

Heavy Quarkonia in Non-Relativistic Quantum Chromodynamics

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Abstract

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Quarkonia are bound states of a quark-antiquark pair having the same flavour. In this work, we go through how the effective field theory of non-relativistic quantum chromodynamics (NRQCD) can be used to describe quarkonia formed by heavy quarks. The Lagrangian describing the theory is derived at lowest orders and used to determine the velocity-scaling of different operators. The velocity-scaling rules are then used to estimate contributions of different Fock states in quarkonia.

We then describe the decay of S-wave quarkonia by writing the decay widths as power series in the velocity of the quark. The equations for the decay widths contain unknown constants that also appear in the inclusive cross sections of quarkonium production, and their connection to the quarkonium wave function is also shown.

The results for the decay widths at different orders of the quark velocity are studied. It is found that the convergence of the power series is slow, with the convergence depending on the decay process.

Keywords: particle physics, quarkonium, effective field theory, quantum field theory, quantum chromodynamics

Tiivistelmä

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Raskaat quarkonium-hiukkaset epärelativistisessa kvanttiväridynamiikassa

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Quarkonium-hiukkaset ovat saman makulajin kvarkki-antikvarkkiparista muodostuvia sidottuja tiloja. Tässä työssä käydään läpi epärelativistiseksi kvanttiväridynamiikaksi kutsuttavaa efektiivistä kenttäteoriaa, jota voidaan käyttää raskaiden kvarkkien muodostamien quarkonium-hiukkasten kuvaamiseen. Teoriaa kuvaava Lagrangen funktio johdetaan alimmissa kertaluvuissa, ja sitä käytetään johtamaan eri operaattorien skaalautuminen kvarkin nopeuden suhteen. Skaalaussääntöjen avulla johdetaan tämän jälkeen arviot eri Fock-tilojen suuruuksille quarkoniumissa.

Orbitaalista kvanttilukua $L = 0$ vastaavien quarkonium-hiukkasten hajoamisleveydet kirjoitetaan potenssisarjana kvarkin nopeuden suhteen. Hajoamisleveyksien yhtälöissä esiintyy tuntemattomia vakioita, jotka esiintyvät myös quarkoniumin inklusiivisen tuoton vaikutusaloissa. Näiden tuntemattomien vakioiden yhteys quarkoniumin aaltofunktioon käydään myös läpi.

Hajoamisleveyksien lausekkeista saatavia arvoja tutkitaan eri kertaluvuissa kvarkin nopeuden suhteen. Havaitaan, että potenssisarjan suppeneminen on hidasta ja riippuu hajoamisprosessista.

Avainsanat: hiukkasfysiikka, quarkonium, efektiivinen kenttäteoria, kvanttikenttäteoria, kvanttiväridynamiikka

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1 Introduction

Quarkonium particles are mesons that are formed by a quark-antiquark pair of the same flavour. The heavy masses of the c - and b -quarks allow us to consider heavy quarkonium particles as bound states of a single flavor. This is in contrast with the light quarkonia, formed by light quarks, that are mixtures of quark-antiquark states of different flavours. This makes the heavy quarkonia simpler, as they can to a good approximation be described by a single $Q\bar{Q}$ Fock state. The quarkonium particles formed by a $c\bar{c}$ -pair are called charmonium, and similarly quarkonia formed by a $b\bar{b}$ -pair are called bottonium. The t -quark cannot form a quarkonium state as it decays before forming a bound state. The charmonium and bottonium particles are the focus of this thesis, and we will from now on mean them when referring to quarkonia.

Quarkonium particles are interesting as they allow us to probe quantum chromodynamics (QCD) at different regions [1, p. vii]. For the physics of the bound $Q\bar{Q}$ state the non-perturbative effects of QCD dominate, whereas the decay and production of the heavy quark-antiquark pair are described by perturbative scattering processes. The quarkonia are also important because of the large amount of data available [2, p. 380].

The non-perturbative effects of QCD, however, are not simple. Therefore it is easier to describe quarkonia using an effective field theory. In quarkonia the velocity of the quark is small, which allows us to write the Lagrangian as a power series in the quark velocity. This is the basis for the non-relativistic QCD (NRQCD) which is an effective field theory used in describing quarkonia. The non-perturbative physics can then be absorbed into unknown constants which are separated from the effects related to the short-distance scattering processes. The separation of the short- and long-distance effects is called factorization, and it is important as it allows us to treat the annihilation and production of the heavy quark-antiquark pair separately from the formation of the bound state [3, p. 3].

Our treatment of quarkonia follows closely reference [3] where NRQCD is discussed thoroughly. In this thesis we focus on the S-wave states of the quarkonia, e.g., particles

η_c and J/ψ in the case of charmonium and η_b and Υ in the case of bottomonium. We especially focus on calculating their decay widths in the framework of NRQCD.

In section 2 we first show how the NRQCD Lagrangian can be derived. We then use the field equations from this Lagrangian to derive estimates for the relevant operators in powers of the quark velocity. These estimates are called the velocity-scaling rules and they are extremely useful in estimating the contributions of different operators and different Fock states. We also introduce the 4-fermion operators that can be linked to the decay of quarkonia. In section 3 we use the velocity-scaling rules to study the Fock state expansion of S-wave quarkonia. In section 4 we match NRQCD to QCD and deduce the coefficients of the 4-fermion operators. In section 5 we then show how the 4-fermion operators can be linked to the decay widths and write the equations for the decay widths in NRQCD. The decay widths can be expressed as power series in the quark velocity in NRQCD. Inclusive production of quarkonia is also briefly discussed along with its connection to decay. In section 6 we study the NRQCD equations for the decay widths and their accuracy at different orders in the quark velocity.

The notation follows the standard notation used in particle physics. We use the natural units where $c = \hbar = 1$, except when deriving the NRQCD Lagrangian where the powers of c are explicit. The metric is defined as $g_{\mu\nu} = \text{diag}(+1, -1, -1, -1)$.

2 NRQCD Lagrangian

2.1 Heavy quark and antiquark terms

The high masses of the c - and b -quarks allow us to treat quarkonium states as approximately pure $Q\bar{Q}$ states. Because of the high mass, the momentum to mass fraction $P/(Mc) \approx v$ is also small. This allows us to write quantities in terms of the first few terms of power series in the velocity v . It is possible to find the NRQCD Lagrangian by starting from the QCD Lagrangian and expanding it as a power series. However, it isn't beforehand clear how each operator in the Lagrangian scales in terms of the velocity. Therefore it is easier to do the expansion first in powers of $1/c$ and then deduce the velocity-scaling rules of the operators from the most dominating terms in the power series. This derivation of the NRQCD Lagrangian follows closely the one presented in reference [4].

The part of the QCD Lagrangian corresponding to heavy quarks and antiquarks is

$$c\mathcal{L}_{\text{heavy}} = c\bar{\Psi}(i\gamma^\mu D_\mu - Mc)\Psi \quad (2.1)$$

where $D_\mu = \partial_\mu + \frac{ig}{c}A_\mu$ is the covariant derivative, g is the strong coupling constant and A_μ is the gluon field. We have not set $c = 1$ in the Lagrangian $\mathcal{L}_{\text{heavy}}$ as keeping it will make the power counting in $1/c$ explicit. We will consider the heavy quark and antiquark parts of the Lagrangian separately. This allows us to write the explicit power counting but in turn we will lose the interaction terms between the quarks and antiquarks. Technically, this corresponds to neglecting the high momentum terms at some momentum cutoff Λ and making NRQCD an effective field theory that has to be matched to QCD [3, p. 8-9]. This will be discussed more in detail once we have done the power series expansion of the Lagrangian.

First let's consider the heavy quark part of the Lagrangian. It will be helpful to write the corresponding fermion field as

$$\Psi = e^{-iMc^2t}\tilde{\Psi} = e^{-iMc^2t} \begin{pmatrix} \psi \\ \chi \end{pmatrix}. \quad (2.2)$$

We want to write the Lagrangian in terms of the field ψ that will be identified with the heavy quark field. This can be done with the help of the Dirac equation [5, p. 102]

$$(i\gamma^\mu D_\mu - Mc)\Psi = 0. \quad (2.3)$$

Substituting the field (2.2) into the Dirac equation we get

$$e^{-iMc^2t} \left(i\gamma^j D_j + \frac{i}{c}\gamma^0 D_t - Mc + Mc\gamma^0 \right) \tilde{\Psi} = 0. \quad (2.4)$$

We can now use the Dirac-Pauli representation of the gamma matrices [5, p. 111]

$$\gamma^0 = \begin{pmatrix} \mathbb{1} & 0 \\ 0 & -\mathbb{1} \end{pmatrix} \quad \gamma^i = \begin{pmatrix} 0 & \sigma^i \\ -\sigma^i & 0 \end{pmatrix} \quad \gamma^5 = \begin{pmatrix} 0 & \mathbb{1} \\ \mathbb{1} & 0 \end{pmatrix} \quad (2.5)$$

to write this as

$$\begin{pmatrix} \frac{i}{c}D_t & i\sigma^j D_j \\ -i\sigma^j D_j & -\frac{i}{c}D_t - 2Mc \end{pmatrix} \begin{pmatrix} \psi \\ \chi \end{pmatrix} = \begin{pmatrix} \frac{i}{c}D_t\psi + i\sigma^j D_j\chi \\ -i\sigma^j D_j\psi - \left(\frac{i}{c}D_t + 2Mc\right)\chi \end{pmatrix} = 0. \quad (2.6)$$

From the lower equation we can solve the χ field:

$$\chi = \frac{1}{\frac{i}{c}D_t + 2Mc} (-i\sigma^j D_j)\psi. \quad (2.7)$$

The operator iD_t here corresponds to the difference $E - Mc^2$ because of the field redefinition (2.2). The energy of the quark is always bigger than the mass, which means that the operator iD_t acting on ψ gives a positive number. Therefore the solution (2.7) for the χ field is sensible as the denominator is always non-zero. Also, because the momentum is small we have $\frac{i}{c}D_t = E/c - Mc \approx Mc \cdot \mathcal{O}((P/Mc)^2) \ll 2Mc$. This allows us to write

$$\frac{1}{\frac{i}{c}D_t + 2Mc} = \frac{1}{2Mc} \left(1 - \frac{i}{2Mc^2} D_t + \mathcal{O}(1/c^3) \right). \quad (2.8)$$

Substituting now (2.2), (2.7) and (2.8) into the heavy quark Lagrangian (2.1) we

get

$$\begin{aligned}
c\mathcal{L}_{\text{quark}} &= c \begin{pmatrix} \psi^\dagger & -\chi^\dagger \end{pmatrix} \left(i\gamma^\mu D_\mu + (\gamma^0 - 1)Mc \right) \begin{pmatrix} \psi \\ \chi \end{pmatrix} \\
&= c\psi^\dagger \begin{pmatrix} 1 & i\sigma^i D_i \frac{1}{\frac{i}{c}D_t + 2Mc} \end{pmatrix} \begin{pmatrix} \frac{i}{c}D_t & i\sigma^j D_j \\ -i\sigma^j D_j & -\frac{i}{c}D_t - 2Mc \end{pmatrix} \begin{pmatrix} 1 \\ \frac{1}{\frac{i}{c}D_t + 2Mc} (-i\sigma^k D_k) \end{pmatrix} \psi \\
&= \psi^\dagger iD_t \psi - \psi^\dagger i\sigma^i D_i \frac{c}{\frac{i}{c}D_t + 2Mc} i\sigma^k D_k \psi \\
&= \psi^\dagger iD_t \psi - \psi^\dagger i\sigma^i D_i \frac{1}{2M} \left(1 - \frac{i}{2Mc^2} D_t \right) i\sigma^k D_k \psi + \mathcal{O}(1/c^3) \\
&= \psi^\dagger iD_t \psi + \frac{1}{2M} \psi^\dagger \sigma^i D_i \sigma^j D_j \psi - \frac{i}{4M^2 c^2} \psi^\dagger \sigma^i D_i D_t \sigma^j D_j \psi + \mathcal{O}(1/c^3).
\end{aligned} \tag{2.9}$$

We can now use the identity

$$\sigma^i \sigma^j = \delta^{ij} + i\epsilon^{ijk} \sigma^k \tag{2.10}$$

to calculate

$$\sigma^i D_i \sigma^j D_j = \left(\delta^{ij} + i\epsilon^{ijk} \sigma^k \right) D_i D_j = \delta^{ij} D_i D_j + \frac{i}{2} \sigma^k \epsilon^{ijk} [D_i, D_j] = \mathbf{D}^2 + \frac{g}{c} \boldsymbol{\sigma} \cdot \mathbf{B} \tag{2.11}$$

where

$$B^k = -\frac{1}{2} \epsilon^{ijk} G_{ij} = -\frac{c}{g} \frac{1}{2} \epsilon^{ijk} [D_i, D_j] \tag{2.12}$$

is the strong interaction equivalent of the magnetic field. Here

$$G_{\mu\nu} = -\frac{ic}{g} [D_\mu, D_\nu] \tag{2.13}$$

is the gluon field strength tensor [6, p. 2]. Similarly, we define

$$E^j = G^{j0} = \frac{c}{g} \left[\frac{1}{c} D_t, D^j \right] \tag{2.14}$$

to correspond to the electric field in QCD. Note that the units of \mathbf{E} and \mathbf{B} fields defined here are the same, which would correspond to Gaussian units in the standard electromagnetic definitions. This choice here has been made to make sure that the fields have similar effect with respect to the power counting in $1/c$. Using the

definition (2.14) we get

$$\begin{aligned}\sigma^i \sigma^j D_i [D_t, D_j] &= (\delta^{ij} + \epsilon^{ijk} \sigma^k) D_i (-g_i) E_j = -g_i (\delta^{ij} D_i E_j + \epsilon^{ijk} \sigma^k D_i E_j) \\ &= g_i (\mathbf{D} \cdot \mathbf{E} + i \boldsymbol{\sigma} \cdot \mathbf{D} \times \mathbf{E}).\end{aligned}\quad (2.15)$$

The signs in the last equality follow from the definitions $\mathbf{D} = D_j$ and $\mathbf{E} = E^j$. In the same way,

$$\sigma^i \sigma^j [D_t, D_i] D_j = (\delta^{ij} + \epsilon^{ijk} \sigma^k) (-g_i) E_i D_j = g_i (\mathbf{E} \cdot \mathbf{D} + i \boldsymbol{\sigma} \cdot \mathbf{E} \times \mathbf{D}).\quad (2.16)$$

Now we can write the Lagrangian (2.9) as

$$\begin{aligned}c\mathcal{L}_{\text{quark}} &= \psi^\dagger i D_t \psi + \frac{1}{2M} \psi^\dagger \sigma^i D_i \sigma^j D_j \psi \\ &\quad - \frac{i}{8M^2 c^2} \psi^\dagger \sigma^i \sigma^j \left(D_i [D_t, D_j] - [D_t, D_i] D_j + \{D_i D_j, D_t\} \right) \psi + \mathcal{O}(1/c^3) \\ &= \psi^\dagger \left(i D_t - \frac{1}{2M} (i \mathbf{D})^2 \right) \psi + \frac{g}{2Mc} \psi^\dagger \boldsymbol{\sigma} \cdot \mathbf{B} \psi \\ &\quad + \frac{g}{8M^2 c^2} \psi^\dagger \left(\mathbf{D} \cdot \mathbf{E} - \mathbf{E} \cdot \mathbf{D} + i \boldsymbol{\sigma} \cdot \mathbf{D} \times \mathbf{E} - i \boldsymbol{\sigma} \cdot \mathbf{E} \times \mathbf{D} \right) \psi^\dagger \\ &\quad - \frac{i}{8M^2 c^2} \psi^\dagger \sigma^i \sigma^j \{D_i D_j, D_t\} \psi + \mathcal{O}(1/c^3).\end{aligned}\quad (2.17)$$

We would like the time derivative to appear only in the first term of the Lagrangian (2.17) or in the field \mathbf{E} . This can be achieved by the following field redefinition:

$$\psi = \left(1 + \frac{A^2}{8M^2 c^2} \right) \psi' \quad (2.18)$$

where $A = \sigma^i D_i$. From this definition of A we notice that

$$A^\dagger = \sigma^i D_i^\dagger = \sigma^i (-D_i) = -A \quad (2.19)$$

and using (2.11) we get

$$A^2 = \sigma^i \sigma^j D_i D_j = \mathbf{D}^2 + \mathcal{O}(1/c). \quad (2.20)$$

The Lagrangian then becomes

$$\begin{aligned}
c\mathcal{L}_{\text{quark}} &= \psi'^{\dagger} \left(iD_t - \frac{1}{2M} (i\mathbf{D})^2 \right) \psi' - \frac{i}{8M^2c^2} \psi'^{\dagger} \{A^2, D_t\} \psi' + \frac{g}{2Mc} \psi'^{\dagger} \boldsymbol{\sigma} \cdot \mathbf{B} \psi' \\
&\quad + \frac{g}{8M^2c^2} \psi'^{\dagger} (\mathbf{D} \cdot \mathbf{E} - \mathbf{E} \cdot \mathbf{D} + i\boldsymbol{\sigma} \cdot \mathbf{D} \times \mathbf{E} - i\boldsymbol{\sigma} \cdot \mathbf{E} \times \mathbf{D}) \\
&\quad + \frac{1}{8M^2c^2} \psi'^{\dagger} \left(iD_t A^2 + iA^2 D_t - \frac{1}{2M} (i\mathbf{D})^2 A^2 - \frac{1}{2M} A^2 (i\mathbf{D})^2 \right) \psi' + \mathcal{O}(1/c^3) \\
&= \psi'^{\dagger} \left(iD_t - \frac{1}{2M} (i\mathbf{D})^2 \right) \psi' + \frac{g}{2Mc} \psi'^{\dagger} \boldsymbol{\sigma} \cdot \mathbf{B} \psi' \\
&\quad + \frac{g}{8M^2c^2} \psi'^{\dagger} (\mathbf{D} \cdot \mathbf{E} - \mathbf{E} \cdot \mathbf{D} + i\boldsymbol{\sigma} \cdot \mathbf{D} \times \mathbf{E} - i\boldsymbol{\sigma} \cdot \mathbf{E} \times \mathbf{D}) \\
&\quad + \frac{1}{8M^3c^2} \psi'^{\dagger} (\mathbf{D}^2)^2 \psi' + \mathcal{O}(1/c^3)
\end{aligned} \tag{2.21}$$

This is the part of the Lagrangian corresponding to the quark field.

We can calculate the antiquark part similarly. We write the antiquark field as

$$\Psi = e^{iMc^2t} \tilde{\Psi} = e^{iMc^2t} \begin{pmatrix} \psi \\ \chi \end{pmatrix} \tag{2.22}$$

which differs from (2.2) by the sign in the exponent. This time, we want to identify the field χ with the antiquark. The Dirac equation becomes now

$$e^{iMc^2t} \left(i\gamma^j D_j + \frac{i}{c} \gamma^0 D_t - Mc - Mc\gamma^0 \right) \tilde{\Psi} = 0, \tag{2.23}$$

and in matrix form

$$\begin{pmatrix} \frac{i}{c} D_t - 2Mc & i\sigma^j D_j \\ -i\sigma^j D_j & -\frac{i}{c} D_t \end{pmatrix} \begin{pmatrix} \psi \\ \chi \end{pmatrix} = \begin{pmatrix} \left(\frac{i}{c} D_t - 2Mc \right) \psi + i\sigma^j D_j \chi \\ -i\sigma^j D_j \psi - \frac{i}{c} D_t \chi \end{pmatrix} = 0. \tag{2.24}$$

This is the same as (2.6) with the substitutions $\psi \rightarrow \chi$ and $M \rightarrow -M$, which allows us to infer from equation (2.7) that we must have

$$\psi = \frac{1}{-\frac{i}{c} D_t + 2Mc} i\sigma^j D_j \chi. \tag{2.25}$$

For the antiquark, $-iD_t$ corresponds to the kinetic energy so that the denominator of equation (2.25) is again positive. Substituting equations (2.22) and (2.25) into

the Lagrangian (2.1) we get

$$\begin{aligned}
c\mathcal{L}_{\text{antiquark}} &= c \begin{pmatrix} \psi^\dagger & -\chi^\dagger \end{pmatrix} (i\gamma^\mu D_\mu - (\gamma^0 + 1)Mc) \begin{pmatrix} \psi \\ \chi \end{pmatrix} \\
&= c\chi^\dagger \begin{pmatrix} i\sigma^i D_i \frac{1}{-\frac{i}{c}D_t + 2Mc} & -1 \end{pmatrix} \begin{pmatrix} \frac{i}{c}D_t - 2Mc & i\sigma^j D_j \\ -i\sigma^j D_j & -\frac{i}{c}D_t \end{pmatrix} \begin{pmatrix} -\frac{1}{\frac{i}{c}D_t + 2Mc} (i\sigma^k D_k) \\ 1 \end{pmatrix} \chi \\
&= \chi^\dagger iD_t \chi - \chi^\dagger i\sigma^i D_i \frac{c}{\frac{i}{c}D_t - 2Mc} i\sigma^k D_k \chi
\end{aligned} \tag{2.26}$$

Again, this is the same as (2.9) with $\psi \rightarrow \chi$ and $M \rightarrow -M$ so we can deduce the antiquark part of the Lagrangian from (2.21):

$$\begin{aligned}
c\mathcal{L}_{\text{antiquark}} &= \chi'^\dagger \left(iD_t + \frac{1}{2M} (i\mathbf{D})^2 \right) \chi' - \frac{g}{2Mc} \chi'^\dagger \boldsymbol{\sigma} \cdot \mathbf{B} \chi' \\
&\quad + \frac{g}{8M^2 c^2} \chi'^\dagger (\mathbf{D} \cdot \mathbf{E} - \mathbf{E} \cdot \mathbf{D} + i\boldsymbol{\sigma} \cdot \mathbf{D} \times \mathbf{E} - i\boldsymbol{\sigma} \cdot \mathbf{E} \times \mathbf{D}) \\
&\quad - \frac{1}{8M^3 c^2} \chi'^\dagger (\mathbf{D}^2)^2 \chi' + \mathcal{O}(1/c^3)
\end{aligned} \tag{2.27}$$

where we have scaled the antiquark field by

$$\chi = \left(1 + \frac{A^2}{8M^2 c^2} \right) \chi'. \tag{2.28}$$

Summing the Lagrangians (2.21) and (2.27) and suppressing the primes we can now write the full heavy quark Lagrangian:

$$\begin{aligned}
c\mathcal{L}_{\text{heavy}} &= \psi^\dagger \left(iD_t - \frac{1}{2M} (i\mathbf{D})^2 \right) \psi + \frac{g}{2Mc} \psi^\dagger \boldsymbol{\sigma} \cdot \mathbf{B} \psi + \frac{1}{8M^3 c^2} \psi^\dagger (\mathbf{D}^2)^2 \psi \\
&\quad + \frac{g}{8M^2 c^2} \psi^\dagger (\mathbf{D} \cdot \mathbf{E} - \mathbf{E} \cdot \mathbf{D}) \psi + \frac{ig}{8M^2 c^2} \psi^\dagger (\boldsymbol{\sigma} \cdot \mathbf{D} \times \mathbf{E} - \boldsymbol{\sigma} \cdot \mathbf{E} \times \mathbf{D}) \psi \\
&\quad + \chi^\dagger \left(iD_t + \frac{1}{2M} (i\mathbf{D})^2 \right) \chi - \frac{g}{2Mc} \chi^\dagger \boldsymbol{\sigma} \cdot \mathbf{B} \chi - \frac{1}{8M^3 c^2} \chi^\dagger (\mathbf{D}^2)^2 \chi \\
&\quad + \frac{g}{8M^2 c^2} \chi^\dagger (\mathbf{D} \cdot \mathbf{E} - \mathbf{E} \cdot \mathbf{D}) \chi + \frac{ig}{8M^2 c^2} \chi^\dagger (\boldsymbol{\sigma} \cdot \mathbf{D} \times \mathbf{E} - \boldsymbol{\sigma} \cdot \mathbf{E} \times \mathbf{D}) \chi \\
&\quad + \mathcal{O}\left(\frac{1}{c^3}\right).
\end{aligned} \tag{2.29}$$

The Lagrangian (2.29) shows the most important terms of the heavy quark Lagrangian.

However, as was discussed earlier the separation of the quarks and antiquarks makes NRQCD an effective field theory that has to be matched to QCD [7]. Therefore each of the terms in (2.29) may have a coefficient that depends on α_s . Setting now $c = 1$ and writing these coefficients, the heavy quark Lagrangian in NRQCD is

$$\begin{aligned}
\mathcal{L}_{\text{heavy}} = & \psi^\dagger \left(iD_t + \frac{1}{2M} \mathbf{D}^2 \right) \psi + \chi^\dagger \left(iD_t - \frac{1}{2M} \mathbf{D}^2 \right) \chi \\
& + \frac{c_1}{8M^3} \left(\psi^\dagger (\mathbf{D}^2)^2 \psi - \chi^\dagger (\mathbf{D}^2)^2 \chi \right) \\
& + \frac{c_2}{8M^2} \left(\psi^\dagger (\mathbf{D} \cdot g\mathbf{E} - g\mathbf{E} \cdot \mathbf{D}) \psi + \chi^\dagger (\mathbf{D} \cdot g\mathbf{E} - g\mathbf{E} \cdot \mathbf{D}) \chi \right) \\
& + \frac{c_3}{8M^2} \left(\psi^\dagger (\boldsymbol{\sigma} \cdot i\mathbf{D} \times g\mathbf{E} - \boldsymbol{\sigma} \cdot g\mathbf{E} \times i\mathbf{D}) \psi \right. \\
& \left. + \chi^\dagger (\boldsymbol{\sigma} \cdot i\mathbf{D} \times g\mathbf{E} - \boldsymbol{\sigma} \cdot g\mathbf{E} \times i\mathbf{D}) \chi \right) + \frac{c_4}{2M} \left(\psi^\dagger \boldsymbol{\sigma} \cdot g\mathbf{B} \psi - \chi^\dagger \boldsymbol{\sigma} \cdot g\mathbf{B} \chi \right).
\end{aligned} \tag{2.30}$$

The first term iD_t in the Lagrangian (2.30) doesn't need to have a coefficient as it can be set to one by field redefinitions similar to (2.18) and (2.28). The term $\mathbf{D}^2/(2M)$ also doesn't have a coefficient because we want to define the mass parameter M to be the coefficient of this term. This is so because then the energy of the quark has the same expansion $E = M + \mathbf{p}^2/(2M) + \dots$ in both NRQCD and QCD and therefore we can identify the mass M with the pole mass M_{pole} in the QCD propagator, as argued in reference [3, p. 11]. The rest of coefficients need to be matched by calculating physical quantities in both QCD and NRQCD. They go as $c_i = 1 + \mathcal{O}(\alpha_s)$ [8], which shows that the Lagrangian (2.29) we derived is correct at the lowest order. As mentioned in reference [4] each of the correction terms has a physical interpretation. The c_1 term is the first relativistic correction to the energy of the particle, the c_2 term is equivalent to the Darwin term in the fine structure of the hydrogen atom, the c_3 term corresponds to the spin-orbit coupling, and the c_4 term arises from the QCD magnetic moment interaction.

The whole NRQCD Lagrangian can be written as

$$\mathcal{L}_{\text{NRQCD}} = \mathcal{L}_{\text{light}} + \mathcal{L}_{\text{gluon}} + \mathcal{L}_{\text{heavy}} \tag{2.31}$$

where

$$\mathcal{L}_{\text{light}} = \bar{\Psi}_{\text{light}} i \not{D} \Psi_{\text{light}} \tag{2.32}$$

is the part concerning the light quarks u , d and s , and

$$\mathcal{L}_{\text{gluon}} = -\frac{1}{2} \text{tr} G_{\mu\nu} G^{\mu\nu} \quad (2.33)$$

is the contribution of the gluon fields. The masses of the light quarks have been neglected in equation (2.32) as they are much smaller than the heavy quark masses. The gluon field can be written as

$$\begin{aligned} G_{\mu\nu} &= -\frac{i}{g} [D_\mu, D_\nu] = -\frac{i}{g} [\partial_\mu + igA_\mu, \partial_\nu + igA_\nu] = \partial_\mu A_\nu - \partial_\nu A_\mu + ig[A_\mu, A_\nu] \\ &\stackrel{A_\mu = A_\mu^a t^a}{=} (\partial_\mu A_\nu^a - \partial_\nu A_\mu^a) t^a + ig A_\mu^b A_\nu^c [t^b, t^c] \\ &= \underbrace{(\partial_\mu A_\nu^a - \partial_\nu A_\mu^a - gf^{abc} A_\mu^b A_\nu^c)}_{G_{\mu\nu}^a} t^a = G_{\mu\nu}^a t^a. \end{aligned} \quad (2.34)$$

Here t^a are the standard basis of the fundamental representation of $\text{SU}(N_c)$, where N_c is the number of colors [9, p. 502]. Substituting this into the gluon Lagrangian we get

$$\begin{aligned} \mathcal{L}_{\text{gluon}} &= -\frac{1}{2} \text{tr} G_{\mu\nu} G^{\mu\nu} = -\frac{1}{2} G_{\mu\nu}^a G^{\mu\nu,b} \text{tr} \{t^a t^b\} = -\frac{1}{2} G_{\mu\nu}^a G^{\mu\nu,b} \frac{1}{2} \delta^{ab} = -\frac{1}{4} G_{\mu\nu}^a G^{\mu\nu,a} \\ &= -\frac{1}{4} (\partial_\mu A_\nu^a - \partial_\nu A_\mu^a - gf^{abc} A_\mu^b A_\nu^c) (\partial^\mu A^{\nu,a} - \partial^\nu A^{\mu,a} - gf^{ade} A^{\mu,d} A^{\nu,e}) \\ &= -\frac{1}{2} (\partial_\mu A_\nu^a \partial^\mu A^{\nu,a} - \partial_\mu A_\nu^a \partial^\nu A^{\mu,a}) + gf^{abc} (\partial_\mu A_\nu^a) A^{\mu,b} A^{\nu,c} \\ &\quad - \frac{1}{4} g^2 f^{abc} f^{ade} A_\mu^b A_\nu^c A^{\mu,d} A^{\nu,e}. \end{aligned} \quad (2.35)$$

2.2 Velocity-scaling rules

We want to estimate how big the expectation values of the operators are to deduce which terms are more relevant than others. It is possible to write how these estimates are related to the powers of the quark velocity v , and these are called the velocity-scaling rules of the operators. The velocity-scaling rules can be calculated from the self-consistency of the field equations corresponding to the NRQCD Lagrangian (2.29) as described in reference [8]. We will follow this derivation of the velocity-scaling rules here.

First of all, we only need to consider the lowest order terms in $1/c$ and the gluon field. We can also leave the antiquark part of the Lagrangian out as the velocity-scaling will be the same for both quarks and antiquarks. This can be seen from the fact that the NRQCD Lagrangian (2.30) is similar for quarks and antiquarks. This means that we can focus on the field equations calculated using the following Lagrangian:

$$\mathcal{L} = \psi^\dagger \left(iD_t + \frac{1}{2M} \mathbf{D}^2 \right) \psi - \frac{1}{2} \text{tr} G_{\mu\nu} G^{\mu\nu} \quad (2.36)$$

It is easier to do the calculations in the Coulomb gauge where $\nabla \cdot \mathbf{A}^a = 0$. Then we get

$$\begin{aligned} \mathcal{L} &= \psi^\dagger \left(i\partial_t - gA_0^a t^a + \frac{1}{2M} \nabla^2 + \frac{ig}{2M} (t^a \mathbf{A}^a + t^b \mathbf{A}^b) \cdot \nabla - \frac{g^2}{2M} \mathbf{A}^a \cdot \mathbf{A}^b t^a t^b \right) \psi \\ &\quad - \frac{1}{2} \text{tr} G_{\mu\nu} G^{\mu\nu} \\ &= \psi^\dagger i\partial_t \psi - gA_0^a \psi^\dagger t^a \psi + \frac{1}{2M} \psi^\dagger \nabla^2 \psi + \frac{ig}{M} \psi^\dagger t^a \mathbf{A}^a \cdot \nabla \psi - \frac{g^2}{2M} \mathbf{A}^a \cdot \mathbf{A}^b \psi^\dagger t^a t^b \psi \\ &\quad - \frac{1}{2} (\partial_\mu A_\nu^a \partial^\mu A^{\nu,a} - \partial_\mu A_\nu^a \partial^\nu A^{\mu,a}) + g f^{abc} (\partial_\mu A_\nu^a) A^{\mu,b} A^{\nu,c} \\ &\quad - \frac{1}{4} g^2 f^{abc} f^{ade} A_\mu^b A_\nu^c A^{\mu,d} A^{\nu,e} \end{aligned} \quad (2.37)$$

For a moment, we will consider the Hamiltonian field equations that can be derived from the Lagrangian. The Hamiltonian density is defined by [10, p. 34]

$$\mathcal{H} = \sum_{\text{fields}} \pi^i \frac{\partial \mathcal{L}}{\partial \dot{\pi}^i} - \mathcal{L} \quad (2.38)$$

where

$$\pi = \frac{\partial \mathcal{L}}{\partial \dot{\phi}} \quad (2.39)$$

is the conjugate momentum density of the field ϕ . Here we have used the notation $\dot{\phi} = \partial_0 \phi$. The Hamiltonian field equations

$$\dot{\pi} = -\frac{\delta \mathcal{H}}{\delta \phi} \quad \dot{\phi} = +\frac{\delta \mathcal{H}}{\delta \pi} \quad (2.40)$$

give us a set of equations equivalent to the Lagrangian field equations [10, p. 35]. In

equations (2.40) one must use the functional derivative

$$\frac{\delta}{\delta\phi} = \frac{\partial}{\partial\phi} - \partial_\mu \frac{\partial}{\partial(\partial_\mu\phi)}. \quad (2.41)$$

The NRQCD Lagrangian (2.31) doesn't depend on $\partial_0 A^0$, as can be seen by considering the parts $\mathcal{L}_{\text{light}}$, $\mathcal{L}_{\text{gluon}}$ and $\mathcal{L}_{\text{heavy}}$ separately. Therefore the conjugate momentum density of A^0 is

$$\pi^0 = \frac{\partial\mathcal{L}}{\partial\dot{A}^0} = 0 \quad (2.42)$$

This is an important result, as the vanishing of the conjugate momentum π^0 tells us that there are no dynamical particles created by A^0 and therefore gluons are created and annihilated by the vector potential \mathbf{A} . The vanishing of the conjugate momentum π^0 also tells us that the Hamiltonian doesn't depend on π^0 . Using this fact we can calculate from the second Hamiltonian field equation (2.40) the time derivative of the scalar potential A^0 :

$$\partial_0 A^0 = \frac{\delta\mathcal{H}}{\delta\pi^0} = 0. \quad (2.43)$$

We can use this result to simplify the field equations.

Let's now turn to the field equations. First of all, we can approximate the strength of the field ψ by considering the expectation value of the heavy quark number operator

$$\left\langle H \left| \int d^3x \psi^\dagger \psi \right| H \right\rangle \approx 1 \quad (2.44)$$

where H is a quarkonium state. This result follows from the fact that for quarkonium the dominating Fock state is $|Q\bar{Q}\rangle$ and the quarkonium state is normalized by $\langle H|H\rangle = 1$. Because the quarkonium is localized to the volume $1/P^3 \approx 1/(Mv)^3$ we get $\psi^\dagger\psi = \mathcal{O}(M^3v^3)$.

Next we can consider the kinetic energy term of the Lagrangian, $\mathbf{D}^2/(2M)$. For this we have the estimate

$$\left\langle H \left| \int d^3x \psi^\dagger \frac{\mathbf{D}^2}{2M} \psi \right| H \right\rangle \approx Mv^2 \quad (2.45)$$

from which it follows that $\mathbf{D} = \mathcal{O}(Mv)$. This is exactly what we would expect from the identification of $-i\mathbf{D}$ as the momentum operator.

The field equation for the field ψ from the Lagrangian (2.36) is

$$\frac{\partial \mathcal{L}}{\partial \psi^\dagger} - \partial_\mu \frac{\partial \mathcal{L}}{\partial (\partial_\mu \psi^\dagger)} = \left(iD_t + \frac{1}{2M} \mathbf{D}^2 \right) \psi = 0. \quad (2.46)$$

This means that D_t must scale as $\mathbf{D}^2/(2M)$ which gives us $D_t = \mathcal{O}(Mv^2)$.

For now, we will assume that the scalar potential A^0 will have a larger contribution than the vector potential \mathbf{A} . This will simplify our equations as we can drop the higher order terms with the vector potential. We will confirm later that this assumption is valid after we have found the velocity-scaling rules for the gluon fields. With this assumption, we can expand equation (2.46) as

$$\left(i\partial_0 - gA_0^a t^a + \frac{1}{2M} \nabla^2 \right) \psi = 0. \quad (2.47)$$

The scaling of gA^0 cannot be faster than the other terms. Therefore we must have $gA^0 = \mathcal{O}(Mv^2)$. The field equation for A^0 is, dropping again the vector potential terms,

$$\begin{aligned} & \frac{\partial \mathcal{L}}{\partial A_0^a} - \partial_\mu \frac{\partial \mathcal{L}}{\partial (\partial_\mu A_0^a)} \\ &= -g\psi^\dagger t^a \psi + \partial_\mu \partial^\mu A^{0,a} - \partial_\mu \partial^0 A^{\mu,a} \\ & \quad - g f^{abc} \left(A^{\nu,c} \partial^0 A_\nu^b + A^{\mu,b} \partial_\mu A^{0,c} + \partial_\mu (A^{\mu,b} A^{0,c}) \right) + g^2 f^{bac} f^{bde} A_\mu^c A^{\mu,d} A^{0,e} \\ &= -g\psi^\dagger t^a \psi - \nabla^2 A^{0,a} \\ & \quad - g f^{abc} \left(A^{\nu,c} \partial^0 A_\nu^b + 2A^{\mu,b} \partial_\mu A^{0,c} + A^{0,c} \partial_0 A^{0,b} \right) + g^2 f^{bac} f^{bde} A_\mu^c A^{\mu,d} A^{0,e} \\ & \stackrel{(*)}{=} -g\psi^\dagger t^a \psi - \nabla^2 A^{0,a} - g f^{abc} \left(A^{i,c} \partial^0 A_i^b + 2A^{i,b} \partial_i A^{c,0} \right) + g^2 f^{bac} f^{bde} A_i^c A^{i,d} A^{0,e} \\ & \approx -g\psi^\dagger t^a \psi - \nabla^2 A^{0,a} = 0 \end{aligned} \quad (2.48)$$

where in (*) we have used the antisymmetry of f^{abc} . From this we see that on the other hand $gA^0 = \mathcal{O}(g^2(Mv)^3/(Mv)^2) = \mathcal{O}(g^2 Mv)$, assuming that the gradient operating on A^0 scales as Mv . This assumption corresponds to the assumption that the gluons have a momentum of order Mv which is the momentum scale for quarks and antiquarks. Comparing this with our previous estimate for gA^0 we see that $g^2 = \mathcal{O}(v)$ and therefore $\alpha_s = g^2/(4\pi) = \mathcal{O}(v)$ at the momentum scales of the quarkonium. It should be noted that in general the magnitude of α_s depends on the

momentum scale. For example, in reference [3, p. 13] it is estimated that $\alpha_s(Mv^2)$ is of order 1. For our purposes the important momentum scale is the momentum of the quarks and antiquarks Mv and for that we can estimate $\alpha_s(Mv) = \mathcal{O}(v)$.

The field equation for A^i is

$$\begin{aligned}
& \frac{\partial \mathcal{L}}{\partial A_i^a} - \partial_\mu \frac{\partial \mathcal{L}}{\partial (\partial_\mu A_i^a)} \\
&= \frac{ig}{M} \psi^\dagger t^a \nabla^i \psi - \frac{g^2}{2M} \mathbf{A}^{i,b} \psi^\dagger \{t^a, t^b\} \psi + \partial_\mu \partial^\mu A^{i,a} - \partial_\mu \partial^i A^{\mu,a} \\
&\quad - g f^{abc} \left(A^{\nu,c} \partial^i A_\nu^b + A^{\mu,b} \partial_\mu A^{i,c} + \partial_\mu (A^{\mu,b} A^{i,c}) \right) + g^2 f^{bac} f^{bde} A_\mu^c A^{\mu,d} A^{i,e} \\
&= \frac{ig}{M} \psi^\dagger t^a \nabla^i \psi - \frac{g^2}{2M} \mathbf{A}^{i,b} \psi^\dagger \{t^a, t^b\} \psi + \partial_\mu \partial^\mu A^{i,a} \\
&\quad - g f^{abc} \left(A^{\nu,c} \partial^i A_\nu^b + 2A^{\mu,b} \partial_\mu A^{i,c} + A^{i,c} \partial_j A^{j,b} \right) + g^2 f^{bac} f^{bde} A_\mu^c A^{\mu,d} A^{i,e} \\
&\approx \frac{ig}{M} \psi^\dagger t^a \nabla^i \psi - \frac{g^2}{2M} \mathbf{A}^{i,b} \psi^\dagger \{t^a, t^b\} \psi + \partial_\mu \partial^\mu A^{i,a} - g f^{abc} A^{0,c} \partial^i A_0^b = 0.
\end{aligned} \tag{2.49}$$

After multiplying this equation by g , the orders of the terms are $M^3 v^5$, $g A^i M^2 v^4$, $g A^i M^2 v^2$ and $M^3 v^5$, from left to right. This means that we must have $g A^i = \mathcal{O}(M v^3)$, which confirms the validity of our assumption $A^0 \gg A^i$. It should be noted that these scalings of A^0 and A^i were calculated only for the Coulomb gauge. Choosing a different gauge we would get a different scaling.

We can also deduce the velocity-scaling of the operators \mathbf{E} and \mathbf{B} . At the lowest order $g\mathbf{E} = -g\nabla A^0 = \mathcal{O}(M^2 v^3)$ and $g\mathbf{B} = \nabla \times g\mathbf{A} = \mathcal{O}(M^2 v^4)$. Even though the velocity-scaling of gA^0 and $g\mathbf{A}$ depends on the selected gauge, the fields $g\mathbf{E}$ and $g\mathbf{B}$ are gauge invariant and therefore the scaling of these operators doesn't depend on the selected gauge. With these, we have calculated the velocity-scaling rules for all of the operators needed. These are collected in table 1.

2.3 4-fermion operators

The NRQCD Lagrangian conserves the quark and antiquark numbers. To consider the decay of a quarkonium particle we need to include 4-fermion operators in the Lagrangian. These operators annihilate and create a quarkonium state and can be used through the optical theorem to examine the annihilation of the quarkonium. These operators cannot be arbitrary, however, as they need to satisfy certain symmetries of NRQCD. These symmetries are the gauge symmetry, rotational symmetry, phase symmetry of the heavy quark and antiquark operators, charge conjugation and

Table 1. Estimates for the magnitudes of the operators

Operator	Scaling
$\alpha_s(Mv)$	v
ψ	$(Mv)^{3/2}$
χ	$(Mv)^{3/2}$
D_t	Mv^2
\mathbf{D}	Mv
gA^0 (Coulomb gauge)	Mv^2
$g\mathbf{A}$ (Coulomb gauge)	Mv^3
$g\mathbf{E}$	M^2v^3
$g\mathbf{B}$	M^2v^4

parity [11]. This narrows down the possible operators to certain combinations of the quark and antiquark fields, spin matrices, color matrices, the covariant derivatives, and the \mathbf{E} and \mathbf{B} fields. The extra terms to the Lagrangian can be written as

$$\delta\mathcal{L} = \sum_{\text{dim}=6} \frac{f_i}{M^2} \mathcal{O}_i + \sum_{\text{dim}=8} \frac{f_i}{M^4} \mathcal{O}_i + \text{higher order} \quad (2.50)$$

where \mathcal{O}_i are the added operators and f_i are coefficients that have to be matched to QCD. The mass dimensions of the operators are matched with the powers of the quark mass so that the coefficients f_i are dimensionless. Note that there are no dimension 7 terms as these would violate the conservation of parity by the inclusion of a single covariant derivative in the term. These are also the operators with velocity-scaling up to v^8 , as according to table 1 each power of mass adds at least one power of velocity.

The possible dimension 6 operators are [3, p. 24]:

$$\begin{aligned} \mathcal{O}_1(^1S_0) &= \psi^\dagger \chi \chi^\dagger \psi & \mathcal{O}_1(^3S_1) &= \psi^\dagger \boldsymbol{\sigma} \chi \cdot \chi^\dagger \boldsymbol{\sigma} \psi \\ \mathcal{O}_8(^1S_0) &= \psi^\dagger t^a \chi \chi^\dagger t^a \psi & \mathcal{O}_8(^3S_1) &= \psi^\dagger \boldsymbol{\sigma} t^a \chi \cdot \chi^\dagger t^a \boldsymbol{\sigma} \psi, \end{aligned} \quad (2.51)$$

where the operators are understood to be normal-ordered. The naming of the operators is as follows: the subscripts 1 and 8 refer to color singlet and color octet operators, respectively. The color octet operators are given by the t^a matrices of the fundamental representation of $\text{SU}(N_c)$. The $^{2S+1}L_J$ part refers to the spin S , orbital angular momentum L and total angular momentum J quantum numbers of the $Q\bar{Q}$ state that the operator annihilates and creates. For example, the action of the

operator $\mathcal{O}_1(^1S_0)$ is non-vanishing only on the quarkonium state where the $Q\bar{Q}$ pair is in the color singlet with the quantum numbers 1S_0 .

At dimension 8, the number of possible operators is a lot larger. Our main interest is to study operators that act on $|Q\bar{Q}\rangle$ Fock states in the center-of-mass frame. Therefore we will list here the only dimension 8 operators that have a non-vanishing contribution to $Q\bar{Q}$ scattering in center-of-mass frame. These are [3, p. 25]:

$$\begin{aligned}
\mathcal{O}_1(^1P_1) &= \psi^\dagger \left(-\frac{i}{2} \overleftrightarrow{\mathbf{D}} \right) \chi \cdot \chi^\dagger \left(-\frac{i}{2} \overleftrightarrow{\mathbf{D}} \right) \psi \\
\mathcal{O}_1(^3P_0) &= \frac{1}{3} \psi^\dagger \left(-\frac{i}{2} \overleftrightarrow{\mathbf{D}} \cdot \boldsymbol{\sigma} \right) \chi \chi^\dagger \left(-\frac{i}{2} \overleftrightarrow{\mathbf{D}} \cdot \boldsymbol{\sigma} \right) \psi \\
\mathcal{O}_1(^3P_1) &= \frac{1}{2} \psi^\dagger \left(-\frac{i}{2} \overleftrightarrow{\mathbf{D}} \times \boldsymbol{\sigma} \right) \chi \cdot \chi^\dagger \left(-\frac{i}{2} \overleftrightarrow{\mathbf{D}} \times \boldsymbol{\sigma} \right) \psi \\
\mathcal{O}_1(^3P_2) &= \psi^\dagger \left(-\frac{i}{2} D^{(i\overleftrightarrow{\sigma}j)} \right) \chi \chi^\dagger \left(-\frac{i}{2} D^{(i\overleftrightarrow{\sigma}j)} \right) \psi \\
\mathcal{P}_1(^1S_0) &= \frac{1}{2} \left[\psi^\dagger \chi \chi^\dagger \left(-\frac{i}{2} \overleftrightarrow{\mathbf{D}} \right)^2 \psi + \text{h.c.} \right] \\
\mathcal{P}_1(^3S_1) &= \frac{1}{2} \left[\psi^\dagger \boldsymbol{\sigma} \chi \cdot \chi^\dagger \boldsymbol{\sigma} \left(-\frac{i}{2} \overleftrightarrow{\mathbf{D}} \right)^2 \psi + \text{h.c.} \right] \\
\mathcal{P}_1(^3S_1, ^3D_1) &= \frac{1}{2} \left[\psi^\dagger \sigma^i \chi \chi^\dagger \sigma^j \left(-\frac{i}{2} \right)^2 D^{(i\overleftrightarrow{\sigma}j)} \psi + \text{h.c.} \right]
\end{aligned} \tag{2.52}$$

Here we have defined the derivative operator

$$\chi^\dagger i \overleftrightarrow{\mathbf{D}} \psi = (i \mathbf{D} \chi)^\dagger \psi + \chi^\dagger (i \mathbf{D} \psi) \tag{2.53}$$

which is the only combination of derivatives that doesn't vanish in the center-of-mass frame. For example the derivative $(i \mathbf{D} \chi)^\dagger \psi - \chi^\dagger (i \mathbf{D} \psi)$ would be proportional to the total momentum of $Q\bar{Q}$ pair and therefore such a derivative doesn't contribute in the center-of-mass frame of the $Q\bar{Q}$ pair. However, a quarkonium particle may have contributions from states $|Q\bar{Q}g\rangle$ in which case the total momentum of $Q\bar{Q}$ pair doesn't vanish in the rest frame of the quarkonium. For such states other types of derivative operators could have non-vanishing contributions. We will talk about contributions of these kinds of states to the quarkonium in section 3 and see that they are suppressed by powers of velocity, meaning that omitting these terms is

justified. The notation $M^{(ij)}$ means the traceless symmetric tensor

$$M^{(ij)} = \frac{1}{2}(M^{ij} + M^{ji}) - \frac{1}{3}\delta^{ij}. \quad (2.54)$$

It should also be mentioned that the operator $\mathcal{P}_1({}^3S_1, {}^3D_1)$ is non-vanishing only for states with the initial quark-antiquark pair in 3S_1 state and the final state in 3D_1 or vice versa. In addition to the singlet operators (2.52) there are also the corresponding octet operators where the color matrices t^a are added between the quark and antiquark fields, similarly as with the dimension 6 operators in equation (2.51). These are then denoted by the subscript 8.

2.4 Field Operators

To do the actual calculations, we need to consider the field operators ψ and χ in more detail. First of all, we will use the non-relativistic normalization where the states are normalized by

$$\langle H(\mathbf{k}_1)|H(\mathbf{k}_2)\rangle = (2\pi)^3\delta(\mathbf{k}_1 - \mathbf{k}_2) \quad (2.55)$$

as opposed to the standard relativistic normalization where there is an extra factor $2E$. This is the standard normalization used in NRQCD and will be make comparing the results to the literature easier.

The field operators are defined as the solutions to the equations of motion from the free field Lagrangian. In our case we define the free field Lagrangian for the heavy quarks with the Lagrangian (2.29) where α_s has been set to zero. In this limit the covariant derivatives become standard partial derivatives that commute. This allows us to write the heavy quark part of the free Lagrangian at all orders using equations (2.9) and (2.26)

$$\begin{aligned} \mathcal{L}_0 &= \tilde{\psi}^\dagger i\partial_t \tilde{\psi} - \tilde{\psi}^\dagger i\sigma^i \partial_i \frac{1}{i\partial_t + 2M} i\sigma^k \partial_k \tilde{\psi} + \tilde{\chi}^\dagger i\partial_t \tilde{\chi} - \tilde{\chi}^\dagger i\sigma^i \partial_i \frac{1}{i\partial_t - 2M} i\sigma^k \partial_k \tilde{\chi} \\ &= \tilde{\psi}^\dagger i\partial_t \tilde{\psi} + \tilde{\psi}^\dagger \frac{1}{i\partial_t + 2M} \nabla^2 \tilde{\psi} + \tilde{\chi}^\dagger i\partial_t \tilde{\chi} + \tilde{\chi}^\dagger \frac{1}{i\partial_t - 2M} \nabla^2 \tilde{\chi} \end{aligned} \quad (2.56)$$

Here we denote the fields by $\tilde{\psi}$ and $\tilde{\chi}$ to remind us that the field redefinition (2.18) needs to be done, so that $\tilde{\psi} = (1 + \nabla^2/(8M^2))\psi$ and similarly for $\tilde{\chi}$. The field

equations are then

$$\left(i\partial_t + \frac{1}{i\partial_t + 2M}\nabla^2\right)\tilde{\psi} = 0 \quad \text{and} \quad \left(i\partial_t + \frac{1}{i\partial_t - 2M}\nabla^2\right)\tilde{\chi} = 0. \quad (2.57)$$

The actual fields ψ and χ also satisfy the same field equations as can be verified by opening $\tilde{\psi}$ and $\tilde{\chi}$. The solutions to the field equations can then be written as

$$\psi(x) = \int \frac{d^3\mathbf{q}}{(2\pi)^3} e^{-ix\cdot q + itM} \sum_{s,c} \xi_s \psi_{s,c}(\mathbf{q}) \quad (2.58)$$

and

$$\chi(x) = \int \frac{d^3\mathbf{q}}{(2\pi)^3} e^{ix\cdot q - itM} \sum_{s,c} \eta_s \chi_{s,c}(\mathbf{q}) \quad (2.59)$$

as can be seen by substituting these into the field equations (2.57). Here $\psi_{s,c}(\mathbf{q})$ is the quark annihilation operator, $\chi_{s,c}(\mathbf{q})$ is the antiquark creation operator and s and c are the spin and color indices, respectively. For the creation and annihilation operators we have the anticommutation relations defined by

$$\{\psi_{s_1,c_1}(\mathbf{q}_1), \psi_{s_2,c_2}^\dagger(\mathbf{q}_2)\} = (2\pi)^3 \delta^{s_1 s_2} \delta^{c_1 c_2} \delta(\mathbf{q}_1 - \mathbf{q}_2) \quad (2.60)$$

for the quark creation operator ψ^\dagger and

$$\{\chi_{s_1,c_1}^\dagger(\mathbf{q}_1), \chi_{s_2,c_2}(\mathbf{q}_2)\} = (2\pi)^3 \delta^{s_1 s_2} \delta^{c_1 c_2} \delta(\mathbf{q}_1 - \mathbf{q}_2) \quad (2.61)$$

for the antiquark creation operator χ , in similar way as in QCD. The quark and antiquark spinors ξ_s and η_s are defined here so that they both form an orthogonal basis. Their normalization is required to be $\eta_s^\dagger \eta_s = \chi_s^\dagger \chi_s = 1$ by the non-relativistic normalization convention (2.55). For the quark spinors it is most convenient to choose the basis as

$$\xi_\uparrow = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \quad \xi_\downarrow = \begin{pmatrix} 0 \\ 1 \end{pmatrix}. \quad (2.62)$$

These are the eigenvectors of the Pauli matrix σ^3 which means that they correspond to the spin up and down states in the z -direction. For the antiquark spinors we choose instead

$$\eta_\uparrow = \begin{pmatrix} 0 \\ -1 \end{pmatrix} \quad \eta_\downarrow = \begin{pmatrix} 1 \\ 0 \end{pmatrix}. \quad (2.63)$$

The reasoning behind this is that the charge conjugation symmetry requires us to have [9, p. 70]

$$\eta_s = i\sigma^2(\xi_s)^* \tag{2.64}$$

which gives us the definition (2.63).

3 Quarkonium States

3.1 Fock state expansion

Any quarkonium state vector can be written as a linear combination of states with the quark, antiquark and gluons. That is, a state for a particle H can be written schematically as

$$|H\rangle = c_{Q\bar{Q}}|Q\bar{Q}\rangle + c_{Q\bar{Q}g}|Q\bar{Q}g\rangle + c_{Q\bar{Q}gg}|Q\bar{Q}gg\rangle + \dots \quad (3.1)$$

We can estimate the contribution of each of these terms. The first term involving only the quark-antiquark pair should be the most dominant one. The contribution of the terms with additional gluons can be estimated by the energy shift of the quarkonium state that they produce. The quarkonium states are eigenstates of the Hamiltonian such that $\hat{H}|H\rangle = E_H|H\rangle$. On the other hand, the Hamiltonian can be divided into “free” and “interaction” parts such that $\hat{H} = \hat{H}_{\text{free}} + \hat{H}_I$. The free field Hamiltonian is the Hamiltonian corresponding to the free field Lagrangian (2.56), and the rest of the Hamiltonian is defined to be in the interaction part. Then we can write the expectation value of the energy as

$$E_H = \langle H|\hat{H}|H\rangle = \langle H|\hat{H}_{\text{free}}|H\rangle + \langle H|\hat{H}_I|H\rangle = \sum_{\text{Fock states}} E_i P_i + \langle H|\hat{H}_I|H\rangle \quad (3.2)$$

where E_i is the expectation value of the energy for the Fock state i , P_i is the probability of finding a state i in the quarkonium and we have also assumed that the states are normalized such that $\langle H|H\rangle = 1$. Now can write

$$\langle H|\hat{H}_I|H\rangle = E_H - \sum_{\text{Fock states}} E_i P_i = \sum_{\text{Fock states}} (E_H - E_i) P_i \quad (3.3)$$

so that each interaction term in the Hamiltonian contributes to the energy shift $\Delta E = \sum_{\text{Fock states}} E_i P_i - E_H$. We can estimate the total energy of the quarkonium by $E_H = 2M + \mathcal{O}(Mv^2)$ because it should be mainly given by the masses of the quark-antiquark pair and their kinetic energies.

As discussed in section 2.2, the gluons are created by the vector potential \mathbf{A} . This means that at leading order in v the gluons are produced by the term $(ig/M)\psi^\dagger \mathbf{A} \cdot \nabla \psi$ in the NRQCD Lagrangian (2.30). This kind of a term keeps the heavy quark spins unchanged, as it doesn't depend on the Pauli spin matrices that would cause a difference in spins between the Fock states. The contribution to the energy shift by this term is

$$\Delta E_{Q\bar{Q}g} = -\frac{ig}{M} \left\langle H \left| \int d^3x \psi^\dagger \mathbf{A} \cdot \nabla \psi \right| H \right\rangle = \mathcal{O}(Mv^4) \quad (3.4)$$

by the velocity-scaling rules of section 2.2. On the other hand, the energy shift can also be written as the product

$$\Delta E_{Q\bar{Q}g} = P_{Q\bar{Q}g} (E_{Q\bar{Q}g} - E_H) \quad (3.5)$$

and we can estimate the energy difference $E_{Q\bar{Q}g} - E_H$ to be of the order of the kinetic energy of the particles. In the case of a gluon with energy of order Mv , the kinetic energy of the gluon dominates and the probability must be $P_{Q\bar{Q}g} = \mathcal{O}(v^3)$ to agree with equation (3.4). In the case of gluons with low energy of order Mv^2 , the kinetic energy is $\mathcal{O}(Mv^2)$ and we have $P_{Q\bar{Q}g} = \mathcal{O}(v^2)$ instead. We then see that these low energy gluons are more dominant. This interaction creates or annihilates a gluon with orbital angular momentum $L = 1$, and it can be thought of as an analogue to the electric dipole transition E1 in nuclear physics. This kind of an interaction requires the orbital angular momentum of the $Q\bar{Q}$ pair to change by $\Delta L = \pm 1$ [11], and is called an *electric transition*.

These estimates only apply if the spin-states of the quark-antiquark pairs are the same both in Fock-states $Q\bar{Q}$ and $Q\bar{Q}g$. If the spin states are different, then the dominant term for gluon production is $(1/2M)\psi^\dagger \boldsymbol{\sigma} \cdot g\mathbf{B}\psi = (1/2M)\psi^\dagger \boldsymbol{\sigma} \cdot \nabla \times g\mathbf{A}\psi$. This term changes the spins of the $Q\bar{Q}$ pair by $\Delta S = \pm 1$ because of the Pauli spin matrix involved. For gluons with momenta of order Mv we can use the velocity-scaling rules from table 1 to estimate the energy shift caused by this term to be $\mathcal{O}(Mv^4)$. This tells us that the probability of finding the corresponding $|Q\bar{Q}g\rangle$ state is $P = \mathcal{O}(v^3)$.

For gluons with momenta of order $k = Mv^2$, however, the arguments for the velocity-scaling do not apply. We can determine the velocity-scaling of the vector potential \mathbf{A} corresponding to these gluons using a different reasoning. Gluons

with momentum Mv^2 have a wavelength of $1/(Mv^2)$ which is a lot larger than the separation between the quark-antiquark pair that is of order $r \approx 1/P \approx 1/(Mv)$. Therefore the gluon sees the $Q\bar{Q}$ -pair as a color dipole, and the interaction between the gluon and the $Q\bar{Q}$ -pair is proportional to the separation r . The interaction cannot depend on any other mass-dimensional parameter of the quarkonium as the gluon sees it as a color dipole. We can therefore write

$$\langle H | \psi^\dagger (g\mathbf{A})^2 \psi | H \rangle \approx f(k) \langle H | \psi^\dagger r^2 \psi | H \rangle \approx \frac{f(k)}{(Mv)^2} \quad (3.6)$$

where $f(k)$ is some function of the gluon's momentum. Here we have two powers of r , one from each gluon field, and the expectation value of r^2 can be approximated by $1/P^2$. On the other hand, we know that the gluon field $g\mathbf{A}$ has dimensions of mass so that the expectation value (3.6) has dimensions of mass squared. This means that we must have $f(k) \propto k^4 = M^2v^8$, as the gluon momentum k is the only mass-dimensional parameter it depends on. Therefore we get the estimate $g\mathbf{A} = \mathcal{O}(Mv^4/(Mv)) = \mathcal{O}(Mv^3)$ for gluons with momentum Mv^2 . Then we also get the estimate $\mathbf{B} = \mathcal{O}(k\mathbf{A}) = \mathcal{O}(M^2v^5)$ and $\Delta E_{Q\bar{Q}g} = \mathcal{O}(Mv^5)$. This means that for such a state we have the probability $P = \mathcal{O}(v^3)$. This is the same as for gluons with momenta $\mathcal{O}(Mv)$, so the probability is $P = \mathcal{O}(v^3)$ for the $Q\bar{Q}g$ state with the spin difference $\Delta S = \pm 1$ from the dominating $Q\bar{Q}$ state. In this case the orbital angular momentum of the $Q\bar{Q}$ pair doesn't change so that $\Delta L = 0$. This type of a transition is called a *magnetic transition*.

Of course, there are also states with a higher number of gluons and even with light quark pairs $q\bar{q}$ included in the Fock state expansion (3.1). However, these states can only be reached from the dominating $|Q\bar{Q}\rangle$ state by either higher order interaction terms or multiple transitions. This also applies to $Q\bar{Q}g$ states that differ by $\Delta L > 1$ from the dominating state. This means that they are suppressed even further by velocity. It is argued in [3, p. 18] that we can generalize the previous estimates for $Q\bar{Q}g$ states to even higher order Fock states by the multipole expansion. This means that we can estimate the probability of finding a state by considering how many electric and magnetic transitions we need to make to reach it from the dominating $Q\bar{Q}$ state. Each electric transition changes the quantum numbers of the $Q\bar{Q}$ pair by $\Delta L = \pm 1$ and $\Delta S = 0$ and adds a suppression factor of v^2 , while each magnetic transition changes the quantum numbers by $\Delta L = 0$ and $\Delta S = \pm 1$ and suppresses

the state by v^3 . In both of these transitions the color state of the pair can change, so that a color-singlet state always changes to a color-octet state while the color-octet may change either to a color-singlet or a color-octet state [11]. For example, if the dominating state is a $|^1S_0\rangle$ color-singlet state, the state $|^3P_1gg\rangle$ is suppressed by $v^{2+3} = v^5$ and the $Q\bar{Q}$ pair can be in either color-singlet or color-octet state.

There is one addition that has to be made to these probability estimates of the Fock states. In the Fock state expansion (3.1), the states can carry different quantum numbers and therefore we can have different $|Q\bar{Q}\rangle$ Fock states contributing to the quarkonium state. However, the heavy quark Lagrangian (2.29) conserves the total angular momentum J , parity P and charge conjugation C quantum numbers which allows us to deduce the possible $Q\bar{Q}$ states [3, p. 17]. These are the same quantum numbers that are also conserved in QCD, which means that we can label the quarkonium states by J^{PC} . If the quark-antiquark pair has the angular momentum L and the total spin quantum number $S = 0, 1$ in the Fock state $|Q\bar{Q}\rangle$, the conserved quantum numbers are

$$J = |L - S|, \dots, L + S \quad P = (-1)^{L+1} \quad C = (-1)^{L+S}. \quad (3.7)$$

If we now have a $Q\bar{Q}$ state with different quantum numbers but the same J^{PC} , the conservation of parity P implies that we must have $L' = L \pm 2, L \pm 4, \dots$ for the other state. Because the total spin S can only have values 0 and 1, the C parity conservation implies that $S' = S$ so that the total spin doesn't change. If the spin is $S = S' = 0$, the conservation of angular momentum J tells us that we must also have $J = L = L'$ which means that the quantum numbers of the $|Q\bar{Q}\rangle$ are uniquely defined. For the case $S = S' = 1$, the conservation of angular momentum implies that we can have $L = J + 1$ and $L' = J - 1$ or vice versa. This means that only $^3(J+1)_J$ and $^3(J-1)_J$ states can mix in the pure quark-antiquark states of the quarkonium. For example, the states 3S_1 and 3D_1 can be mixed in the $J^{PC} = 1^{--}$ quarkonium states. However, this mixing is suppressed because the orbital angular momentum can change only through terms that contain powers of ∇ [3, p. 18]. The change of two units of orbital angular momentum needs at least two powers of ∇ , meaning that this mixing is suppressed by v^2 . This mixing could cause problem when trying to figure out the quantum numbers of the dominating $|Q\bar{Q}\rangle$ state, but usually we can use the quarkonium spectra to determine the quantum numbers. This

relies on the fact that in general states with higher L have a higher mass.

We can now determine the Fock state expansion for the charmonium particles η_c and J/ψ . The spin parities of these are 0^{-+} and 1^{--} , respectively. These are the lowest-lying charmonium states so we can expect them to be dominated by the $L = 0$ orbital angular momentum $|c\bar{c}\rangle$ state. The spin parities then tell us that at the lowest order, $|\eta_c\rangle \approx |^1S_0\rangle$ and $|J/\psi\rangle \approx |^3S_1\rangle$. Using the previous arguments for the probabilities of the states and considering the possible quantum numbers for the $c\bar{c}$ pair, we can write these to higher orders by

$$|\eta_c\rangle = |^1S_0^{[1]}\rangle + \mathcal{O}(v) |^1P_0^{[8]}g\rangle + \mathcal{O}(v^{3/2}) |^3S_1^{[8]}g\rangle + \mathcal{O}(v^2) \quad \text{and} \quad (3.8)$$

$$|J/\psi\rangle = |^3S_1^{[8]}\rangle + \mathcal{O}(v) |^3P_1^{[8]}g\rangle + \mathcal{O}(v^{3/2}) |^1S_0^{[8]}g\rangle + \mathcal{O}(v^2). \quad (3.9)$$

Here the $c\bar{c}$ pair has been denoted using the spectroscopic notation, with the addition that the superscript [1] denotes a color-singlet and [8] a color-octet state. Similar expansions can also be written for the lowest-lying bottomonium states: η_b has the same Fock state expansion as η_c except that the $c\bar{c}$ pair has been replaced by a $b\bar{b}$ pair, and in the same way Υ has an identical expansion with J/ψ .

3.2 S-wave Fock states

In a similar way as in equation (5.43) of reference [9, p. 149], we can write the 1S_0 quark-antiquark Fock state as

$$|^1S_0(\mathbf{p})\rangle = \int \frac{d^3\mathbf{k}}{(2\pi)^3} \tilde{\psi}(\mathbf{k}) \frac{\epsilon^{s_1 s_2} \delta^{c_1 c_2}}{\sqrt{2} \sqrt{N_c}} \left| Q_{s_1 c_1} \left(\frac{\mathbf{p}}{2} + \mathbf{k} \right) \bar{Q}_{s_2 c_2} \left(\frac{\mathbf{p}}{2} - \mathbf{k} \right) \right\rangle \quad (3.10)$$

Here $\tilde{\psi}$ is the wave function in momentum space, ϵ is the two-dimensional Levi-Civita symbol and s_i and c_i are the spin and color indices. The wave function can be written as

$$\tilde{\psi}(\mathbf{k}) = Y_0^0(\theta, \phi) \varphi(k) = \frac{1}{\sqrt{4\pi}} \varphi(k) \quad (3.11)$$

where Y_0^0 is the spherical harmonic with quantum numbers $l = 0$, $m = 0$ and $\varphi(k)$ is the radial wave function in momentum space, normalized in such a way that

$$\int d^3\mathbf{k} |\tilde{\psi}(\mathbf{k})|^2 = \int dk k^2 |\varphi(k)|^2 = 1. \quad (3.12)$$

The 3S_1 state can be similarly written as

$$\left|{}^3S_1(\mathbf{p}, m_S)\right\rangle = \int \frac{d^3\mathbf{k}}{(2\pi)^3} \frac{1}{\sqrt{4\pi}} \varphi(k) S^{s_1 s_2}(m_S) \frac{\delta^{c_1 c_2}}{\sqrt{N_c}} \left| Q_{s_1 c_1} \left(\frac{\mathbf{p}}{2} + \mathbf{k} \right) \bar{Q}_{s_2 c_2} \left(\frac{\mathbf{p}}{2} - \mathbf{k} \right) \right\rangle. \quad (3.13)$$

Here m_S is the polarization of the state, which can be -1 , 0 or $+1$. It corresponds to the projection of spin in the z -direction. Consequently, the coupling of the spins depends on the polarization, which is indicated in the spin matrix $S^{s_1 s_2}(m_S)$. The spins are combined using the standard Clebsch-Gordan coefficients:

$$\begin{aligned} |m_S = +1\rangle &= |s_1 = \uparrow, s_2 = \uparrow\rangle \\ |m_S = 0\rangle &= \frac{1}{\sqrt{2}} \left(|s_1 = \uparrow, s_2 = \downarrow\rangle + |s_1 = \downarrow, s_2 = \uparrow\rangle \right) \\ |m_S = -1\rangle &= |s_1 = \downarrow, s_2 = \downarrow\rangle \end{aligned} \quad (3.14)$$

Other $|Q\bar{Q}\rangle$ states could be written in a similar way as (3.10), taking into account the coupling of the spins and orbital angular momentum.

In the following calculations we need to explicitly calculate how operators act on the $|Q\bar{Q}\rangle$ Fock state. It is instructive to see how these calculations can often be simplified by separating the spin and color parts of the operator. Let us now consider an operator $\chi^\dagger \hat{A} \hat{S} \hat{C} \psi$ acting on a 1S_0 or 3S_1 state where \hat{S} and \hat{C} are the spin and color parts of the operator, respectively. Then we can write

$$\begin{aligned} \chi^\dagger \hat{A} \hat{S} \hat{C} \psi |Q\bar{Q}\rangle &= \int \frac{d^3\mathbf{k}_1 d^3\mathbf{k}_2}{(2\pi)^6} \sum_{s_1 s_2} \eta_{s_2}^\dagger \hat{S} \xi_{s_1} M^{s_1 s_2} \sum_{c_1 c_2} \hat{C}^{c_1 c_2} \frac{\delta^{c_1 c_2}}{\sqrt{N_c}} \\ &\cdot \chi^\dagger(\mathbf{k}_1) \hat{A} \psi(\mathbf{k}_2) \left| Q \left(\frac{\mathbf{p}}{2} + \mathbf{k} \right) \bar{Q} \left(\frac{\mathbf{p}}{2} - \mathbf{k} \right) \right\rangle. \end{aligned} \quad (3.15)$$

Here the notation has been changed so that operators $\chi^\dagger(\mathbf{k})$ and $\psi(\mathbf{k})$ annihilate a state with momentum \mathbf{k} irrespective of the spin or color and $M^{s_1 s_2}$ is the matrix for coupling the spins. For the Fock state 1S_0 we have $M^{s_1 s_2} = \epsilon^{s_1 s_2}$ and for 3S_1 we have $M^{s_1 s_2} = S^{s_1 s_2}(m_S)$. We have assumed that the quark-antiquark pair is in the color-singlet state so that colors are coupled by the $\delta^{c_1 c_2}$ matrix. In the case of a color-octet state this would be a linear combination of the Gell-Mann matrices t^a . From equation (3.15) we can see that the color and spin parts can be treated separately. In this case, the color part gives us simply the trace of the operator \hat{C} .

The spin part we write in the following way:

$$\sum_{s_1 s_2} \eta_{s_2}^\dagger \hat{S} \xi_{s_1} M^{s_1 s_2} = \text{Tr} \left(\sum_{s_1 s_2} M^{s_1 s_2} \xi_{s_1} \eta_{s_2}^\dagger \hat{S} \right). \quad (3.16)$$

By using the definitions for the spinors (2.62) and (2.63) with the spin matrices from equations (3.10) and (3.13), we can write the spin sums as

$${}^1S_0 : \sum_{s_1 s_2} M^{s_1 s_2} \xi_{s_1} \eta_{s_2}^\dagger = \frac{1}{\sqrt{2}} \mathbb{1}_2 \quad \text{and} \quad {}^3S_1 : \sum_{s_1 s_2} M^{s_1 s_2} \xi_{s_1} \eta_{s_2}^\dagger = \frac{1}{\sqrt{2}} \epsilon_\lambda \cdot \boldsymbol{\sigma}, \quad (3.17)$$

with $\mathbb{1}_2$ being 2×2 identity matrix and ϵ_λ the polarization vectors [5, p. 137]

$$\begin{aligned} \epsilon_{+1} &= -\frac{1}{\sqrt{2}} \begin{pmatrix} 1 & i & 0 \end{pmatrix} \\ \epsilon_0 &= \begin{pmatrix} 0 & 0 & 1 \end{pmatrix} \\ \epsilon_{-1} &= \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & -i & 0 \end{pmatrix}. \end{aligned} \quad (3.18)$$

Equation (3.15) now simplifies to

$$\begin{aligned} \psi^\dagger \hat{A} \hat{S} \hat{C} \chi |Q\bar{Q}\rangle &= \text{Tr} (M_S \hat{S}) \text{Tr} \left(\frac{1}{\sqrt{N_c}} \hat{C} \right) \\ &\cdot \int \frac{d^3 \mathbf{k}_1 d^3 \mathbf{k}_2}{(2\pi)^6} \psi^\dagger(\mathbf{k}_1) \hat{A} \chi(\mathbf{k}_2) \left| Q \left(\frac{\mathbf{P}}{2} + \mathbf{k} \right) \bar{Q} \left(\frac{\mathbf{P}}{2} - \mathbf{k} \right) \right\rangle \end{aligned} \quad (3.19)$$

where $M_S = \sum_{s_1 s_2} M^{s_1 s_2} \xi_{s_1} \eta_{s_2}^\dagger$ is the matrix for the spin part from equation (3.17) depending on the total spin and the polarization of the $|Q\bar{Q}\rangle$ state.

4 Matching NRQCD to QCD

We want to determine the coefficients of the 4-fermion operators in equation (2.50). This can be done by requiring that invariant amplitudes calculated both in NRQCD and QCD give the same results. We will calculate the invariant amplitude for the process $Q\bar{Q} \rightarrow Q\bar{Q}$ to do the matching.

4.1 Invariant amplitudes from NRQCD

The operators in equation (2.50) correspond to a 4-fermion interaction shown in figure 1 and their Feynman rules are straightforward to calculate. For the lowest order diagrams shown in figure 1 with only one interaction vertex, we can get their contribution to the invariant amplitude $Q\bar{Q} \rightarrow Q\bar{Q}$ by the substitutions $\psi \rightarrow \xi$, $\chi \rightarrow \eta$, $-\frac{i}{2}\overleftrightarrow{\mathbf{D}} \rightarrow M\mathbf{v}(1 + \mathcal{O}(v^2))$. Here ξ and η are the quark and antiquark spinors and \mathbf{v} is the velocity of the quark in the center-of-mass frame. The velocity of the antiquark in the center-of-mass frame is then $-\mathbf{v}$. Using these substitutions the invariant amplitude from the 4-fermion operators (2.51) and (2.52) is then

$$\begin{aligned} \mathcal{M} = & \frac{1}{M^2} \mathbb{1}_c \otimes \mathbb{1}_c \left[f_1(^1S_0) \xi'^\dagger \eta' \eta^\dagger \xi + f_1(^3S_1) \xi'^\dagger \boldsymbol{\sigma} \eta' \cdot \eta^\dagger \boldsymbol{\sigma} \xi + f_1(^1P_1) \xi'^\dagger \mathbf{v}' \eta' \cdot \eta^\dagger \mathbf{v} \xi \right. \\ & + \frac{1}{3} f_1(^3P_0) \xi'^\dagger \mathbf{v}' \cdot \boldsymbol{\sigma} \eta' \eta^\dagger \mathbf{v} \cdot \boldsymbol{\sigma} \xi + \frac{1}{2} f_1(^3P_1) \xi'^\dagger \mathbf{v}' \times \boldsymbol{\sigma} \eta' \cdot \eta^\dagger \mathbf{v} \times \boldsymbol{\sigma} \xi \\ & + f_1(^3P_2) \xi'^\dagger v'^{(i} \sigma^{j)} \eta' \eta^\dagger v^{(i} \sigma^{j)} \xi + \mathbf{v}^2 g_1(^1S_0) \xi'^\dagger \eta' \eta^\dagger \xi + \mathbf{v}^2 g_1(^3S_1) \xi'^\dagger \boldsymbol{\sigma} \eta' \cdot \eta^\dagger \boldsymbol{\sigma} \xi \\ & \left. + \frac{1}{2} (v^{(i} v^{j)}) v'^{(i} v'^{j)}) g_1(^3S_1, ^3D_1) \xi'^\dagger \sigma^i \eta' \eta^\dagger \sigma^j \xi + \mathcal{O}(v^3) \right] + \text{color-octet operators.} \end{aligned} \quad (4.1)$$

Here f_i are the coefficients for the \mathcal{O}_i operators and g_i coefficients for the \mathcal{P}_i operators, ξ and η are the 2-spinors of the incoming quark and antiquark, and v^i is the velocity of the incoming quark. The corresponding quantities for the outgoing quark-antiquark pair are denoted by primes. The notation $\mathbb{1}_c \otimes \mathbb{1}_c$ is a shorthand notation for $\xi_c'^\dagger \mathbb{1}_c \eta_c' \eta_c^\dagger \mathbb{1}_c \xi_c$ where ξ_c and η_c are the vectors describing the color state of the incoming quark and antiquark. As argued in section 3.2, these can be written as a

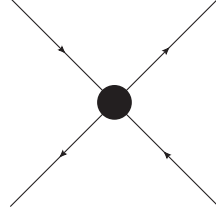


Figure 1. 4-fermion interaction in NRQCD that corresponds to the 4-fermion operators in section 2.3

trace of the color identity matrix $\mathbb{1}_c$ times the color matrix $\eta_c \xi_c^\dagger$ of the quark-antiquark pair. This is non-zero only if the pair is in the color-singlet state. We define similarly the notations $\xi'^\dagger \eta' \eta^\dagger \xi = \mathbb{1}_s \otimes \mathbb{1}_s$ and $\xi'^\dagger \sigma^i \eta' \eta^\dagger \sigma^j \xi = \sigma^i \otimes \sigma^j$ to simplify the equations. Rearranging the terms, equation (4.1) now becomes

$$\begin{aligned}
 \mathcal{M} = & \frac{1}{M^2} \mathbb{1}_c \otimes \mathbb{1}_c \left[\mathbb{1}_s \otimes \mathbb{1}_s \left(f_1(^1S_0) + \mathbf{v} \cdot \mathbf{v}' f_1(^1P_1) + \mathbf{v}^2 g_1(^1S_0) \right) \right. \\
 & + \sigma^i \otimes \sigma^i \left(f_1(^3S_0) + \mathbf{v}^2 \frac{3g_1(^3S_1) - g_1(^3S_1, ^3D_1)}{3} + \mathbf{v} \cdot \mathbf{v}' \frac{f_1(^3P_1) + f_1(^3P_2)}{2} \right) \\
 & + \sigma^i \otimes \sigma^j \left(v^j v'^i \frac{f_1(^3P_0) - f_1(^3P_2)}{3} + v^i v'^j \frac{f_1(^3P_2) - f_1(^3P_1)}{2} \right. \\
 & \left. \left. + (v^i v^j + v'^i v'^j) g_1(^3S_1, ^3D_1) \right) + \mathcal{O}(v^3) \right] + \text{color-octet operators}.
 \end{aligned} \tag{4.2}$$

It should be also noted that the initial and final states may be superpositions of different color and spin combinations of the quark and antiquark. For example, if the initial $Q\bar{Q}$ -pair has total spin $S = 1$ and polarization $m_S = 0$ the initial state would consist of a linear combination of $|s_1 = \uparrow, s_2 = \downarrow\rangle$ and $|s_1 = \downarrow, s_2 = \uparrow\rangle$ spin states. In this case, we need to sum over these different combinations in the invariant amplitude. These sums are left implicit in equation (4.2).

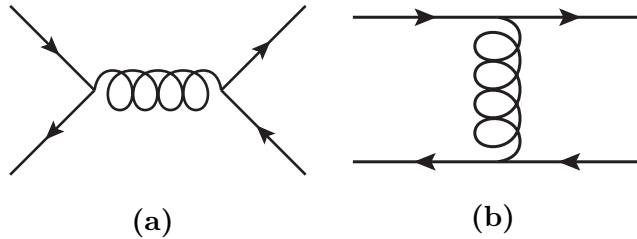


Figure 2. Lowest order $Q\bar{Q} \rightarrow Q\bar{Q}$ diagrams. These do not contribute to the decay of the quarkonium.

4.2 Invariant amplitudes in QCD

We can calculate the invariant amplitude corresponding to the $Q\bar{Q} \rightarrow Q\bar{Q}$ process also in QCD. This invariant amplitude needs to match with the one from NRQCD as physical quantities can be calculated from these and they need to be the same for both theories. We can then calculate the coefficients in (2.50) by matching invariant amplitudes of NRQCD to QCD. Our goal is to calculate quarkonium decay widths using NRQCD, and it will turn out that only the imaginary parts of the coefficients will affect the decay widths. Therefore we are interested only in matching the imaginary parts of the coefficients, which allows us to consider only the imaginary part of the invariant amplitude. This will greatly simplify calculations.

To do the matching, we need to consider all the Feynman diagrams of the process $Q\bar{Q} \rightarrow Q\bar{Q}$ in QCD. The lowest order diagrams for this process are shown in figure 2. By the Cutkosky rules [9, p. 236], the imaginary part of the invariant amplitude corresponds to on-shell particles in the intermediate state. The intermediate gluon in figure 2a has to be a virtual one because of the energy-momentum conservation, and therefore the corresponding invariant amplitude doesn't have an imaginary part. Figure 2b doesn't have intermediate particles and the imaginary part corresponding to this invariant amplitude also vanishes. Neither of the diagrams in figure 2 then contributes to the imaginary parts of the 4-fermion operator coefficients and we need to consider higher-order diagrams.

At higher orders in α_s we have actual contributions to the decay width. All contributing diagrams of order α_s^2 are in figure 3. It should be noted that diagrams where the imaginary part comes from an on-shell heavy quark pair in the intermediate state are not included, as these diagrams do not describe an annihilation process of the quarkonium. In practice, this means that all diagrams where the initial $Q\bar{Q}$ -pair

isn't annihilated at some point can be neglected.

We will from now on focus only on η_c and J/ψ charmonium particles and their decay. The corresponding results for bottonia particles η_b and Υ can be deduced by simple substitutions. As we will discuss in section 5.3, only the color-singlet $|c\bar{c}\rangle$ states will contribute to the decay of η_c and J/ψ at the lowest orders of v . This means that we can neglect most of the diagrams in figure 3, as they contain a $c\bar{c}(\text{singlet}) \rightarrow g$ vertex that requires us to take the trace of the product of the color singlet and octet matrices $\delta_{ij}T_{ji}^a = \text{Tr}(T^a) = 0$. Therefore we will calculate only the contributions from the diagrams 3a and 3b as the other diagrams do not contribute to the decay widths at the order of v we are considering in section 5.3.

Because we have used the non-relativistic normalization for the NRQCD states, we should use that same normalization for the QCD invariant amplitude calculations to match the coefficients correctly. That is, we define the Dirac spinors to be

$$u_s(\mathbf{p}) = \sqrt{\frac{E+m}{2E}} \begin{pmatrix} \xi_s \\ \frac{\boldsymbol{\sigma}\cdot\mathbf{p}}{E+m}\xi_s \end{pmatrix} \quad v_s(-\mathbf{p}) = \sqrt{\frac{E+m}{2E}} \begin{pmatrix} -\frac{\boldsymbol{\sigma}\cdot\mathbf{p}}{E+m}\eta_s \\ \eta_s \end{pmatrix}. \quad (4.3)$$

The invariant amplitude can then be calculated using the standard QCD Feynman rules in the Feynman gauge [12, p. 505]. We also choose to do the calculations in the center-of-mass frame where the incoming quark and antiquark have momenta in opposite directions, as this is also the momentum frame used in NRQCD. Then all the incoming and outgoing quarks and antiquarks in diagrams 3 have the same energy E .

We can now proceed to calculate the invariant amplitude for the diagram 3a. Using the notation in figure 4, the invariant amplitude is

$$\begin{aligned} i\mathcal{M}_{3a} &= \int \frac{d^4k}{(2\pi)^4} \bar{u}_{s_3}(p_3) \left(-ig_s t_{ji}^a \gamma^\alpha \right) \frac{i(\not{q}_2 + m)}{q_2^2 - m^2 + i\varepsilon} \left(-ig_s t_{ih}^b \gamma^\beta \right) v_{s_4}(p_4) \\ &\quad \cdot \bar{v}_{s_2}(p_2) \left(-ig_s t_{gf}^b \gamma^\nu \right) \frac{i(\not{q}_1 + m)}{q_1^2 - m^2 + i\varepsilon} \left(-ig_s t_{fe}^a \gamma^\mu \right) u_{s_1}(p_1) \cdot \left(\frac{-ig_{\mu\alpha}}{k_1^2 + i\varepsilon} \right) \left(\frac{-ig_{\nu\beta}}{k_2^2 + i\varepsilon} \right) \\ &= \int \frac{d^4k}{(2\pi)^4} \frac{1}{(k^2 + i\varepsilon) \left((p_1 + p_2 - k)^2 + i\varepsilon \right) \left((p_1 - k)^2 - m^2 + i\varepsilon \right)} \\ &\quad \cdot \frac{1}{(p_3 - k)^2 - m^2 + i\varepsilon} \cdot g_s^4 t_{ji}^a t_{ih}^b t_{gf}^b t_{fe}^a \cdot \underbrace{\bar{u}_3 \gamma_\mu (\not{q}_2 + m) \gamma_\nu v_4}_{L'_{\mu\nu}} \underbrace{\bar{v}_2 \gamma^\nu (\not{q}_1 + m) \gamma^\mu u_1}_{L^{\mu\nu}} \end{aligned} \quad (4.4)$$

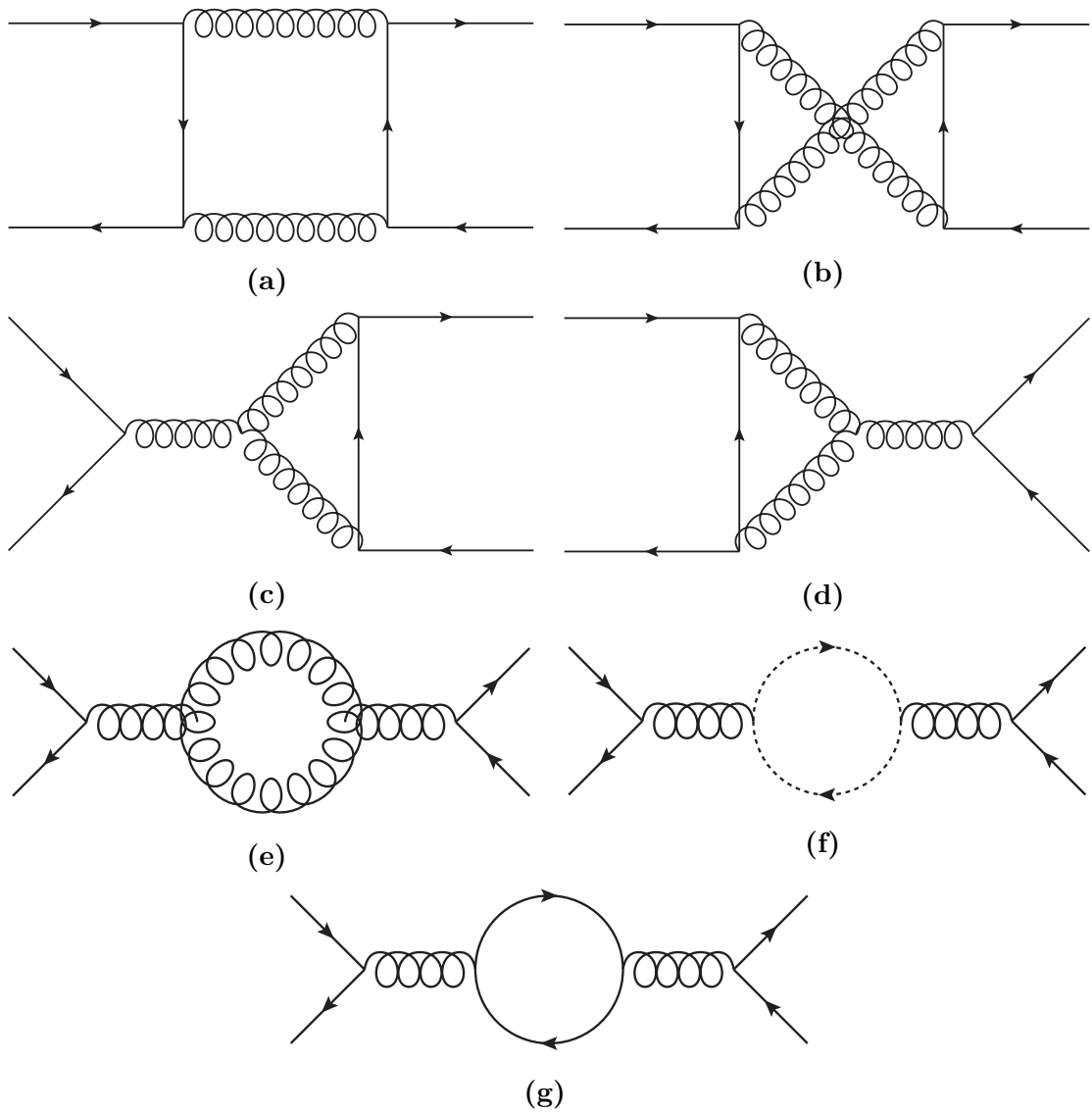


Figure 3. Lowest order diagrams contributing to the decay of $c\bar{c}$.

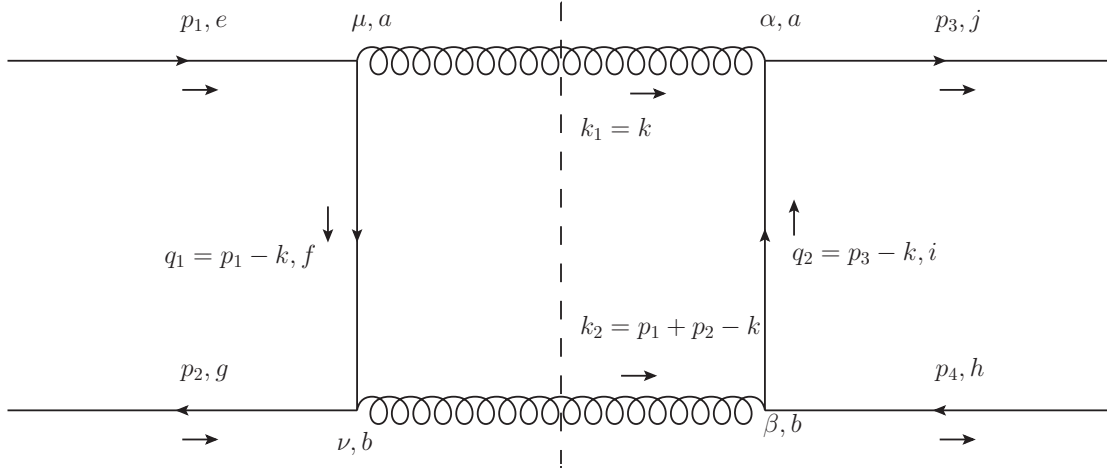


Figure 4. Diagram for calculating the invariant amplitude \mathcal{M}_{3a}

Here m is the physical mass of the heavy quark which can be identified with the NRQCD mass parameter M at the lowest order. The loop integral can be simplified by noting that we are only interested in the imaginary part of invariant amplitude. Only the imaginary parts of the operators have a contribution to the decay widths, so we are interested in matching only those. The imaginary part of the invariant amplitude can be obtained by using the Cutkosky cutting rules for simplifying the loop integral. According to the cutting rules, we can calculate the loop integral by “cutting” propagators that can correspond to on-shell particles. In the case of figure 4 this corresponds to cutting the diagram at the gluon propagators as shown in the figure. The Cutkosky rules tell us that such a diagram gives us $2 \text{Im} \mathcal{M}$ after we have done the substitution

$$\frac{1}{k^2 + i\varepsilon} \rightarrow -2\pi i \delta(k^2) \quad (4.5)$$

for the cut gluon propagators in the loop integral. We then get

$$\begin{aligned} & \int \frac{d^4k}{(2\pi)^4} \frac{1}{(k^2 + i\varepsilon) \left((p_1 + p_2 - k)^2 + i\varepsilon \right) \left((p_1 - k)^2 - m^2 + i\varepsilon \right) \left((p_3 - k)^2 - m^2 + i\varepsilon \right)} \\ & \rightarrow \int \frac{d^4k}{(2\pi)^2} \frac{-\delta(k^2) \delta\left((p_1 + p_2 - k)^2 \right)}{\left((p_1 - k)^2 - m^2 \right) \left((p_3 - k)^2 - m^2 \right)} \end{aligned} \quad (4.6)$$

and therefore

$$\begin{aligned}
2 \operatorname{Im} \mathcal{M}_{3a} &= \int \frac{d^4 k}{(2\pi)^2} \frac{\delta(k^2) \delta((p_1 + p_2 - k)^2)}{((p_1 - k)^2 - m^2)((p_3 - k)^2 - m^2)} f(k) \\
&= \int \frac{d^4 k}{(2\pi)^2} \frac{\delta(k_0^2 - \mathbf{k}^2) \delta(4E^2 - 4Ek_0)}{(-2Ek_0 + 2\mathbf{p}_1 \cdot \mathbf{k})(-2Ek_0 + 2\mathbf{p}_3 \cdot \mathbf{k})} f(k) \\
&= \int \frac{d^3 \mathbf{k}}{(2\pi)^2} \frac{\delta(E^2 - \mathbf{k}^2)}{16E(-E^2 + \mathbf{p}_1 \cdot \mathbf{k})(-E^2 + \mathbf{p}_3 \cdot \mathbf{k})} f(k_0 = E, \mathbf{k}) \\
&= \int \frac{d\Omega d|\mathbf{k}|}{(2\pi)^2} \frac{|\mathbf{k}|^2 \delta(E - |\mathbf{k}|)}{32E|\mathbf{k}|(-E^2 + \mathbf{p}_1 \cdot \mathbf{k})(-E^2 + \mathbf{p}_3 \cdot \mathbf{k})} f(k_0 = E, \mathbf{k}) \\
&= \int \frac{d\Omega}{(2\pi)^2} \frac{f(k_0 = E, |\mathbf{k}| = E, \Omega)}{32E^2(E - |\mathbf{p}_1| \cos \theta_1)(E - |\mathbf{p}_3| \cos \theta_3)} \\
&= \frac{1}{2^7 \pi^2 E^4} \int d\Omega \frac{f(k_0 = E, |\mathbf{k}| = E, \Omega)}{(1 - v \cos \theta_1)(1 - v \cos \theta_3)}.
\end{aligned} \tag{4.7}$$

Here $f(k)$ is the rest of the integral and θ_i is the angle between \mathbf{k} and \mathbf{p}_i .

We can write the quark spinor part $L'_{\mu\nu} L^{\mu\nu}$ of the integral (4.4) in a different way. First of all, we can use the momentum forms of the Dirac equation [9, p. 803]

$$(\not{p} - m)u(p) = \bar{u}(p)(\not{p} - m) = 0 \quad \text{and} \quad (\not{p} + m)v(p) = \bar{v}(p)(\not{p} + m) = 0 \tag{4.8}$$

to simplify it. For this we need to use the anticommutation relation of the gamma matrices

$$\{\gamma^\mu, \gamma^\nu\} = 2g^{\mu\nu}. \tag{4.9}$$

The anticommutation relation (4.9) now allows us to write

$$\begin{aligned}
L'_{\mu\nu} L^{\mu\nu} &= \bar{u}_3 \gamma_\mu (\not{q}_2 + m) \gamma_\nu v_4 \bar{v}_2 \gamma^\nu (\not{q}_1 + m) \gamma^\mu u_1 \\
&= \bar{u}_3 (-\not{q}_2 \gamma_\mu + m \gamma_\mu + 2q_{2,\mu}) \gamma_\nu v_4 \bar{v}_2 \gamma^\nu (-\gamma^\mu \not{q}_1 + \gamma^\mu m + 2q_1^\mu) u_1 \\
&= (\bar{u}_3 (-\not{p}_3 + m) \gamma_\mu + \bar{u}_3 (\not{k} \gamma_\mu + 2q_{2,\mu})) \gamma_\nu v_4 \\
&\quad \cdot \bar{v}_2 \gamma^\nu ((-\gamma^\mu \not{p}_1 + m) u_1 + (\gamma^\mu \not{k} + 2q_1^\mu) u_1) \\
&\stackrel{(*)}{=} \bar{u}_3 (\not{k} \gamma_\mu + 2p_{3,\mu} - 2k_\mu) \gamma_\nu v_4 \bar{v}_2 \gamma^\nu (\gamma^\mu \not{k} + 2p_1^\mu - 2k^\mu) u_1 \\
&= \bar{u}_3 (-\gamma_\mu \not{k} + 2p_{3,\mu}) \gamma_\nu v_4 \bar{v}_2 \gamma^\nu (-\not{k} \gamma^\mu + 2p_1^\mu) u_1.
\end{aligned} \tag{4.10}$$

where the Dirac equations (4.8) were used at (*). We can also use the same trick as

in (3.16), allowing us to write:

$$\begin{aligned} & \bar{u}_3(-\gamma_\mu \not{k} + 2p_{3,\mu})\gamma_\nu v_4 \bar{v}_2 \gamma^\nu (-\not{k}\gamma^\mu + 2p_1^\mu) u_1 \\ & = \text{Tr}(v_4 \bar{u}_3(-\gamma_\mu \not{k} + 2p_{3,\mu})\gamma_\nu) \text{Tr}(u_1 \bar{v}_2 \gamma^\nu (-\not{k}\gamma^\mu + 2p_1^\mu)). \end{aligned} \quad (4.11)$$

In general, we might have a sum over different spin combinations for the incoming and outgoing $Q\bar{Q}$ states. In that case, to get the total invariant amplitude we need to sum the expression (4.7) over these combinations. The spins of the quarks and antiquarks appear only in the spinors, meaning that the invariant amplitude becomes

$$\begin{aligned} \text{Im } \mathcal{M}_{3a} &= \frac{1}{2^8 \pi^2 E^4} \int d\Omega \frac{1}{(1 - v \cos \theta_1)(1 - v \cos \theta_3)} \cdot g_s^4 t_{ji}^a t_{ih}^b t_{gf}^b t_{fe}^a \\ & \cdot \text{Tr} \left(\sum_{\text{outgoing spins}} v_4 \bar{u}_3(-\gamma_\mu \not{k} + 2p_{3,\mu})\gamma_\nu \right) \text{Tr} \left(\sum_{\text{incoming spins}} u_1 \bar{v}_2 \gamma^\nu (-\not{k}\gamma^\mu + 2p_1^\mu) \right). \end{aligned} \quad (4.12)$$

By substituting the expressions for the spinors from (4.3), the spinor sum can also be written as

$$\begin{aligned} \sum_{\text{spins}} u_{s_1}(p_1) \bar{v}_{s_2}(p_2) &= \sum_{\text{spins}} \frac{E+m}{2E} \begin{pmatrix} \xi_{s_1} \\ \frac{\boldsymbol{\sigma} \cdot \mathbf{p}_1}{E+m} \xi_{s_1} \end{pmatrix} \begin{pmatrix} \eta_{s_2}^\dagger \frac{\boldsymbol{\sigma} \cdot \mathbf{p}_2}{E+m} & -\eta_{s_2}^\dagger \end{pmatrix} \\ &= \sum_{\text{spins}} \frac{E+m}{2E} \begin{pmatrix} \xi_{s_1} \eta_{s_2}^\dagger \frac{\boldsymbol{\sigma} \cdot \mathbf{p}_2}{E+m} & -\xi_{s_1} \eta_{s_2}^\dagger \\ \frac{\boldsymbol{\sigma} \cdot \mathbf{p}_1}{E+m} \xi_{s_1} \eta_{s_2}^\dagger \frac{\boldsymbol{\sigma} \cdot \mathbf{p}_2}{E+m} & -\frac{\boldsymbol{\sigma} \cdot \mathbf{p}_1}{E+m} \xi_{s_1} \eta_{s_2}^\dagger \end{pmatrix} = \frac{E+m}{2E} \begin{pmatrix} A \frac{\boldsymbol{\sigma} \cdot \mathbf{p}_2}{E+m} & -A \\ \frac{\boldsymbol{\sigma} \cdot \mathbf{p}_1}{E+m} A \frac{\boldsymbol{\sigma} \cdot \mathbf{p}_2}{E+m} & -\frac{\boldsymbol{\sigma} \cdot \mathbf{p}_1}{E+m} A \end{pmatrix}. \end{aligned} \quad (4.13)$$

In the last equality we have written $A = \sum \xi_{s_1} \eta_{s_2}^\dagger$. The Pauli spin matrices along with the identity matrix form a linear basis for the 2×2 matrices [12, p. 110], which means that we can write A as a sum

$$A = a \mathbb{1} + \mathbf{b} \cdot \boldsymbol{\sigma} \quad (4.14)$$

where a is a complex number and \mathbf{b} is a 3-component complex vector. We now want to use this to write the spinor sum (4.13) as a combination of Dirac gamma matrices. Using the Pauli spin matrix identity (2.10) along with the fact that in the

center-of-mass frame $\mathbf{p}_2 = -\mathbf{p}_1$, we get

$$\begin{aligned}
& \sum_{\text{spins}} u_{s_1}(p_1) \bar{v}_{s_2}(p_2) \\
&= \frac{E+m}{2E} \left[a \begin{pmatrix} -\frac{\boldsymbol{\sigma} \cdot \mathbf{p}_1}{E+m} & -\mathbb{1} \\ -\frac{\boldsymbol{\sigma} \cdot \mathbf{p}_1}{E+m} \frac{\boldsymbol{\sigma} \cdot \mathbf{p}_1}{E+m} & -\frac{\boldsymbol{\sigma} \cdot \mathbf{p}_1}{E+m} \end{pmatrix} + b^i \begin{pmatrix} -\sigma^i \frac{\boldsymbol{\sigma} \cdot \mathbf{p}_1}{E+m} & -\sigma^i \\ -\frac{\boldsymbol{\sigma} \cdot \mathbf{p}_1}{E+m} \sigma^i \frac{\boldsymbol{\sigma} \cdot \mathbf{p}_1}{E+m} & -\frac{\boldsymbol{\sigma} \cdot \mathbf{p}_1}{E+m} \sigma^i \end{pmatrix} \right] \\
&= \frac{E+m}{2E} \left[-a \begin{pmatrix} \frac{\boldsymbol{\sigma} \cdot \mathbf{p}_1}{E+m} & \mathbb{1} \\ \frac{\mathbf{p}_1^2}{(E+m)^2} & \frac{\boldsymbol{\sigma} \cdot \mathbf{p}_1}{E+m} \end{pmatrix} - b^i \begin{pmatrix} \frac{p_1^i}{E+m} + i\epsilon^{ijk} \frac{\sigma^k p_1^j}{E+m} & \sigma^i \\ -\frac{\mathbf{p}_1^2}{(E+m)^2} \sigma^i + 2p_1^i \frac{\boldsymbol{\sigma} \cdot \mathbf{p}_1}{(E+m)^2} & \frac{p_1^i}{E+m} - i\epsilon^{ijk} \frac{\sigma^k p_1^j}{E+m} \end{pmatrix} \right] \\
&= -\frac{1}{2E} \left[a \begin{pmatrix} \boldsymbol{\sigma} \cdot \mathbf{p}_1 & E+M \\ E-M & \boldsymbol{\sigma} \cdot \mathbf{p}_1 \end{pmatrix} + b^i \begin{pmatrix} p_1^i + i\epsilon^{ijk} \sigma^k p_1^j & (E+m)\sigma^i \\ (-E+m)\sigma^i + 2p_1^i \frac{\boldsymbol{\sigma} \cdot \mathbf{p}_1}{E+m} & p_1^i - i\epsilon^{ijk} \sigma^k p_1^j \end{pmatrix} \right] \\
&= -\frac{1}{2E} \left[a \begin{pmatrix} \boldsymbol{\sigma} \cdot \mathbf{p}_1 & 0 \\ 0 & \boldsymbol{\sigma} \cdot \mathbf{p}_1 \end{pmatrix} + a \begin{pmatrix} 0 & E \\ E & 0 \end{pmatrix} + a \begin{pmatrix} 0 & m \\ -m & 0 \end{pmatrix} \right. \\
&\quad \left. + b^i \begin{pmatrix} p_1^i & 0 \\ 0 & p_1^i \end{pmatrix} + b^i \begin{pmatrix} i\epsilon^{ijk} \sigma^k p_1^j & 0 \\ 0 & -i\epsilon^{ijk} \sigma^k p_1^j \end{pmatrix} \right. \\
&\quad \left. + b^i \begin{pmatrix} 0 & E\sigma^i - p_1^i \frac{\boldsymbol{\sigma} \cdot \mathbf{p}_1}{E+m} \\ -E\sigma^i + p_1^i \frac{\boldsymbol{\sigma} \cdot \mathbf{p}_1}{E+m} & 0 \end{pmatrix} + b^i \begin{pmatrix} 0 & m\sigma^i + p_1^i \frac{\boldsymbol{\sigma} \cdot \mathbf{p}_1}{E+m} \\ m\sigma^i + p_1^i \frac{\boldsymbol{\sigma} \cdot \mathbf{p}_1}{E+m} & 0 \end{pmatrix} \right] \\
&= -\frac{1}{2E} \left[a(p_1^i \gamma^0 \gamma^i \gamma^5 + E\gamma^5 + m\gamma^0 \gamma^5) \right. \\
&\quad \left. + b^i \left(p_1^i \mathbb{1} + i\epsilon^{ijk} p_1^j \gamma^k \gamma^5 + E\gamma^i - \frac{p_1^i p_1^j}{E+m} \gamma^j + m\gamma^0 \gamma^i + \frac{p_1^i p_1^j}{E+m} \gamma^0 \gamma^j \right) \right] \\
&= -\frac{1}{2E} \left[a(p_1^i \gamma^0 \gamma^i \gamma^5 + m\gamma^0 \gamma^5) \right. \\
&\quad \left. + b^i \left(p_1^i \mathbb{1} + i\epsilon^{ijk} p_1^j \gamma^k \gamma^5 + E\gamma^i - \frac{p_1^i p_1^j}{E+m} \gamma^j + m\gamma^0 \gamma^i + \frac{p_1^i p_1^j}{E+m} \gamma^0 \gamma^j \right) \right].
\end{aligned} \tag{4.15}$$

Here we have used the Dirac-Pauli representation of the gamma matrices (2.5). The repeated indices are summed over, as usual.

We can now calculate the trace part of equation (4.12) for the incoming particles. To do this, we need the following trace properties of the gamma matrices [9, p. 805]:

- Trace of an odd number of gamma matrices γ^μ is zero.
- Trace of γ^5 times an odd number gamma matrices γ^μ is zero.

- $\text{Tr}(\gamma^\mu \gamma^\nu) = 4g^{\mu\nu}$
- $\text{Tr}(\gamma^5) = \text{Tr}(\gamma^5 \gamma^\mu \gamma^\nu) = 0$
- $\text{Tr}(\gamma^\mu \gamma^\nu \gamma^\rho \gamma^\sigma) = 4(g^{\mu\nu} g^{\rho\sigma} + g^{\mu\sigma} g^{\rho\nu} - g^{\mu\rho} g^{\sigma\nu})$
- $\text{Tr}(\gamma^\mu \gamma^\nu \gamma^\rho \gamma^\sigma \gamma^5) = -4i\epsilon^{\mu\nu\rho\sigma}$

Using these, the trace can be written as

$$\begin{aligned}
& \text{Tr} \left(\sum_{\text{incoming spins}} u_1 \bar{v}_2 \gamma^\nu (-\not{k} \gamma^\mu + 2p_1^\mu) \right) \\
&= -\frac{1}{2E} \text{Tr} \left(\gamma^\nu (-\not{k} \gamma^\mu + 2p_1^\mu) \cdot \left[a(p_1^i \gamma^0 \gamma^5 + M \gamma^0 \gamma^5) \right. \right. \\
&\quad \left. \left. + b^i \left(p_1^i \mathbb{1} + i\epsilon^{ijk} p_1^j \gamma^k \gamma^5 + E \gamma^i - \frac{p_1^i p_1^j}{E+m} \gamma^j + m \gamma^0 \gamma^i + \frac{p_1^i p_1^j}{E+m} \gamma^0 \gamma^j \right) \right] \right) \\
&= -\frac{1}{2E} \left(4aim k_\alpha \epsilon^{\nu\alpha\mu 0} + b^i \left(-4\epsilon^{ijk} \epsilon^{\nu\alpha\mu k} p_1^j k_\alpha - 4Ek_\alpha (g^{\nu\alpha} g^{\mu i} + g^{\nu i} g^{\alpha\mu} - g^{\mu\nu} g^{\alpha i}) \right. \right. \\
&\quad \left. \left. + 8Ep_1^\mu g^{\nu i} + 4\frac{p_1^i p_1^j}{E+m} (k^\nu g^{\mu j} + k^\mu g^{\nu j} - k^j g^{\mu\nu} - 2p_1^\mu g^{\nu j}) \right) \right). \tag{4.16}
\end{aligned}$$

Denoting the coefficients in (4.14) by a' and \mathbf{b}' for the outgoing quark-antiquark pair, we can also write the trace for the outgoing particles as

$$\begin{aligned}
& \text{Tr} \left(\sum_{\text{outgoing spins}} v_4 \bar{u}_3 (-\gamma_\mu \not{k} + 2p_{3,\mu}) \gamma_\nu \right) = \text{Tr} \left(\left(\sum_{\text{outgoing spins}} u_3 \bar{v}_4 \gamma_\nu (-\not{k} \gamma_\mu + 2p_{3,\mu}) \right)^\dagger \right) \\
&= \text{Tr} \left(\sum_{\text{outgoing spins}} u_3 \bar{v}_4 \gamma_\nu (-\not{k} \gamma_\mu + 2p_{3,\mu}) \right)^* \\
&= -\frac{1}{2E} \left(-4a'^* im k^\beta \epsilon_{\nu\beta\mu 0} + b'^* i \left(-4\epsilon^{ijk} \epsilon_{\nu\beta\mu}^k p_3^j k^\beta - 4Ek^\beta (g_{\nu\beta} \delta_\mu^i + \delta_\nu^i g_{\beta\mu} - g_{\mu\nu} \delta_\beta^i) \right. \right. \\
&\quad \left. \left. + 8Ep_{3,\mu} \delta_\nu^i + 4\frac{p_3^i p_3^j}{E+m} (k_\nu \delta_\mu^j + k_\mu \delta_\nu^j - k^j g_{\mu\nu} - 2p_{3,\mu} \delta_\nu^j) \right) \right). \tag{4.17}
\end{aligned}$$

We can now calculate the spinor part $L'_{\mu\nu}L^{\mu\nu}$:

$$\begin{aligned}
L'_{\mu\nu}L^{\mu\nu} &= \text{Tr} \left(\sum_{\text{outgoing spins}} v_4 \bar{u}_3 (-\gamma_\mu \not{k} + 2p_{3,\mu}) \gamma_\nu \right) \text{Tr} \left(\sum_{\text{incoming spins}} u_1 \bar{v}_2 \gamma^\nu (-\not{k} \gamma^\mu + 2p_1^\mu) \right) \\
&= \frac{4}{E^2} \left[a'^* a m^2 k_\alpha k^\beta \epsilon^{\nu\alpha\mu 0} \epsilon_{\nu\beta\mu 0} + i m b'^* a k_\alpha \epsilon^{\nu\alpha\mu 0} \left(-\epsilon^{ijk} \epsilon_{\nu\beta\mu} k p_3^j k^\beta + 2E p_{3,\mu} \delta_\nu^i \right) \right. \\
&\quad + i m a'^* b^i k^\beta \epsilon_{\nu\beta\mu 0} \left(\epsilon^{ijk} \epsilon^{\nu\alpha\mu k} p_1^j k_\alpha - 2E p_1^\mu g^{\nu i} \right) \\
&\quad + b'^* i b^j \left(\epsilon^{jkl} \epsilon^{\nu\alpha\mu l} p_1^k k_\alpha \left(\epsilon^{imn} \epsilon_{\nu\beta\mu} p_3^m k^\beta - 2E p_{3,\mu} \delta_\nu^i + 2 \frac{p_3^i p_3^m}{E+m} p_{3,\mu} \delta_\nu^m \right) \right. \\
&\quad + 2E^2 k^\beta k_\alpha \left(\delta_\beta^\alpha g^{ij} + g^{i\alpha} \delta_\beta^j \right) - 2E^2 \left(k^i p_3^j - k^j p_3^i + k^j p_1^i - k^i p_1^j + k_\alpha (p_3^\alpha + p_1^\alpha) g^{ij} \right) \\
&\quad + \epsilon^{imn} \epsilon_{\nu\beta\mu} p_3^m k^\beta \left(-2E p_1^\mu g^{j\nu} + 2 \frac{p_1^j p_1^m}{E+m} p_1^\mu g^{m\nu} \right) + 4E^2 p_{1,\mu} p_3^\mu g^{ij} \\
&\quad + 2 \frac{E}{E+m} p_3^i p_3^m \left(k^j p_1^m + p_1^\mu k_\mu g^{mj} - k^m p_1^j - 2p_{3,\mu} p_1^\mu g^{jm} \right) \\
&\quad + 2 \frac{E}{E+m} p_1^j p_1^m \left(k^i p_3^m + p_3^\mu k_\mu g^{mi} - k^m p_3^i - 2p_{1,\mu} p_3^\mu g^{im} \right) \\
&\quad - \frac{E}{E+m} \left(p_1^j p_1^m \left(2k_\alpha k^\alpha g^{im} + 2k^m k^i - 2p_1^i k^m + p_1^m k^i \right) \right. \\
&\quad + p_3^i p_3^m \left(2k_\alpha k^\alpha g^{jm} + 2k^m k^j - 2p_3^j k^m + p_3^m k^j \right) \left. \right) \\
&\quad + \frac{p_1^j p_1^l p_3^i p_3^m}{(E+m)^2} \left(2k_\mu k^\mu g^{ml} + 4k^m k^l - 2p_1^m k^l + 2p_1^l k^m \right) \\
&\quad \left. - 2p_3^l k^m + 2p_3^m k^l - 2p_1^\mu k_\mu g^{ml} - 2p_3^\mu k_\mu g^{ml} 4p_{1,\mu} p_3^\mu g^{ml} \right) \left. \right]
\end{aligned} \tag{4.18}$$

Our ultimate goal here is to match the QCD invariant amplitude (4.12) to the NRQCD one (4.2). The NRQCD invariant amplitude is calculated only to the accuracy $\mathcal{O}(v^3)$, so we need to consider the QCD invariant amplitude only to that order. By noting that $\mathbf{p} = m\mathbf{v}(1 + \mathcal{O}(v^2))$ and by equation (4.7) $k^0 = E$ and $|\mathbf{k}| = E$,

we can simplify equation (4.18):

$$\begin{aligned}
L'_{\mu\nu}L^{\mu\nu} &= \frac{4}{E^2} \left[a'^* am^2 (-k_i k^i) 2 + b'^* i b^j \left(\epsilon^{jkl} \epsilon^{\nu\alpha\mu l} p_1^k k_\alpha \left(\epsilon^{imn} \epsilon_{\nu\beta\mu}{}^n p_3^m k^\beta - 2E p_{3,\mu} \delta_\nu^i \right) \right. \right. \\
&\quad + 2E^2 k^\beta k_\alpha \left(\delta_\beta^\alpha g^{ij} + g^{i\alpha} \delta_\beta^j \right) - 2E^2 \left(k^i p_3^j - k^j p_3^i + k^j p_1^i - k^i p_1^j + k_\alpha (p_3^\alpha + p_1^\alpha) g^{ij} \right) \\
&\quad + \epsilon^{imn} \epsilon_{\nu\beta\mu}{}^n p_3^m k^\beta \left(-2E p_1^\mu g^{j\nu} \right) + 4E^2 p_{1,\mu} p_3^\mu g^{ij} \\
&\quad \left. \left. - \frac{E}{E+m} \left(p_1^j p_1^m \left(2k_\alpha k^\alpha g^{im} + 2k^m k^i \right) + p_3^i p_3^m \left(2k_\alpha k^\alpha g^{jm} + 2k^m k^j \right) \right) \right) \right] \\
&\quad + \mathcal{O}(v^3) \Bigg] \\
&= \frac{4}{E^2} \left[2a'^* am^2 E^2 + b'^* i b^j \left(2\epsilon^{jkl} \epsilon^{imn} k^l k^n p_1^k p_3^m \right. \right. \\
&\quad - 2E^2 \left(2\mathbf{p}_1 \cdot \mathbf{p}_3 \delta^{ij} - 2p_1^i p_3^j - \mathbf{p}_1 \cdot \mathbf{k} \delta^{ij} - \mathbf{p}_3 \cdot \mathbf{k} \delta^{ij} + k^j p_1^i + k^i p_3^j \right) \\
&\quad + 2E^2 k^i k^j - 2E^2 \left(k^i p_3^j - k^j p_3^i + k^j p_1^i - k^i p_1^j - 2E^2 \delta^{ij} + \mathbf{p}_1 \cdot \mathbf{k} \delta^{ij} + \mathbf{p}_3 \cdot \mathbf{k} \delta^{ij} \right) \\
&\quad \left. \left. - 4E^4 \delta^{ij} + 4E^2 \mathbf{p}_1 \cdot \mathbf{p}_3 \delta^{ij} - p_1^j p_1^m k^m k^i - p_3^i p_3^m k^m k^j + \mathcal{O}(v^3) \right) \right]. \tag{4.19}
\end{aligned}$$

Here we have also used properties of the Levi-Civita symbols to simplify the results.

Let's now denote the velocity of the incoming quark by \mathbf{v} and the velocity of the outgoing quark by \mathbf{v}' . We then have $\mathbf{p}_1 = \mathbf{v}E$ and $\mathbf{p}_3 = \mathbf{v}'E$. Because the incoming and outgoing quarks have the same energy, we must have $|\mathbf{v}| = |\mathbf{v}'| = v$. We can also denote $\mathbf{k} = E\hat{\mathbf{k}}$ where $\hat{\mathbf{k}}$ is the unit vector pointing in the direction of \mathbf{k} . Now

we get

$$\begin{aligned}
L'_{\mu\nu}L^{\mu\nu} &= \frac{4}{E^2} \left[2a'^*am^2E^2 \right. \\
&+ b'^*ib^j \left(2\epsilon^{jkl}\epsilon^{imn}k^lk^np_1^kp_3^m + 2E^2(2p_1^ip_3^j - 2k^jp_1^i - 2k^ip_3^j + k^jp_3^i + k^ip_1^j) \right. \\
&+ \left. \left. 2E^2k^ik^j - p_1^jp_1^mk^mk^i - p_3^ip_3^mk^mk^j + \mathcal{O}(v^3) \right) \right] \quad (4.20) \\
&= 4 \left[2a'^*am^2 + b'^*ib^j E^2 \left(2\epsilon^{jkl}\epsilon^{imn}\hat{k}^l\hat{k}^nv^kv'^m + 4v^iv'^j - 4\hat{k}^jv^i - 4\hat{k}^iv'^j \right. \right. \\
&+ \left. \left. 2\hat{k}^jv'^i + 2\hat{k}^iv^j + 2\hat{k}^i\hat{k}^j - v^jv^mv^m\hat{k}^i - v^iv^mv^m\hat{k}^j + \mathcal{O}(v^3) \right) \right].
\end{aligned}$$

We can now go on to perform the angular integral of (4.12). First of all, we note that

$$\begin{aligned}
&\int d\Omega \frac{f(\Omega)}{(1-v\cos\theta_1)(1-v\cos\theta_3)} \\
&= \int d\Omega f(\Omega) \left(1 + v(\cos\theta_1 + \cos\theta_3) + v^2(\cos^2\theta_1 + \cos^2\theta_3 + \cos\theta_1\cos\theta_3) + \mathcal{O}(v^3) \right) \\
&= \int d\Omega f(\Omega) \left(1 + \hat{k}^i(v^i + v'^i) + \hat{k}^i\hat{k}^j(v^iv^j + v'^iv'^j + v^iv'^j) + \mathcal{O}(v^3) \right). \quad (4.21)
\end{aligned}$$

By looking at this and equation (4.20), we see that the angular dependence is in the $\hat{\mathbf{k}}$ vector. To evaluate the integral, we need to use the formula

$$\int d\Omega \hat{k}^{i_1}\hat{k}^{i_2}\dots\hat{k}^{i_{2n}} = \frac{4\pi}{(2n+1)!!} \sum_{\text{combinations}} \delta^{i_1i_2}\delta^{i_3i_4}\dots\delta^{i_{2n-1}i_{2n}} \quad (4.22)$$

where \hat{k}^i are the components of the unit vector over which we integrate. If the number of \hat{k}^i is odd the integral is zero by symmetry. Here i_j can be any index 1,2,3. This equation can be derived from a similar formula [13, p. 80]

$$\begin{aligned}
&\int d\Omega (\hat{k}^1)^{2\alpha_1} (\hat{k}^2)^{2\alpha_2} (\hat{k}^3)^{2\alpha_3} = \frac{2\Gamma(\alpha_1 + \frac{1}{2})\Gamma(\alpha_2 + \frac{1}{2})\Gamma(\alpha_3 + \frac{1}{2})}{\Gamma(\alpha_1 + \alpha_2 + \alpha_3 + \frac{3}{2})} \\
&= 4\pi \frac{(2\alpha_1 - 1)!!(2\alpha_2 - 1)!!(2\alpha_3 - 1)!!}{(2n + 1)!!} \quad (4.23)
\end{aligned}$$

where α_i are positive integers, $n = \alpha_1 + \alpha_2 + \alpha_3$ and the identity $\Gamma(z/2 + 1) = z!!\sqrt{\pi/2^{z+1}}$ has been used. The difference between equations (4.22) and (4.23) is that in equation (4.22) we don't know how many of the indices are the same. We can prove it using equation (4.23) by noting that if the number of indices with $i = 1, 2, 3$ is $2\alpha_1, 2\alpha_2, 2\alpha_3$, respectively, then the left side of equation (4.22) is simply equation (4.23). The right side of equation (4.22) can on the other hand be written as

$$\begin{aligned} & \frac{4\pi}{(2n+1)!!} \sum_{\text{combinations}} \delta^{i_1 i_2} \delta^{i_3 i_4} \dots \delta^{i_{2n-1} i_{2n}} \\ &= \frac{4\pi}{(2n+1)!!} \cdot (2\alpha_1 - 1)!! (2\alpha_2 - 1)!! (2\alpha_3 - 1)!! \end{aligned} \quad (4.24)$$

which is also the same as (4.23). Because this is true for all numbers of same indices α_i , equation (4.22) holds in general. We can then use it to calculate for example:

$$\begin{aligned} \int d\Omega \hat{k}^i &= \int d\Omega \hat{k}^i \hat{k}^j \hat{k}^k = 0, \\ \int d\Omega \hat{k}^i \hat{k}^j &= \frac{4\pi}{3} \delta^{ij}, \quad \text{and} \\ \int d\Omega \hat{k}^i \hat{k}^j \hat{k}^k \hat{k}^l &= \frac{4\pi}{15} (\delta^{ij} \delta^{kl} + \delta^{ik} \delta^{jl} + \delta^{il} \delta^{jk}). \end{aligned} \quad (4.25)$$

Using these, we get from the angular integral

$$\begin{aligned}
& \int d\Omega \frac{1}{(1-v\cos\theta_1)(1-v\cos\theta_3)} L'_{\mu\nu} L'^{\mu\nu} \\
&= \int d\Omega \left(1 + \hat{k}^a(v^a + v'^a) + \hat{k}^a \hat{k}^b (v^a v^b + v'^a v'^b + v^a v'^b) + \mathcal{O}(v^3) \right) \\
&\quad \cdot 4 \left[2a'^* a m^2 + b'^* b^j E^2 \left(2\epsilon^{jkl} \epsilon^{imn} \hat{k}^l \hat{k}^n v^k v'^m + 4v^i v'^j - 4\hat{k}^j v^i - 4\hat{k}^i v'^j + 2\hat{k}^j v'^i \right. \right. \\
&\quad \left. \left. + 2\hat{k}^i v^j + 2\hat{k}^i \hat{k}^j - v^j v^m \hat{k}^m \hat{k}^i - v'^i v'^m \hat{k}^m \hat{k}^j + \mathcal{O}(v^3) \right) \right] \\
&= \int d\Omega 4 \left[2a'^* a m^2 \left(1 + \hat{k}^a(v^a + v'^a) + \hat{k}^a \hat{k}^b (v^a v^b + v'^a v'^b + v^a v'^b) \right) \right. \\
&\quad \left. + b'^* b^j E^2 \left(2\hat{k}^i \hat{k}^j \left(1 + \hat{k}^a(v^a + v'^a) + \hat{k}^a \hat{k}^b (v^a v^b + v'^a v'^b + v^a v'^b) \right) \right. \right. \\
&\quad \left. \left. + \left(-4\hat{k}^j v^i - 4\hat{k}^i v'^j + 2\hat{k}^j v'^i + 2\hat{k}^i v^j \right) \left(1 + \hat{k}^a(v^a + v'^a) \right) \right. \right. \\
&\quad \left. \left. - v^j v^m \hat{k}^m \hat{k}^i + 2\epsilon^{jkl} \epsilon^{imn} \hat{k}^l \hat{k}^n v^k v'^m + 4v^i v'^j - v'^i v'^m \hat{k}^m \hat{k}^j \right) + \mathcal{O}(v^3) \right] \\
&= 16\pi \left[2a'^* a m^2 \left(1 + \frac{2}{3}v^2 + \frac{1}{3}v^i v'^i \right) \right. \\
&\quad \left. + b'^* b^j E^2 \left(\frac{2}{3}\delta^{ij} + \frac{2}{15} \left(2v^2 \delta^{ij} + v^a v'^a \delta^{ij} + 2v^i v^j + 2v'^i v'^j + v^i v'^j + v^j v'^i \right) \right. \right. \\
&\quad \left. \left. + \frac{1}{3} \left(-2v^i v^j - 2v'^i v'^j - 8v^i v'^j + 4v'^i v^j \right) \right. \right. \\
&\quad \left. \left. - \frac{1}{3}v^j v^i + \frac{2}{3}\epsilon^{jkl} \epsilon^{iml} v^k v'^m + 4v^i v'^j - \frac{1}{3}v'^i v'^j \right) + \mathcal{O}(v^3) \right] \\
&= 32\pi \left[a'^* a m^2 \left(1 + \frac{2}{3}v^2 + \frac{1}{3}\mathbf{v} \cdot \mathbf{v}' \right) + b'^* b^j E^2 \left(\frac{1}{3}\delta^{ij} + \frac{2}{15}\delta^{ij}v^2 + \frac{2}{5}\delta^{ij}\mathbf{v} \cdot \mathbf{v}' \right. \right. \\
&\quad \left. \left. - \frac{11}{30} \left(v^i v^j + v'^i v'^j \right) + \frac{2}{5}v^i v'^j + \frac{11}{15}v'^i v^j \right) + \mathcal{O}(v^3) \right].
\end{aligned} \tag{4.26}$$

For the energy of the quark we have $E = m \left(1 + \frac{1}{2}v^2 + \mathcal{O}(v^4) \right)$, so we can write the

whole invariant amplitude as

$$\begin{aligned}
\text{Im}\mathcal{M}_{3a} &= \frac{1}{2^8\pi^2 E^4} \cdot g_s^4 t_{ji}^a t_{ih}^b t_{gf}^b t_{fe}^a \cdot 32\pi \left[a'^* a m^2 \left(1 + \frac{2}{3}v^2 + \frac{1}{3}\mathbf{v} \cdot \mathbf{v}' \right) \right. \\
&\quad \left. + b'^* i b^j E^2 \left(\frac{1}{3}\delta^{ij} + \frac{2}{15}\delta^{ij}v^2 + \frac{2}{5}\delta^{ij}\mathbf{v} \cdot \mathbf{v}' - \frac{11}{30}(v^i v^j + v'^i v'^j) + \frac{2}{5}v^i v'^j + \frac{11}{15}v'^i v^j \right) \right. \\
&\quad \left. + \mathcal{O}(v^3) \right] \\
&= \frac{g_s^4}{2^3\pi m^2} \cdot t_{ji}^a t_{ih}^b t_{gf}^b t_{fe}^a \left[a'^* a (1 - 2v^2) \left(1 + \frac{2}{3}v^2 + \frac{1}{3}\mathbf{v} \cdot \mathbf{v}' \right) \right. \\
&\quad \left. + b'^* i b^j (1 - v^2) \left(\frac{1}{3}\delta^{ij} + \frac{2}{15}\delta^{ij}v^2 + \frac{2}{5}\delta^{ij}\mathbf{v} \cdot \mathbf{v}' - \frac{11}{30}(v^i v^j + v'^i v'^j) + \frac{2}{5}v^i v'^j \right. \right. \\
&\quad \left. \left. + \frac{11}{15}v'^i v^j \right) + \mathcal{O}(v^3) \right] \\
&= \frac{g_s^4}{2^3\pi m^2} \cdot t_{ji}^a t_{ih}^b t_{gf}^b t_{fe}^a \left[a'^* a \left(1 - \frac{4}{3}v^2 + \frac{1}{3}\mathbf{v} \cdot \mathbf{v}' \right) \right. \\
&\quad \left. + b'^* i b^j \left(\frac{1}{3}\delta^{ij} - \frac{1}{5}\delta^{ij}v^2 + \frac{2}{5}\delta^{ij}\mathbf{v} \cdot \mathbf{v}' - \frac{11}{30}(v^i v^j + v'^i v'^j) + \frac{2}{5}v^i v'^j + \frac{11}{15}v'^i v^j \right) \right. \\
&\quad \left. + \mathcal{O}(v^3) \right].
\end{aligned} \tag{4.27}$$

The color matrix part can be simplified further into color-singlet and color-octet operators. Using the Fierz identity [12, p. 110]

$$t_{bc}^a t_{de}^a = \frac{1}{2} \left(\delta_{be} \delta_{cd} - \frac{1}{N_c} \delta_{bc} \delta_{de} \right) \tag{4.28}$$

we can write

$$\begin{aligned}
t_{ji}^a t_{ih}^b t_{gf}^b t_{fe}^a &= \frac{1}{4} \left(\delta_{je} \delta_{fi} - \frac{1}{N_c} \delta_{ji} \delta_{fe} \right) \left(\delta_{if} \delta_{gh} - \frac{1}{N_c} \delta_{ih} \delta_{fg} \right) \\
&= \frac{1}{4} \left[\left(N_c - \frac{2}{N_c} \right) \delta_{je} \delta_{gh} + \frac{1}{N_c^2} \delta_{jh} \delta_{eg} \right] \\
&= \frac{1}{4} \left[\left(N_c - \frac{2}{N_c} \right) \left(\delta_{je} \delta_{gh} - \frac{1}{N_c} \delta_{jh} \delta_{ge} \right) + \left(1 - \frac{1}{N_c^2} \right) \delta_{jh} \delta_{ge} \right] \quad (4.29) \\
&= \frac{N_c^2 - 1}{4N_c^2} \delta_{jh} \delta_{ge} + \frac{N_c^2 - 2}{2N_c} t_{jh}^a t_{ge}^a = \frac{C_F}{2N_c} \delta_{jh} \delta_{ge} + \frac{N_c^2 - 2}{2N_c} t_{jh}^a t_{ge}^a \\
&= \frac{C_F}{2N_c} \mathbb{1}_c \otimes \mathbb{1}_c + \frac{N_c^2 - 2}{2N_c} t^a \otimes t^a
\end{aligned}$$

where $C_F = (N_c^2 - 1)/(2N_c)$ is the Casimir invariant for the fundamental representation [9, p. 501]. We have used here the same notation for $\mathbb{1}_c \otimes \mathbb{1}_c$ and $t^a \otimes t^a$ as in section 4.1.

We can also identify the parts with the coefficients a and b^i to correspond to the identity spin matrix and Pauli matrices acting on the $Q\bar{Q}$ state. This can be seen by noting that

$$\sum_{\substack{\text{incoming} \\ \text{spins}}} \xi_{s_1}^\dagger \mathbb{1}_s \eta_{s_2} = \text{Tr} \left(\sum_{\substack{\text{incoming} \\ \text{spins}}} \eta_{s_2} \xi_{s_1}^\dagger \right) = \text{Tr}(a\mathbb{1} + \mathbf{b} \cdot \boldsymbol{\sigma}) = 2a, \quad (4.30)$$

$$\sum_{\substack{\text{incoming} \\ \text{spins}}} \xi_{s_1}^\dagger \sigma^i \eta_{s_2} = \text{Tr} \left(\sum_{\substack{\text{incoming} \\ \text{spins}}} \eta_{s_2} \xi_{s_1}^\dagger \sigma^i \right) = \text{Tr}((a\mathbb{1} + \mathbf{b} \cdot \boldsymbol{\sigma}) \sigma^i) = 2b^i \quad (4.31)$$

and similarly for the outgoing spins. With this, we can identify $4a^*a = \eta_{s_4}^\dagger \mathbb{1}_s \xi_{s_3} \xi_{s_1}^\dagger \mathbb{1}_s \eta_{s_2}$ and $4b^{i*}b^j = \eta_{s_4}^\dagger \sigma^i \xi_{s_3} \xi_{s_1}^\dagger \sigma^j \eta_{s_2}$. We can again use the same notation as in section 4.1, for example $\eta_{s_4}^\dagger \mathbb{1}_s \xi_{s_3} \xi_{s_1}^\dagger \mathbb{1}_s \eta_{s_2} = \mathbb{1}_s \otimes \mathbb{1}_s$.

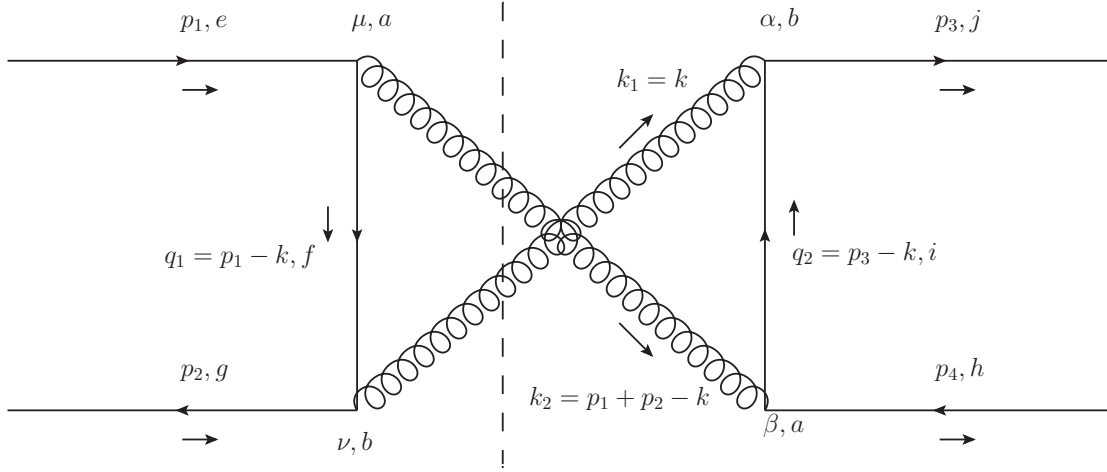


Figure 5. Diagram for calculating the invariant amplitude \mathcal{M}_{3b}

Using these substitutions along with (4.29) the invariant amplitude becomes

$$\begin{aligned}
\text{Im}\mathcal{M}_{3a} &= \frac{g_s^4}{2^5\pi m^2} \cdot \left(\frac{C_F}{2N_c} \mathbb{1}_c \otimes \mathbb{1}_c + \frac{N_c^2 - 2}{2N_c} t^a \otimes t^a \right) \left[\mathbb{1}_s \otimes \mathbb{1}_s \left(1 - \frac{4}{3}v^2 + \frac{1}{3}\mathbf{v} \cdot \mathbf{v}' \right) \right. \\
&\quad \left. + \sigma^i \otimes \sigma^j \left(\frac{1}{3}\delta^{ij} - \frac{1}{5}\delta^{ij}v^2 + \frac{2}{5}\delta^{ij}\mathbf{v} \cdot \mathbf{v}' - \frac{11}{30}(v^i v^j + v'^i v'^j) + \frac{2}{5}v^i v'^j + \frac{11}{15}v'^i v^j \right) \right. \\
&\quad \left. + \mathcal{O}(v^3) \right] \\
&= \frac{\pi\alpha_s^2}{2m^2} \cdot \left(\frac{C_F}{2N_c} \mathbb{1}_c \otimes \mathbb{1}_c + \frac{N_c^2 - 2}{2N_c} t^a \otimes t^a \right) \left[\mathbb{1}_s \otimes \mathbb{1}_s \left(1 - \frac{4}{3}v^2 + \frac{1}{3}\mathbf{v} \cdot \mathbf{v}' \right) \right. \\
&\quad \left. + \sigma^i \otimes \sigma^i \left(\frac{1}{3} - \frac{1}{5}v^2 + \frac{2}{5}\mathbf{v} \cdot \mathbf{v}' \right) \right. \\
&\quad \left. + \sigma^i \otimes \sigma^j \left(\frac{2}{5}v^i v'^j + \frac{11}{15}v'^i v^j - \frac{11}{30}(v^i v^j + v'^i v'^j) \right) + \mathcal{O}(v^3) \right].
\end{aligned} \tag{4.32}$$

Now we also need to calculate the invariant amplitude for the diagram 3b. We can proceed with this in the same way as with the diagram 3a. Using the notation

in figure 5, we get

$$\begin{aligned}
i\mathcal{M}_{3b} &= \int \frac{d^4k}{(2\pi)^4} \bar{u}_{s_3}(p_3) (-ig_s t_{ji}^a \gamma^\alpha) \frac{i(q_2 + m)}{q_2^2 - m^2 + i\varepsilon} (-ig_s t_{ih}^b \gamma^\beta) v_{s_4}(p_4) \\
&\quad \cdot \bar{v}_{s_2}(p_2) (-ig_s t_{gf}^a \gamma^\nu) \frac{i(q_1 + m)}{q_1^2 - m^2 + i\varepsilon} (-ig_s t_{fe}^b \gamma^\mu) u_{s_1}(p_1) \cdot \left(\frac{-ig_{\mu\beta}}{k_1^2 + i\varepsilon} \right) \left(\frac{-ig_{\nu\alpha}}{k_2^2 + i\varepsilon} \right) \\
&= \int \frac{d^4k}{(2\pi)^4} \frac{1}{(k^2 + i\varepsilon) \left((p_1 + p_2 - k)^2 + i\varepsilon \right) \left((p_1 - k)^2 - m^2 + i\varepsilon \right)} \\
&\quad \cdot \frac{1}{(k - p_4)^2 - m^2 + i\varepsilon} \cdot \underbrace{g_s^4 t_{ji}^a t_{ih}^b t_{gf}^a t_{fe}^b}_{L'_{\nu\mu}} \cdot \underbrace{\bar{u}_3 \gamma_\nu (q_2 + m) \gamma_\mu v_4 \bar{v}_2 \gamma^\nu (q_1 + m) \gamma^\mu u_1}_{L^{\mu\nu}}.
\end{aligned} \tag{4.33}$$

Again, the Cutkosky rules tell us to cut the gluon propagators and we get

$$\begin{aligned}
\text{Im } \mathcal{M}_{3b} &= \int \frac{d^4k}{(2\pi)^2} \frac{\delta(k^2) \delta((p_1 + p_2 - k)^2)}{\left((p_1 - k)^2 - m^2 \right) \left((p_4 - k)^2 - m^2 \right)} f(k) \\
&= \frac{1}{2^7 \pi^2 E^4} \int d\Omega \frac{f(k_0 = E, |\mathbf{k}| = E, \Omega)}{(1 - v \cos \theta_1)(1 - v \cos \theta_4)} \\
&= \frac{1}{2^7 \pi^2 E^4} \int d\Omega \frac{f(k_0 = E, |\mathbf{k}| = E, \Omega)}{(1 - \hat{\mathbf{k}} \cdot \mathbf{v}_1)(1 - \hat{\mathbf{k}} \cdot \mathbf{v}_4)}
\end{aligned} \tag{4.34}$$

as the only difference to equation (4.7) is that now we have p_4 instead of p_3 . The Dirac equations (4.8) allow us to simplify the spinor part of the integral:

$$\begin{aligned}
L'_{\nu\mu} L^{\mu\nu} &= \bar{u}_3 \gamma_\nu (q_2 + m) \gamma_\mu v_4 \bar{v}_2 \gamma^\nu (q_1 + m) \gamma^\mu u_1 \\
&= \bar{u}_3 \gamma_\nu (\not{k} \gamma_\mu + \gamma_\mu \not{p}_4 - 2p_{4,\mu} + \gamma_\mu m) v_4 \bar{v}_2 \gamma^\nu (-\not{k} \gamma^\mu - \gamma^\mu \not{p}_1 + 2p_1^\mu + \gamma^\mu m) u_1 \\
&= \bar{u}_3 \gamma_\nu (\not{k} \gamma_\mu - 2p_{4,\mu}) v_4 \bar{v}_2 \gamma^\nu (-\not{k} \gamma^\mu + 2p_1^\mu) u_1 \\
&= -\bar{u}_3 \gamma_\nu (-\not{k} \gamma_\mu + 2p_{4,\mu}) v_4 \bar{v}_2 \gamma^\nu (-\not{k} \gamma^\mu + 2p_1^\mu) u_1
\end{aligned} \tag{4.35}$$

We see that the incoming quark part is the same as in the diagram 3a and therefore we get equation (4.16) also in this case. For the part corresponding to the outgoing

quark-antiquark pair, we get instead

$$\begin{aligned}
& \text{Tr} \left(\sum_{\text{outgoing spins}} v_4 \bar{u}_3 \gamma_\nu (-\not{k} \gamma_\mu + 2p_{4,\mu}) \right) = \text{Tr} \left(\sum_{\text{outgoing spins}} u_3 \bar{v}_4 (-\not{k} \gamma_\mu + 2p_{4,\mu}) \gamma_\nu \right)^* \\
& = -\frac{1}{2E} \left(-4a^{*i} i m k^\beta \epsilon_{\mu\beta\nu 0} + b^{*i} \left(-4\epsilon^{ijk} \epsilon_{\mu\beta\nu}^k p_3^j k^\beta - 4E k^\beta (g_{\nu\beta} \delta_\mu^i + \delta_\nu^i g_{\beta\mu} - g_{\mu\nu} \delta_\beta^i) \right. \right. \\
& \left. \left. + 8E p_{4,\mu} \delta_\nu^i + 4 \frac{p_3^i p_3^j}{E+m} (k_\nu \delta_\mu^j + k_\mu \delta_\nu^j - k^j g_{\mu\nu} - 2p_{4,\mu} \delta_\nu^j) \right) \right).
\end{aligned} \tag{4.36}$$

by using equation (4.15) and the gamma matrix properties. In the center-of-mass frame $\mathbf{p}_3 = -\mathbf{p}_4$ so that this can be written as

$$\begin{aligned}
& \text{Tr} \left(\sum_{\text{outgoing spins}} v_4 \bar{u}_3 \gamma_\nu (-\not{k} \gamma_\mu + 2p_{4,\mu}) \right) \\
& = \frac{1}{2E} \left(-4a^{*i} i m k^\beta \epsilon_{\nu\beta\mu 0} \right. \\
& \quad \left. + (-b^{*i}) \left(-4\epsilon^{ijk} \epsilon_{\nu\beta\mu}^k p_4^j k^\beta - 4E k^\beta (g_{\nu\beta} \delta_\mu^i + \delta_\nu^i g_{\beta\mu} - g_{\mu\nu} \delta_\beta^i) \right. \right. \\
& \quad \left. \left. + 8E p_{4,\mu} \delta_\nu^i + 4 \frac{p_4^i p_4^j}{E+m} (k_\nu \delta_\mu^j + k_\mu \delta_\nu^j - k^j g_{\mu\nu} - 2p_{4,\mu} \delta_\nu^j) \right) \right)
\end{aligned} \tag{4.37}$$

where we have also permuted indices on the Levi-Civita symbols. This equation can be compared with equation (4.17) that is the corresponding one for the diagram 3a. We see that that equations (4.37) and (4.17) are the same with the substitutions $p_3 \rightarrow p_4$ and $b^{*i} \rightarrow -b^{*i}$, except for the overall minus sign. The minus sign is cancelled by the one in equation (4.35) so that we can read $L'_{\nu\mu} L^{\mu\nu}$ from equation (4.20) with the substitution $p_3, b^{*i} \rightarrow p_4, -b^{*i}$. In fact, we can read the angular integral over $L'_{\nu\mu} L^{\mu\nu}$ using these same substitutions as we also have v_4 instead of v_3

in the integral (4.34). We then get

$$\begin{aligned}
\text{Im}\mathcal{M}_{3b} &= \frac{1}{27\pi^2 E^4} \cdot g_s^4 t_{ji}^a t_{ih}^b t_{gf}^a t_{fe}^b \int d\Omega \frac{L'_{\nu\mu} L^{\mu\nu}}{(1 - \hat{\mathbf{k}} \cdot \mathbf{v}_1)(1 - \hat{\mathbf{k}} \cdot \mathbf{v}_4)} \\
&= \frac{g_s^4}{2^3 \pi m^2} \cdot t_{ji}^a t_{ih}^b t_{gf}^a t_{fe}^b \left[a'^* a \left(1 - \frac{4}{3} v^2 + \frac{1}{3} \mathbf{v}_1 \cdot \mathbf{v}_4 \right) \right. \\
&\quad \left. + b'^* b^j \left(\frac{1}{3} \delta^{ij} - \frac{1}{5} \delta^{ij} v^2 + \frac{2}{5} \delta^{ij} \mathbf{v}_1 \cdot \mathbf{v}_4 - \frac{11}{30} (v_1^i v_1^j + v_4^i v_4^j) + \frac{2}{5} v_1^i v_4^j + \frac{11}{15} v_4^i v_1^j \right) \right. \\
&\quad \left. + \mathcal{O}(v^3) \right].
\end{aligned} \tag{4.38}$$

The color part can again be separated into color-singlet and color-octet operators, using the identity (4.28). This allows us to write

$$\begin{aligned}
t_{ji}^a t_{ih}^b t_{gf}^a t_{fe}^b &= \frac{1}{4} \left(\delta_{jf} \delta_{gi} - \frac{1}{N_c} \delta_{ji} \delta_{gf} \right) \left(\delta_{ie} \delta_{fh} - \frac{1}{N_c} \delta_{ih} \delta_{fe} \right) \\
&= \frac{1}{4} \left[\left(1 + \frac{1}{N_c^2} \right) \delta_{jh} \delta_{ge} - \frac{2}{N_c} \delta_{je} \delta_{gh} \right] \\
&= \frac{1}{4} \left[-\frac{2}{N_c} \left(\delta_{je} \delta_{gh} - \frac{1}{N_c} \delta_{jh} \delta_{ge} \right) + \left(\frac{N_c^2 + 1}{N_c^2} - \frac{2}{N_c^2} \right) \delta_{jh} \delta_{ge} \right] \\
&= \frac{N_c^2 - 1}{4N_c^2} \delta_{jh} \delta_{ge} - \frac{1}{N_c} t_{jh}^a t_{ge}^a = \frac{C_F}{2N_c} \mathbb{1}_c \otimes \mathbb{1}_c - \frac{1}{N_c} t^a \otimes t^a.
\end{aligned} \tag{4.39}$$

By substituting this into (4.38) and writing $\mathbf{v} = \mathbf{v}_1$, $\mathbf{v}' = \mathbf{v}_3 = -\mathbf{v}_4$, $g_s^2 = 4\pi\alpha_s$, $4a'^* a = \mathbb{1}_s \otimes \mathbb{1}_s$ and $4b'^* b^j = \sigma^i \otimes \sigma^j$, we get final expressions for the invariant amplitude of the diagram 3b:

$$\begin{aligned}
\text{Im}\mathcal{M}_{3b} &= \frac{\pi\alpha_s^2}{2m^2} \cdot \left(\frac{C_F}{2N_c} \mathbb{1}_c \otimes \mathbb{1}_c - \frac{1}{N_c} t^a \otimes t^a \right) \left[\mathbb{1}_s \otimes \mathbb{1}_s \left(1 - \frac{4}{3} v^2 - \frac{1}{3} \mathbf{v} \cdot \mathbf{v}' \right) \right. \\
&\quad \left. + \sigma^i \otimes \sigma^i \left(-\frac{1}{3} + \frac{1}{5} v^2 + \frac{2}{5} \mathbf{v} \cdot \mathbf{v}' \right) \right. \\
&\quad \left. + \sigma^i \otimes \sigma^j \left(\frac{2}{5} v^i v'^j + \frac{11}{15} v^i v^j + \frac{11}{30} (v^i v^j + v'^i v'^j) \right) + \mathcal{O}(v^3) \right].
\end{aligned} \tag{4.40}$$

These are the only two diagrams that contribute to the color-singlet part of the invariant amplitude at the lowest order, as discussed previously. We can then

calculate the imaginary part of the total invariant amplitude for the color-singlet part:

$$\begin{aligned} \text{Im } \mathcal{M} = & \sum_{\text{diagrams}} \text{Im } \mathcal{M}_i = \frac{\pi\alpha_s^2}{m^2} \cdot \frac{C_F}{2N_c} \mathbb{1}_c \otimes \mathbb{1}_c \left[\mathbb{1}_s \otimes \mathbb{1}_s \left(1 - \frac{4}{3}v^2 \right) \right. \\ & \left. + \sigma^i \otimes \sigma^i \frac{2}{5} \mathbf{v} \cdot \mathbf{v}' + \sigma^i \otimes \sigma^j \left(\frac{2}{5} v^i v'^j + \frac{11}{15} v'^i v^j \right) + \mathcal{O}(v^3) \right] + \text{color-octet terms.} \end{aligned} \quad (4.41)$$

By comparing this with (4.2) we can read the coefficients of the operators at order $\mathcal{O}(\alpha_s^2)$:

$$\text{Im } f_1(^1S_0) = \frac{\pi C_F}{2N_c} \alpha_s^2, \quad (4.42a)$$

$$\text{Im } g_1(^1S_0) = -\frac{2\pi C_F}{3N_c} \alpha_s^2, \quad (4.42b)$$

$$\text{Im } f_1(^3P_0) = \frac{3\pi C_F}{2N_c} \alpha_s^2 \quad \text{and} \quad (4.42c)$$

$$\text{Im } f_1(^3P_2) = \frac{2\pi C_F}{5N_c} \alpha_s^2. \quad (4.42d)$$

All the other coefficients are zero at this order. These agree with reference [3, p. 96].

4.3 Electromagnetic decays

The coefficients of the operators include contributions from all $Q\bar{Q} \rightarrow Q\bar{Q}$ processes. By considering only certain diagrams we can calculate the part of the coefficient that corresponds to that diagram. In this way, the coefficients (4.42) can be seen to correspond to a gluonic decay of quarkonium. This means that we can also calculate separately the part that comes from the electromagnetic interactions and is therefore linked to the electromagnetic decay. At the lowest order, these diagrams are shown in figure 6. The figures 6a and 6b have their strong interaction counterparts in figures 3a and 3b. Therefore the invariant amplitudes for these processes are simple to calculate from the results we got in the case of strong interaction processes. Calculating the invariant amplitude we only need to make a substitution $t_{ij}^a g_s \rightarrow \delta_{ij} e Q$ for each QQg -vertex, where Q is the fractional charge of the heavy quark. In this way we

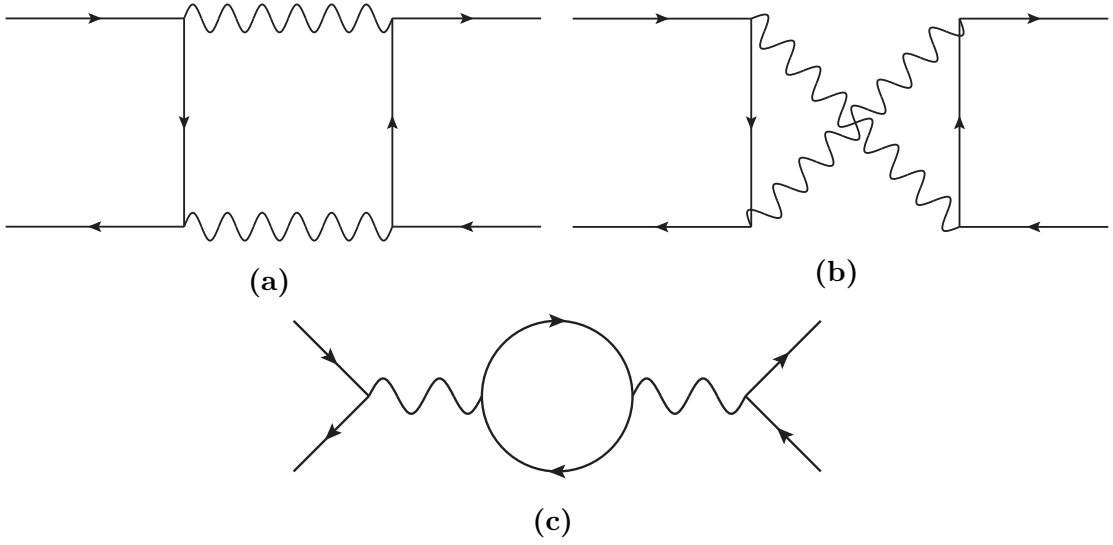


Figure 6. Lowest order diagrams contributing to the electromagnetic decay of $c\bar{c}$.

easily get the invariant amplitudes for the diagrams 6a and 6b:

$$\begin{aligned}
 \text{Im } \mathcal{M}_{6a} = & \frac{\pi\alpha^2 Q^4}{2m^2} \cdot \mathbb{1}_c \otimes \mathbb{1}_c \left[\mathbb{1}_s \otimes \mathbb{1}_s \left(1 - \frac{4}{3}v^2 + \frac{1}{3}\mathbf{v} \cdot \mathbf{v}' \right) \right. \\
 & + \sigma^i \otimes \sigma^i \left(\frac{1}{3} - \frac{1}{5}v^2 + \frac{2}{5}\mathbf{v} \cdot \mathbf{v}' \right) \\
 & \left. + \sigma^i \otimes \sigma^j \left(\frac{2}{5}v^i v'^j + \frac{11}{15}v'^i v^j - \frac{11}{30}(v^i v^j + v'^i v'^j) \right) + \mathcal{O}(v^3) \right] \quad \text{and}
 \end{aligned} \tag{4.43}$$

$$\begin{aligned}
 \text{Im } \mathcal{M}_{6b} = & \frac{\pi\alpha^2 Q^4}{2m^2} \cdot \mathbb{1}_c \otimes \mathbb{1}_c \left[\mathbb{1}_s \otimes \mathbb{1}_s \left(1 - \frac{4}{3}v^2 - \frac{1}{3}\mathbf{v} \cdot \mathbf{v}' \right) \right. \\
 & + \sigma^i \otimes \sigma^i \left(-\frac{1}{3} + \frac{1}{5}v^2 + \frac{2}{5}\mathbf{v} \cdot \mathbf{v}' \right) \\
 & \left. + \sigma^i \otimes \sigma^j \left(\frac{2}{5}v^i v'^j + \frac{11}{15}v'^i v^j + \frac{11}{30}(v^i v^j + v'^i v'^j) \right) + \mathcal{O}(v^3) \right].
 \end{aligned} \tag{4.44}$$

From this we can calculate the imaginary parts of the coefficients that correspond to the process where there is a $\gamma\gamma$ intermediate state, as the third diagram 6c doesn't

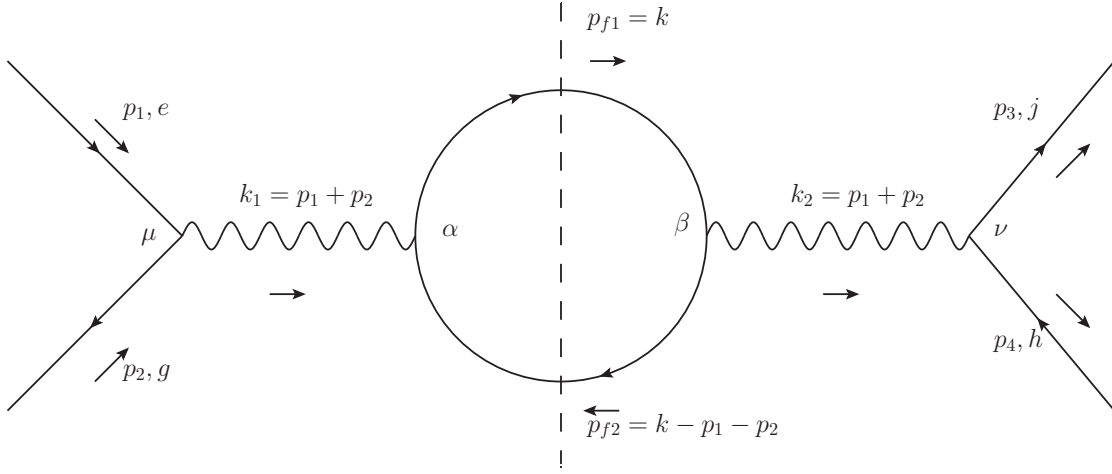


Figure 7. Diagram for calculating the invariant amplitude \mathcal{M}_{6c}

have such an intermediate state. The non-zero coefficients are then:

$$\text{Im } f_{\gamma\gamma}({}^1S_0) = \pi Q^4 \alpha^2, \quad (4.45a)$$

$$\text{Im } g_{\gamma\gamma}({}^1S_0) = -\frac{4}{3}\pi Q^4 \alpha^2, \quad (4.45b)$$

$$\text{Im } f_{\gamma\gamma}({}^3P_0) = 3\pi Q^4 \alpha^2 \quad \text{and} \quad (4.45c)$$

$$\text{Im } f_{\gamma\gamma}({}^3P_2) = \frac{4}{5}\pi Q^4 \alpha^2. \quad (4.45d)$$

Figure 6c also has a corresponding strong interaction diagram in figure 3g. In the case of strong interaction, this figure doesn't contribute to the invariant amplitudes for a color-singlet $|Q\bar{Q}\rangle$ state. However, figure 6c does have a non-zero invariant amplitude in the color-singlet state and therefore it is useful to calculate its contribution to the operator coefficients. This will correspond to a process where the decay happens through a virtual photon. Using the notation in figure 7, we get

the QCD invariant amplitude for diagram 6c:

$$\begin{aligned}
i\mathcal{M}_{6c} &= (-1) \int \frac{d^4k}{(2\pi)^4} \bar{u}_{s_3}(p_3) (iQe\delta_{jh}\gamma^\nu) v_{s_4}(p_4) \bar{v}_{s_2}(p_2) (iQe\delta_{ge}\gamma^\mu) u_{s_1}(p_1) \\
&\cdot \left(\frac{-ig_{\mu\alpha}}{k_1^2 + i\epsilon} \right) \left(\frac{-ig_{\nu\beta}}{k_2^2 + i\epsilon} \right) \text{Tr} \left((iQ_f e \delta_{kl} \gamma^\beta) \frac{-i(\not{p}_{f1} + m_f)}{p_{f1}^2 - m_f^2 + i\epsilon} (iQ_f e \delta_{lk} \gamma^\alpha) \frac{-i(\not{p}_{f2} + m_f)}{p_{f2}^2 - m_f^2 + i\epsilon} \right) \\
&= \int \frac{d^4k}{(2\pi)^4} \frac{-1}{\left(k^2 - m_f^2 + i\epsilon\right) \left((k - p_1 - p_2)^2 - m_f^2 + i\epsilon\right) \left((p_1 + p_2)^2\right)^2} \cdot \delta_{jh} \delta_{ge} \cdot \delta_{kl} \delta_{lk} \\
&\cdot e^4 Q^2 Q_f^2 \cdot \bar{u}_{s_3}(p_3) \gamma^\nu v_{s_4}(p_4) \bar{v}_{s_2}(p_2) \gamma^\mu u_{s_1}(p_1) \text{Tr} \left(\gamma_\nu (\not{p}_{f1} + m_f) \gamma_\mu (\not{p}_{f2} + m_f) \right).
\end{aligned} \tag{4.46}$$

Here $\delta_{kl}\delta_{lk}$ corresponds to possible color charges in the fermion loop. In the case of leptons there is no color charge associated with the fermion loop and we have $\delta_{kl}\delta_{lk} = 1$. For quarks this simply gives us $\delta_{kl}\delta_{lk} = N_c$.

To calculate the imaginary part of the invariant amplitude we can again use the Cutkosky cutting rules. This forces the fermions in the loop to be on the mass-shell with the cut shown in figure 7. In principle one could also cut the photon propagators, but the photons cannot be on the mass-shell and therefore the contribution from these cuts vanishes. The on-shell condition for the intermediate fermions reduces the possible particles in the fermion loop. For a quarkonium particle with mass m_H to decay into a fermion pair we must have $m_H > 2m_f$. For example, for charmonium particles J/ψ and η_c we have $m_H \approx 3.1\text{ GeV}$ so that the possible intermediate fermions are u -, d -, s - and c -quarks and electrons and muons. Of these, the c -quark intermediate state doesn't correspond to a decay process. The rest of the fermions have $m_f \ll m_c$ so that in this case we can approximate $m_f/m_c \approx 0$. This kind of approximation can also be made for the bottomonium particles, with the addition that they can decay also into $c\bar{c}$ - and $\tau\bar{\tau}$ -pairs. The Cutkosky rules then allow us to

simplify the propagator part of the integral:

$$\begin{aligned}
\text{Im } \mathcal{M}_{6c} &= \frac{(2\pi)^2}{2} \int \frac{d^4k}{(2\pi)^4} \frac{-\delta(k^2 - m_f^2) \delta((k - p_1 - p_2)^2 - m_f^2)}{((p_1 + p_2)^2)^2} \cdot f(k) \\
&= -\frac{1}{2^7 \pi^2 E^4} \int d^4k \delta(k^2 - m_f^2) \delta(4E^2 - 4k^0 E) f(k) \\
&= -\frac{1}{2^9 \pi^2 E^5} \int d^3\mathbf{k} \delta(E^2 - \mathbf{k}^2 - m_f^2) f(k^0 = E, \mathbf{k}) \\
&= -\frac{\sqrt{E^2 - m_f^2}}{2^{10} \pi^2 E^5} \int d\Omega f(k^0 = E, |\mathbf{k}| = \sqrt{E^2 - m_f^2}, \Omega) \\
&\approx -\frac{1}{2^{10} \pi^2 E^4} \int d\Omega f(k^0 = E, |\mathbf{k}| = E, \Omega)
\end{aligned} \tag{4.47}$$

where again $f(k)$ is rest of the integral (4.46).

We write spinor product for the incoming quark-antiquark pair as in equation (4.15) and use the properties of gamma matrices to write

$$\sum_{\text{spins}} \bar{v}_{s_2} \gamma^\mu u_{s_1} = \text{Tr} \left(\sum_{\text{spins}} u_{s_1} \bar{v}_{s_2} \gamma^\mu \right) = -\frac{2}{E} b^i \left(E g^{i\mu} - \frac{p_1^i p_1^j}{E + m} g^{j\mu} \right). \tag{4.48}$$

For the outgoing state we get

$$\begin{aligned}
\sum_{\text{spins}} \bar{u}_{s_3} \gamma^\nu v_{s_4} &= \text{Tr} \left(\gamma^\nu \sum_{\text{spins}} v_{s_4} \bar{u}_{s_3} \right) = \text{Tr} \left(\sum_{\text{spins}} u_{s_3} \bar{v}_{s_4} \gamma^\nu \right)^* \\
&= -\frac{2}{E} b^{i*} \left(E g^{i\nu} - \frac{p_3^i p_3^j}{E + m} g^{j\nu} \right).
\end{aligned} \tag{4.49}$$

The trace of the propagators in equation (4.46) can also be simplified using properties of the gamma matrices:

$$\begin{aligned}
\text{Tr} \left(\gamma_\nu (\not{p}_{f_1} + m_f) \gamma_\mu (\not{p}_{f_2} + m_f) \right) &= p_{f_1}^\alpha p_{f_2}^\beta \text{Tr}(\gamma_\nu \gamma_\alpha \gamma_\mu \gamma_\beta) + m_f^2 \text{Tr}(\gamma_\nu \gamma_\mu) \\
&= 4 p_{f_1}^\alpha p_{f_2}^\beta (g_{\nu\alpha} g_{\mu\beta} + g_{\mu\alpha} g_{\nu\beta} - g_{\nu\mu} g_{\alpha\beta}) + 4 m_f^2 g_{\mu\nu} \\
&= 4 \left(2k_\mu k_\nu - k_\nu (p_1 + p_2)_\mu - k_\mu (p_1 + p_2)_\nu + g_{\mu\nu} (-k^2 + m_f^2 + k^\alpha (p_1 + p_2)_\alpha) \right) \\
&= 4 \left(2k_\mu k_\nu - k_\nu (p_1 + p_2)_\mu - k_\mu (p_1 + p_2)_\nu + 2g_{\mu\nu} E^2 \right)
\end{aligned} \tag{4.50}$$

In total we get then

$$\begin{aligned}
& \sum_{\text{incoming spins}} \bar{v}_{s_2} \gamma^\mu u_{s_1} \sum_{\text{outgoing spins}} \bar{u}_{s_3} \gamma^\nu v_{s_4} \text{Tr} \left(\gamma_\nu (\not{p}_{f_1} + m_f) \gamma_\mu (\not{p}_{f_2} + m_f) \right) \\
&= \frac{16}{E^2} b^{i*} b^j \left(E g^{j\mu} - \frac{p_1^j p_1^k}{E+m} g^{k\mu} \right) \left(E g^{i\nu} - \frac{p_3^i p_3^l}{E+m} g^{l\nu} \right) \\
&\quad \cdot \left(2k_\mu k_\nu - k_\nu (p_1 + p_2)_\mu - k_\mu (p_1 + p_2)_\nu + 2g_{\mu\nu} E^2 \right) \\
&= \frac{16}{E^2} b^{i*} b^j \left(2E^2 k^i k^j + 2E^4 g^{ij} - \frac{2E^3}{E+m} (p_1^k p_1^j g^{ik} + p_3^i p_3^l g^{jl}) \right. \\
&\quad \left. - \frac{2E}{E+m} (p_1^j p_1^k k^k k^i + p_3^i p_3^l k^l k^j) + \mathcal{O}(v^3) \right) \\
&= 32E^2 b^{i*} b^j \left(\hat{k}^i \hat{k}^j - \delta^{ij} + \frac{1}{2} (v^i v^j + v'^i v'^j) - \frac{1}{2} (v^j v^k \hat{k}^k \hat{k}^i + v'^i v'^l \hat{k}^l \hat{k}^j) + \mathcal{O}(v^3) \right)
\end{aligned} \tag{4.51}$$

where again \mathbf{v} is the velocity of the incoming quark and \mathbf{v}' velocity of the outgoing quark. Using equations (4.25) we can perform the angular integral:

$$\begin{aligned}
& \int d\Omega 32E^2 b^{i*} b^j \left(\hat{k}^i \hat{k}^j - \delta^{ij} + \frac{1}{2} (v^i v^j + v'^i v'^j) - \frac{1}{2} (v^j v^k \hat{k}^k \hat{k}^i + v'^i v'^l \hat{k}^l \hat{k}^j) + \mathcal{O}(v^3) \right) \\
&= 32E^2 b^{i*} b^j \cdot 4\pi \left(\frac{1}{3} \delta^{ij} - \delta^{ij} + \frac{1}{2} (v^i v^j + v'^i v'^j) - \frac{1}{6} (v^j v^i + v'^i v'^j) + \mathcal{O}(v^3) \right) \\
&= -2^7 \pi E^2 b^{i*} b^j \left(\frac{2}{3} \delta^{ij} - \frac{1}{3} (v^i v^j + v'^i v'^j) + \mathcal{O}(v^3) \right)
\end{aligned} \tag{4.52}$$

In total, the invariant amplitude is then

$$\begin{aligned}
\text{Im } \mathcal{M}_{6c} &= \frac{1}{2^3 \pi E^2} \delta_{ji} \delta_{gf} \cdot \delta_{kl} \delta_{lk} \cdot g^4 Q^2 Q_f^2 b^{i*} b^j \left(\frac{2}{3} \delta^{ij} - \frac{1}{3} (v^i v^j + v'^i v'^j) + \mathcal{O}(v^3) \right) \\
&= \frac{(4\pi\alpha)^2 Q^2 Q_f^2}{2^3 \pi m^2} \delta_{ji} \delta_{gf} \cdot \delta_{kl} \delta_{lk} \cdot b^{i*} b^j \frac{2}{3} \left(\delta^{ij} (1 - v^2) - \frac{1}{2} (v^i v^j + v'^i v'^j) + \mathcal{O}(v^3) \right) \\
&= \frac{4\pi\alpha^2 Q^2 Q_f^2}{3m^2} \delta_{ji} \delta_{gf} \cdot \delta_{kl} \delta_{lk} \cdot b^{i*} b^j \left(\delta^{ij} (1 - v^2) - \frac{1}{2} (v^i v^j + v'^i v'^j) + \mathcal{O}(v^3) \right) \\
&= \frac{\pi\alpha^2 Q^2 Q_f^2}{3m^2} \cdot \delta_{kl} \delta_{lk} \cdot \mathbb{1}_c \otimes \mathbb{1}_c \cdot \sigma^i \otimes \sigma^j \left(\delta^{ij} (1 - v^2) - \frac{1}{2} (v^i v^j + v'^i v'^j) + \mathcal{O}(v^3) \right).
\end{aligned} \tag{4.53}$$

By comparing this with equation (4.2) we can read off the parts of the coefficients that

are related to the decay through a virtual photon. For the decay of the quarkonium into a lepton pair this is the leading order process and we get:

$$\text{Im } f_{l+l-}({}^3S_1) = \frac{\pi Q^2 \alpha^2}{3} \quad \text{and} \quad (4.54a)$$

$$\text{Im } g_{l+l-}({}^3S_1) = -\frac{4\pi Q^2 \alpha^2}{9} \quad (4.54b)$$

with the rest of the coefficients being zero. For the decay of the quarkonium into light hadrons (LH) through a virtual photon we need to sum over the intermediate quarks. The non-zero coefficients are then

$$\text{Im } f_{\gamma^* \rightarrow \text{LH}}({}^3S_1) = \frac{\pi N_c \alpha^2 Q^2}{3} \sum_i Q_i^2 \quad \text{and} \quad (4.55a)$$

$$\text{Im } g_{\gamma^* \rightarrow \text{LH}}({}^3S_1) = -\frac{4\pi N_c \alpha^2 Q^2}{9} \sum_i Q_i^2. \quad (4.55b)$$

For example, for J/ψ we have $\sum_i Q_i^2 = \sum_{i=u,d,s} Q_i^2 = 2/3$.

5 Quarkonium Decay and Production

5.1 Connection between the decay and the 4-fermion operators

We have now demonstrated how to calculate the coefficients of the 4-fermion operators. With the explicit forms of the 4-fermion operators, we can go on to connect them to the decay widths. This is done using the optical theorem. The optical theorem allows us to link the invariant amplitude of the forward scattering to the sum of all possible scattering processes [9, p. 231]:

$$2 \operatorname{Im} \mathcal{M}(a \rightarrow a) = \sum_f \int d\Pi_f |\mathcal{M}(a \rightarrow f)|^2 \quad (5.1)$$

where $d\Pi_f$ is the phase space element corresponding to the final state f . On the other hand, the decay width of a particle H with mass M is [9, p. 237]

$$\Gamma = 2M \cdot \frac{1}{2M} \sum_f \int d\Pi_f |\mathcal{M}(H \rightarrow f)|^2 = 2 \operatorname{Im} \mathcal{M}(H \rightarrow H). \quad (5.2)$$

The prefactor $2M$ comes from the non-relativistic normalization of the states (2.55).

In equation (5.2) we sum over all final states. We can use this to distinguish the parts of the decay width that correspond to different particles in the final state. In QCD this is easily accomplished as we can calculate the invariant amplitudes corresponding to decay processes $H \rightarrow f$ directly. In NRQCD however, the heavy quark and antiquark numbers are conserved so that calculating the invariant amplitudes $\mathcal{M}(Q\bar{Q} \rightarrow f)$ isn't possible unless the final state f has exactly one heavy quark and antiquark. In this work, we are interested in calculating the quarkonium decay widths for processes where the final states don't contain heavy quarks. Therefore we need to calculate the width using the imaginary part of the forward scattering amplitude $\mathcal{M}(H \rightarrow H)$. At the lowest orders in α_s , the NRQCD diagrams that contribute to the imaginary part either have continuous heavy quark lines from the initial state to the final state or a 4-fermion vertex. The first type we can identify

with decays where the final state also contains heavy quarks. For decays with no heavy quarks in the final state we can then identify that the whole contribution to the decay width comes from the 4-fermion vertices.

Let us calculate the invariant amplitude corresponding to the 4-fermion vertices in an operator form. The LSZ reduction theorem allows us to connect the transition matrix to the interaction part of the Hamiltonian [9, p. 109]:

$$\langle H | iT | H \rangle = \lim_{T \rightarrow \infty (1-i\epsilon)} \left(\left\langle H \left| T \left(\exp \left[-i \int_{-T}^T dt H_I(t) \right] \right) \right| H \right\rangle_I \right)_{\text{connected amputated}}. \quad (5.3)$$

The left side of this equation is defined as the forward scattering amplitude

$$\langle H(K') | iT | H(K) \rangle = (2\pi)^4 \delta^4(K - K') i\mathcal{M}(H(K) \rightarrow H(K')). \quad (5.4)$$

If we now expand the exponential in equation (5.3) to the first order and consider only the 4-fermion vertex interactions, we get

$$\begin{aligned} & (2\pi)^4 \delta^4(K - K') i\mathcal{M}(H(K) \rightarrow H(K'))_{4\text{-fermion}} \\ = & i \int d^4x \sum_{\text{dim}=6} \frac{f_i}{M^2} \langle H(K') | \mathcal{O}_i(x) | H(K) \rangle + \sum_{\text{dim}=8} \frac{f_i}{M^4} \langle H(K') | \mathcal{O}_i(x) | H(K) \rangle \quad (5.5) \\ & + \text{higher order.} \end{aligned}$$

This can be simplified by noting that the x -dependence of the operators can be written in terms of momentum operators [9, p. 26]:

$$\mathcal{O}_i(x) = e^{i\hat{P}\cdot x} \mathcal{O}_i(0) e^{-i\hat{P}\cdot x}. \quad (5.6)$$

We can then write

$$\begin{aligned} \int d^4x \langle H(K') | \mathcal{O}_i(x) | H(K) \rangle &= \int d^4x \langle H(K') | e^{i\hat{P}\cdot x} \mathcal{O}_i(0) e^{-i\hat{P}\cdot x} | H(K) \rangle \\ &= \int d^4x \langle H(K') | e^{iK'\cdot x} \mathcal{O}_i(0) e^{-iK\cdot x} | H(K) \rangle \quad (5.7) \\ &= (2\pi)^4 \delta^4(K - K') \langle H(K') | \mathcal{O}_i(0) | H(K) \rangle, \end{aligned}$$

and comparing to equation (5.5) we can identify

$$\begin{aligned} & \mathcal{M}(H(K) \rightarrow H(K'))_{4\text{-fermion}} \\ &= \sum_{\text{dim}=6} \frac{f_i}{M^2} \langle H(K') | \mathcal{O}_i(0) | H(K) \rangle + \sum_{\text{dim}=8} \frac{f_i}{M^4} \langle H(K') | \mathcal{O}_i(0) | H(K) \rangle + \dots \end{aligned} \quad (5.8)$$

As we argued above, this invariant amplitude can be linked to quarkonium decays where there are no heavy quarks in the final state. The optical theorem now gives us the corresponding decay width:

$$\Gamma(H \rightarrow \text{no heavy quarks}) = \sum_{\text{dim}=6} \frac{2 \text{Im } f_i}{M^2} \langle H | \mathcal{O}_i | H \rangle + \sum_{\text{dim}=8} \frac{2 \text{Im } f_i}{M^4} \langle H | \mathcal{O}_i | H \rangle + \dots \quad (5.9)$$

The matrix elements $\langle H | \mathcal{O}_i | H \rangle$ are called *long-distance matrix elements* (LDME), as they are linked to the non-perturbative effects of QCD. This is in contrast with the coefficients $\text{Im } f_i$ that can be calculated from point-like scattering processes.

Depending on the particle, the matrix elements in (5.9) have different scalings in powers of velocity. From now on, we will focus explicitly on η_c and J/ψ particles. Higher charmonium states can be treated similarly by estimating the contributions of different Fock states as in section 3.1 and using the corresponding velocity-scaling rules from table 1 for the operators. For η_c and J/ψ we have the Fock state expansions (3.8) and (3.9). We can now use the fact that the 4-fermion operators vanish for most Fock states, and remember that they are labeled by the one Fock state for which they give a non-vanishing contribution. Then we can write the η_c decay schematically as

$$\begin{aligned} \Gamma(\eta_c) &= \frac{2 \text{Im } f_1(^1S_0)}{M^2} \langle ^1S_0^{[1]} | \mathcal{O}_1(^1S_0) | ^1S_0^{[1]} \rangle + \frac{2 \text{Im } g_1(^1S_0)}{M^4} \langle ^1S_0^{[1]} | \mathcal{P}_1(^1S_0) | ^1S_0^{[1]} \rangle \\ &+ \mathcal{O}(v^2) \cdot \frac{2 \text{Im } f_8(^1P_0)}{M^2} \langle ^1P_0^{[8]} g | \mathcal{O}_8(^1P_0) | ^1P_0^{[8]} g \rangle \\ &+ \mathcal{O}(v^3) \cdot \frac{2 \text{Im } f_8(^3S_1)}{M^2} \langle ^3S_1^{[8]} | \mathcal{O}_8(^3S_1) | ^3S_1^{[8]} g \rangle + \dots \end{aligned} \quad (5.10)$$

In section 4 we calculated the imaginary parts of the coefficients $f_1(^1S_0)$ and $g_1(^1S_0)$, finding that they are proportional to α_s^2 . The other coefficients also have to be at least of order $\mathcal{O}(\alpha_s^2)$, so that we can use the velocity-scaling rules and the Fock state expansion of η_c to see that the first term in the decay width has the least order in velocity. We can similarly deduce that the following terms scale as v^2 , v^4 and v^3

compared to the first one. This allows us to write

$$\Gamma(\eta_c) = \frac{2 \operatorname{Im} f_1(^1S_0)}{M^2} \langle \eta_c | \mathcal{O}_1(^1S_0) | \eta_c \rangle + \frac{2 \operatorname{Im} g_1(^1S_0)}{M^4} \langle \eta_c | \mathcal{P}_1(^1S_0) | \eta_c \rangle + \mathcal{O}(v^3\Gamma), \quad (5.11)$$

where the notation $\mathcal{O}(v^3\Gamma)$ means that the discarded terms scale as v^3 compared to the dominant term in the decay width. For J/ψ we can similarly use the Fock state expansion and the velocity-scaling rules to get the following expression for the decay width:

$$\begin{aligned} \Gamma(J/\psi) &= \frac{2 \operatorname{Im} f_1(^3S_1)}{M^2} \langle J/\psi | \mathcal{O}_1(^3S_1) | J/\psi \rangle + \frac{2 \operatorname{Im} g_1(^3S_1)}{M^4} \langle J/\psi | \mathcal{P}_1(^3S_1) | J/\psi \rangle \\ &+ \mathcal{O}(v^3\Gamma). \end{aligned} \quad (5.12)$$

5.2 Quarkonium wave functions

The matrix elements $\langle \mathcal{O}_i \rangle$ that we get can be related to the wave function of the particle. This can be done by noting that the 4-fermion operators can be written as $\mathcal{O}_i = \psi^\dagger \mathcal{K}'_n \chi \chi^\dagger \mathcal{K}_n \psi$, where the operators \mathcal{K} consist of spin and color matrices, derivative operators, and fields \mathbf{E} and \mathbf{B} . This form allows us to see that the 4-fermion operators can be divided into parts with the initial state and the final state by inserting a sum over a complete set of states X :

$$\langle H | \mathcal{O}_i | H \rangle = \sum_X \langle H | \psi^\dagger \mathcal{K}'_n \chi | X \rangle \langle X | \chi^\dagger \mathcal{K}_n \psi | H \rangle \approx \langle H | \psi^\dagger \mathcal{K}'_n \chi | 0 \rangle \langle 0 | \chi^\dagger \mathcal{K}_n \psi | H \rangle. \quad (5.13)$$

In the last step we approximated that the contribution to the sum comes mostly from the vacuum state. This is called the *vacuum-saturation approximation*. For 4-fermion operators that annihilate and create the dominant $Q\bar{Q}$ -pair this is a reasonable assumption, as the next-to-leading contribution comes from the term $\langle H | \psi^\dagger \mathcal{K}'_n \chi | gg \rangle \langle gg | \chi^\dagger \mathcal{K}_n \psi | H \rangle$. Fock states $|Q\bar{Q}gg\rangle$ are generally suppressed by v^4 according to the multipole expansion, which means that the vacuum-saturation approximation also holds up to order v^4 for matrix elements $\langle H | \mathcal{O}_i | H \rangle$. For operators that annihilate the $Q\bar{Q}$ -pair in a non-dominant state the vacuum-saturation approximation is less justified.

We can now calculate the matrix element $\langle \eta_c | \mathcal{O}_1(^1S_0) | \eta_c \rangle$ using the vacuum

saturation approximation:

$$\langle \eta_c | \mathcal{O}_1(^1S_0) | \eta_c \rangle \approx \langle \eta_c | \psi^\dagger \chi | 0 \rangle \langle 0 | \chi^\dagger \psi | \eta_c \rangle = \left| \langle 0 | \chi^\dagger \psi | \eta_c \rangle \right|^2. \quad (5.14)$$

Following reference [3, p. 40], we define the radial wave function of η_c by

$$R_{\eta_c}(r) = \sqrt{\frac{2\pi}{N_c}} \langle 0 | \chi^\dagger(-\mathbf{r}/2) \psi(\mathbf{r}/2) | \eta_c \rangle. \quad (5.15)$$

Let us justify this definition. If η_c were a pure 1S_0 state, we could use the explicit form (3.10) to calculate this quantity. We would then get

$$\begin{aligned} & \frac{\sqrt{2\pi}}{\sqrt{N_c}} \langle 0 | \chi^\dagger(-\mathbf{r}/2) \psi(\mathbf{r}/2) | ^1S_0(\mathbf{0}) \rangle \\ &= \sqrt{\frac{2\pi}{N_c}} \text{Tr} \left(\frac{1}{\sqrt{2}} \mathbb{1}_2 \right) \text{Tr} \left(\frac{1}{\sqrt{N_c}} \mathbb{1}_{N_c} \right) \int \frac{d^3\mathbf{q}}{(2\pi)^3} \frac{1}{\sqrt{4\pi}} \varphi(\mathbf{q}) \int \frac{d^3\mathbf{q}_1 d^3\mathbf{q}_2}{(2\pi)^6} e^{i\mathbf{r}/2 \cdot \mathbf{q}_1} e^{-i\mathbf{r}/2 \cdot \mathbf{q}_2} \\ & \quad \cdot \langle 0 | \chi_{j,b}^\dagger(\mathbf{q}_2) \psi_{i,a}(\mathbf{q}_1) \psi_{i,a}^\dagger(\mathbf{q}) \chi_{j,b}(-\mathbf{q}) | 0 \rangle \\ &= \int \frac{d^3\mathbf{q}}{(2\pi)^3} \varphi(\mathbf{q}) \int \frac{d^3\mathbf{q}_1 d^3\mathbf{q}_2}{(2\pi)^6} e^{i\mathbf{r}/2 \cdot \mathbf{q}_1} e^{-i\mathbf{r}/2 \cdot \mathbf{q}_2} (2\pi)^6 \delta(\mathbf{q}_2 + \mathbf{q}) \delta(\mathbf{q}_1 - \mathbf{q}) \\ &= \int \frac{d^3\mathbf{q}}{(2\pi)^3} \varphi(\mathbf{q}) e^{i\mathbf{r}/2 \cdot \mathbf{q}} e^{-i\mathbf{r}/2 \cdot (-\mathbf{q})} = \int \frac{d^3\mathbf{q}}{(2\pi)^3} \varphi(\mathbf{q}) e^{i\mathbf{r} \cdot \mathbf{q}} = R(r) \end{aligned} \quad (5.16)$$

which shows that the definition (5.15) is reasonable. With this definition for the η_c wave function we can write the expectation value as

$$\langle \eta_c | \mathcal{O}_1(^1S_0) | \eta_c \rangle = |R_{\eta_c}(0)|^2 (1 + \mathcal{O}(v^4)), \quad (5.17)$$

remembering that the vacuum-saturation approximation used in equation (5.14) holds at relative order v^4 . In general, however, the wave function or its derivative defined in this way may be singular at the origin. Therefore we should instead use regularized operators χ_Λ and ψ_Λ that can be defined by dimensional regularization with scale Λ or with some other regularization scheme. We then define

$$\overline{R_{\eta_c}}(\Lambda) = \sqrt{\frac{2\pi}{N_c}} \langle 0 | \chi_\Lambda^\dagger(0) \psi_\Lambda(0) | \eta_c \rangle. \quad (5.18)$$

The interpretation of this is that instead of taking the value of the wave function at

the origin we take the average over a sphere of size $1/\Lambda$.

We can similarly define the renormalized Laplacian of the wave function by

$$\overline{\nabla^2 R_{\eta_c}}(\Lambda) = \sqrt{\frac{2\pi}{N_c}} \langle 0 | \chi_\Lambda^\dagger(0) \left(\frac{1}{2} \overleftrightarrow{\nabla} \right)^2 \psi_\Lambda(0) | \eta_c \rangle. \quad (5.19)$$

Let's show again that this definition is justified. First of all, using the non-regularized operators we can write

$$\begin{aligned} & \chi^\dagger(\mathbf{r}_2) \left(\frac{1}{2} \overleftrightarrow{\nabla} \right)^2 \psi(\mathbf{r}_1) \\ &= \frac{1}{4} \left[\left(\nabla_{\mathbf{r}_2}^2 \chi(\mathbf{r}_2) \right)^\dagger \psi(\mathbf{r}_1) + \chi(\mathbf{r}_2)^\dagger \nabla_{\mathbf{r}_1}^2 \psi(\mathbf{r}_1) - 2 \left(\nabla_{\mathbf{r}_2} \chi(\mathbf{r}_2) \right)^\dagger \nabla_{\mathbf{r}_1} \psi(\mathbf{r}_1) \right] \\ &= \frac{1}{4} \int \frac{d^3 \mathbf{q}_1 d^3 \mathbf{q}_2}{(2\pi)^6} \chi^\dagger(\mathbf{q}_2) \psi(\mathbf{q}_1) \\ & \quad \cdot \left[\left(\nabla_{\mathbf{r}_2}^2 e^{-i\mathbf{q}_2 \cdot \mathbf{r}_2} \right)^\dagger e^{i\mathbf{q}_1 \cdot \mathbf{r}_1} + e^{i\mathbf{q}_2 \cdot \mathbf{r}_2} \nabla_{\mathbf{r}_1}^2 e^{i\mathbf{q}_1 \cdot \mathbf{r}_1} - 2 \left(\nabla_{\mathbf{r}_2} e^{-i\mathbf{q}_2 \cdot \mathbf{r}_2} \right)^\dagger \cdot \nabla_{\mathbf{r}_1} e^{i\mathbf{q}_1 \cdot \mathbf{r}_1} \right] \\ &= \frac{1}{4} \int \frac{d^3 \mathbf{q}_1 d^3 \mathbf{q}_2}{(2\pi)^6} \chi^\dagger(\mathbf{q}_2) \psi(\mathbf{q}_1) e^{i(\mathbf{q}_1 \cdot \mathbf{r}_1 + \mathbf{q}_2 \cdot \mathbf{r}_2)} \left(-\mathbf{q}_2^2 - \mathbf{q}_1^2 + 2\mathbf{q}_1 \cdot \mathbf{q}_2 \right). \end{aligned} \quad (5.20)$$

Now it is easy to calculate to action of this operator on the 1S_0 state:

$$\begin{aligned} & \sqrt{\frac{2\pi}{N_c}} \langle 0 | \chi^\dagger(-\mathbf{r}/2) \left(\frac{1}{2} \overleftrightarrow{\nabla} \right)^2 \psi(\mathbf{r}/2) | ^1S_0(\mathbf{0}) \rangle \\ &= \frac{1}{4} \sqrt{\frac{2\pi}{N_c}} \text{Tr} \left(\frac{1}{\sqrt{2}} \mathbb{1}_2 \right) \text{Tr} \left(\frac{1}{\sqrt{N_c}} \mathbb{1}_{N_c} \right) \int \frac{d^3 \mathbf{q}}{(2\pi)^3} \frac{1}{\sqrt{4\pi}} \varphi(\mathbf{q}) \int \frac{d^3 \mathbf{q}_1 d^3 \mathbf{q}_2}{(2\pi)^6} \\ & \quad \cdot e^{i(\mathbf{q}_1 \cdot \mathbf{r}/2 - \mathbf{q}_2 \cdot \mathbf{r}/2)} \cdot \left(-\mathbf{q}_2^2 - \mathbf{q}_1^2 + 2\mathbf{q}_1 \cdot \mathbf{q}_2 \right) \cdot \langle 0 | \chi_{j,b}^\dagger(\mathbf{q}_2) \psi_{i,a}(\mathbf{q}_1) \psi_{i,a}^\dagger(\mathbf{q}) \chi_{j,b}(-\mathbf{q}) | 0 \rangle \\ &= \frac{1}{4} \int \frac{d^3 \mathbf{q}}{(2\pi)^3} \varphi(\mathbf{q}) \int \frac{d^3 \mathbf{q}_1 d^3 \mathbf{q}_2}{(2\pi)^6} e^{i\mathbf{r}/2 \cdot (\mathbf{q}_1 - \mathbf{q}_2)} \left(-\mathbf{q}_2^2 - \mathbf{q}_1^2 + 2\mathbf{q}_1 \cdot \mathbf{q}_2 \right) \\ & \quad \cdot (2\pi)^6 \delta(\mathbf{q}_2 + \mathbf{q}) \delta(\mathbf{q}_1 - \mathbf{q}) \\ &= \int \frac{d^3 \mathbf{q}}{(2\pi)^3} \varphi(\mathbf{q}) e^{i\mathbf{r} \cdot \mathbf{q}} \left(-\mathbf{q}^2 \right) = \nabla^2 R(r). \end{aligned} \quad (5.21)$$

This shows that the definition (5.19) is reasonable. We can now write the second

matrix element in the equation for the η_c decay width (5.11) as

$$\begin{aligned} \langle \eta_c | \mathcal{P}_1(^1S_0) | \eta_c \rangle &\approx \frac{1}{2} \left[\langle \eta_c | \psi_\Lambda^\dagger \chi_\Lambda | 0 \rangle \langle 0 | \chi_\Lambda^\dagger \left(\frac{i \overleftrightarrow{\mathbf{D}}}{2} \right)^2 \psi_\Lambda | \eta_c \rangle + \text{h.c.} \right] \\ &\approx -\frac{1}{2} \left[\langle \eta_c | \psi_\Lambda^\dagger \chi_\Lambda | 0 \rangle \langle 0 | \chi_\Lambda^\dagger \left(\frac{1 \overleftrightarrow{\nabla}}{2} \right)^2 \psi_\Lambda | \eta_c \rangle + \text{h.c.} \right] \approx -\frac{N_c}{2\pi} \text{Re} \left(\overline{R_{\eta_c}^*} \overleftrightarrow{\nabla}^2 R_{\eta_c} \right). \end{aligned} \quad (5.22)$$

In the first equivalence we used the vacuum-saturation approximation, which holds at order v^4 . In the second one we used the approximation $\overleftrightarrow{\mathbf{D}}^2 = \overleftrightarrow{\nabla}^2(1 + \mathcal{O}(v^2))$. Therefore this holds in total up to relative order v^2 , and we can use these approximations in the expression for the decay width (5.11).

We can similarly define the wave functions for J/ψ . In this case we need to take into account the polarization $\boldsymbol{\epsilon}$ of the particle, and we define

$$\overline{R_{J/\psi}}(\Lambda) = \boldsymbol{\epsilon}^* \cdot \sqrt{\frac{2\pi}{N_c}} \langle 0 | \chi_\Lambda^\dagger(0) \boldsymbol{\sigma} \psi_\Lambda(0) | J/\psi(\boldsymbol{\epsilon}) \rangle \quad (5.23)$$

and

$$\overleftrightarrow{\nabla}^2 \overline{R_{J/\psi}}(\Lambda) = \boldsymbol{\epsilon}^* \cdot \sqrt{\frac{2\pi}{N_c}} \langle 0 | \chi_\Lambda^\dagger(0) \boldsymbol{\sigma} \left(\frac{1 \overleftrightarrow{\nabla}}{2} \right)^2 \psi_\Lambda(0) | J/\psi(\boldsymbol{\epsilon}) \rangle. \quad (5.24)$$

The reasoning here is that J/ψ is mainly a 3S_1 state, so that the only difference to the 1S_0 case of η_c comes from the spin matrix. We can now write the matrix elements in the J/ψ decay width (5.12) using the vacuum-saturation approximation, and we get similar results as for η_c :

$$\langle J/\psi | \mathcal{O}_1(^3S_1) | J/\psi \rangle = \frac{N_c}{2\pi} |\overline{R_{J/\psi}}|^2 (1 + \mathcal{O}(v^4)) \quad \text{and} \quad (5.25)$$

$$\langle J/\psi | \mathcal{P}_1(^3S_1) | J/\psi \rangle = -\frac{N_c}{2\pi} \text{Re} \left(\overline{R_{J/\psi}^*} \overleftrightarrow{\nabla}^2 R_{J/\psi} \right) (1 + \mathcal{O}(v^2)). \quad (5.26)$$

Having the η_c and J/ψ wave functions, we can also construct a spin-averaged wave function. Spin effects come from terms like $1/M^2 \psi^\dagger \boldsymbol{\sigma} \cdot i\mathbf{D} \times \mathbf{E} \psi$ and $1/M \psi^\dagger \boldsymbol{\sigma} \cdot g\mathbf{B}$ in the heavy quark Lagrangian (2.29). These scale as $\mathcal{O}(M^4 v^7)$ which is suppressed by a factor of v^2 compared to the leading order terms that scale as $\mathcal{O}(M^4 v^5)$. Therefore we also expect the wave functions to be similar up to this accuracy, meaning that we have

$$R_{\eta_c}(r) = R_{J/\psi}(r) (1 + \mathcal{O}(v^2)). \quad (5.27)$$

If we only need the wave function at order $\mathcal{O}(v^2)$ we can then combine these wave functions into a spin-averaged wave function

$$R_S(r) = \frac{1}{4} \left(3R_{J/\psi}(r) + R_{\eta_c}(r) \right). \quad (5.28)$$

This is the same definition as in reference [3, p. 41]. The coefficients have been chosen to minimize the effects of the spin: in the quantum mechanical perturbation theory, the effects of the spin for $L = 0$ states come from the spin-spin coupling which is proportional to the inner product of the spin vectors $\langle \mathbf{S}_c \cdot \mathbf{S}_{\bar{c}} \rangle$ [14, p. 286]. This has the value $+1/4$ for a spin-triplet state and $-3/4$ for a spin-singlet state, so the combination in equation (5.28) is chosen in such a way that the spin-spin coupling terms cancel each other.

5.3 Decay widths

Writing the matrix elements in terms of the wave functions, we can write the decay widths of η_c and J/ψ as

$$\Gamma(\eta_c) = \frac{N_c \text{Im } f_1(^1S_0)}{\pi M^2} |\overline{R_{\eta_c}}|^2 - \frac{N_c \text{Im } g_1(^1S_0)}{\pi M^4} \text{Re} \left(\overline{R_S^*} \nabla^2 R_S \right) + \mathcal{O}(v^3 \Gamma) \quad (5.29)$$

and

$$\Gamma(J/\psi) = \frac{N_c \text{Im } f_1(^3S_1)}{\pi M^2} |\overline{R_{J/\psi}}|^2 - \frac{N_c \text{Im } g_1(^3S_1)}{\pi M^4} \text{Re} \left(\overline{R_S^*} \nabla^2 R_S \right) + \mathcal{O}(v^3 \Gamma). \quad (5.30)$$

By looking at the different diagrams that contribute to the imaginary parts of the coefficients we can then conclude the equations for different partial widths. For example, for the partial width $\Gamma(\eta_c \rightarrow \text{light hadrons})$ we can substitute the values for the coefficients (4.42a) and (4.42b) that we calculated in section 4.2. Similarly for the decay $J/\psi \rightarrow l^+ l^-$ we can take the values for the coefficients from equations (4.54a) and (4.54b). However, to use the equations (5.29) and (5.30) we would need to know the values for the coefficient $\text{Im } f$ at order v^2 higher than the first non-vanishing order in v . For example, we would need to calculate $\text{Im } f_{\text{LH}}(^1S_0)$ at order α_s^4 and $\text{Im } f_{ee}(^3S_1)$ at order $\alpha^2 \alpha_s^2$. So far, these have been calculated only up to order α_s relative to the first non-vanishing order. A complete collection of these for the 1S_0 and 3S_1 and states can be found in reference [15], and they are shown in table 2. These can be calculated in a similar way as we have done here by including higher

order diagrams when calculating the imaginary part of the invariant amplitude in QCD.

Even though the coefficients $\text{Im } f$ have not been calculated in the required accuracy, we will still use the equations (5.29) and (5.30) also in this order when comparing to experimental data. The reason for this is that in reference [3, p. 8] it is argued that we should expect v to be greater than or of order $\alpha_s(Q)$, where Q is the energy scale associated with the process. This comes from the fact that the velocity-scaling rules state that $\alpha(Mv) \approx v$, and because α_s is a decreasing function in terms of energy then we must have $v > \alpha_s(Q)$ if $Q > Mv$. The natural energy scale depends on the process, but here it is natural to take it as either the mass of the heavy quark or the quarkonium particle. Therefore we could expect powers of velocity to be more relevant than $\alpha_s(M)$ in equations (5.29) and (5.30), and it is somewhat justifiable to leave the α_s^2 corrections to $\text{Im } f$ out. For the coefficients $\text{Im } g$ it is enough to calculate them in the order of v where the coefficient $\text{Im } f$ is non-vanishing. In this case it means that the order of $\text{Im } g$ we have calculated is enough. They also agree with the corresponding equations in reference [15], except for the case $^3S_1 \rightarrow \text{LH}$ where they have been calculated to orders α_s^3 and $\alpha\alpha_s^2$ in the reference as this is lowest order where the corresponding coefficient $\text{Im } f$ is non-vanishing.

We can also write the equations for the decay widths at lower order in v , in which case we have

$$\Gamma(\eta_c) = \frac{N_c \text{Im } f_1(^1S_0)}{\pi M^2} |\overline{R}_{\eta_c}|^2 + \mathcal{O}(v^2\Gamma) \quad (5.31)$$

and

$$\Gamma(J/\psi) = \frac{N_c \text{Im } f_1(^3S_1)}{\pi M^2} |\overline{R}_\psi|^2 + \mathcal{O}(v^2\Gamma). \quad (5.32)$$

Here we should include the α_s corrections to the coefficients $\text{Im } f$. If we don't include these corrections, these equations hold only at order $\mathcal{O}(v\Gamma)$.

Table 2. Decay coefficients for quarkonium, from reference [15].

Channel	Coefficient
${}^3S_1 \rightarrow ggg$	$\text{Im } f = \frac{(\pi^2 - 9)(N_c^2 - 4)C_F}{54N_c} \alpha_s^3 \left[1 + (-9.46C_F + 4.13C_A - 1.161n_f) \frac{\alpha_s}{\pi} \right]$ $\text{Im } g = -4 \cdot 4.33 \frac{(\pi^2 - 9)(N_c^2 - 4)C_F}{54N_c} \alpha_s^3$
${}^3S_1 \rightarrow \gamma gg$	$\text{Im } f = \frac{2(\pi^2 - 9)C_F Q^2 \alpha}{3N_c} \alpha_s^2 \left[1 + (-9.46C_F + 2.75C_A - 0.774n_f) \frac{\alpha_s}{\pi} \right]$ $\text{Im } g = -4 \cdot 4.33 \frac{2(\pi^2 - 9)C_F Q^2 \alpha}{3N_c} \alpha_s^2$
${}^3S_1 \rightarrow \gamma^* \rightarrow \text{LH}$	$\text{Im } f = \pi Q^2 \left(\sum_i Q_i^2 \right) \alpha^2 \left[1 - \frac{13}{4} C_F \frac{\alpha_s}{\pi} \right]$ $\text{Im } g = -\frac{4}{3} \pi Q^2 \left(\sum_i Q_i^2 \right) \alpha^2$
${}^3S_1 \rightarrow l^+ l^-$	$\text{Im } f = \frac{\pi Q^2 \alpha^2}{3} \left[1 - 4C_F \frac{\alpha_s}{\pi} \right]$ $\text{Im } g = -\frac{4}{3} \frac{\pi Q^2 \alpha^2}{3}$
${}^1S_0 \rightarrow gg$	$\text{Im } f = \frac{\pi C_F}{2N_c} \alpha_s^2 \left[1 + \left(\left(\frac{\pi^2}{4} - 5 \right) C_F + \left(\frac{199}{18} - \frac{13\pi^2}{24} \right) C_A - \frac{8}{9} n_f \right) \frac{\alpha_s}{\pi} \right]$ $\text{Im } g = -\frac{4}{3} \frac{\pi C_F}{2N_c} \alpha_s^2$
${}^1S_0 \rightarrow \gamma\gamma$	$\text{Im } f = \pi Q^4 \alpha^2 \left[1 + \left(\frac{\pi^2}{4} - 5 \right) C_F \frac{\alpha_s}{\pi} \right]$ $\text{Im } g = -\frac{4}{3} \pi Q^4 \alpha^2$

5.4 Quarkonium production

We will briefly mention the treatment of quarkonium production in NRQCD. This is similar to the quarkonium decay in the way that we can define quarkonium production operators and link these to the cross section for inclusive production. This treatment of quarkonium production follows section IV of reference [3].

The production operators can be written in terms of the produced quarkonium particle and the same operators that appear in the 4-fermion operators. A general production operator can be written as

$$\mathcal{O}_n^H = \sum_X \sum_{m_J} \chi^\dagger \mathcal{K}'_n \psi |H_{m_J} + X\rangle \langle H_{m_J} + X| \psi^\dagger \mathcal{K}_n \chi \quad (5.33)$$

where \mathcal{K} and \mathcal{K}' are combinations of the derivatives, spin and color matrices and fields \mathbf{E} and \mathbf{B} , and H is the quarkonium particle that is produced. Here the sum goes over all additional particles X and the polarizations m_J of the particle H . These operators can also be labeled by the quark-antiquark pair that they create and annihilate. For example, a production operator that creates and annihilates the $Q\bar{Q}$ pair in the state $^1S_0^{[1]}$ can be written as

$$\mathcal{O}_1^H(^1S_0) = \sum_X \sum_{m_J} \chi^\dagger \psi |H_{m_J} + X\rangle \langle H_{m_J} + X| \psi^\dagger \chi. \quad (5.34)$$

These production operators appear in the cross section for the inclusive production of the quarkonium. The idea is that the cross section formula factorizes so that we can think of it as first producing the $Q\bar{Q}$ -pair which then forms the bound quarkonium state [3, p. 72]. We can then write the differential cross section in the following way [16]:

$$d\sigma_{a+b \rightarrow H+X} = \sum_n d\sigma_{a+b \rightarrow Q\bar{Q}[n]+X} \langle 0 | \mathcal{O}_n^H | 0 \rangle. \quad (5.35)$$

Here n denotes the different quantum numbers of the $Q\bar{Q}$ -pair. We can again use the vacuum-saturation approximation to simplify the expectation value $\langle 0 | \mathcal{O}_i^H | 0 \rangle$. If we approximate that the contribution in the sum of equation (5.33) comes mostly

from the pure quarkonium state, we get

$$\begin{aligned}
\langle 0 | \mathcal{O}_n^H | 0 \rangle &= \sum_X \sum_{m_J} \langle 0 | \chi^\dagger \mathcal{K}'_n \psi | H_{m_J} + X \rangle \langle H_{m_J} + X | \psi^\dagger \mathcal{K}_n \chi | 0 \rangle \\
&\approx \sum_{m_J} \langle 0 | \chi^\dagger \mathcal{K}'_n \psi | H_{m_J} \rangle \langle H_{m_J} | \psi^\dagger \mathcal{K}_n \chi | 0 \rangle = (2J + 1) \langle 0 | \chi^\dagger \mathcal{K}'_n \psi | H \rangle \langle H | \psi^\dagger \mathcal{K}_n \chi | 0 \rangle \\
&\approx (2J + 1) \sum_X \langle H | \psi^\dagger \mathcal{K}_n \chi | X \rangle \langle X | \chi^\dagger \mathcal{K}'_n \psi | H \rangle = (2J + 1) \langle H | \mathcal{O}_i | H \rangle
\end{aligned} \tag{5.36}$$

where \mathcal{O}_i is the 4-fermion operator with the same \mathcal{K}_n and \mathcal{K}'_n operators between the quark and antiquark fields. Here it should be noted that this does not hold for all possible production operators, as the vacuum-saturation approximation cannot be justified in all cases. For example, in the case of a color-octet operator, the vacuum state cannot be the dominant one as the particle H has to be a color-singlet in total. Therefore in that case states like $|H + g\rangle\langle H + g|$ would be more dominant in the sum and the vacuum-saturation approximation isn't applicable. However, if the production operators creates and annihilates the $Q\bar{Q}$ -pair with the same quantum numbers as the dominant state in the particle H , the vacuum-saturation approximation is justified and holds at relative order v^4 , in the similar way as we argued with equation (5.13). The vacuum-saturation approximation is useful as it allows us to link some of the production matrix elements to the decay matrix elements. For example, we can link the leading-order matrix elements in the decay of η_c and J/ψ to the following production matrix elements:

$$\langle \eta_c | \mathcal{O}_1(^1S_0) | \eta_c \rangle = \langle 0 | \mathcal{O}_1^{\eta_c} (^1S_0) | 0 \rangle (1 + \mathcal{O}(v^4)) \quad \text{and} \tag{5.37}$$

$$\langle J/\psi | \mathcal{O}_1(^3S_1) | J/\psi \rangle = 3 \langle 0 | \mathcal{O}_1^{J/\psi} (^3S_1) | 0 \rangle (1 + \mathcal{O}(v^4)). \tag{5.38}$$

6 Phenomenology

The long-distance matrix elements that appear in the equations for decay widths and cross sections can be determined from lattice QCD simulations or by fitting to corresponding experimental data. When doing that, one must keep in mind that the quarkonium velocity can be rather large and therefore the convergence of the power series may not be fast. Therefore we will not try to determine the LDMEs by the decay width data ourselves, but instead refer to the literature where these matrix elements have been determined to a good precision. We will then use these LDMEs to study the convergence of the power series. Only the decay widths will be considered here for two reasons: our focus has been mainly on calculating the decay widths for quarkonia, and the cross sections would involve color-octet matrix elements that are not significant for decay widths [17]. Thus the decay widths allow us to study NRQCD phenomenology with a minimal amount of unknown parameters.

6.1 Charmonium decay widths

For charmonium, we will use the LDME values from reference [18]. Following their notation we will denote $\langle \mathcal{O}_1 \rangle_{J/\psi} = \langle J/\psi | \mathcal{O}_1(^3S_1) | J/\psi \rangle$ and $\langle \mathcal{O}_1 \rangle_{\eta_c} = \langle \eta_c | \mathcal{O}_1(^1S_0) | \eta_c \rangle$ and similarly for the matrix elements $\langle J/\psi | \mathcal{P}_1(^3S_1) | J/\psi \rangle$ and $\langle \eta_c | \mathcal{P}_1(^1S_0) | \eta_c \rangle$. Their estimates are:

$$\begin{aligned} \langle \mathcal{O}_1 \rangle_{J/\psi} &= 0.440 \text{ GeV}^3, & \frac{\langle \mathcal{P}_1 \rangle_{J/\psi}}{\langle \mathcal{O}_1 \rangle_{J/\psi}} &= 0.441 \text{ GeV}^2, \\ \langle \mathcal{O}_1 \rangle_{\eta_c} &= 0.437 \text{ GeV}^3, \quad \text{and} & \frac{\langle \mathcal{P}_1 \rangle_{\eta_c}}{\langle \mathcal{O}_1 \rangle_{\eta_c}} &= 0.442 \text{ GeV}^2. \end{aligned} \tag{6.1}$$

These values were evaluated using experimental data for the decays $\eta_c \rightarrow \gamma\gamma$ and $J/\psi \rightarrow e^+e^-$. The equations they used in determining these values were based on equations (5.29) and (5.30) but also included some of the higher order terms in velocity and α_s . Therefore substituting the values (6.1) to the equations (5.29) and (5.30) is not expected to give an exact match with the experimental value. In

determining these values, they also used the fact that the LDMEs can be defined using the wave functions of the particle. This way, they were able to use a potential model to calculate the wave functions with suitable regularizations and link the matrix elements $\langle \mathcal{O}_1 \rangle$ and $\langle \mathcal{P}_1 \rangle$.

Using these values for the matrix elements, we have calculated the decay widths from the equations (5.29) and (5.30) for various channels. The decay widths were calculated at relative orders $\mathcal{O}(v\Gamma)$, $\mathcal{O}(v^2\Gamma)$ and $\mathcal{O}(v^3\Gamma)$. As discussed in section 5.3, the order $\mathcal{O}(v\Gamma)$ corresponds to equations (5.31) and (5.32) with the coefficient $\text{Im } f$ at the lowest non-vanishing order, order $\mathcal{O}(v^2\Gamma)$ has α_s -corrections added to $\text{Im } f$, and $\mathcal{O}(v^3\Gamma)$ also has coefficient $\text{Im } g$ at the order where $\text{Im } f$ is non-vanishing. The results are presented in table 3, with the explicit orders of $\text{Im } f$ and $\text{Im } g$ shown. The different decay channels used were $J/\psi \rightarrow ggg$, $J/\psi \rightarrow \gamma gg$, $J/\psi \rightarrow \gamma^* \rightarrow \text{LH}$, $J/\psi \rightarrow l^+l^-$, $\eta_c \rightarrow \text{LH}$ and $\eta_c \rightarrow \gamma\gamma$. Of these, the decays of J/ψ into ggg , γgg and the virtual photon are only intermediates states that in the end are observed as light hadrons. Therefore one could also combine these to calculate the width $J/\psi \rightarrow \text{LH}$. The mass of the charm quark used is $m_c = 1.4 \text{ GeV}$, and the values for the coupling constants were also the same as in reference [18]. The coupling constants were taken to be $\alpha_s(m_{J/\psi}) = 0.25$ and $\alpha(m_{J/\psi}) = 1/132.6$ for processes $J/\psi \rightarrow \gamma^* \rightarrow \text{LH}$ and $J/\psi \rightarrow l^+l^-$, and $\alpha_s(m_{\eta_c}/2) = 0.35$ and $\alpha(m_{\eta_c}/2) = 1/133.6$ for processes $J/\psi \rightarrow ggg$, $J/\psi \rightarrow \gamma gg$, $\eta_c \rightarrow \text{LH}$ and $\eta_c \rightarrow \gamma\gamma$. The reason for taking the coupling constants at different energy scales is that for processes $Q\bar{Q} \rightarrow \gamma^*$ the energy transfer should correspond to the mass of the quarkonium particle, and for the other processes one can estimate the energy transfer to be of the order of the quark mass. As the difference between the masses of η_c and J/ψ is small compared to their mass, at this accuracy it doesn't make a difference which of these particles is used for the energy scale of the coupling constant. Therefore it is justified to use the energy scale m_{η_c} also for the coupling constants for the processes $J/\psi \rightarrow ggg$ and $J/\psi \rightarrow \gamma gg$. The experimental values are from Particle Data Group (2018) [19]. For the decay $J/\psi \rightarrow l^+l^-$ we used the experimental value of $J/\psi \rightarrow e^+e^-$, but we could as well have used the corresponding muon channel as the experimental values for these are almost identical.

Table 3 shows that the convergence of the power series is slow. For the decays of J/ψ into ggg and γgg the results are especially suspicious, as it makes no sense to say that the decay width is negative. This shows that for these decays the NRQCD

Table 3. Charmonium decay widths calculated for different channels and at different orders using NRQCD. The last column shows the ratio of the NRQCD value to the experimental data.

Channel	Accuracy		Decay width (keV)	NRQCD/Experiment
$J/\psi \rightarrow ggg$	$\text{Im } f: \alpha_s^3,$	$\text{Im } g: 0$	689	11.6
	$\text{Im } f: \alpha_s^4,$	$\text{Im } g: 0$	404	6.79
	$\text{Im } f: \alpha_s^4,$	$\text{Im } g: \alpha_s^3$	-2280	-38.3
$J/\psi \rightarrow \gamma gg$	$\text{Im } f: \alpha\alpha_s^2,$	$\text{Im } g: 0$	424	51.9
	$\text{Im } f: \alpha\alpha_s^3,$	$\text{Im } g: 0$	108	13.2
	$\text{Im } f: \alpha\alpha_s^3,$	$\text{Im } g: \alpha\alpha_s^2$	-718	-87.9
$J/\psi \rightarrow \gamma^* \rightarrow \text{LH}$	$\text{Im } f: \alpha^2,$	$\text{Im } g: 0$	23.8	1.90
	$\text{Im } f: \alpha^2\alpha_s,$	$\text{Im } g: 0$	15.6	1.24
	$\text{Im } f: \alpha^2\alpha_s,$	$\text{Im } g: \alpha^2$	8.44	0.673
$J/\psi \rightarrow l^+l^-$	$\text{Im } f: \alpha^2,$	$\text{Im } g: 0$	11.9	2.14
	$\text{Im } f: \alpha^2\alpha_s,$	$\text{Im } g: 0$	6.84	1.22
	$\text{Im } f: \alpha^2\alpha_s,$	$\text{Im } g: \alpha^2$	3.28	0.590
$\eta_c \rightarrow \text{LH}$	$\text{Im } f: \alpha_s^2,$	$\text{Im } g: 0$	38 100	1.20
	$\text{Im } f: \alpha_s^3,$	$\text{Im } g: 0$	85 200	2.67
	$\text{Im } f: \alpha_s^3,$	$\text{Im } g: \alpha_s^2$	73 600	2.31
$\eta_c \rightarrow \gamma\gamma$	$\text{Im } f: \alpha^2,$	$\text{Im } g: 0$	15.5	3.10
	$\text{Im } f: \alpha^2\alpha_s,$	$\text{Im } g: 0$	9.67	1.93
	$\text{Im } f: \alpha^2\alpha_s,$	$\text{Im } g: \alpha^2$	4.98	0.994

decay widths are unreliable. For the other decays the results are more reasonable, but even in these cases the results differ greatly order by order. It is especially notable that the value of $\Gamma(J/\psi \rightarrow e^+e^-)$ differs from the experimental value even though this was used in determining the LDMEs. This is because of additional higher order contributions included in reference [18]. The other decay width used in determining LDMEs, $\Gamma(\eta_c \rightarrow \gamma\gamma)$, agrees with the experimental data almost exactly as for this one the differences between our equation and the one in reference [18] are smaller.

In total, the electromagnetic decays and the decay $\eta_c \rightarrow \text{LH}$ seem to behave more nicely. This can also be seen from the equations in table 2 for the coefficients $\text{Im } f$ and $\text{Im } g$. For these decays, we have $\text{Im } g \approx -4/3 \text{Im } f$ in contrast with $\text{Im } g \approx -17.32 \text{Im } f$ that holds for the processes $J/\psi \rightarrow ggg$ and $J/\psi \rightarrow \gamma gg$. For the power counting of equations (5.29) and (5.30) to work, we would need to have $|\text{Im } g \cdot v^2| \ll |\text{Im } f|$. As we have the estimate $v^2 \approx 0.23$ [18], we see that in the case of the processes $J/\psi \rightarrow ggg$ and $J/\psi \rightarrow \gamma gg$ we have $|\text{Im } g \cdot v^2| \approx 4|\text{Im } f|$ and the assumptions of the power counting do not hold. For the other processes we have $|\text{Im } g \cdot v^2| \approx 0.3|\text{Im } f| \ll |\text{Im } f|$, but even then the convergence of the power series is poor.

6.2 Bottonium decay widths

We also studied the convergence of the power series for bottonium. The bottonium LDMEs were calculated in reference [20], in a similar way as for charmonium. This time they were fitted using $\Upsilon(nS) \rightarrow e^+e^-$ data, giving us for the $1S$ state $\langle \mathcal{O}_1 \rangle_\Upsilon = 3.069 \text{ GeV}^3$ and $\langle \mathcal{P}_1 \rangle_\Upsilon / \langle \mathcal{O}_1 \rangle_\Upsilon = -0.193 \text{ GeV}^2$. It is interesting that the ratio of LDMEs is negative, as it should roughly correspond to the expectation value $\langle \mathbf{p}^2 \rangle$ where \mathbf{p} is the momentum of the quark [18]. One should, however, remember that these quantities have been renormalized, meaning that the necessary subtractions can make these quantities negative.

The bottonia states η_b and Υ can be handled in NRQCD in exactly the same way as η_c and J/ψ . The only differences from equations (5.29) and (5.30) are that one must remember to use the b -quark mass and charge instead of the corresponding quantities for the c -quark. In table 4 we have calculated the bottonia decay widths using NRQCD in the same way as we did for charmonium. Here we have used the above LDME values for both Υ and η_b , as the corresponding LDMEs for η_b have not been calculated. As discussed in section 5.2, the wave functions and therefore

the LDMEs of Υ and η_b should be the same up to accuracy $\mathcal{O}(v^2)$ so that we can use the LDMEs from Υ to estimate the ones for η_b . For the mass of the b -quark we used $m_b = 4.6$ GeV, and for the couplings $\alpha_s(m_\Upsilon) = 1/131$ and $\alpha(m_\Upsilon) = 0.18$ for all processes. These are the values used in reference [20] when determining the LDMEs. It would be preferable to use the coupling constants at the energy scale $m_\Upsilon/2$ for the processes $\Upsilon \rightarrow ggg$, $\Upsilon \rightarrow \gamma gg$ and $\eta_b \rightarrow \text{LH}$, but the results do not differ much between the energy scales m_Υ and $m_\Upsilon/2$ because the running of the couplings is slow enough at these scales. Again, the NRQCD results have also been compared to the experimental data from the Particle data group [19]. The experimental value for $\Upsilon \rightarrow l^+l^-$ is from the decay $\Upsilon \rightarrow e^+e^-$. One could also use the experimental values from the decays $\Upsilon \rightarrow \mu^+\mu^-$ and $\Upsilon \rightarrow \tau^+\tau^-$ but the differences are not remarkable.

Apart from the channel $\Upsilon \rightarrow \gamma gg$, the convergence and accuracy of the NRQCD results seems good. The width $\Gamma(\Upsilon \rightarrow l^+l^-)$ is expected to agree with the experimental data, as this the decay used in determining the LDME. It is surprising that the width $\Gamma(\Upsilon \rightarrow ggg)$ convergences rather well, as this channel gave non-sensical results for charmonium. For the width $\Gamma(\eta_b \rightarrow \text{LH})$, we also have surprisingly good agreement with the experimental data, even though the LDMEs used were for Υ and not η_b . One should, however, remember that the measured width $\Gamma(\eta_b \rightarrow \text{LH})_{\text{exp}} \approx \Gamma(\eta_c)_{\text{exp}} = 10_{-4}^{+5} \text{MeV}$ is not very precise so that the agreement is unreliable. Nevertheless, the width $\Gamma(\eta_b \rightarrow \text{LH})$ is at least correct order of magnitude and the convergence seems to be good. The width $\Gamma(\Upsilon \rightarrow \gamma gg)$ is the only one of these that differs greatly from experimental value. The power series seems to converge quickly also in this case, however. This is puzzling as we would expect it to approach the experimental value when we continue power series, which does not seem to be the case here. One possible cause for this could be that the α_s^2 corrections to the coefficient $\text{Im } f$ are big and needed to take into account. In fact, table 4 shows that the α_s corrections to the coefficient $\text{Im } f$ are significant whereas the terms with the coefficient $\text{Im } g$ do not have a big impact in the bottonium case.

Table 4. Bottomonium decay widths calculated for different channels and at different orders using NRQCD. The last column shows the ratio of the NRQCD value to the experimental data.

Channel	Accuracy	Decay width (keV)	NRQCD/Experiment
$\Upsilon \rightarrow ggg$	$\text{Im } f: \alpha_s^3, \quad \text{Im } g: 0$	60.5	1.37
	$\text{Im } f: \alpha_s^4, \quad \text{Im } g: 0$	43.7	0.989
	$\text{Im } f: \alpha_s^4, \quad \text{Im } g: \alpha_s^3$	53.2	1.21
$\Upsilon \rightarrow \gamma gg$	$\text{Im } f: \alpha\alpha_s^2, \quad \text{Im } g: 0$	18.5	15.6
	$\text{Im } f: \alpha\alpha_s^3, \quad \text{Im } g: 0$	10.6	8.91
	$\text{Im } f: \alpha\alpha_s^3, \quad \text{Im } g: \alpha\alpha_s^2$	10.1	10
$\Upsilon \rightarrow l^+l^-$	$\text{Im } f: \alpha^2, \quad \text{Im } g: 0$	1.96	1.47
	$\text{Im } f: \alpha^2\alpha_s, \quad \text{Im } g: 0$	1.37	1.02
	$\text{Im } f: \alpha^2\alpha_s, \quad \text{Im } g: \alpha^2$	1.39	1.04
$\eta_b \rightarrow \text{LH}$	$\text{Im } f: \alpha_s^2, \quad \text{Im } g: 0$	6560	0.656
	$\text{Im } f: \alpha_s^3, \quad \text{Im } g: 0$	10 400	1.04
	$\text{Im } f: \alpha_s^3, \quad \text{Im } g: \alpha_s^2$	10 500	1.05

7 Conclusions

Non-relativistic QCD is an effective field theory that is particularly useful in studying quarkonia. The primary assumption of NRQCD is that the heavy quarks and antiquarks have velocities $v \ll 1$, so that they are non-relativistic and we can separate the field operators of the heavy quarks from antiquarks. This is what we did in section 2 where we wrote the NRQCD Lagrangian for the heavy quarks in terms of the heavy quark and antiquark fields. We then were able to deduce the velocity-scaling of each operator that appears in Lagrangian by the use of the field equations. This is extremely useful, as it allows us to write quantities of interest as a power series in velocity by using the velocity-scaling rules. In particular, it allows us to write $\alpha_s(Mv) = \mathcal{O}(v)$, which means that we don't need to treat the power counting in α_s and v separately. The desired quantities can then be written systematically as a power series in the quark velocity.

In NRQCD, we get equations for decay widths and cross sections that can be written in terms of long-distance matrix elements and coefficients which can be determined by perturbative matching. The LDMEs are unknown constants that have to be fitted from experimental data or calculated either from potential models or lattice QCD simulations. The decay and production LDMEs are not independent: we can often use the vacuum-saturation approximation and find that they are proportional to each other, as shown in equation (5.36). NRQCD thus allows us to use the same universal constants in quarkonium decay and production.

Our focus has been on calculating the decay widths of quarkonia using NRQCD. We showed how the LDMEs arise from the 4-fermion operators and how the operator coefficients can be calculated by matching invariant amplitudes to QCD. The matching was done for color-singlet operators at order α_s^2 for gluonic decays and α^2 for electromagnetic decays. At this order, the operator coefficients agree with the ones in the literature where they have been calculated to higher orders [15]. It can then be seen from the equations of decay widths (5.29) and (5.30) that for η_c and J/ψ the decay widths depend only on the pure $|c\bar{c}\rangle$ Fock state at lowest orders. The corresponding result holds also for the bottomonium particles η_b and Υ , for which the

decay widths depend mostly on the $|b\bar{b}\rangle$ state.

These equations for the decay widths are written as a power series of the quark velocity v . We therefore studied the convergence and the accuracy of these power series for charmonium particles J/ψ and η_c and bottonium particles Υ and η_b . In general, the power series do not seem to converge fast. This can be understood by the fact that the quantities with respect to which we are expanding, α_s and v , are not particularly small. For charmonium, it is estimated that $\alpha_s(m_{J/\psi}) \approx 0.25$ and $v \approx \sqrt{0.23} \approx 0.48$ [18]. For bottonium these are a little smaller, with $\alpha_s(m_\Upsilon) \approx 0.18$ and the estimate $v \approx \sqrt{0.1} \approx 0.3$. Another reason for the poor convergence is that the coefficient $\text{Im } g$ for the higher order terms is often bigger than coefficient $\text{Im } f$ for the leading order terms. This is especially true for processes $Q\bar{Q}(^3S_1) \rightarrow ggg$ and $Q\bar{Q}(^3S_1) \rightarrow \gamma gg$, for which the power series fails completely in the case of charmonium. The electromagnetic processes, along with the process $Q\bar{Q}(^1S_0) \rightarrow \text{LH}$, behave more nicely and are more reliable. For bottonium, the convergence of the power series is better in general, which is to be expected. To fully evaluate the decay widths up to relative order $\mathcal{O}(v^3\Gamma)$, however, one would need to calculate the coefficients $\text{Im } f$ with α_s^2 corrections relative to the first non-vanishing order. Unfortunately, these corrections have not been calculated so far.

In total, NRQCD offers us a framework for a systematic treatment of quarkonia. It allows us to treat the decay and production of quarkonium particles in a similar way, with a few unknown constants that can also be linked to the quarkonium wave function. While the magnitude of the quark velocity and α_s means that the equations do not give accurate results at lowest orders, in principle we can get better results by continuing the power series. All in all, the factorization of non-perturbative effects into LDMEs simplifies the treatment of quarkonia and allows us to quantify the contributions of different Fock states.

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