4}, \end{aligned} \quad \text{(A.41)}$$

$$\Rightarrow iM_{spin} = 3!\; ig_s^4 \int_0^1 dx \int_0^x dy \int \frac{d^4q}{(2\pi)^4} \frac{(1-x)C^{\mu\nu} q_\mu q_\nu}{\left[(q^2-\lambda^2)+(2mq_0+\lambda^2+i\epsilon)x-4mq_0y\right]^4} \quad \text{(A.42)}$$

We will make the following change of variable $q_0 \to q_0' = q_0 + m(x-2y)$

$\rightarrow {q_0'}^2 = q_0^2 + 2mq_0(x-2y) + m^2(x-2y)^2.$

$$iM_{spin} = 3!\ ig_s^4 \int_0^1 dx \int_0^x dy \int \frac{d^4q}{(2\pi)^4} \frac{(1-x)\left[C^{\mu\nu}q_\mu q_\nu + C^{00}m^2(x-2y)^2\right]}{\left[q^2 - \{m^2(x-2y)^2 + \lambda^2(1-x) - i\epsilon x\}\right]^4}$$

$$= \quad 3!\ ig_s^4 \int_0^1 dx \int_0^x dy \int \frac{d^4q}{(2\pi)^4} \frac{(1-x)\left[C^{\mu\nu}q_\mu q_\nu + C^{00}m^2(x-2y)^2\right]}{\left[q^2 - \Delta\right]^4}$$

$$= \quad -\frac{g_s^4}{4\pi^2} \int_0^1 dx \int_0^x dy\ (1-x) \left[\frac{-\frac{1}{2}C^{\mu\nu}g_{\mu\nu}\Delta + C^{00}m^2(x-2y)^2}{\Delta^2}\right]$$

$$= \quad -\frac{\alpha_s^2}{2m^2} \int_0^1 dx \int_0^x dy\ \ (1-x) \left[\frac{C^{00}[(x-2y)^2 - \delta^2(1-x) + i\epsilon x)]}{{\Delta'}^2} + \frac{C^{ii}}{\Delta'}\right], \tag{A.43}$$

where $\Delta' \equiv (x-2y)^2 + \delta^2(1-x) - i\epsilon x.$

Interestingly enough, evaluation of the y-integral in the first term gives

$$\frac{\alpha_s^2\ C^{00}}{2m^2} \int_0^1 dx\ \frac{(1-x)x}{x^2 + \delta^2(1-x) - i\epsilon x}, \tag{A.44}$$

which we know from (A.12) is just

$$iM_{spin}^a = -\frac{\alpha_s^2\ C^{00}}{2m^2}\Big(1 + \ln(\lambda/m)\Big). \tag{A.45}$$

Evaluation of the second term is a little more interesting, it is this term that will give us a singular pole term in $\frac{1}{\lambda}$, along with another set of logarithmic and constant terms contributing to the spin. It is nearly identical to the second term in eqn. (9), except for the extra integral, and missing x-term in the numerator.

But as we will see these minor changes create large differences in the answers.

$$iM^b_{spin} = -C^{ii}\frac{\alpha_s^2}{2m^2}\int_0^1 dx \int_0^x dy \quad \frac{1-x}{(x-2y)^2+\delta^2(1-x)-i\epsilon x} \tag{A.46}$$

$$= \quad -C^{ii}\frac{\alpha_s^2}{2m^2}\int_0^1 dx \quad \frac{1-x}{\delta\sqrt{1-x(1+i\epsilon)}} \quad \tan^{-1}\left(\frac{x}{\delta\sqrt{1-x(1+i\epsilon)}}\right), \tag{A.47}$$

the epsilons will be left in until we're sure there's no danger of a divergence, but to save space $b \equiv 1 + i\epsilon$. Evaluation of the x-integral gives

$$\begin{aligned} I^b_{spin} = \quad & -\tfrac{1}{2}ln(1-i\epsilon) + \frac{2}{3\delta\sqrt{-b^2}}\tanh^{-1}\left(\frac{\delta^2-2}{2\delta\sqrt{-b^2}}\right) \\ & + \ln(\delta) - \frac{2}{3\delta\sqrt{-b^2}}\tanh^{-1}\left(\frac{\delta}{2\sqrt{-b^2}}\right) + \frac{1}{3}. \end{aligned} \tag{A.48}$$

We can now easily see that the $\sqrt{-b^2}$ terms can safely be set to i.

$$I^b_{spin} = -\frac{2i}{3\delta}\tanh^{-1}\left(\frac{i}{\delta}\right) + \frac{2i}{3\delta}\tanh^{-1}\left(\frac{-i\delta}{2}\right) + \ln(\delta) + \frac{1}{3}$$

$$= \quad \frac{2}{3\delta}\left[\tan^{-1}\left(\frac{1}{\delta}\right) + \tan^{-1}\left(\frac{\delta}{2}\right)\right] + \ln(\delta) + \frac{1}{3}, \tag{A.49}$$

where the identity $\quad i\tanh^{-1}(z) = \tan^{-1}(iz)$, was used. Now we have that

$$\begin{aligned}\tan^{-1}(1/x) &= \frac{\pi}{2} - \tan^{-1}(x) \;\; \forall x : [0,1) \\ \tan^{-1}(x) &\approx x, \;\; x << 1.\end{aligned}$$

Thus upon using the expansion in our expression we get that

$$\begin{aligned}I^b_{spin} &= \frac{\pi}{3\delta} + \frac{2}{3\delta}\left(\frac{-\delta}{2}\right) + \ln(\delta) + \frac{1}{3} \\ &= \frac{\pi}{3\delta} + \ln(\delta) \\ &= \frac{\pi m}{3\lambda} + \ln\left(\tfrac{\lambda}{m}\right) \qquad \text{(A.50)}\end{aligned}$$

.

So now, all in all, we have

$$iM^{p.b.}_{spin} = -\frac{C_F^2}{2m^2}\,\alpha_s^2\left[C^{00}\Big(\,1 + \ln\left(\tfrac{\lambda}{m}\,\right)\Big) + C^{ii}\Big(\,\frac{\pi m}{3\lambda} + \ln\left(\tfrac{\lambda}{m}\right)\,\Big)\right], \qquad \text{(A.51)}$$

$$iM^{c.b.}_{spin} = \frac{C_F^2 - \frac{1}{2}C_A C_F}{2m^2}\,\alpha_s^2\left[C^{00}\left(2 + \ln(\lambda/m)\right) + C^{ii}\left(1 + \ln(\lambda/m)\right)\right]. \qquad \text{(A.52)}$$

Plugging in the definitions of the coefficients:

$$C^{ii} = -4\,[\xi_r^\dagger\,\zeta_t^\dagger\,(\sigma_{\mathbf{1}}\cdot\sigma_{\mathbf{2}})\xi_s\zeta_w] = -8\mathbf{S}^2 \;\;;\;\; C^{00} = 2\,[\xi_r^\dagger\,\zeta_t^\dagger\,(\sigma_{\mathbf{1}}\cdot\sigma_{\mathbf{2}})\xi_s\zeta_w] = 4\mathbf{S}^2$$

$$V^{p.b.}_{spin} = \frac{C_F^2}{m^2}\,\alpha_s^2\,\Big[\,-2 + 2\ln\big(\lambda/m\big) + \,\frac{4\pi}{3}\frac{m}{\lambda}\,\Big]\mathbf{S}^2, \qquad \text{(A.53)}$$

$$V_{spin}^{c.b.} = -\frac{C_F^2 - \frac{1}{2}C_A C_F}{m^2}\,\alpha_s^2\,\big[\,2\ln\big(\lambda/m\big)\,\big]\mathbf{S}^2. \tag{A.54}$$

The equations (A.53) and (A.54) constitute our final result for these diagrams. This result will be checked by a more modern analytical technique, known as expansion by regions, later.

A.3 Pauli Form-Factor

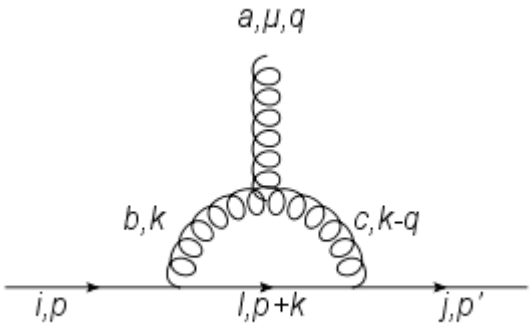

Figure A.3: Non-Abelian Vertex

If we perform this calculation in the background field formulation it will make things considerably easier to carry out. Following the Feynman rules for the background formalism [16]

$$i\Gamma^{\mu} \sim \int d^D\hat{k}\frac{\gamma^{\beta}\Big[g_{\alpha\beta}(2k-q)^{\mu} - g_{\alpha}^{\mu}\big(k+q+\frac{1}{\xi}(q-k)\big)_{\beta} + g_{\beta}^{\mu}\big(2q-k+\frac{1}{\xi}k\big)_{\alpha}\Big](\not{p}+\not{k}+m)\gamma^{\alpha}}{[(p+k)^2-m^2][(k-q)^2-\lambda^2][k^2-\lambda^2]}. \tag{A.55}$$

In the above, constant prefactors have been temporarily omitted in the interest

of space. Then, in the Feynman gauge the numerator simplifies substantially

$$i\Gamma^{\mu}_{NA}(p,p') = ig_s^3 C^a_{ji}\int d^D\hat{k}\frac{\gamma^\beta\Big[g_{\alpha\beta}(2k-q)^\mu - 2g^\mu_\alpha q_\beta + 2g^\mu_\beta q_\alpha\Big](\not{p}+\not{k}+m)\gamma^\alpha}{[(p+k)^2-m^2][(k-q)^2-\lambda^2][k^2-\lambda^2]}. \tag{A.56}$$

where $\frac{i}{2}C_A\,T^a_{ji} \equiv C^a_{ji}$. The work of Manohar [17] will be invaluable in this calculation. The denominator of his calculation of this vertex reads (Eq.'s 31 & 32)

$$m^2(x+y-1)^2 - q^2xy. \tag{A.57}$$

We can reproduce precisely this denominator in our work if we use the following Feynman parametrization (working first without the gluon mass)

$$\int_0^1 dx\int_0^{1-x} dy\int d^D\hat{k}\frac{N^\mu}{k^2+2p\cdot k+\big[q^2-2(q+p)\cdot k\big]x-2p\cdot ky}. \tag{A.58}$$

From the above expression it is clear that the necessary change of variables is $k\to l = k+[p(1-y)-p'x]$. The quantity in the square brackets then goes back into the denominator squared which gives $m^2(1-y)^2+m^2x^2-2p\cdot p'x(1-y)$, then upon noting that $-2p\cdot p' = q^2-2m^2$ we recover the required denominator. Finally we see that by including a gluon-mass term we incorporate into the denominator a term of the form $\lambda^2(x+y)$. Thus inserting this factor into Manohar's expression for the non-abelian F_2 we get

$$F_2^g = -\frac{\alpha_s}{4\pi}C_A\int_0^1 dx\int_0^{1-x} dy\frac{2(x+y)(1-x-y)m^2}{m^2(x+y-1)^2-q^2xy+\lambda^2(x+y)}. \tag{A.59}$$

We are interested only in the limit $q\to 0$, so for us

$$F_2^g = -\frac{\alpha_s}{4\pi}C_A\int_0^1 dx\int_0^{1-x} dy\frac{2(x+y)(1-x-y)}{(x+y-1)^2+\frac{\lambda^2}{m^2}(x+y)}. \tag{A.60}$$

Evaluation of this integral gives us

$$F_2^g = \frac{\alpha_s}{4\pi} C_A \Big[3 + 2 \ \ln\big(\lambda/m\big) \Big] + \mathcal{O}(q^2/m^2). \tag{A.61}$$

We must add to this the contribution of the abelian vertex, which Schwinger tells us (up to colour factors) is

$$F_2^V = \ \frac{\alpha_s}{2\pi}\big(C_F - \tfrac{1}{2}C_A\big) + \mathcal{O}(q^2/m^2). \tag{A.62}$$

We can thus write out the final result[1]

$$\begin{aligned} F_2 = \ & F_2^V + F_2^g \\ = \ & \frac{\alpha_s}{2\pi}\Big[C_F + C_A\Big(1 + \ln\big(\lambda/m\big)\Big)\Big]. \end{aligned} \tag{A.63}$$

[1]Note that we will have to multiply this result by two when inserting it into the Born result, to account for the two separate insertions of the vertex corrections

Appendix B

Expansion By Regions

Expansion by regions is a technique for asymptotic expansion of loop integrals with several momentum scales [19], [20]. It involves three main steps

- (i) Separate the momentum integral into regions where the loop momentum is characterized by one of the scales.
- (ii) In each region perform Taylor expansion in the parameters that are small there.
- (iii) Extend the integration limits of each region to the whole virtual momentum space and use dimensional regularization for IR and UV divergences.

The sum of the contributions of all the regions then recovers the asymptotic series for the loop integral.

B.1 Application to the Crossed Box Diagram

$$iM = ig_s^4 \int \frac{d^4q}{(2\pi)^4} \frac{C^{\mu\nu} q_\mu q_\nu}{(q^2-\lambda^2)^2(q^2-2mq_0+i\epsilon)^2} \tag{B.1}$$

We will omit the colour factors in this demonstration for brevity. The hard modes mean setting the gluon mass to zero ($\lambda \to 0$), thus

$$I_{hard} \equiv \; ig_s^4 \int \frac{d^d q}{(2\pi)^d} \; \frac{C^{\mu\nu} q_\mu q_\nu}{(q^2)^2 (q^2 - 2p\cdot q + i\epsilon)^2}. \tag{B.2}$$

Then combining this in a Feynman parametrization gives

$$\begin{aligned} I_{hard} = \; & 3!\, ig_s^4 \int_0^1 dx\; x(1-x) \int \frac{d^d q}{(2\pi)^d} \; \frac{C^{\mu\nu} q_\mu q_\nu}{\big[q^2 - 2p\cdot qx\big]^4} \\ = \; & -\frac{\alpha_s^2}{m^2} \int_0^1 dx\; x(1-x)\; \frac{C^{00} - \frac{1}{2} C^{\mu\nu} g_{\mu\nu}}{x^2} \\ = \; & \frac{\alpha_s^2}{2m^2} C_{\mu\mu} \Big(1 + \frac{1}{\epsilon}\Big). \end{aligned} \tag{B.3}$$

The soft modes are then characterized by $m \to \infty$,

$$I_{soft} \equiv \; ig_s^4 \int \frac{d^d q}{(2\pi)^d} \; \frac{C_{\mu\nu} q^\mu q^\nu}{(q^2 - \lambda^2)^2 (2mq_0 - i\epsilon)^2}. \tag{B.4}$$

We can again use a Feynman-parametrization to get

$$I_{soft} = 3!\, ig_s^4 \int_0^1 dx\; \frac{x}{(1-x)^3} \int \frac{d^d q}{(2\pi)^d} \; \frac{C_{\mu\nu} q^\mu q^\nu}{\big[q^2 - \lambda^2 + 2m(\frac{x}{1-x}) q_0\big]^4}. \tag{B.5}$$

Then we perform the change of variables to $q_0' = q_0 + m\big(\frac{x}{1-x}\big)$,

$$I_{soft} = 3!\, ig_s^4 \int_0^1 dx\; \frac{x}{(1-x)^3} \int \frac{d^d q}{(2\pi)^d} \; \frac{C_{\mu\nu} q^\mu q^\nu + C^{00} m^2 \big(\frac{x}{1-x}\big)^2}{\big[q^2 - \lambda^2 - m^2 (\frac{x}{1-x})^2\big]^4}. \tag{B.6}$$

We carry out the standard loop integral to get

$$-\frac{\alpha_s^2}{m^2} \int_0^1 dx \left[\frac{x^3 C^{00}}{(1-x)^5 \big[\big(\frac{x}{1-x}\big)^2 + \delta^2\big]^2} - \frac{\frac{1}{2}\big[C^{00} - C^{ii}\big] x}{(1-x)^3 \big[\big(\frac{1-x}{x}\big)^2 + \delta^2\big]} \right]. \tag{B.7}$$

The respective Feynman parameter integrals give

$$
\begin{aligned}
&= \frac{\alpha_s^2}{m^2}\left[C^{00}\Big(\frac{1}{2}+\ln\big(\lambda/m\big)-\frac{1}{\epsilon}\Big)-\frac{1}{2}\big[C^{00}-C^{ii}\big]\Big(\ln\big(\lambda/m\big)-\frac{1}{\epsilon}\Big)\right] \\
&= \frac{\alpha_s^2}{2m^2}\left[C^{00}+C_{\mu\mu}\ln\big(\lambda/m\big)-\frac{1}{\epsilon}C_{\mu\mu}\right]. \qquad \text{(B.8)}
\end{aligned}
$$

We add the two regions together, and recover our original result (without the colour factor)

$$
\frac{\alpha_s^2}{2m^2}\left[2C^{00}+C^{ii}+C_{\mu\mu}\ln\big(\lambda/m\big)\right]. \qquad \text{(B.9)}
$$

B.2 Application to the Planar Box Diagram

$$iM_{p.b} \;=\; ig_s^4 C_F^2 \int \frac{d^4q}{(2\pi)^4}\, \frac{C^{\mu\nu} q_\mu q_\nu}{(q^2-\lambda^2)^2 (q^2 - 2p\cdot q)(q^2+2p\cdot q)} \tag{B.10}$$

The analysis of the planar box is nearly identical, and therefore we will omit many details, as they add nothing to the discourse. There is a new effect in the planar box however, that we do wish to address via the expansion.

As before, we take the limit as $m \to \infty$ in the soft region. This gives us exactly the negative of the crossed box soft region, except that in addition there are now poles at both $+i\epsilon$ *and* $-i\epsilon$. This means we can no longer adjust the contour of the integral to remove the pole at $q_0 = 0$. This effect is the evaluation of Coulomb poles and is typical of threshold expansions. We start by noticing that this integral will be completely dominated by the pole value and thus terms of order q_0^2 can be dropped without further thought. This new piece is called the potential contribution, and will give rise to the λ-pole which was obtained in the original analysis.

$$\begin{aligned}
I_{potential} &= -\frac{1}{4m^2} \int \frac{d^4q}{(2\pi)^4}\, \frac{C^{ij} q_i q_j}{(\vec{q}^{\,2}+\lambda^2)^2 (q_0 + \frac{\vec{q}^{\,2}}{2m} + i\epsilon)(q_0 - \frac{\vec{q}^{\,2}}{2m} - i\epsilon)} && \text{(B.11)}\\
&= -\frac{i\,C^{ii}}{12m^2} \int \frac{d^3q}{(2\pi)^3}\, \frac{\vec{q}^{\,2}}{(\vec{q}^{\,2}+\lambda^2)^2 \left(\frac{\vec{q}^{\,2}}{m}\right)} && \text{(B.12)}\\
&= -\frac{i\,C^{ii}}{12m} \frac{4\pi}{(2\pi)^2} \int \frac{d|\vec{q}|}{2\pi}\, \frac{\vec{q}^{\,2}}{(\vec{q}^{\,2}+\lambda^2)^2} && \text{(B.13)}\\
&= -\frac{C^{ii}}{2m^2} \frac{i}{(4\pi)^2} \frac{\pi m}{3\lambda}. && \text{(B.14)}
\end{aligned}$$

Thus in total we get exactly the same pole as we got originally,

$$iM^{p.b.}_{pot.} = -\frac{C_F^2}{2m^2}\, \alpha_s^2 \left(\frac{\pi m}{3\lambda}\right) C^{ii}. \tag{B.15}$$

Appendix C

Colour Factors of Feynman Diagrams

We will be interested in the group $SU(N)$, which is known as the special unitary group. It is not the purpose of this appendix to give a full account of the details of the group theory involved, and as such, will include a short introduction that should serve as a good reminder. The interested reader is referred to the very readable account in [18].

The group $SU(N)$ has the simple defining properties of containing unitary operators that have unit norm (i.e. any matrix representation must contain elements of determinant one). It is also a Lie-group, and thus all elements of the group can represented as an exponential of a linear combination of generators, where the exponential is realized by its Taylor series. The generators themselves form a representation for a local vector space, and as the group is continuous, it can be shown that all Lie-groups describe a differentiable manifold. To make this more concrete, we can write

$$\left\{ \forall\, G_j \;\in\; SU(N) \;\exists\; \{\alpha_i\} \;\;|\;\; G_j = exp(i\,\alpha_i T^i) \right\} \quad i = 1, 2, ..., N, \qquad \text{(C.1)}$$

where the T^i are the generators which form a basis for the vector space. If we then form an algebra with these generators under commutation

$$\left[\, T^i \,,\, T^j \,\right] = \, f^{ijk}\, T^k, \tag{C.2}$$

we obtain a Lie-Algebra for the group[1], where summation over k is implied and the antisymmetric[2] f^{ijk} are known as the structure constants. The theory of QCD is based off the non-abelian gauge theory SU(3), and the quarks and anti-quarks each take on one of three different possibilities of colour and anticolour: Red, Green, Blue.

$$q = R, G, B \quad ; \quad \bar{q} = \bar{R}, \bar{G}, \bar{B} \tag{C.3}$$

The colour factors for quark (antiquark) lines are transformed in the fundamental representation $F(\bar{F}) = 3(\bar{3})$. A quark and antiquark can scatter of eachother via the exchange of a gluon between them. By the postulate of colour conservation, each gluon must carry one unit of colour and one unit of anticolour. As such we say that the gluons are in the adjoint representation $A = 3 \otimes \bar{3} = 8 \oplus 1$. The colour singlet of the adjoint representation could potentially be measured as a free particle, being colourless. This possibility seems to be excluded by experiment, which is why gluons are a colour $SU(3)$ instead of $U(3)$.

We can give a much more concrete definition to the adjoint representation through the use of the Jacobi identity. The matrices of the adjoint representation are given by the structure constants $(T^a)_{bc} = if^{abc}$, and the proof that this forms a representation is just a regurgitation of the Jacobi identity where the matrix elements are written explicitly. The Jacobi identity states that $\Big(\big[A,\, [B, C]\,\big]\Big)_{ABC} = 0$, where the round brackets indicate the sum of all even

[1]Strictly speaking, the Lie group is only a continuous group until an algebra is specified for its generators

[2]switching i and j in the commutator gives the negative of the original commutator.

interchanges of the labels ABC. Explicitly: $(ABC)_{ABC} = ABC+BCA+CAB$,

$$\left[T^a_{ij}, [T^b_{jk}, T^c_{kl}]\right] = \left[T^a_{ij}, f^{bcd}T^d_{jl}\right] = f^{bcd}f^{ade}T^e_{jl}. \tag{C.4}$$

Then applying the symmetric interchange sum and using anti-symmetry of the structure constants

$$f^{ade}f^{bcd} + f^{bde}f^{cad} - f^{cde}f^{bad} = 0,$$

$$-if^{bcd}T^d_{ea} + [T^b, T^c]_{ea} = 0 \quad \Rightarrow \quad [T^b, T^c]_{ea} = if^{bcd}T^d_{ea}. \tag{C.5}$$

With the notation now set, we give the rules for assigning colour to the various diagrams that arise from terms in the expansion of the interaction part of the QCD Lagrangian.

Figure C.1: Quark-Gluon Vertex: $-igT^a_{ij}$

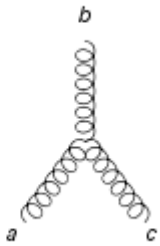

Figure C.2: 3-Gluon Vertex: $-gf^{abc}$

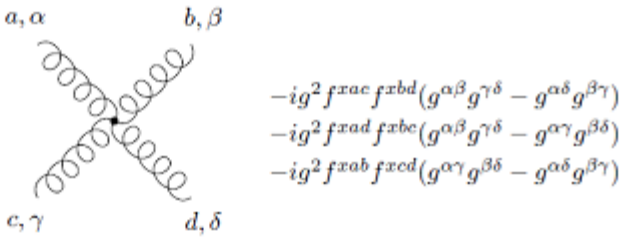

Figure C.3: 4 Gluon Vertex