Abstract

This is the first in a series of papers, in which we compute the third-order QCD corrections to top-antitop production near threshold in $e^+e^-$ collisions. The present paper provides a detailed outline of the strategy of computation in the framework of non-relativistic effective theory and the threshold expansion, applicable more generally to heavy-quark pair production near threshold. It summarizes matching coefficients and potentials relevant to the next-to-next-to-next-to-leading order and ends with the master formula for the computation of the third-order Green function. The master formula is evaluated in part II of the series.
1 Introduction

Many of the most accurate heavy-quark mass determinations are related to the spectral functions of the heavy-quark vector current, which can be measured in $e^+e^-$ collisions. The energy region near the pair production threshold is particularly sensitive to the mass value. The bottom and charm masses are usually inferred from suitable averages of the pair production cross section. Looking to the future, the measurement of the top quark pair production cross section in the threshold region at the planned International Linear Collider (ILC) would lead to a very precise knowledge of the top mass directly from the energy dependence of the cross section, even though the toponium resonances are smeared out due to the large top quark width [1]. To put this into perspective, the current top mass value from direct production at the Fermilab Tevatron is $m_t = 173.18 \pm 0.56 \text{ (stat.)} \pm 0.75 \text{ (syst.) GeV}$ [2], and $m_t = 173.3 \pm 0.5 \text{ (stat.)} \pm 1.3 \text{ (syst.) GeV}$ from the Large Hadron Collider (LHC) run at 7 TeV centre-of-mass energy [3]. A less precise value can be obtained from the total production cross section as illustrated for example in [4]. Further reduction of the uncertainty below the one of the Tevatron result is very difficult due to the complicated theoretical systematics of top jet mass reconstruction at hadron colliders. The above numbers should be compared to a precision of 30 MeV that can be achieved experimentally [5,6,7] from the $t\bar{t}$ threshold scan at the ILC. In particular, while it is not evident which renormalized top mass parameter is determined with the quoted accuracy at the Tevatron and LHC, the threshold cross section in $e^+e^-$ collisions provides an observable that can be unambiguously related to a particular top mass definition.

Aside from determining a fundamental parameter of the Standard Model (SM), accurate top mass measurements are of interest for extrapolating the SM or its TeV scale extension to higher energies, either in the context of “electroweak precision tests” or a theory of the Yukawa couplings. Furthermore, the recent discovery of a Higgs boson [8,9] with a mass of about 125 GeV if interpreted as the SM Higgs boson determines the Higgs self-coupling and leads to the conclusion that the SM vacuum becomes metastable at scales above $10^{10}$ GeV [10]. The precise value of this scale turns out to depend very sensitively on the value of the top quark mass. Finally, the absence of any hint on physics beyond the SM in high-energy collisions at LHC has renewed the interest in performing precision measurements of properties of SM particles, including the top quark mass, width and Yukawa coupling. Measurements at the top pair production threshold are uniquely suited for this purpose.

The challenge is thus to calculate the heavy-quark spectral functions precisely in the threshold region. This kinematic region is characterized by two features, which make the theoretical calculation of QCD corrections rather different from standard loop calculations: the small three-velocity $v$ of the heavy quarks, which allows to expand Feynman diagrams in $v$ rather than calculate them exactly, and the strong colour-Coulomb force.

\footnote{In the following we will often refer to the heavy quark as the “top quark”, since this covers the most general case. For charm and bottom quarks, one simply sets the decay width $\Gamma$ to zero in the top-quark expressions.}
which on the other hand requires certain diagrams to be summed to all orders in the strong coupling $\alpha_s$ similar to bound-state calculations in quantum electrodynamics. The expansion of the cross section relative to the ultra-relativistic point-particle cross section $\sigma_0$ is then organized as

$$R = \sigma_{\text{tot}}/\sigma_0 \sim v \sum_k \left( \frac{\alpha_s}{v} \right)^k \{1(\text{LO}); \alpha_s, v (\text{NLO}); \alpha_s^2, \alpha_s v, v^2 (\text{NNLO}); \alpha_s^3, \alpha_s^2 v, \alpha_s v^2, v^3 (\text{NNNLO}); \ldots \},$$

where the overall factor of $v$ arises from the phase-space of the two produced massive particles, and the order of the various terms is indicated explicitly. To perform the expansion and the required summation of perturbation theory to all orders beyond the next-to-leading order (NLO), non-relativistic effective field theory $^{11,12,13}$ and the threshold expansion of Feynman diagrams $^{14}$ are the methods of choice. The cross section is then obtained from the expression

$$R = 12\pi e_t^2 \text{Im} \left[ \frac{N_c}{2m^2} \left( c_v - \frac{E}{m} \left( c_v + \frac{d_v}{3} \right) \right) G(E) + \ldots \right], \quad (1.2)$$

where $c_v, d_v$ denote certain relativistic matching corrections, $E = \sqrt{s} - 2m$, $N_c = 3$ the number of colours, and $G(E)$ represents a two-point function of heavy-quark currents in the non-relativistic effective theory. The purpose of this paper is to present results of the part of the third-order (NNNLO) QCD corrections to the heavy quark anti-quark pair production cross section near threshold related to the correlation function $G(E)$, which contains the all-order summation. Since this concludes the non-relativistic third-order calculation, we also present details of the methods and calculations that have been used but not given in earlier publications.

For the top pair production threshold the leading order (LO) and next-to-leading order (NLO) approximations to the cross section $^{11}$ have been examined long ago $^{15,16,17}$. Several other aspects of the threshold such as top momentum distributions and polarization have been computed at this order $^{18,19,20,21}$. Beyond NLO, matching the non-relativistic approximation to QCD is non-trivial, because the separation between relativistic and non-relativistic physics is no longer unambiguous. A consistent field theoretical approach based on non-relativistic effective QCD is now required. The second-order (NNLO) QCD corrections to the total pair production cross section have been computed in this framework about ten years ago $^{22,23,24,25,26,27,28}$ and turned out to be surprisingly large even for top quarks. While some of the large corrections can be understood as being due to mass renormalization $^{29}$, and can be avoided by a change of renormalization convention, there remains an apparently slow convergence of successive approximations to the normalization of the cross section, which necessitates the calculation of the NNNLO term. An alternative approach that sums logarithms of $v$ has also been pursued, and an improvement of convergence has been found in a (still partially incomplete)
next-to-next-to-leading logarithmic (NNLL) approximation \([30,31,32,33]\). Nonetheless, the NNNLO non-logarithmic terms not included in the NNLL approximation are required to be certain that the theoretical calculation is sufficiently accurate for the proposed mass measurement at the ILC. This is the main motivation for the present work. Over the past years a significant number of results relevant to a NNNLO calculation or partial results for third-order quarkonium energy levels and wave-functions at the origin have already appeared \([34,35,36,37,38,39,40,41,42,43,44,45,46,47,48,49,50,51,52,53,54,55,56,57]\).

In the following we summarize the status of the NNNLO top cross section calculation, the contribution of the present paper, and what remains to be done to complete the NNNLO calculation.

Matching calculations

While the resummed cross section is calculated in an effective field theory (EFT), a number of matching calculations has to be performed to guarantee that the EFT reproduces QCD to the required accuracy. This is done in two steps. Hard matching (scale \(k \sim m\)) yields the coefficients of the non-relativistic QCD (NRQCD) interactions and heavy-quark currents; soft matching (scale \(k \sim mv\)) the quark-anti-quark potentials. At NNNLO the coefficients of several subleading NRQCD interactions must be determined with one-loop precision. This calculation has been performed in \([58]\). However, as shall be explained, the calculation of the cross section requires the \(O(\epsilon)\) terms of the coefficient functions. We therefore repeated the NRQCD matching calculation, confirm the results of \([58]\) and provide the expressions for the \(O(\epsilon)\) terms in this paper (see also \([59]\)). Hard matching of the non-relativistic currents at NNNLO is needed at the one-loop level for the sub-leading currents and at the three-loop level for the leading current. The former are known \([60]\), and will be rederived in the present paper, but only the fermionic contributions to the three-loop matching coefficient \(c_3\) have been calculated up to now \([47]\). As discussed in \([51]\), the incomplete result for \(c_3\) presently constitutes the most important missing NNNLO contribution to the cross section.

As concerns soft matching, the potentials of order \(1/(m^2r^3)\) must be determined with one-loop precision, the \(1/(mr^2)\) potential with two-loop precision, and the \(1/r\) Coulomb potential at three loops, since \(r\) counts as the Bohr radius \(1/(ma_s)\). Except for the Coulomb potential, the coefficients of the other potentials have been calculated in \([40,41]\), but again these results are not sufficient for the cross section calculations, since the \(O(\epsilon)\) terms of all these potentials are needed. We repeated the calculation of the one-loop \(1/(m^2r^3)\) potentials, confirm the results of \([41]\) and provide the expressions for the \(O(\epsilon)\) terms in this paper (see also \([59]\)). The \(O(\epsilon)\) term of the two-loop \(1/(mr^2)\) potential coefficient \(b_2\) remains presently unknown. As concerns the three-loop Coulomb potential, the fermionic contributions to the three-loop coefficient \(a_3\) have been calculated first in \([53]\) and the full result is now also known \([55,56]\).

To summarize: the matching coefficients required for the NNNLO calculation of the heavy-quark production cross section near threshold are known except for the non-fermionic contributions to \(c_3\), and the \(O(\epsilon)\) terms of \(b_2\). Out of these, only \(c_3\) is expected
to have a major impact on the final result \[48\]. Work on these missing contributions is in progress.

**Matrix element calculations**

After matching the heavy-quark currents and Lagrangians the cross section calculation is mapped to the calculation of the imaginary part of the two-point function \(G(E)\) of non-relativistic currents in (1.2). The leading-order colour Coulomb potential is now part of the leading-order effective Lagrangian, since the Coulomb interaction is strong near threshold. The propagators to be used in the perturbative calculation of the two-point function are the Coulomb Green functions, making this part of the computation similar to QED bound-state problems. The calculation can be divided into three parts: contributions up to the third order involving only the Coulomb potential, already completed in \[45\]; the ultrasoft contribution, appearing first at NNNLO, which has been computed in \[52\]; and finally, contributions involving at least one potential other than the Coulomb potential (“non-Coulomb potential contribution”), which are not yet known.

The main result of this paper is the missing non-Coulomb potential contribution. Compared to the Coulomb contributions the major complication is the singular nature of the potential insertions. The ultraviolet divergences must be regulated in dimensional regularization in a scheme consistent with the calculation of the matching coefficients order by order in the strong coupling, while retaining the resummation of infinitely many Coulomb gluon exchanges by the use of Coulomb Green functions, whose \(d\)-dimensional expression is unknown. The techniques we apply are an extension of those used in the NNLO calculation \[24\]. Since the method of that calculation was never written up (though some results are scattered in \[32,45\]), we devote some effort to presenting the third-order calculation in some technical detail.

In addition to the dominant production of the top-quark pair though a virtual photon there is also a \(Z\)-boson contribution. The contribution from the vector-coupling of the \(Z\) is trivially inferred from the photon-mediated cross section, while the axial-vector coupling contribution is suppressed near threshold and begins only at NNLO. Thus, only the first-order correction to the axial-vector in non-relativistic perturbation theory is needed. Some results at this order are available \[28,61,62\], but none of these results are given in dimensional regularization. We recalculated these small contributions, and will present them elsewhere, since in this paper we focus on the missing third-order terms in the vector current contribution.

To summarize: together with the results of this paper, the matrix element calculation is complete to NNNLO.

**Electroweak and electromagnetic corrections**

Much less work has been done on electroweak and electromagnetic corrections. Counting the electromagnetic and electroweak coupling as two powers of the strong coupling, electromagnetic corrections contribute from NLO through the electromagnetic Coulomb potential. This effect is easily included and has been discussed in \[32,63\]. Electroweak
contributions to the matching coefficients of NRQCD currents and production operators have been calculated in \cite{65,66,67,68,69}. The formalism for calculating initial-state radiation, and soft and collinear photon corrections in general, simultaneous with summing Coulomb exchange has been worked out in \cite{70} for $W$-boson pair production. Its application to top quarks is straightforward. It remains to be done to put all these electroweak effects together.

For top quarks the sizeable decay width $\Gamma_t$ introduces further complications. In leading order the width is correctly included by evaluating the current two-point functions in PNRQCD at complex energy argument $E + i\Gamma_t$, \cite{15,16}, where $E = \sqrt{s} - 2m_t$. We adopt this prescription as the \textit{definition} of the pure QCD contributions to the cross section. Beginning at NLO there exist further contributions related to the finite width. Since the physical final state is $W^+W^-b\bar{b}$ there exist irreducible “backgrounds” related to off-shell and single or non-resonant top-quark pair production. In fact, the QCD contribution as defined above cannot be unambiguously separated from electroweak effects at this order – perhaps not surprisingly, since the top quark width itself is such an effect – and the fact that a physical scattering cross section should refer only to stable (or sufficiently long-lived) particles in the final state, must be taken into account. The incompleteness of the QCD cross section is signaled explicitly by the presence of uncanceled singularities in dimensional regularization with coefficients proportional to $\Gamma_t$ starting at NNLO.\footnote{To the extent that we focus on top width effects, the $W$ boson may be regarded as stable.} The origin and consistent cancellation of these singularities is discussed in \cite{52,66} and the corresponding calculations of electroweak effects and non-resonant contributions to a physical final state such as $W^+W^-b\bar{b}$ can in principle be performed in the framework of unstable-particle effective field theory \cite{71,72} as already done for $W$ pair production \cite{70,73}. The corresponding calculation of the non-resonant NLO correction for top production has been performed in \cite{64} and confirmed by a different method in \cite{74}. Rather than embarking on the rather difficult computation of non-resonant contributions up to NNNLO, however, a more promising approach suppresses them by appropriate invariant mass cuts \cite{70,75}, which will anyway be applied experimentally. Calculations of top quark pair production near threshold with cuts on the final-state $Wb$ invariant masses have appeared recently \cite{63,64} in the non-relativistic QCD and unstable particle effective theory frameworks. As should be expected, the non-resonant contributions to the $W^+W^-b\bar{b}$ are sizeable below the nominal top pair production threshold, and hence can change the shape of the threshold cross section in the region of interest for the top-quark mass determination. In the present paper, we focus only on the QCD part of the problem. We shall, however, make the finite-width $1/\epsilon$ poles explicit, so that they can be canceled analytically with future computations of electroweak effects. Indeed, the pole parts of the NNLO non-resonant contribution have recently been computed \cite{76} and the cancelation has been verified.\footnote{At NLO these finite-width divergences are linear and therefore do not show up as poles in dimensional regularization. Nevertheless, this implies an implicit dependence of the result of the regularization scheme, which is cancelled by computing the non-resonant contributions consistently in the same scheme, as was done in \cite{64}.}
To summarize: while the formalism for computing electroweak and finite-width effects consistently is in place, and bits and pieces have already been calculated, significant work remains to be done on electroweak effects at NNNLO. With the third-order QCD calculation now being nearly complete, improvements in the prediction of realistic cross sections (including electroweak effects and cuts) must be made.

Since our intention to present the concepts, techniques and calculations in some detail resulted in a rather lengthy text, we have split it into two parts. Part I presents the effective field theory set-up, the NRQCD and PNRQCD matching coefficients and ends with a master formula for the third-order heavy-quark pair production cross sections. This part could also be read as a review of non-relativistic effective theory in the weak-coupling regime complementary to [77]. Part II contains the actual PNRQCD matrix element calculation together with a numerical estimate of the new contributions to the top cross section. (A preliminary version has been presented in [51].) The small P-wave contributions to the cross section from the axial-vector coupling of the Z-boson will be presented separately in [78].

The outline of the paper I is as follows: In section 2 we review the effective field theory framework and discuss the power-counting arguments that lead to the identification of the matching coefficients needed for the NNNLO calculation. The subsequent two sections deal with matching QCD to a sequence of two non-relativistic effective theories, NRQCD and PNRQCD. Section 3 discusses the NRQCD aspects of the calculation. In particular, we calculate the relevant one-loop matching coefficients including the new $O(\epsilon)$ terms and collect all other results that feed into the cross section calculation. The second matching step from NRQCD to PNRQCD is discussed at length in section 4 since a coherent summary is not yet available in the literature. Among the new results of this section are the path-integral derivation of the PNRQCD Lagrangian (neglecting ultrasoft gluons), the $O(\epsilon)$ terms of the one-loop potentials, and a discussion on the non-renormalization of currents in the NRQCD to PNRQCD matching.

PNRQCD perturbation theory in the pole-mass scheme provides a poor approximation to the top-quark pair production cross section near threshold. The top quark decay width is obviously an important effect, as is the conversion from the pole mass renormalization scheme that is employed in the primary calculations to renormalization schemes that absorb large corrections into the mass counterterm, which is a prerequisite for reliable perturbative calculations [29,79]. Furthermore, a resummation of PNRQCD perturbation theory for the Green function is necessary in the vicinity of the bound state poles despite the sizeable top quark width. These refinements will be explained in paper II. In section 5 we conclude paper I by providing the master formula for the computation of the third-order cross section in PNRQCD.
2 Top pair production near threshold in effective field theory

In this section we present the relation of the pair production cross section to correlation functions of heavy quark currents together with the arguments, why this relation holds true at NNNLO. We review the scales and momentum regions relevant to the problem both of which are central to the systematics of the effective theory approach.

2.1 Heavy-quark correlation function

The basic top pair production mechanisms in $e^+e^-$ annihilation are shown in the upper part of figure 1. Since we work to lowest order in the electromagnetic and electroweak couplings, the optical theorem allows us to relate the total cross section $\sigma_{t\bar{t}X}$ of the process $e^+e^- \rightarrow t\bar{t}X$ to the two point functions of the vector and axial-vector heavy quark current. We define

$$\Pi^{(X)}_{\mu\nu}(q^2) = i \int d^4x e^{iq\cdot x} \langle 0 | T(j^{(X)}_{\mu}(x)j^{(X)}_{\nu}(0)) | 0 \rangle = (q_{\mu}q_{\nu} - q^2 g_{\mu\nu}) \Pi^{(X)}(q^2) + q_{\mu}q_{\nu} \Pi_L^{(X)}(q^2),$$

(2.1)

for the vector current $j^{(v)}_{\mu} = \bar{t}\gamma_\mu t$ and the axial vector current $j^{(a)}_{\mu} = \bar{t}\gamma_\mu\gamma_5 t$. The cross section is then given by

$$\sigma_{t\bar{t}X} = \sigma_0 \times 12\pi \text{Im} \left[ e_t^2 \Pi^{(v)}(q^2) - \frac{2q^2}{q^2 - M_Z^2} v_e v_t e_t \Pi^{(v)}(q^2) \right.$$

$$\left. + \left( \frac{q^2}{q^2 - M_Z^2} \right)^2 (v_e^2 + a_e^2)(v_t^2 \Pi^{(v)}(q^2) + a_t^2 \Pi^{(a)}(q^2)) \right],$$

(2.2)

where $\sigma_0 = 4\pi\alpha_{em}^2/(3s)$ is the high-energy limit of the $\mu^+\mu^-$ production cross section, $s = q^2$ the center-of-mass energy squared, and $M_Z$ the Z-boson mass. $e_t = 2/3$ denotes the top quark electric charge in units of positron charge and $\alpha_{em}$ is the electromagnetic coupling. The vector and axial-vector couplings of fermion $f$ to the Z-boson are given by

$$v_f = \frac{T_3^f - 2e_f \sin^2 \theta_w}{2 \sin \theta_w \cos \theta_w}, \quad a_f = \frac{T_3^f}{2 \sin \theta_w \cos \theta_w},$$

(2.3)

with $\theta_w$ the weak mixing angle, $e_f$ the electric charge of fermion $f$ and $T_3^f$ its third component of the weak isospin.

The dominant production mechanism is through the coupling to the virtual photon. The vector coupling of the Z-boson increases the photon-mediated cross section by only about 8% in the threshold region $q^2 \approx 4m_t^2$. The axial-vector contribution is even smaller, since the axial coupling is suppressed near threshold by the small velocity of the top quarks. $\Pi^{(a)}(q^2)$ contributes to (2.2) only at NNLO relative $\Pi^{(v)}(q^2)$. 
Eq. (2.2) which relates the inclusive top cross section to the spectral functions of heavy-quark currents is not exact. There exist top production mechanisms, shown in the lower part of figure 1 which are not captured by the heavy-quark current correlation functions, since the photon or $Z$-boson couples to light quarks. Vice versa, there exist cuts contributing to $\text{Im} \Pi^{(X)}(q^2)$ related to annihilation subdiagrams, see figure 3 below, which do not contain top quarks and hence should be excluded. We shall discuss in the next subsection that these contributions are either highly suppressed and not relevant at third order, or can easily be included.

Energy variables

The characteristic non-relativistic energy in threshold production is much smaller than $\sqrt{s} \approx 2m$. We define $E = \sqrt{s} - 2m$ and the top quark “velocity” $v = (E/m)^{1/2}$. This is related to another often used velocity parameter $\beta = (1 - 4m^2/s)^{1/2}$ by

$$v = \sqrt{\frac{E}{m}} = \left(\frac{2}{(1 - \beta^2)^{1/2}} - 2\right)^{1/2} = \beta + \frac{3\beta^3}{8} + \ldots \quad (2.4)$$

Real values of $s$ and $E$ should be interpreted with a $+i\epsilon$ prescription. We will extensively use another variable $\lambda$ defined by

$$\lambda = \frac{\alpha_s C_F}{2 \sqrt{\frac{E}{m}}} \quad (2.5)$$

Here and below $\alpha_s$ without any argument denotes the strong coupling in the $\overline{\text{MS}}$ scheme at the renormalization scale $\mu$, and $C_F = (N_c^2 - 1)/(2N_c) = 4/3$.

The value of $\lambda$ determines when resummation to all orders in $\alpha_s$ is necessary. Above threshold, the variable $\lambda$ is purely positive-imaginary, below threshold it is real and
positive. The threshold region is characterized by an absolute value of $\lambda$ of order 1 or larger. In particular, the Coulomb bound state poles are found at positive integer values of $\lambda$. Conventional fixed-order perturbation theory can be used only when $\lambda \ll 1$. As will be discussed later the width of the top quark is accounted for by substituting $E \rightarrow E + i \Gamma$. Thus, as $E$ varies from $-\infty$ to $\infty$ the variable $\lambda$ sweeps through a curve in the complex plane that begins at the origin, moves out into the first quadrant into the direction of the positive real axis and returns to the origin from above near the imaginary axis. The absolute value of $\lambda$ along this curve is always smaller than $\alpha_s C_F / 2 \times (m/\Gamma)^{1/2}$, which is about 1.2 for top quarks, with $\alpha_s(15 \text{ GeV}) \approx 0.16$, but since it reaches order one in the threshold region, the perturbation expansion in $\alpha_s$ breaks down and resummation is necessary.

2.2 Momentum regions and effective field theory

Near the heavy-quark pair production threshold only a small kinetic energy $\sqrt{s} - 2m = E = mv^2$ is available to the final state. In the natural frame where $q^\mu = (2m + E, 0)$ this implies that the typical three momentum of a heavy quark is of order $mv$ (about 20 GeV for top quarks), while the energy and momentum of any other nearly massless particle can at most be $mv^2$ (about 2 GeV for tops). The presence of several small scales propagates into the loop diagrams that contribute to the spectral functions and causes a breakdown of the standard perturbation expansion in the strong coupling $\alpha_s$. However, since $v$ is small one does not have to compute the loop integrals exactly – an expansion in $v$ suffices. This leads to a reorganized expansion as shown in (1.1), in which $\alpha_s$ and $v$ are expansion parameters but $\alpha_s/v$ or, equivalently, $\lambda$ is of order one.

For a given Feynman diagram the expansion in $v$ can be constructed without first computing the full expression using the threshold expansion [14]. The method uses that every diagram is the sum of terms, for which each loop momentum is in one of the following four regions:

\begin{align}
\text{hard (h)} & : \quad \ell^0 \sim m, \quad \ell \sim m \\
\text{soft (s)} & : \quad \ell^0 \sim mv, \quad \ell \sim mv \\
\text{potential (p)} & : \quad \ell^0 \sim mv^2, \quad \ell \sim mv \\
\text{ultrasoft (us)} & : \quad \ell^0 \sim mv^2, \quad \ell \sim mv^2
\end{align}

When on-shell, only massless particles (gluons, light quarks and ghosts) can be ultrasoft, and only the heavy quarks can be potential[3]. In each region, the loop integrand is expanded in the terms which are small in the corresponding region and the loop integration of the expanded integrand is carried out over the complete $d$-dimensional space-time volume. The expansion generates ultraviolet and infrared divergences which are regulated

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5 Here and in the following we set the masses of all quarks other than the heavy quark to zero. This is a good approximation for top quarks, but less so for bottom quarks, in which case the charm mass is of order of the soft scale.

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dimensionally \((d = 4 - 2\epsilon)\) and subtracted according to the \(\overline{\text{MS}}\) prescription. However, the divergences generated by the separation of the diagram into regions cancel in the sum over all terms.

The procedure just described is largely equivalent to constructing appropriate effective Lagrangians within dimensional regularization, but it clarifies the correct matching procedure which is subtle in dimensional regularization if the effective theory contains more than one scale as is the case in non-relativistic QCD \([58,81]\). The threshold expansion also synthesizes the non-relativistic velocity power counting rules developed for the different modes (momentum regions) in \([60,82,83,84]\). In the construction of the non-relativistic and resummed expansion of the pair production cross section we derive effective Lagrangians in two steps by integrating out the large momentum modes according to the following scheme:

\[
\begin{align*}
\mathcal{L}_{\text{QCD}}[Q(h,s,p), g(h,s,p,us)] & \quad \mu > m \\
\quad \downarrow \\
\mathcal{L}_{\text{NRQCD}}[Q(s,p), g(s,p,us)] & \quad mv < \mu < m \\
\quad \downarrow \\
\mathcal{L}_{\text{PNRQCD}}[Q(p), g(us)] & \quad \mu < mv
\end{align*}
\]

In square brackets we display the modes of the heavy quarks \((Q)\) and massless particles \((g)\) which are still contained in the effective Lagrangian; the others are integrated out when the energy cut-off \(\mu\) is lowered as indicated on the right. The first step leads to NRQCD \([11,12,13]\), in which all interactions are local, since only the short-distance hard modes have been eliminated. The expansion rules of the threshold expansion define the dimensionally regularized NRQCD Lagrangian. The second step whereby soft modes and potential massless modes are integrated out was suggested in \([14,85]\) in the context of the effective Lagrangian and threshold expansion method. The result is the potential NRQCD (PNRQCD) Lagrangian \([24,79,85,86,87]\). The PNRQCD Lagrangian is not local. It contains spatially non-local but temporally local, i.e. instantaneous interactions of the heavy quarks, since the three-momentum of the potential heavy quark field still present in PNRQCD is of the same order as the one of the modes integrated out. These interactions provide a precise definition of the concept of “heavy-quark potentials”. Perturbation theory in PNRQCD resembles quantum-mechanical perturbation theory closely, since the leading colour-Coulomb interaction is part of the unperturbed theory. Thus, the propagator of PNRQCD includes the leading Coulomb interaction exactly, which effects the required resummation of conventional perturbation theory to all orders.

To illustrate the velocity scaling of Feynman diagrams, we consider the power counting for the loop integrand. Eq. (2.6) implies that the integration measure \(d^4\ell\) scales as
\[ v^0, v^4, v^5 \text{ and } v^8, \text{ when } \ell \text{ is hard, soft, potential and ultrasoft, respectively. The denominator of a gluon (massless) propagator with momentum } \ell = (\ell^0, \ell) \text{ is approximated at leading order in a given region by:} \]

\[
\frac{1}{\ell^2} = \begin{cases} 
\frac{1}{\ell^2} & \text{hard (} v^0 \text{), soft (} v^{-2} \text{), ultrasoft (} v^{-4} \text{)} \\
-\frac{1}{\ell^2} + \ldots & \text{potential (} v^{-2} \text{)}
\end{cases}
\tag{2.8}
\]

The velocity scaling is given in brackets. For the heavy-quark propagator with momentum \( q/2 + \ell = (m + E/2 + \ell^0, \ell) \) the denominators are:

\[
\frac{1}{(q/2 + \ell)^2 - m^2} = \begin{cases} 
\frac{1}{\ell^2 + q \cdot \ell + \ldots} & \text{hard (} v^0 \text{)} \\
\frac{1}{2m} \frac{1}{\ell^0} + \ldots & \text{soft (} v^{-1} \text{)} \\
\frac{1}{2m} \frac{1}{E/2 + \ell^0 - \ell^2/(2m)} + \ldots & \text{potential (} v^{-2} \text{)}
\end{cases}
\tag{2.9}
\]

Using these scaling rules, it is easy to see why an all-order resummation of Feynman diagrams is required in the threshold region. It will become clear from the later systematic derivation that the relevant diagrams are the ladder diagrams shown in figure 2 and that the dominant term in the velocity expansion arises from the loop momentum region when all loop momenta are in the potential region. Adding an additional rung to the ladder adds one potential gluon \( 1/v^2 \) and two potential heavy-quark propagators \( 1/v^2 \times 1/v^2 \) to the diagram. The numerator of the diagram contains no velocity suppression factors, hence accounting for the potential loop measure \( (v^5) \) and strong coupling from the two additional vertices \( (g_s^2) \), we find that each rung provides a factor of order \( \alpha_s/v \), which is unsuppressed in the threshold region. It will be seen below that only potential gluon exchange generates this \( 1/v \) enhancement, which is equivalent to the statement that only the leading Coulomb interaction must be included in the unperturbed effective Lagrangian.

We now return to the discussion of heavy-quark production mechanisms not captured by (2.2), which expresses the cross section in terms of the heavy-quark current spectral functions. In the case of heavy-quark radiation (lower left in figure 1) the final state
Figure 3: Diagram containing cuts not related to top quark production.

consists of $Q\bar{Q}q\bar{q}$, and since the available energy at threshold is limited to $mv^2$, the light quarks must be ultrasoft. In the three-loop diagram that represents the square of the heavy-quark radiation amplitude, the $Q\bar{Q}$ loop must be potential and the two other loops ultrasoft, which leads to a factor of $v^{21}$ from the loop integration measure. The intermediate gluon and light-quark propagators in the amplitude must be hard to produce the $Q\bar{Q}$ pair and hence do not contribute inverse powers of $v$. The two potential heavy quark and the two ultrasoft light quark propagators $(1/\ell)$ supply a factor of $1/v^2$ each, so the heavy-quark radiation contribution to the cross section scales at least as $\alpha_s^2v^{13}$ which should be compared to $v$ for the leading term. Inspection of the analytic expression confirms this result, hence this contribution can be safely neglected. In the case of singlet production (lower right in figure 1) through the coupling of the virtual photon or $Z$-boson to light quarks the dominant term comes from three hard loops, leading to the counting $\alpha_s^3v$, which represents a third-order correction to the cross section. While not part of $\text{Im}\,\Pi^{(v)}(q^2)$ this mechanism can be included in the three-loop short-distance coefficient $c_v^{(3)}$ of the non-relativistic heavy-quark current, which is discussed below, although it is not known at present. Note that this contribution to $c_v^{(3)}$ is complex, but the imaginary part should be discarded, since it corresponds to the three-gluon and light-quark cut, which is not part of the heavy-quark production cross section. A similar singlet-production diagram exists for the axial-vector coupling with only two gluons coupling to the light-quark triangle, but due to velocity suppression this contribution begins only at fourth order.

We have thus argued that the production mechanisms not included in $\text{Im}\,\Pi^{(v,a)}(q^2)$ are either suppressed or easily included at third order. Consider now figure 4 which shows a diagram contained in $\text{Im}\,\Pi^{(v)}(q^2)$, but whose three-gluon cut should not be part of the heavy-quark cross section. The possible loop momentum regions for this diagram are h-h-h-h, p-h-h-p, p-h-h-h and h-h-h-p, where the first and last letter refers to the left and right heavy quark loop, respectively. In the all-hard configuration only the three-gluon cut contributes to $\text{Im}\,\Pi^{(v)}(q^2)$, so the correct prescription is to simply not include this configuration. The p-h-h-p configuration may be interpreted as heavy-quark production followed by rescattering through annihilation. Annihilation is suppressed by $\alpha_s^2v^2$ relative
to Coulomb exchange as can be seen by counting loop integration and propagator factors, so this configuration is relevant only from fourth order as a contribution to the $\alpha_s^3/m^2$ potential. The remaining two configurations with only one potential heavy quark loop are analogous to the singlet production mechanisms. That is, one drops the imaginary part of the h-h-h subdiagram, which comes from the three-gluon cut and associates its real part to $c_3^{(v)}$. There exists a three-loop diagram similar to figure 3 but with two gluon lines only for the axial-vector coupling, but as in the singlet diagram with a light-quark triangle discussed above, the axial-vector coupling implies another factor of $v^2$, so this diagram is never relevant at third order.

3 Non-relativistic QCD

In this section we discuss the matching of the vector current correlation function for $q^2 \approx 4m^2$ to its equivalent representation in non-relativistic QCD. This amounts to integrating out the hard modes, which correspond to “relativistic effects” involving the scale of the heavy-quark mass. Non-relativistic QCD is expressed in terms of a two-component quark field $\psi$ and the corresponding anti-quark field $\chi$ to represent the remaining soft and potential fluctuations of the original quark field. The effective gluon field $A_\mu = A_\mu^AT^A$ can be soft, potential and ultrasoft.

Before going into the details of the Lagrangian and power counting we briefly sketch the result. As will be shown below the expansion of the vector current $j^{(v)_\mu}$ in terms of the non-relativistic fields is given by

$$j^{(v)_\mu} = c_v \psi^\dagger \sigma^i \chi + \frac{d_v}{6m^2} \psi^\dagger \sigma^i D^2 \chi + \ldots,$$

where the hard matching coefficients $c_v$, $d_v$ have perturbative expansions in $\alpha_s$. In the “rest frame” $q^\mu = (2m + E, 0)$, eq. (2.1) implies $\Pi^{(v)}_{ij}(q^2) = \frac{N_c}{(d-1)q^2} \Pi^{(v)}_{ii} = \frac{N_c}{2m^2} c_v \left[ c_v - \frac{E}{m} \left( c_v + \frac{d_v}{3} \right) \right] G(E) + \ldots,$

where the neglected terms on the right-hand side include a subtraction term that does not contribute to the imaginary part of $\Pi^{(v)}(q^2)$ as well as terms beyond the third order (NNNLO). The important quantity is the two-point function of the non-relativistic current

$$G(E) = \frac{i}{2N_c(d-1)} \int d^d x e^{iEx} \langle 0 | T\left( [\chi^\dagger \sigma^i \psi](x) [\psi^\dagger \sigma^i \chi](0) \right) |0\rangle_{\text{NRQCD}},$$

where now the matrix element must be evaluated in non-relativistic QCD (NRQCD). The terms proportional to $E$ in (3.2) arise from expanding the prefactor $1/q^2$ and from

---

6Our convention is to use the anti-particle field from the four-component Dirac field. Alternatively, we could treat particles and anti-particles on the same footing and introduce a particle field in the anti-triplet colour representation for the anti-quark, which corresponds to the charge-conjugate of the convention adopted in this paper.
the $1/m^2$ suppressed current in (3.1), whose matrix element can be reduced to the one of the leading current by an equation-of-motion relation derived later. Thus the main ingredients to the non-relativistic representation are the calculation of $G(E)$ and the current matching coefficients.

Similar relations hold for the axial-vector contribution to the cross section (2.2), which arises from $Z$-boson exchange. The axial-vector current $j^{(a)\mu} = \bar{t}g_{\mu5}t$ is represented in NRQCD by the expansion

$$j^{(a)i} = \frac{c_a}{2m} \psi^i \left[ \sigma^i, (-i)\sigma \cdot D \right] \chi + \ldots,$$

with hard matching coefficient $c_a$. As is the case for the vector current, only the spatial components of the current contribute to the cross section, since the lepton tensor from the $e^+e^-$ initial state is transverse to both initial state momenta when the electron mass is neglected. Only the leading term in the $1/m$ expansion is needed for NNNLO accuracy, since the derivative in the leading current implies the well-known P-wave velocity suppression. The QCD correlation function is then given by the expression

$$\Pi^{(a)}(q^2) = \frac{1}{(d-1)q^2} \Pi^{(a)}_{\text{ii}}$$

where $\Pi^{(a)}_{\text{ii}}$ is the non-relativistic correlation function.

3.1 Lagrangian and Feynman rules

For the present purpose the non-relativistic effective Lagrangian can be divided into five parts,

$$\mathcal{L}_{\text{NRQCD}} = \mathcal{L}_\psi + \mathcal{L}_\chi + \mathcal{L}_{\psi\chi} + \mathcal{L}_g + \mathcal{L}_{\text{light}}.$$  

The gluon field is contained in the gauge-covariant derivative $D^\mu = \partial^\mu - ig_s A^\mu$, field strength tensor $G_{\mu\nu} = (i/g_s) [D_\mu, D_\nu]$, and the chromoelectric and chromomagnetic fields defined as

$$E^i \equiv G^{i0} = -\nabla^i A^0 - \frac{\partial}{\partial t} A^i - ig_s \left[ A^i, A^0 \right],$$

$$\sigma \cdot B \equiv -\frac{1}{2} \sigma^{ij} G^{ij},$$

where $\sigma^{ij} = (-i/2) [\sigma^i, \sigma^j]$ and $D^i = -\nabla^i$. With these definitions the bilinear heavy-quark Lagrangian is given by

$$\mathcal{L}_\psi = \psi^i \left( iD^0 + \frac{D^2}{2m} + \frac{D^i}{8m^3} \right) \psi - \frac{d_1 g_s}{2m} \psi^i \sigma \cdot B \psi,$$

$$\Pi^{(a)}(q^2) = \frac{1}{(d-1)q^2} \Pi^{(a)}_{\text{ii}}$$

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$$\Pi^{(a)}(q^2) = \frac{1}{(d-1)q^2} \Pi^{(a)}_{\text{ii}}$$

where $\Pi^{(a)}_{\text{ii}}$ is the non-relativistic correlation function.
Figure 4: NRQCD Feynman rules for two-quark vertices up to order \(1/m^2\). Dashed (curly) lines denote the \(A^0 (A^i)\) gluon field. \(q = p' - p\).
\[
+ \psi^\dagger \left( \frac{d_2 g_s}{8m^2} [D^i, E^j] + i \frac{d_3 g_s}{8m^2} \sigma^{ij} \{D^i, E^j\} \right) \psi
\]
\[
+ \psi^\dagger \left( -d_W g_s \left[ \frac{\mathbf{D}_2}{8m^3} - \frac{\mathbf{B}^2 - \mathbf{E}^2}{8m^3} \right] + d_A g_s \frac{\mathbf{B}^2 - \mathbf{E}^2}{8m^3} + d_B g_s \frac{\sigma^{ij} (B^i B^j - E^i E^j)}{8m^3} \right) \psi
\]
\[
+ O \left( \frac{1}{m^4} \right), \quad (3.8)
\]

\[
\mathcal{L}_\chi = -\mathcal{L}_\psi \quad \text{with} \quad \psi \to \chi, iD^0 \to -iD^0, E^i \to -E^i. \quad (3.9)
\]

Note that in \( d \) dimensions we cannot define the \( B^i \) individually, since they do not represent the components of a \( d-1 \) dimensional vector. However, all we need are scalars such as \( 3.7 \) and \( B^2, \sigma^{ij} B^i B^j \), which can be consistently defined through the \( d \) dimensional field strength tensor:

\[
B^2 \equiv \frac{1}{2} \mathbf{G}^{ij} \mathbf{G}^{ij}, \quad \sigma^{ij} B^i B^j \equiv -\frac{1}{2} \sigma^{ij} [\mathbf{G}^{ik}, \mathbf{G}^{kj}]. \quad (3.10)
\]

The four-fermion quark-antiquark terms in the effective Lagrangian read

\[
\mathcal{L}_{\psi \chi} = \frac{d_{ss}}{m^2} \psi^\dagger \psi \chi^\dagger \chi - \frac{d_{sv}}{8m^2} \psi^\dagger [\sigma^i, \sigma^j] \psi \chi^\dagger [\sigma^i, \sigma^j] \chi +
\]
\[
+ \frac{d_{\bar{v}s}}{m^2} \psi^\dagger T^a \psi \chi^\dagger T^a \chi - \frac{d_{wv}}{8m^2} \psi^\dagger T^a [\sigma^i, \sigma^j] \psi \chi^\dagger T^a [\sigma^i, \sigma^j] \chi + O \left( \frac{1}{m^3} \right), \quad (3.11)
\]

where the factor \(-1/8\) in the definition of the spin-triplet operators has been inserted, since in four dimensions \([\sigma^i, \sigma^j] \otimes [\sigma^i, \sigma^j] = -8 \sigma^i \otimes \sigma^i \). The pure gluon Lagrangian takes the form

\[
\mathcal{L}_g = -\frac{d_4}{4} \mathbf{G}^{\mu \nu} \mathbf{G}^{\mu \nu} + \frac{d_5}{m^2} \mathbf{G}^{\mu \nu} \mathbf{D}^2 \mathbf{G}^{\mu \nu} + \frac{d_6}{m^2} g_s f^{ABC} \mathbf{G}^{\mu \nu} \mathbf{G}^{\mu \nu} + O \left( \frac{1}{m^4} \right). \quad (3.12)
\]

Finally, \( \mathcal{L}_{\text{light}} \) is the same as the light-quark Lagrangian in full QCD. The Feynman rules for the \( 1/m \) and \( 1/m^2 \) terms in \( \mathcal{L}_\psi \) are given in figure 4. The hard matching coefficients \( d_{1-4}, d_W, d_A, d_B \) equal one at tree level, while the others vanish. All coefficients obtain one-loop corrections, which must be determined by matching the QCD diagrams to the NRQCD diagrams order by order in the non-relativistic expansion. For reasons which will be explained later, the matching coefficients are needed to order \( \epsilon \) in the dimensional regularization parameter. In writing (3.8) we did not include \( 1/m^3 \) interactions with vanishing tree-level coefficients as well as mixed heavy-light quark operators of the form \( \psi^\dagger \bar{q} q \) in \( \mathcal{L}_\psi \), since they are irrelevant for the NNNLO calculation, as we discuss now.

---

8 The vertices involving \( q^0 \) in the fifth row can be eliminated using the heavy-quark equation of motion. This generates \( 1/m^3 \) terms not shown in the figure and modifies the \( 1/m^2 \) four-point vertices in the last row of the figure as follows: drop the \( \mathbf{p} \) and \( \mathbf{p}' \) terms and multiply the remaining terms by two.
The velocity scaling of the fields depends on the momentum region. Heavy quark fields can be potential or soft. From the scaling rules of the propagator (compare (2.9)) and the integration measure, it follows that in both cases the field scales as $v^{3/2}$. The same power counting can be done with the gluon field, which is either soft, potential or ultrasoft and one finds that $g_s A$ scales as $v^{3/2}$, $v^2$ and $v^{5/2}$ respectively, which includes a factor of $v^{1/2}$ from the coupling constant $g_s$.

Turning to the effective Lagrangian, we first consider the bilinear terms in the heavy Lagrangian $\mathcal{L}_\psi$. For potential quarks, the bilinear terms in the kinetic term $\bar{\psi}(i D^0 + D^2/(2m))\psi$ are both of order $v^5$. The relativistic correction $\bar{\psi}(\partial^4/(8m^3))\psi$ scales as $v^7$. Being suppressed by $v^2$ relative to the leading terms it contributes from NNLO. The next term in the expansion of the relativistic energy-momentum relation would be of order $v^9$ and is beyond NNNLO. For soft quarks, the quadratic kinetic energy term is an order $v$ correction to the leading-order static Lagrangian $\bar{\psi}iD^0\psi$, which scales as $v^4$. This explains why static heavy-quark propagators can be used in the calculation of the heavy-quark potentials. For soft heavy quarks the quartic kinetic energy correction is a NNLO effect.

Consider now the interactions of the heavy quark with the gauge field, i.e. terms of the form $\bar{\psi}\psi (g_s A)^n$, potentially with derivatives on the quark and gluon fields. The $g_s \bar{\psi}\psi A^0$ interaction that arises from $\bar{\psi}i D^0\psi$ scales as $v^5$ when all fields are potential. Therefore it is not suppressed relative to the bilinear terms that persist as $g_s \to 0$. In the potential region, this interaction has to be treated non-perturbatively; this is why the cross section near threshold requires a summation of some loop momentum contributions to all orders in $\alpha_s$. When the gluon field is soft, the velocity scaling of the $g_s \bar{\psi}\psi A^0$ interaction is $v^{9/2}$, but since in this case the leading term $\bar{\psi}iD^0\psi$ scales as $v^4$, this interaction is now a perturbation. It follows that all soft interactions can be treated in conventional perturbation theory. Further three-point interactions of the form above carry derivatives. Each derivative gives at least a suppression of $v$ so interactions with up to three derivatives in $g_s \bar{\psi}\psi A$ may contribute at NNNLO. The requirement of gauge invariance restricts the possible interaction terms to the so-called chromomagnetic interaction $g_s \bar{\psi}\sigma \cdot B \psi$ at order $v^6$ (NLO), and the Darwin and spin-orbit interactions at order $v^7$ (NNLO), multiplied by the short-distance coefficients $d_1$, $d_2$, and $d_3$, respectively. However, a single chromomagnetic interaction contributes only in connection with a $v$ suppressed quark-gluon vertex from the $\bar{\psi}D^2/(2m)\psi$ interaction, and not at all to the current correlation function, since the trace over an odd number of Pauli matrices vanishes. Thus the chromomagnetic, Darwin and spin-orbit interaction all start to contribute at NNLO (with two insertions of the chromomagnetic term). Hence, at NNNLO one needs the coefficient functions $d_1$, $d_2$ and $d_3$ in the one-loop approximation. Beyond order $v^7$ only the interactions with non-vanishing tree-level coefficient functions given in (3.3) can potentially contribute to NNNLO. None of them does, however, since single insertions of interactions with Pauli matrices vanish, as discussed above, while the terms with two electric or magnetic field strengths are of the form $\bar{\psi}\psi(g_s A)^2$ with two derivatives, which is smaller than NNNLO in both, the potential and soft region.

Bilinear heavy quark operators in conjunction with light quarks, $\bar{\psi}\psi \bar{q}q$, are of order
\( v^6 \). For these operators to contribute to the heavy-quark current correlation function at least one interaction of the form \( g_s \bar{q}qA \) is required, which costs a factor of \( v \) or, equivalently \( \alpha_s \). Thus, a \( \psi \dagger \psi \bar{q}q \) operator is relevant at NNLO, if its short-distance coefficient function is of order \( \alpha_s \). The only operator that may have a tree-level coefficient is \( \psi \dagger T^A\psi \bar{q} \gamma^0 T^A q \), since in this case the intermediate potential gluon propagator can be cancelled, making the operator local. This operator is generated at tree level from the Darwin term in the Lagrangian (3.8) by the use of the field equation for the chromo-electric field. Our convention is that we do not eliminate the Darwin term by the field equation, hence \( \psi \dagger \psi \bar{q}q \) operators must be added to the Lagrangian only with coefficients of order \( \alpha_s^2 \) producing corrections to the heavy-quark current correlation function beyond NNLO.

We therefore conclude that only the terms in the first two lines of (3.8) are needed for the NNNLO calculation, the same as in NNLO. The only difference to NNLO is that the short-distance coefficients \( d_1, d_2 \) and \( d_3 \) are required at the one-loop order. We also see that only the \( g_s \psi \dagger \psi A_0 \) interaction in the potential region is non-perturbative, and this explains why only ladder diagrams of Coulomb gluons must be summed to all orders.

The four-quark operator Lagrangian \( \mathcal{L}_{\psi \chi} \) (3.11) is generated by hard scattering of quarks and anti-quarks, or by quark anti-quark annihilation. Hard scattering with momentum exchange of order \( m \) requires the exchange of at least two gluons, corresponding to one-loop diagrams so the coefficient functions are of order \( \alpha_s^2 \). The four-quark operator counts as \( v^6 \). Including the one-loop coefficient function gives the counting \( \alpha_s^2 v^6 \), which is a NNNLO effect relative to the leading-order Lagrangian of order \( v^5 \) for the scattering of potential quarks. The annihilation contribution is present already at order \( \alpha_s \) (tree-level), but the operator has the colour structure \( \psi \dagger T^a \chi \chi \dagger T^a \psi \), which does not contribute to the current correlation function due to \( \text{tr} T^a = 0 \). Similarly, annihilation into two gluons does not contribute to the vector correlation function, since it leads to fermion loops with three vector couplings that vanish by charge conjugation. Thus, at NNLO, we can restrict ourselves to the four-fermion operators generated by hard quark-anti-quark scattering. For this reason we write the operators in the “scattering ordering” \( (\psi \dagger \psi)(\chi \dagger \chi) \) rather than the “annihilation ordering” \( (\psi \dagger \chi)(\chi \dagger \psi) \). Although the two orderings are related by a Fierz transformation in four space-time dimensions, the two are inequivalent in dimensional regularization. In general, we would have to introduce the difference of the two as evanescent operators. This complication is avoided here, since there are no annihilation contributions at NNLO. Adopting the “scattering ordering” in the Lagrangian, we do not need to perform any Fierz transformations.

The necessity to avoid relations that hold only in four dimensions is also the reason for introducing the definition (3.7) that does not make use of the three-dimensional \( \epsilon^{ijk} \) symbol, which is not defined in \( d - 1 \) dimensions. In particular, the commutator

\[
\sigma^{ij} = \frac{1}{2i} [\sigma^i, \sigma^j], \tag{3.13}
\]

\(^9\)Once again, this holds only because we do not eliminate the Darwin term by the chromo-electric field equation, which would otherwise generate a local four-quark operator with a tree-level coefficient function.
must be considered as an independent element of the $d$-dimensional algebra of Pauli matrices. This poses no difficulty in the calculation of the vector current correlation function, since in the end all expressions can be evaluated using the $d$-dimensional identities

\begin{align}
\sigma^i \sigma^i &= d - 1, \\
\sigma^i \sigma^j \sigma^i &= (3 - d) \sigma^j,
\end{align}

where $d = 4 - 2\epsilon$ and $\text{tr}(1) = 2$.

The pure gauge field Lagrangian (3.12) follows from integrating out heavy-quark loops with small momentum gluon lines attached. The renormalization of the standard kinetic term by the coefficient $d_4$ is well-known to be related to the matching of the strong coupling from the $n_f + 1$ flavour theory including the heavy quark to the theory with $n_f$ light flavours. In the following we express all results in terms of the strong coupling in the $\overline{\text{MS}}$ scheme in the $n_f$ flavour theory, which is the appropriate coupling for calculations in NRQCD, where the heavy quark short-distance fluctuations have been integrated out. After redefining the strong coupling, $d_4$ should be set to one in (3.12), so that the kinetic term is canonically normalized. The next term, $G^A_{\mu\nu} D^2 G^{A\mu\nu}$, in the gauge field Lagrangian involves two derivatives and a coefficient function $d_5 \propto \alpha_s \sim v$. Therefore it must be included at NNNLO. On the other hand, the term involving three gluon field strengths can be neglected at this order.

Having collected the relevant terms in the effective Lagrangian, we are now in the position to discuss the matching calculations. Most of the results required at NNNLO are available in the literature. However, many of the matching coefficients multiply NRQCD correlation functions, which exhibit $1/\epsilon$ poles. Thus, as will be explained in section 3.5 below, we also need the $O(\epsilon)$ terms of the matching coefficients, which have not been calculated or presented up to now. We therefore had to repeat these matching calculations and extend them to the $O(\epsilon)$ terms. The matching calculation is performed in the center-of-mass frame, so that the three-momenta of the heavy quark and anti-quark are of opposite sign. The external heavy quark spinors in QCD are given by

\begin{align}
u(p) &= \frac{1}{(E_p + m)^{1/2}} \left( \frac{(E_p + m) \xi}{\sigma \cdot p \xi} \right), \\
u(p) &= \frac{1}{(E_p + m)^{1/2}} \left( \frac{\sigma \cdot p \eta}{(E_p + m) \eta} \right),
\end{align}

for external momentum $p = (E_p, p)$ with $E_p \equiv (m^2 + p^2)^{1/2}$. The variables $\xi$ and $\eta$ denote the quark and anti-quark two-spinors, respectively. They are normalized according to $\xi^\dagger \xi = \eta^\dagger \eta = 1$.

### 3.2 Bilinear heavy-quark operators

The coefficient functions of the interactions of heavy quarks with a single gauge field in $\mathcal{L}_\psi$ can be deduced from the heavy quark form factors in background field gauge. The finite part of the one-loop form factors was calculated in [58]. However, the order $\epsilon$
coefficients were not computed there. The on-shell form factors can be brought into the general form
\[ ig_s T^a \bar{u}(p') \begin{bmatrix} \gamma^\mu F_1(q^2) + \frac{i\sigma^\mu\nu q_\nu}{2m} F_2(q^2) \end{bmatrix} u(p), \] (3.17)
where \( q = p' - p \). For the one-loop diagrams shown in figure 5 we obtain the following result for the expansion of the ultraviolet-renormalized form factors in \( \alpha_s \) and \( q^2 \) up to order \( \alpha_s q^2/m^2 \):

\[ F_1 = 1 + \frac{\alpha_s}{\pi} \left( \frac{\mu}{m} \right)^{2\epsilon} \frac{\Gamma(\epsilon)\epsilon^{\gamma\epsilon} \epsilon}{48(4\epsilon^2 - 1)} \frac{q^2}{m^2} \left[ C_A (-12\epsilon^3 + 4\epsilon^2 + 3\epsilon + 5) 
+ 2C_F(12\epsilon^3 - 4\epsilon^2 + 3\epsilon + 4) \right], \] (3.18)

\[ F_2 = \frac{\alpha_s}{\pi} \left( \frac{\mu}{m} \right)^{2\epsilon} \frac{\Gamma(\epsilon)\epsilon^{\gamma\epsilon} \epsilon}{24(4\epsilon^2 - 1)} \left[ C_A \left( 6(2\epsilon + 1)(2\epsilon^2 - 1) + \frac{q^2}{m^2}(4\epsilon^4 + 8\epsilon^3 + 5\epsilon^2 - 2\epsilon - 6) \right)
+ C_F \left( -12\epsilon(2\epsilon + 1)^2 - \frac{q^2}{m^2} 2\epsilon(\epsilon + 1)(2\epsilon + 1)^2 \right) \right]. \] (3.19)

Here and below we use the standard colour factors \( T_F = 1/2, \ C_F = 4/3, \ C_A = 3 \). The remaining divergences are infrared divergences of the on-shell form factors. By calculation of the corresponding form factors in the effective theory we obtain the relations between the coefficients \( d_i \) and the form factors:

\[ d_1 = F_1(0) + F_2(0), \] (3.20)
\[ d_2 = F_1(0) + 2F_2(0) + 8F_1'(0), \] (3.21)
\[ d_3 = F_1(0) + 2F_2(0), \] (3.22)

where \( F_i(0) = F_i|_{q^2=0} \) and \( F_1'(0) = dF_1/d(q^2/m^2)|_{q^2=0} \). Since \( F_1(0) = 1 \) exactly, this implies the well-known relation \( d_3 = 2d_1 - 1 \). The \( \overline{\text{MS}} \) renormalized coefficient functions follow by subtracting the \( 1/\epsilon \) poles from the above expressions. The \( O(\epsilon) \) terms of the above expressions are in agreement with [59].

### 3.3 Gauge field operators

To obtain the bilinear pure gauge field Lagrangian \( L_g \), the gluon self energy has to be matched. In the one-loop order the relevant diagram is the heavy-quark loop, which gives:

\[ d_4 = 1 + \frac{\alpha_s}{\pi} \left( \frac{\mu}{m} \right)^{2\epsilon} \frac{T_F \Gamma(\epsilon)\epsilon^{\gamma\epsilon} \epsilon}{3}, \] (3.23)
Figure 5: One-loop form factor diagrams: wavefunction renormalization and vertex corrections.

Figure 6: QCD diagrams for the four-fermion operators at one loop.

\[ d_5 = \frac{\alpha_s}{\pi} \left( \frac{\mu}{m} \right)^2 \frac{e^{\gamma_E} \Gamma(1 + \epsilon) e^{\gamma_E} \Gamma(1 + \epsilon)}{60}. \]  

(3.24)

The results agree for \( d = 4 \) with the ones in [58]. As mentioned above, the operator with coefficient \( d_6 \) is not needed, because it can contribute to the heavy quark correlation function only with an additional loop, which is beyond NNNLO. Recall that \( d_4 = 1 \) should be used after having normalized the fields canonically.

3.4 Four-fermion operators

The remaining part of the Lagrangian to be matched to QCD is the one containing the four-fermion operators. As discussed in section 2.1 we do not need the annihilation contributions and therefore restrict ourselves to the scattering diagrams shown in figure 6.

The results in \( d = 4 \) can be obtained from the equal mass limit of the unequal mass case given in [89]. Here we present the \( d \)-dimensional matching coefficients:

\[ d_{ss} = \alpha_s^2 C_F (C_A - 2C_F) \left( \frac{\mu}{m} \right)^2 \frac{e^{\gamma_E} (2\epsilon - 3)(2\epsilon^2 + \epsilon + 1) \Gamma(2 + \epsilon)}{2\epsilon \left( 8\epsilon^3 + 12\epsilon^2 - 2\epsilon - 3 \right)}. \]  

(3.25)

\[ d_{sv} = \alpha_s^2 C_F (C_A - 2C_F) \left( \frac{\mu}{m} \right)^2 \frac{e^{\gamma_E} \Gamma(1 + \epsilon)}{2(1 + 2\epsilon)}. \]  

(3.26)

\[ d_{vs} = \alpha_s^2 \left( \frac{\mu}{m} \right)^2 \frac{e^{\gamma_E} (3 - 2\epsilon)(C_A(\epsilon + 2\epsilon + 1)(4\epsilon + 3) + 5) - 8C_F(1 + \epsilon)(2\epsilon^2 + \epsilon + 1)) \Gamma(\epsilon)}{4(2\epsilon - 1)(2\epsilon + 1)(2\epsilon + 3)}. \]  

(3.27)

\[ d_{vv} = \alpha_s^2 \left( \frac{\mu}{m} \right)^2 \frac{e^{\gamma_E} (-C_A(1 + 4\epsilon) + 8C_F \epsilon) \Gamma(\epsilon)}{4(1 + 2\epsilon)}. \]  

(3.28)
This agrees with the finite part of the unequal mass case in [89]. The $O(\epsilon)$ terms of the above expressions are in agreement with [59] 10.

### 3.5 Matching of the vector current

We finally need an expression for the heavy quark vector current $j_\mu^{(v)}$ to NNNLO accuracy in the effective theory. The perturbative matching coefficients of the NRQCD currents come from diagrams where the hard loop connects to one of the external current vertices. Since the zero component of the vector current is irrelevant, we focus on matching the operator $\bar{t}\gamma^i t$.

At leading order in the velocity expansion the unique NRQCD vector current is $\psi^\dagger \sigma^i \chi$ with coefficient function $c_v$ as given by the first term on the right-hand side of (3.1). The precise definition of the matching coefficient is [90]

$$Z_{2,\text{QCD}} \Gamma_{\text{QCD}} = c_v Z_{2,\text{NRQCD}} Z_J^{-1} \Gamma_{\text{NRQCD}},$$

(3.29)

where $Z_2$ are the on-shell wave function renormalization constants in QCD and NRQCD, respectively. $\Gamma$ represents the amputated, bare electromagnetic current vertex function evaluated for on-shell heavy quarks directly at threshold, i.e. with zero relative momentum, expressed in terms of the renormalized QCD coupling and pole mass. In dimensional regularization, $Z_{2,\text{NRQCD}} = 1$, and $\Gamma_{\text{NRQCD}}$, the corresponding NRQCD vertex function, equals its tree-level expression $\xi^\dagger \sigma^i \eta$, since the NRQCD integrals for zero external relative momentum are scaleless. Here it is important that the threshold expansion is employed to define NRQCD in dimensional regularization. Thus, $c_v$ equals the UV renormalized on-shell QCD vertex directly at threshold with infrared divergences subtracted recursively by the NRQCD renormalization factor $Z_J$. This definition is equivalent at order $\alpha_s^n$ to extracting the purely hard (h-h-...-h) momentum regions in the threshold expansion of the $n$-loop vertex function with external heavy quark momenta in the potential region.

The coefficient $c_v$ is needed to three-loop accuracy to achieve NNNLO precision. While the two-loop expression has been known for some time [90,91], the three-loop correction is not yet completed and constitutes one of the missing pieces in the complete third-order calculation of the cross section. The three-loop diagrams involving at least one fermion loop are, however, already known [92,93,94], as are the logarithmic terms related to the anomalous dimension of the current and strong coupling renormalization [95]. Defining

$$L_m = \ln(\mu/m),$$

(3.30)

de the coefficients of perturbative expansions of any quantity $S$ in $\alpha_s = \alpha_s(\mu)$, through

$$S = 1 + \sum_n S^{(n)} \left(\frac{\alpha_s}{4\pi}\right)^n,$$

(3.31)

10. The short-distance coefficients $d_{sv}$ and $d_{vv}$ defined in [59] are $(1 - \epsilon)$ times those above.
11. Except for the “singlet diagrams” where the fermion loop attaches to the external vertex (see lower right figure [1]).
and the coefficients of the QCD $\beta$ function in the $\overline{\text{MS}}$ scheme with $n_f$ light flavours (not including the heavy quark) \cite{92}

\[
\begin{align*}
\beta_0 &= \frac{11}{3}C_A - \frac{4}{3}T_F n_f, \\
\beta_1 &= \frac{34}{3}C_A^2 - \frac{20}{3}C_AT_F n_f - 4C_F T_F n_f, \\
\beta_2 &= \frac{2857}{54}C_A^3 - \frac{1415}{27}C_A^2 T_F n_f - \frac{205}{9}C_A C_F T_F n_f + 2C_F^2 T_F n_f \\
&\quad + \frac{158}{27}C_A T_F^2 n_f^2 + \frac{44}{9}C_F T_F^2 n_f,
\end{align*}
\tag{3.32}
\]

the known results for the vector current matching coefficients are given by:

\[
\begin{align*}
c_v^{(1)}(\mu) &= c_v^{(1)}(m) = -8C_F, \\
c_v^{(2)}(\mu) &= 2\beta_0 L_m c_v^{(1)}(m) + L_m C_F \pi^2 \left[ -\frac{16}{3}C_F - 8C_A \right] + c_v^{(2)}(m), \\
c_v^{(3)}(\mu) &= \left( 4\beta_0^2 L_m^2 + 2\beta_1 L_m \right) c_v^{(1)}(m) \\
&\quad + 4\beta_0 L_m \left\{ L_m C_F \pi^2 \left[ -\frac{16}{3}C_F - 8C_A \right] + c_v^{(2)}(m) \right\} \\
&\quad + L_m^2 C_F \pi^2 \left[ -40C_F^2 - \frac{188}{9}C_F C_A + \frac{128}{3}C_A^2 \\
&\quad \quad \quad - \frac{128}{9}C_F T_F n_f - \frac{64}{3}C_A T_F n_f \right] \\
&\quad + L_m C_F \pi^2 \left[ (-72 + 192 \ln 2) C_F^2 + \left( -\frac{1888}{27} - 96 \ln 2 \right) C_F C_A \\
&\quad \quad \quad + \left( -\frac{256}{9} - 96 \ln 2 \right) C_A^2 + \frac{800}{27}C_F T_F n_f \\
&\quad \quad \quad + \frac{296}{9}C_A T_F n_f - \frac{32}{5}C_F T_F \right] + c_v^{(3)}(m),
\end{align*}
\tag{3.35}
\]

where $c_v^{(i)}(m)$ is the matching coefficient evaluated at $\mu = m$. The two-loop non-logarithmic terms are fully known but the three-loop ones only for the fermionic contributions. They read:

\[
c_v^{(2)}(m) = 16 \left[ C_F^2 \left( \frac{23}{8} - \frac{1}{2} \zeta_3 - \frac{79}{36} \pi^2 + \pi^2 \ln 2 \right) \right]
\]
\[ +C_F C_A \left( -\frac{151}{72} - \frac{13}{4} \zeta_3 + \frac{89}{144} \pi^2 - \frac{5}{6} \pi^2 \ln 2 \right) \]
\[ + \frac{11}{18} C_F T_F n_f + C_F T_F \left( \frac{22}{9} - \frac{2}{9} \pi^2 \right), \quad (3.36) \]

\[ c_v^{(3)}(m) = 64 \left[ C_F T_F n_f \left[ C_F (46.692(1)) + C_A (39.623(1)) \right. \right. \]
\[ + T_F n_f \left( -\frac{163}{162} - \frac{4}{27} \pi^2 \right) + T_F \left( -\frac{557}{162} + \frac{26}{81} \pi^2 \right) \]
\[ + C_F T_F \left[ C_F (-0.840(2)) + C_A (-0.09(2)) \right. \]
\[ \left. \left. + T_F \left( -\frac{427}{162} + \frac{158}{2835} \pi^2 + \frac{16}{9} \zeta_3 \right) \right] \right] + c_{v,g}^{(3)}(m). \quad (3.37) \]

where the last term \( c_{v,g}^{(3)}(m) \) is the unknown gluonic and singlet contribution and \( \zeta_3 \) is a short-hand for the Riemann zeta function value \( \zeta(3) \). We recall our convention that \( \alpha_s \) denotes the strong coupling in the \( \overline{\text{MS}} \) scheme with \( n_f \) light flavours.

Turning to the next orders in the velocity expansion, we find the operators

\[ O_a = \frac{1}{2m^2} \psi^+ \sigma \cdot D D^i \chi, \]
\[ O_b = \frac{1}{m^2} \psi^i \sigma^i \nabla^2 \chi, \quad (3.38) \]

which are suppressed by \( O(v^2) \) relative to the leading NRQCD current. Further operators of dimension five contain the ultrasoft gauge field strength \( g_s F_{\mu \nu} \) of order \( v^9/2 \). Thus up to NNNLO all production vertices contain only the quark-antiquark pair. The on-shell heavy quark-antiquark production vertex in full QCD can be decomposed into the expression

\[ V^\mu = \bar{u}(p_1) \left[ \gamma^\mu \hat{F}_1(q^2) + \frac{i \sigma^{\mu \nu} q^\nu}{2m} \hat{F}_2(q^2) \right] v(p_2), \quad (3.39) \]

where now \( p_1 = (E_p, \mathbf{p}), p_2 = (E_p, -\mathbf{p}), \) and \( q = p_1 + p_2 = (2E_p, \mathbf{0}) = (2m + E, \mathbf{0}). \) Inserting (3.16) for the external spinors, we obtain the exact expression

\[ V^i = 2E_p \left[ \hat{F}_1(q^2) + \hat{F}_2(q^2) \right] \xi^i \sigma^i \eta - 2E_p \left[ \frac{m}{E_p} \hat{F}_1(q^2) - \hat{F}_2(q^2) \right] \frac{p^i}{m(E_p + m)} \xi^\dagger \sigma \cdot \mathbf{p} \eta. \quad (3.40) \]

This shows explicitly that only quark-antiquark operators with a sigma matrix can appear as assumed in (3.38). Expanding this expression in \( q^2 - 4m^2 = 4\mathbf{p}^2 \) we find

\[ c_v = [\hat{F}_1 + \hat{F}_2]_{q^2=4m^2, \text{hard;}} \]
\begin{align}
d_{va} &= [\hat{F}_1 - \hat{F}_2]_{\mu^2=4m^2, \text{hard}}, \\
d_{vb} &= (-4) \frac{d}{d(\mu^2/m^2)} [\hat{F}_1 + \hat{F}_2]_{\mu^2=4m^2, \text{hard}}.
\end{align}

The subscript “hard” means that only the hard regions should be included in the computation. The one-loop hard form factors can be extracted from [93], by dropping the non-analytic terms in the expansion in \( p^2 \), which originate from the potential region. We obtain \( c_v^{(1)} \) given in (3.33) above and

\begin{align}
d_{va} &= 1 - \frac{\alpha_s C_F}{4\pi} \cdot 4 + O(\alpha_s^2), \\
d_{vb} &= \frac{\alpha_s C_F}{4\pi} \left[ \frac{8}{3} \ln \frac{m^2}{\mu^2} - \frac{2}{9} \right] + O(\alpha_s^2).
\end{align}

The logarithm in \( d_{vb} \) arises as the consequence of mixing with the leading order current through sub-leading NRQCD interactions, see (4.129) below. These results agree with the computation of the one-loop corrected matching coefficients of the sub-leading current operators through explicit NRQCD matching [60].

At NNNLO the correlation functions of velocity-suppressed currents will be evaluated only with the leading and next-to-leading order Coulomb potential, which is spin-independent. Hence, only the traces \( \text{tr} (O_{a,b}\sigma^i) \) appear. This allows us to combine

\begin{align}
d_{va} O_a + d_{vb} O_b \rightarrow \frac{d_v}{6m^2} \psi^\dagger \sigma^i D^2 \chi
\end{align}

such that the QCD vector current is now represented by

\begin{align}
j_i^{(v)} = c_v \psi^\dagger \sigma_i \chi + \frac{d_v}{6m^2} \psi^\dagger \sigma_i D^2 \chi + O(1/m^4),
\end{align}

as anticipated in (3.1). From (3.42) and (3.43) we obtain

\begin{align}
d_v(\mu) = \frac{3}{3 - 2\epsilon} d_{va} + 6d_{vb} = 1 - \frac{\alpha_s C_F}{4\pi} \left[ 32 L_m + \frac{16}{3} \right] + O(\alpha_s^2).
\end{align}

The explicit scale dependence of the matching coefficients is due to evolution of the strong coupling and the factorization of the hard scale. It must cancel when all contributions to the cross section are combined. We have checked explicitly that this is indeed the case.

Note that we do not need the \( O(\epsilon) \) terms of the coefficient functions \( c_v \) and \( d_v \) to compute the heavy-quark current correlation function, since they multiply the finite, renormalized NRQCD correlation function in (3.2). One may wonder then what is the difference between the NRQCD current and the NRQCD Lagrangian matching coefficients \( d_1, d_2 \) etc., since for the latter we need the \( O(\epsilon) \) terms as stated and given above. The reason is the particular definition (3.29) of the current matching coefficient. Imagine
that we calculate the QCD and NRQCD vertex functions $\Gamma$ with non-vanishing external relative momentum. Then the NRQCD diagrams are no longer scaleless and $\Gamma_{\text{NRQCD}}$ is the sum of potential, soft and ultrasoft loop momentum contributions. Because of the $1/v$ factors from potential gluon exchange, the higher-dimensional NRQCD interactions contribute to the leading current matching equation at some order in perturbation theory. As a result $\Gamma_{\text{NRQCD}}$ will be different whether one uses the NRQCD Lagrangian with four-dimensional or with $d$-dimensional short-distance coefficients. The difference is, however, a local term that can be absorbed into the matching coefficients of the external currents. Which definition does (3.29) correspond to? Suppose we follow the more conventional path to define the renormalized effective Lagrangian with $d = 4$ short-distance coefficients. In this case $\Gamma_{\text{NRQCD}}$ does not represent the sum of all potential, soft and ultrasoft loop momentum regions plus the hard ones not connected to the external vertex (encapsulated in the Lagrangian matching coefficients $d_1$ etc.), since one misses some $O(\epsilon)$ terms from hard subgraphs that multiply divergent soft, potential or ultrasoft loops. These missing local contributions can be and must be added back by adapting the external current matching coefficient. Hence the matching coefficient $c_v$ defined by this prescription does not correspond to (3.29). On the other hand, the NRQCD Lagrangian with $d$-dimensional short-distance coefficients reproduces these missing terms directly, so the matching coefficient corresponding to this case is simply the contribution from the purely hard (h-h-...-h) regions as it was defined in (3.29). Moreover, the purely hard regions can now be computed directly at zero external relative momentum, which simplifies the calculation.

The same discussion applies to the matching of the potentials in PNRQCD, to which we turn next. However, while the $O(\epsilon)$ terms of the NRQCD Lagrangian are relevant only at NNNLO, the difference between four- and $d$-dimensional potentials in the PNRQCD Lagrangian matters already at NNLO. The $d$-dimensional ones must be used in conjunction with (3.29) as was done in [24].

3.6 Matching of the axial-vector current

Due to the $v^2$ suppression of the P-wave correlation function [35] relative to the S-wave case (3.3), the hard matching coefficient $c_a$ of the axial-vector current is needed only with one-loop accuracy for the NNNLO calculation of the top-quark pair production cross section near threshold. The relevant expression is

$$c_a = 1 - 4C_F \cdot \frac{\alpha_s}{4\pi} + O(\alpha_s^2).$$

(3.46)

The two-loop correction is also known [94].

4 Potential NRQCD

As discussed in Section 2.2 to perform the all-order resummation, a second matching procedure is required, by which the soft region and potential light fields (gluons and
light quarks) are integrated out. This results in the potential NRQCD (PNRQCD) effective field theory \[24,79,85,86,87\]. In PNRQCD the light fields are purely ultrasoft and the heavy quarks are potential, hence the terms in the effective Lagrangian can be assigned a unique scaling in the velocity expansion. The effective Lagrangian relevant to the third-order calculation takes the simple form

\[
\mathcal{L}_{\text{PNRQCD}} = \psi^\dagger \left( i\partial_0 + g_s A_0(t,0) + \frac{\partial^2}{2m} + \frac{\partial^4}{8m^3} \right) \psi + \chi^\dagger \left( i\partial_0 + g_s A_0(t,0) - \frac{\partial^2}{2m} - \frac{\partial^4}{8m^3} \right) \chi \\
+ \int d^{d-1}r \left[ \psi^\dagger_a \psi^\dagger_b \right] (x + r) V_{abcd}(r, \partial) \left[ \chi^\dagger c \chi_d \right] (x) \\
- g_s \psi^\dagger (x) \mathbf{E}(t,0) \psi(x) - g_s \chi^\dagger (x) \mathbf{E}(t,0) \chi(x),
\]

(4.1)

where

\[
V_{abcd}(r, \partial) = T_{ab}^A T_{cd}^A V_0(r) + \delta V_{abcd}(r, \partial)
\]

(4.2)

with \( V_0 = -\alpha_s/r \) the tree-level colour Coulomb potential. The PNRQCD Lagrangian consists of kinetic terms (first line; including the relativistic corrections proportional to \( \partial^4/m^3 \)), heavy-quark potential interactions (second line) and an ultrasoft interaction that contributes first at third order. The heavy-quark potentials generated in the matching to PNRQCD should be considered as short-distance coefficients of the PNRQCD interactions. They are split into the tree-level Coulomb potential, which must be treated non-perturbatively and a remainder \( \delta V_{abcd}(r, \partial) \), which represents a perturbation. To achieve a homogeneous velocity scaling the position argument of ultrasoft fields should be multipole-expanded in interactions with heavy quarks \[82,84,95\], which explains the space-time argument of \( A_0 \) and the chromo-electric field in the ultrasoft interaction terms.

As will be discussed below no further matching of the non-relativistic vector current is needed, that is \( \psi^\dagger \sigma^i \chi|_{\text{NRQCD}} = \psi^\dagger \sigma^i \chi|_{\text{PNRQCD}} \) to the required accuracy. Thus, instead of (3.3), we have to calculate

\[
G(E) = \frac{i}{2N_c(d-1)} \int d^d x e^{iE_0x} \langle 0| T(\left[ \chi^\dagger \sigma^i \psi \right](x) \left[ \psi^\dagger \sigma^i \chi \right](0))|0\rangle_{\text{PNRQCD}},
\]

(4.3)

where now the matrix element must be evaluated to third-order in PNRQCD perturbation theory.

The dimensionally regulated PNRQCD Lagrangian required for second-order calculations of heavy-quark pair production near threshold was provided in \[24\], and the explicit derivation of the ultrasoft interaction in the third line of (4.1) from NRQCD was given in \[95\]. The only new piece that is needed is the third-order heavy-quark potential in \( \delta V_{abcd}(r, \partial) \). In the remainder of this subsection we first give the PNRQCD Feynman rules (when the ultrasoft interactions are neglected) and then sketch several ways of deriving these rules and the form of the propagator. Subsequently, we summarize the heavy-quark potentials. We also derive equation-of-motion relations that allow us to reduce the number of potential insertions to be calculated and briefly discuss the ultrasoft contribution already calculated in \[52\].
Figure 7: PNRQCD Feynman rules.

4.1 Feynman rules

We begin by summarizing the rules for calculating PNRQCD diagrams with insertions of potential interactions, but no ultrasoft interactions. Since the leading-order Lagrangian includes the Coulomb potential $V_0(r)$, the propagator is the one for a heavy quark antiquark pair. We draw the propagator as in the left diagram of figure 7, where the blob stands for the sum of all potential (Coulomb) ladder diagrams, which is included in the propagator. For a pair in a colour-singlet state each propagator gives a factor

$$\frac{1}{N_c} \delta_{bc} \delta_{da} i G_0^{(1)}(p, p'; E),$$

where $E = \sqrt{s} - 2m$ is the non-relativistic energy of the pair and $p$ ($p'$) the three-momentum of the in-coming (out-going) quark. For the colour-octet state the propagator is $2 T_{bc} T_{da} i G_0^{(8)}(p, p'; E)$. The function $G_0^{(R)}(p, p'; E)$ is the solution to the $d$-dimensional Lippmann-Schwinger equation for a pair in irreducible SU(3) colour representation $R$,

$$\left(\frac{p^2}{m} - E\right) G_0^{(R)}(p, p'; E) + \tilde{\mu}^{2\varepsilon} \int \frac{d^{d-1}k}{(2\pi)^{d-1}} \frac{4\pi D_R \alpha_s}{k^2} G_0^{(R)}(p - k, p'; E)
= (2\pi)^{d-1} \delta^{(d-1)}(p - p'),$$

where the $D_R = -C_F$ and $D_R = -(C_F - C_A/2)$ for the colour-singlet and colour-octet representation, respectively. Explicit expressions will be given below. The scale $\tilde{\mu} = \mu \left[e^{\gamma_E}/(4\pi)\right]^{1/2}$ is defined such that minimal subtraction of $1/\varepsilon$ poles corresponds to the $\overline{\text{MS}}$ rather than MS scheme [28]. The Fourier transform

$$G_0^{(R)}(r, r'; E) = \int \frac{d^{d-1}p}{(2\pi)^{d-1}} \frac{d^{d-1}p'}{(2\pi)^{d-1}} e^{ip\cdot r} e^{-ip'\cdot r'} G_0^{(R)}(p, p'; E)$$

satisfies in $d = 4$ dimensions the Schrödinger equation

$$\left(-\nabla^2_{[r]} + \frac{D_R \alpha_s}{r} - E\right) G_0^{(R)}(r, r'; E) = \delta^{(3)}(r - r').$$
In the following, when the superscript is left out, the propagator refers to the colour-singlet representation.

The vertex associated with the insertion of a perturbation potential \( \delta V_{abcd}(p, p') \) in momentum space is given by

\[
i \delta V_{abcd}(p, p'), \tag{4.8}
\]

and internal relative momenta \( p_i \) are integrated over with measure \( \tilde{\mu}^2 \int d^{d-1}p_i/(2\pi)^{d-1} \).

Note that the insertion of a potential does not change the colour-state of the quark-antiquark pair, when it is in an irreducible representation, that is the colour-singlet or the colour-octet state. The reason for this is that \( \frac{1}{N_c} \delta_{bc} \delta_{da} \) and \( 2 T_A^c T_A^d \) constitute a complete set of orthogonal projectors.\(^{12}\)

If the in-coming pair is, for example, in the colour-singlet state, all propagators will be colour-singlet propagators and the potential insertions are effectively projected to the colour-singlet potential

\[
\delta V(p, p') = \frac{1}{N_c} \delta_{bc} \delta_{da} \delta V_{abcd}(p, p'). \tag{4.9}
\]

This is different when an ultrasoft gluon is emitted, in which case the pair changes its colour state, as explicitly seen in (4.126) below.

A general PNRQCD diagram with multiple insertions of perturbation potentials is therefore an expression of the form

\[
\int \left[ \prod_i \frac{d^{d-1}p_i}{(2\pi)^{d-1}} \right] iG_0(p_1, p_2; E)i\delta V_1(p_2, p_3)iG_0(p_3, p_4; E)i\delta V_2(p_4, p_5)iG_0(p_5, p_6; E) \ldots \tag{4.10}
\]

(for the case of a colour-singlet state). For convenience of notation here and below we often leave out factors of \( \tilde{\mu}^{2c} \) required in dimensional regularization to restore the proper dimension of the given expression.

### 4.2 Three derivations of the PNRQCD rules

In this section we sketch three derivations of the rules for PNRQCD perturbation theory: diagrammatic, quantum-mechanical, and by path-integral methods. For simplicity we assume the colour-singlet representation, but the derivation is easily generalized to an arbitrary irreducible representation.

#### 4.2.1 Diagrammatic

Consider the amputated amplitude of the heavy-quark scattering process \( Q(p_1)\bar{Q}(p_2) \rightarrow Q(p'_1)\bar{Q}(p'_2) \) with non-relativistic external momenta \( p_1 = (E/2, p), p_2 = (E/2, -p) \) and \( p'_1 = (E/2, p'), p'_2 = (E/2, -p') \) in the rest frame of the \( Q\bar{Q} \) pair. The sum of all (ladder)

\(^{12}\)See \cite{96,97} for a general discussion of the colour decomposition in arbitrary representations.
diagrams with any number (greater than zero) of leading-order potential insertions \( V_0(r) \) is given in momentum space by

\[
H(p, p'; E) = \sum_{n=0}^{\infty} C_F^{n+1} \int \prod_{i=1}^{n} \frac{d^d k_i}{(2\pi)^d} \frac{(ig_s)^2i}{(k_1 - k_0)^2} \frac{(ig_s)^2i}{(k_2 - k_1)^2} \cdots \frac{(ig_s)^2i}{(k_{n+1} - k_n)^2} \]

\[
\times \prod_{i=1}^{n} \frac{i}{E + k_i^0 - \frac{(p+k_i)^2}{2m} + i\epsilon} \frac{-i}{E - k_i^0 - \frac{(p+k_i)^2}{2m} + i\epsilon},
\]

where we define \( k_{n+1} = p' - p \) and \( k_0 \equiv 0 \). We perform the integrations over the loop momentum zero components \( k_i^0 \) by closing the contour in the upper half plane, and pick up the residues from the poles at \( k_i^0 = E/2 - (p + k_i)^2/(2m) + i\epsilon \), which results in

\[
H(p, p'; E) = i \sum_{n=0}^{\infty} (-g_s^2 C_F)^{n+1} \int \prod_{i=1}^{n} \frac{d^{d-1} k_i}{(2\pi)^{d-1}} \frac{1}{k_i^2} \]

\[
\times \prod_{i=1}^{n} \frac{1}{(k_{i+1} - k_i)^2(E - \frac{(p+k_i)^2}{2m} + i\epsilon)}. \tag{4.12}
\]

The \( n = 0 \) term in this and the previous sum is understood as \( (-ig_s^2 C_F)/(p' - p)^2 \), which is the expression for the exchange of a single potential (Coulomb) gluon. \( H(p, p'; E) \) sums the leading \( p-p-\cdots-p \) region to all orders.

Next we multiply the propagator factors \( (-i)/(E + i\epsilon - p^2/m) \) for the external pairs of lines and add the zero-Coulomb exchange graph. Multiplying by \( (-i) \) this defines

\[
G_0(p, p'; E) = -\frac{(2\pi)^{d-1}\delta^{(d-1)}(p' - p)}{E + i\epsilon - \frac{p^2}{m}} + \frac{1}{E + i\epsilon - \frac{p^2}{m}} \frac{iH(p, p'; E)}{1}{E + i\epsilon - \frac{p^2}{m}}. \tag{4.13}
\]

It is straightforward to show that this expression satisfies the \( d \)-dimensional Lippmann-Schwinger equation \((4.13)\), and hence represents the colour-singlet Coulomb Green function. The summation of ladder diagrams is therefore accomplished by associating the quantity \( ig_0(p, p'; E) \) with the propagator of the quark anti-quark pair and the vertex \( i\delta V(p, p') \) with the interaction potentials. It is understood that the integrations over the zero-components of loop momenta are already done.

Note that while no closed expression for the Green function is known in \( d \) dimensions, it is important that the above expression is defined in dimensional regularization, and that it can be expanded perturbatively in \( g_s^2 \) in \( d \) dimensions. This guarantees the consistency of the dimensional regularization procedure, which requires subtracting terms with a finite number of Coulomb exchanges from \( G_0(p, p'; E) \) in \( d \) dimensions as will be seen in part II of the paper.

The PNRQCD correlation function \((4.13)\) describes a quark anti-quark pair created in a colour-singlet, spin-triplet state at point 0, which propagates and is destroyed locally at point \( x \). In terms of the momentum-space propagator it is given by

\[
G(E) = \int \frac{d^{d-1}p}{(2\pi)^{d-1}} \frac{d^{d-1}p'}{(2\pi)^{d-1}} \left[ G_0^{(1)}(p, p'; E) \right]
\]

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\[ + \int \frac{d^{d-1}p_1}{(2\pi)^{d-1}} \frac{d^{d-1}p_1'}{(2\pi)^{d-1}} G_0^{(1)}(p, p_1; E) i\delta V(p_1, p_1') iG_0^{(1)}(p_1', p'; E) + \ldots \], \ (4.14)\]

where the potential refers to the colour-singlet potential \[ (4.9) \], and the ellipses to terms with multiple potential insertions. Both the propagator and the potential carry spin-indices in general. However, the unperturbed PNRQCD Lagrangian is spin-independent, so the propagator is diagonal in the spin indices and we drop the \[ \delta_{\alpha\beta'}\delta_{\alpha'\beta} \] spin factor.

The spin-dependence of the perturbation potential enters only at NNLO, hence up to \[ N^3\text{LO} \] only one of the \( \delta V \) insertions can carry a non-trivial spin-dependence. When this insertion appears in \[ (4.14) \], \( \delta V \) is understood as
\[ \delta V = \frac{1}{2(d-1)} \sigma^i_{\alpha\alpha'} \delta V_{\alpha\beta';\alpha'\beta} \sigma^i_{\beta\beta'} \] \ (4.15).

The trace must be carried out in \( d \) dimensions. Greek indices of the potential refer to spin (rather than colour). The normalization factor and Pauli matrices result from the definition of \[ (4.3) \] and correspond to the spin-triplet projection of the potential. For the insertions of spin-independent potentials the spin-factor
\[ \frac{1}{2(d-1)} \sigma^i_{\alpha\alpha'} \delta_{\alpha\beta'} \delta_{\alpha'\beta} \sigma^i_{\beta\beta'} = 1 \] \ (4.16)
is included in \[ (4.14) \].

### 4.2.2 Quantum-mechanical

With only potential interactions the PNRQCD Lagrangian can be projected onto the Fock states with a single quark and a single anti-quark without loss of content, since potential interactions do not change particle number. We define the centre-of-mass wave function of a quark anti-quark state \( |\psi\rangle \) in the position-space representation via
\[ \psi(t, r) = \langle 0 | [\psi(t, r/2)\chi^\dagger(t, -r/2)]^\dagger |\psi\rangle, \] \ (4.17)

which is a matrix in colour and spin indices. For simplicity, we assume again a projection on the colour-singlet representation. By reversing the steps that lead from the Schrödinger equation to a second-quantized Schrödinger field theory, making use of the field equation and the canonical commutation relations, we find that
\[ i\partial_t \psi(t, r) = H \psi(t, r) = \left[ -\frac{\nabla^2}{m} + C_F V_0(r) + \delta V(r) \right] \psi(t, r). \] \ (4.18)

The Green function of the Schrödinger operator is given by \( \langle r | [H - E - i\epsilon]^{-1} | r' \rangle \) with \( |r\rangle \) a quark anti-quark separation eigenstate with eigenvalue \( r \). In operator notation the Green function is \( \hat{G}_H(E) = [H - E - i\epsilon]^{-1} \) such that
\[ \hat{G}_H(E) = \hat{G}_0(E) + \hat{G}_0(E)i\delta Vi\hat{G}_0(E) + \ldots, \] \ (4.19)
where \( \hat{G}_0(E) = [H_0 - E - i\epsilon]^{-1} \) and \( H = H_0 + \delta V \). Since \( G_0^{(1)}(r, r'; E) = \langle r | \hat{G}_0(E) | r' \rangle \), the previous equation verifies the PNRQCD Feynman rules. In this notation the correlation function (4.3) is given by

\[
G(E) = \langle 0 | \hat{G}_H(E) | 0 \rangle ,
\]

which is equivalent to (4.14) upon using (4.19) and inserting complete sets of momentum eigenstates,

\[
1 = \int \frac{d^{d-1}p}{(2\pi)^{d-1}} |p\rangle \langle p| ,
\]

leaving the spin-average being implicit.

4.2.3 Path integral derivation

In [85,86,87] the PNRQCD Lagrangian is expressed in terms of composite colour-singlet and colour-octet fields. Here we provide a path-integral derivation of this formulation. We focus on the colour-singlet field and drop the colour and spin indices of the composite field

\[
[S(x, y)]_{x^0 = y^0} = [\psi \dagger(x) \chi(y)]_{x^0 = y^0}, \quad [S^\dagger(y, x)]_{x^0 = y^0} = [\chi \dagger(y) \psi(x)]_{x^0 = y^0} .
\]

The partition function \( Z_{PNRQCD} \) of PNRQCD is defined as

\[
Z_{PNRQCD} = \int D\psi D\psi \dagger D\chi D\chi \dagger \exp \left\{ i \int d^4x \mathcal{L}_{PNRQCD}(x) \right\} ,
\]

where we use the leading-order PNRQCD Lagrangian

\[
\mathcal{L}_{PNRQCD}(x) = \psi \dagger(x) \left[ i\partial_0 + \frac{\partial^2}{2m} \right] \psi(x) + \chi \dagger(x) \left[ i\partial_0 - \frac{\partial^2}{2m} \right] \chi(x)
\]

\[
- \int d^4y \left[ \psi \dagger(x) \chi(y) \right] V(x, y) \left[ \chi \dagger(y) \psi(x) \right] ,
\]

with the quark anti-quark potential \( V(x, y) = V_0(x - y)\delta(x^0 - y^0) \). The derivation remains however valid with an arbitrary potential, not just the leading-order Coulomb potential. The different sign of the potential term relative to (4.1) is due to the different order of fermion fields. The composite field is introduced by means of

\[
1 = \int D\sigma \delta \left( [S(x, y)]_{x^0 = y^0} - \left[ \psi \dagger(x) \chi(y) \right]_{x^0 = y^0} \right)
\]

\[
= \int D\sigma \exp \left\{ i \int d^4x \int d^4y \sigma(x, y) \delta(x^0 - y^0) \left( S(x, y) - \left[ \psi \dagger(x) \chi(y) \right] \right) \right\} ,
\]

where the second line is the Fourier representation of the functional delta-function which introduces the auxiliary field \( \sigma \). With a similar formula for the complex conjugate field we can rewrite the partition function as

\[
Z_{PNRQCD} = \int D\psi D\psi \dagger D\chi D\chi \dagger D\sigma D\sigma \dagger \exp \left\{ i \int d^4x \int d^4y \mathcal{L}_{\psi, \chi, S, \sigma}(x, y) \right\} ,
\]
where

\[ L_{\psi,\chi,S,\sigma}(x,y) = \psi^{\dagger}(x)K_{Q}(x,y)\psi(y) + \chi^{\dagger}(x)K_{q}(y) - S(x,y)V(x,y)S^{\dagger}(y,x) + \Sigma(x,y)\left(S(x,y) - [\psi^{\dagger}(x)\chi(y)]\right) + \Sigma^{\dagger}(y,x)\left(S^{\dagger}(y,x) - [\chi^{\dagger}(y)\psi(x)]\right). \]  

(4.27)

To make equations concise we introduced \( \Sigma(x,y) = \sigma(x,y)\delta(x^{0} - y^{0}) \) and

\[ K_{Q}(x,y) = \delta^{4}(x - y)\left(i\partial_{0} + \frac{\partial^{2}}{2m}\right)_{y}, \]

\[ K_{\bar{Q}}(x,y) = \delta^{4}(x - y)\left(i\partial_{0} - \frac{\partial^{2}}{2m}\right)_{y}. \]  

(4.28)

Our task is to integrate over \( \psi, \chi, \sigma \) and their conjugates to obtain the Lagrangian for the \( S \) field. In the following we do this step by step obtaining the sequence of Lagrangians

\[ L_{\psi,\chi,S,\sigma} \rightarrow L_{\chi,S,\sigma} \rightarrow L_{\sigma,S} \rightarrow L_{S}. \]  

(4.29)

We drop field-independent factors which can be absorbed into the path-integral measure. First we integrate out \( \psi \) and its conjugate by completing squares in the exponent:

\[ \int d^{4}x \int d^{4}y L_{\psi,\chi,S,\sigma}(x,y) = \int d^{4}x \int d^{4}y [L_{\psi,\chi,S,\sigma}(x,y)]_{\psi=0} + (\psi^{\dagger} - \chi^{\dagger} \cdot \Sigma^{\dagger} \cdot K_{Q}^{-1}) \cdot K_{Q} \cdot (\psi - K_{Q}^{-1} \cdot \Sigma \cdot \chi) - \chi^{\dagger} \cdot \Sigma^{\dagger} \cdot K_{Q}^{-1} \cdot \Sigma \cdot \chi. \]  

(4.30)

In the second line the abbreviation \( (\cdot) \) stands for the integration of the adjoining variables, such that, for example, the last term reads explicitly

\[ \chi^{\dagger} \cdot \Sigma^{\dagger} \cdot K_{Q}^{-1} \cdot \Sigma \cdot \chi = \int d^{4}x \int d^{4}z_{1} \int d^{4}z_{2} \int d^{4}y \chi^{\dagger}(x)\Sigma^{\dagger}(x,z_{1})K_{Q}^{-1}(z_{1},z_{2})\Sigma(z_{2},y)\chi(y). \]  

(4.31)

The inverse operators are given by

\[ K_{Q}^{-1}(x,y) = \int \frac{d^{4}p}{(2\pi)^{4}} \frac{e^{-ip(x-y)}}{p^{0} - \frac{p^{2}}{2m} + i\epsilon}, \]

\[ K_{\bar{Q}}^{-1}(x,y) = \int \frac{d^{4}p}{(2\pi)^{4}} \frac{e^{-ip(x-y)}}{p^{0} + \frac{p^{2}}{2m} - i\epsilon}. \]  

(4.32)

Changing variables to \( \psi' = \psi - K_{Q}^{-1} \cdot \Sigma \cdot \chi \) (similarly for \( \psi'^{\dagger} \)) and integrating over \( \psi, \psi'^{\dagger} \) we obtain

\[ \int d^{4}x \int d^{4}y L_{\chi,S,\sigma}(x,y) = \int d^{4}x \int d^{4}y [L_{\psi,\chi,S,\sigma}(x,y)]_{\psi=0} - \chi^{\dagger} \cdot \Sigma^{\dagger} \cdot K_{Q}^{-1} \cdot \Sigma \cdot \chi. \]  

(4.33)
The integration over $\chi, \chi^\dagger$ is done analogously resulting in the partition function
\[
Z_{PNRQCD} = \int D\sigma D\sigma^\dagger \det(1 - K^{-1}_Q \cdot \Sigma \cdot K^{-1}_Q \cdot \Sigma) \tag{4.34}
\]
\[
\times \exp \left( i \int d^4 x d^4 y \left\{ S(x,y)\Sigma(x,y) + S^\dagger(y,x)\Sigma^\dagger(y,x) - S(x,y)V(x,y)S^\dagger(y,x) \right\} \right).
\]
The determinant contains the $\sigma$ field. To write it as a term in the Lagrangian we use
\[
\det(1 - K^{-1}_Q \cdot \Sigma \cdot K^{-1}_Q \cdot \Sigma) = \exp \left\{ \text{Tr} \ln \left( 1 - K^{-1}_Q \cdot \Sigma \cdot K^{-1}_Q \cdot \Sigma \right) \right\}
\]
\[
= \exp \left\{ -\text{Tr} K^{-1}_Q \cdot \Sigma \cdot K^{-1}_Q \cdot \Sigma + \ldots \right\}, \tag{4.35}
\]
and keep only the bilinear term in the $\Sigma$ field in the expansion of the logarithm. We comment on the other terms below. The Lagrangian after this procedure is
\[
\int d^4 x \int d^4 y \mathcal{L}_{S,\sigma}(x,y) =
\int d^4 x \int d^4 y \left( S(x,y)\Sigma(x,y) + S^\dagger(y,x)\Sigma^\dagger(y,x) - S(x,y)V(x,y)S^\dagger(y,x) \right)
+ \int d^4 x \int d^4 y \int d^4 x' \int d^4 y' \Sigma^\dagger(y',x') iK^{-1}_Q(x',x)K^{-1}_Q(y',y')\Sigma(x,y). \tag{4.36}
\]
Now we integrate over the delta-functions in the time coordinates implicit in the definition of the $\Sigma$ field and obtain
\[
\int d^4 x \int d^4 y \mathcal{L}_{S,\sigma}(x,y) = \int d^7 z \left( S(z)\sigma(z) + S^\dagger(z)\sigma^\dagger(z) - S^\dagger(z)V(z)S(z) \right)
+ \int d^7 z d^7 z' \sigma^\dagger(z') iK_{\sigma}(z';z)\sigma(z), \tag{4.37}
\]
where $z = (t, x, y)$ represents the coordinates of the quark and anti-quark at coincident time $t = x^0 = y^0$. The fields with argument $z$ are defined as
\[
S(z) = [S(x,y)]_{x^0 = y^0},
\]
\[
\sigma(z) = [\sigma(x,y)]_{x^0 = y^0},
\]
\[
K_{\sigma}(z',z) = [K^{-1}_Q(x',x)K^{-1}_Q(y',y')]_{t = x^0 = y^0, t' = x^0 = y^0}. \tag{4.38}
\]
The last step consists of performing the Gaussian integral over $\sigma$. The inverse of $K_{\sigma}$ is defined by
\[
\delta^{(7)}(z_1 - z_2) = \int d^7 z K^{-1}_{\sigma}(z_1, z) K_{\sigma}(z, z_2), \tag{4.39}
\]
resulting in
\[ \int d^7z \mathcal{L}_S(z) = \int d^7z d^7z' S(z') iK^{-1}_\sigma(z', z) S^\dagger(z) - \int d^7z S^\dagger(z) V(z) S(z). \tag{4.40} \]

To compute \( iK^{-1}_\sigma(z', z) \) we use (4.38) and the definitions (4.32). The integrals over the zero-components of the two momenta can be written as integrals over relative momentum \( q^0 \) and total momentum \( P^0 \). Since the exponentials are independent of \( P^0 \), the \( P^0 \) integral can be performed by contour integration which gives
\[ K_\sigma(z', z) = \int \frac{d^7K}{(2\pi)^7} e^{-iK(z'-z)} \frac{i}{q^0 - \frac{p^2}{2m} - \frac{p'^2}{2m}}, \tag{4.41} \]
where \( K = (q^0, p, p') \). It follows that
\[ K^{-1}_\sigma(z, z') = \delta^{(7)}(z - z') (-i) \left[ i\partial_0 + \frac{\partial^2_x}{2m} + \frac{\partial^2_y}{2m} \right], \tag{4.42} \]
and therefore
\[ Z_{PNRQCD} = \int \mathcal{D}S \mathcal{D}S^\dagger \exp \left\{ i \int d^7z \mathcal{L}_S(z) \right\} \tag{4.43} \]
with
\[ \mathcal{L}_S(z) = \int d^7z S^\dagger(z) \left\{ i\partial^0 + \frac{\partial^2}{2m} - V(z) \right\} S(z). \tag{4.44} \]

After separating the free centre-of-mass motion this represents the PNRQCD Lagrangian expressed in terms of the composite quark anti-quark field.

When one keeps the higher-order terms in the expansion of the logarithm in (4.35) the path-integral over \( \sigma \) can no longer be done exactly. Expanding the quartic and higher-order terms in the exponential, we obtain vertices involving four and more \( S \) fields, which describe scattering of composite fields. These terms are clearly not relevant to the threshold dynamics of a single quark anti-quark pair.

### 4.3 Explicit forms of the propagator (Coulomb Green function)

In four dimensions explicit solutions for the the Schrödinger equation (4.7) can be found, equivalent to the sum of diagrams (4.13). We quote the results for the colour-singlet Green function. The general case is obtained by substituting \( C_F \rightarrow -D_R \) everywhere.

The momentum space PNRQCD propagator (Coulomb Green function) can be expressed in the form
\[ G_0(p, p'; E) = -\frac{(2\pi)^3\delta^{(3)}(p' - p)}{E - \frac{p^2}{m}} + \frac{1}{E - \frac{p^2}{m}} \frac{g_s^2C_F}{(p - p')^2} \frac{1}{E - \frac{p'^2}{m}} \]
\[ + \frac{1}{E - \frac{p^2}{m}} \int_0^1 dt \frac{g_s^2 C_F \lambda t^{-\lambda}}{(p - p')^2 t - \frac{m}{4E}(E - \frac{p^2}{m})(E - \frac{p'^2}{m})(1 - t)^2} \frac{1}{E - \frac{p'^2}{m}}, \]

which closely resembles \[4.13\] and shows that the sum from \( n = 1 \) to infinity in \[4.12\] can be transformed into a remarkably simple integral.\(^{13}\) At this point we omit the \(+i\varepsilon\) prescription on \( E \) and regard \( G_0(p, p'; E) \) as a function of a complex energy variable, which has a cut for \( E > 0 \) and isolated poles on the negative real axis. The variable \( \lambda \) equals \( \alpha_s C_F/(2\sqrt{-E/m}) \) as defined in \((2.5)\). The first line of \((4.45)\) separates the zero- and one-Coulomb gluon exchange terms. In practice, we find it simpler to perform the all-order summation in the position space representation, where the potential insertions take a simple multiplicative (rather than convolutive) form, and therefore we do not make use of the above representation in the calculation in paper II.

An integral representation for the position space Coulomb Green function is

\[
G_0(r, r'; E) = -\frac{m}{4\pi \Gamma(1 + \lambda)\Gamma(1 - \lambda)} \int_0^1 dt \int_{-1}^1 ds [s(1 - t)]^\lambda [t(s - 1)]^{-\lambda}
\times \frac{\partial^2}{\partial t \partial s} \left( \frac{ts}{|s r - t r'|} e^{-\sqrt{-mE}((1-t)r'+(s-1)r+|sr-tr'|)} \right), \tag{4.46}
\]

valid for \( r > r' \), where \( r = |r|, r' = |r'| \). \(^9\) For \( r < r' \) exchange \( r \leftrightarrow r' \) in the above expression. Putting one of the arguments to zero, this simplifies to

\[
G_0(0, r; E) = -\frac{m\sqrt{-mE}}{2\pi} e^{-\sqrt{-mE}r} \int_0^\infty ds e^{-2rs\sqrt{-mE}} \left( \frac{1 + s}{s} \right)^\lambda, \tag{4.47}
\]

which depends only on \( r = |r| \). We use this form of the Coulomb Green function mainly for propagators connecting to the external current vertex, in which case \((4.47)\) applies.

For the general case of a propagator in between two potential insertions the representation of the position-space Green function in terms of Laguerre polynomials \( L_n^{(2l+1)}(x) \) turns out to be most useful. In this representation one first performs a partial wave expansion

\[
G_0(r, r'; E) = \sum_{l=0}^{\infty} (2l + 1) P_l \left( \frac{r \cdot r'}{rr'} \right) G_{[l]}(r, r'; E), \tag{4.48}
\]

where \( P_l(z) \) are the Legendre polynomials. The partial-wave Green functions read

\[
G_{[l]}(r, r'; E) = \frac{m p}{2\pi} (2pr)^l (2pr')^l e^{-p(r+r')} \sum_{s=0}^{s} \frac{s! L_s^{(2l+1)}(2pr)L_s^{(2l+1)}(2pr')}{(s + 2l + 1)!(s + l + 1 - \lambda)}, \tag{4.49}
\]

where \( p = \sqrt{-mE} \), and the Laguerre polynomials are defined by

\[
L_s^{(\alpha)}(z) = \frac{e^z z^{-\alpha}}{s!} \left( \frac{d}{dz} \right)^s \left[ e^z z^{s+\alpha} \right]. \tag{4.50}
\]

\(^{13}\)Note the sign change compared to \[108\], since Schwinger defines the Green function with an opposite sign.
Since at NNNLO accuracy the potential insertions cannot change the angular momentum of the quark anti-quark pair and since the production current $\psi^{\dagger}\sigma^{i}\chi$ creates an S-wave state, we only need the $l = 0$ Green function to compute the potential contributions to the PNRQCD correlation function (4.3). The P-wave Green function is required to compute the ultrasoft contribution [49,52] and the contribution (3.3) from the P-wave production current.

A general property of the Coulomb interaction is that the ultraviolet behaviour of the technical diagrams improves with the number of exchanges. Thus, when the external current or potential insertions cause UV divergences, it is necessary to subtract only the first few terms in the sum of ladder diagrams. The divergent diagrams must be done in $d$ dimensions using standard methods, while for the convergent remainder one of the above expressions, properly subtracted, can be used. We therefore use the notation $^{14}$

$$ G_0(\ldots; E) = G_0^{(0ex)}(\ldots; E) + G_0^{(1ex)}(\ldots; E) + \ldots + G_0^{(n_{ex})}(\ldots; E) + G_0^{(>n_{ex})}(\ldots; E) \quad (4.51) $$

For example, the three terms in (4.45) correspond to $G_0^{(0ex)}(\ldots; E) + G_0^{(1ex)}(\ldots; E) + G_0^{(>1ex)}(\ldots; E)$.

From (1.14) it follows that the leading term in $G(E)$ equals $G_0(r = 0, r' = 0; E)$, which is, however, divergent as can be seen from (4.47). To compute $G_0(0, 0; E)$ in dimensional regularization, we note that the zero-Coulomb exchange term is linearly divergent, the one-Coulomb exchange logarithmically, and the remainder is convergent. We therefore compute $G_0^{(0ex)}(0, 0; E) + G_0^{(1ex)}(0, 0; E)$ from the first line of (4.45), which yields

$$ G_0^{(0+1ex)}(0, 0; E) = \int \frac{d^{d-1}p}{(2\pi)^{d-1}} \frac{-1}{E - \frac{p^2}{m}} + \int \frac{d^{d-1}p}{(2\pi)^{d-1}} \frac{d^{d-1}p'}{(2\pi)^{d-1}} \frac{1}{E - \frac{p^2}{m} (p - p')^2} \frac{1}{E - \frac{p'^2}{m}} $$

$$ = \frac{m^2}{4\pi} \left[ -\sqrt{\frac{E}{m}} - \alpha_s C_F \left\{ -\frac{1}{4\epsilon} + \frac{1}{2} \ln \left( \frac{-4mE}{\mu^2} \right) - \frac{1}{2} \right\} + O(\epsilon) \right]. \quad (4.52) $$

The remaining terms can be calculated from a modified version of (4.47) with $r = 0$ and integrand $(1 + s)^{\lambda} s^{-\lambda - \delta}$. After subtracting the first two terms of the $\alpha_s$ expansion the result is finite as the regulator $\delta \to 0$ and gives the remaining contribution $G^{(>1ex)}(0, 0; E)$. The final result for the MS subtracted zero-distance Green function [95,102] is

$$ G_0^{\text{MS}}(0, 0; E) = \frac{m^2}{4\pi} \left[ -\sqrt{\frac{E}{m}} - \alpha_s C_F \left\{ \frac{1}{2} \ln \left( \frac{-4mE}{\mu^2} \right) - \frac{1}{2} + \gamma_E + \Psi(1 - \lambda) \right\} \right]. \quad (4.53) $$

The poles of the Euler Psi-function at positive integer $\lambda$ correspond to the S-wave quark anti-quark bound states. Near the bound-state poles the Green function takes the form

$$ G_0(0, 0; E) \stackrel{E \to E_n}{\longrightarrow} \frac{1}{E_n - E - i\epsilon} + \text{regular}, \quad (4.54) $$

$^{14}$In an abuse of notation we now use a superscript on the Green function to denote a) the colour representation and b) the number of Coulomb exchanges. What is meant should be clear from the context.
where \( \psi_n(0) \) is the wave-function at the origin of the \( n \)th bound state with energy \( E_n = -(m \alpha_s^2 C_F^2) / (4n^2) \). The imaginary part of the Green function for \( E > 0 \) is known as the Sommerfeld factor \([103]\). Explicitly, the imaginary part below and above threshold is given by

\[
\text{Im} G_0(0, 0; E) = \sum_{n=1}^{\infty} \frac{1}{8} \left( \frac{\alpha_s C_F m}{n} \right)^3 \delta(E - E_n) + \theta(E) \frac{m^2}{4\pi} \frac{\pi \alpha_s C_F}{1 - e^{-\pi \alpha_s C_F}},
\]

for real energies \( E = m v^2 \). This expression can be used in (1.2) to obtain the leading-order approximation to the resummed top pair production cross section in the threshold region for zero width of the top quark.

### 4.4 Potentials

We now summarize the momentum-space potentials required for the NNLO calculation with the PNRQCD Lagrangian (4.1). Only the colour-singlet projection

\[
V(p, p') = \frac{1}{N_c} \delta_{ab} \delta_{cd} V_{ab|cd}(p, p') = V_1(p, p') + C_F V_T(p, p')
\]

of the general quark anti-quark potential \( V_{1,ab|cd} + V_T^A T^A_{ab|cd} \) is relevant to top-quark pair production through the electromagnetic and electroweak current, and this will be given in the following.

The various potential terms can be ordered in a \( 1/m \) expansion, beginning with the Coulomb potential of order \( 1/m^0 \). Allowing for the spin-dependence from order \( 1/m^2 \), we write the singlet-potential in the general form:

\[
V(p, p') = -V_C(\alpha_s) \frac{4\pi C_F \alpha_s}{q^2} + V_{1/m}(\alpha_s) \frac{\pi^2(4\pi) C_F \alpha_s}{m|q|}
\]

\[
+ V_\delta(\alpha_s) \frac{2\pi C_F \alpha_s}{m^2} \quad - V_s(\alpha_s) \frac{\pi C_F \alpha_s}{4m^2} \quad [\sigma_i, \sigma_j] \otimes [\sigma_i, \sigma_j]
\]

\[
- V_p(\alpha_s) \frac{2\pi C_F \alpha_s (p^2 + p'^2)}{m^2 q^2} + V_{hf}(\alpha_s) \frac{\pi C_F \alpha_s}{4m^2 q^2} \quad [\sigma_i, \sigma_j] q_j \otimes [\sigma_i, \sigma_k] q_k
\]

\[
- V_{so}(\alpha_s) \frac{3\pi C_F \alpha_s}{2m^2 q^2} \quad [\sigma_i, \sigma_j] q_i p_j \otimes 1 - 1 \otimes [\sigma_i, \sigma_j] q_i p_j \quad + \ldots
\]

The coefficients \( V_X \) of the potentials are \( \alpha_s \) dependent:

\[
V_i(\alpha_s) = V_i^{(0)} \quad + \frac{\alpha_s}{4\pi} V_i^{(1)} \quad + \left( \frac{\alpha_s}{4\pi} \right)^2 V_i^{(2)} \quad + O(\alpha_s^3).
\]
The term is of order $\alpha_s/q^2 \sim 1/v$. The ellipses denote terms of order $\alpha_s^2|q|/m^3, \alpha_s q^2/m^4 \sim v^3$, which would contribute from $N^3$LO. A notation has been used which is valid in $d$ dimensions by avoiding the use of vector products or the totally antisymmetric $\epsilon$ tensor that would arise from using the three-dimensional identity for the commutator of Pauli matrices. The coefficients of the potentials are chosen such that the leading-order coefficients are either one or zero. The tensor products $a \otimes b$ refer to the spin matrices on the quark ($a$) and anti-quark line ($b$). For the first three and the fifth terms of (4.57), which are spin-independent, we omitted the trivial $1 \otimes 1$ factor.

The on-shell matching calculation of the potential coefficients $V_{C}^{(3)}, V_{1/m}, V_{\delta}^{(1)}, V_{p}^{(1)}$ results in infrared (IR) divergences [36,41,104], which are related to ultraviolet divergences in the calculation of the ultrasoft correction. It is convenient to subtract these divergences in the results given below and add them back to the ultrasoft calculation (see [49,52] and section 4.8). The subtraction term, which is added to the potential, is

$$\delta V_{c.t.} = \frac{\alpha_s C_F}{6\epsilon} \left[ C_A^3 \frac{\alpha_s^3}{q^2} + 4 \left( C_A^2 + 2C_A C_F \right) \frac{\pi \alpha_s^2}{m|q|} \right.$$ 

$$+ 16 \left( C_F - \frac{C_A}{2} \right) \frac{\alpha_s}{m^2} + 16C_A \frac{\alpha_s}{m^2} \frac{p^2 + p'^2}{2q^2} \right]. \quad (4.59)$$

In addition to potential insertions, the relativistic correction to the kinetic energy term $\pm \partial^4/(8m^3)$ in (4.1) needs to be included in PNRQCD perturbation theory. Formally, this can be done by adding

$$V_{\text{kin}} = -\frac{p^4}{4m^3} (2\pi)^{d-1} \delta^{(d-1)}(p - p'). \quad (4.60)$$

to the potential. Since $V_{\text{kin}} \sim v$, it counts as a NNLO potential. The delta function eliminates the momentum integration that is associated with a potential insertion, but which is not present for the kinetic energy correction to a (anti-)quark propagator.

We now present the results for the potential coefficients, starting with the Coulomb potential.

### 4.4.1 The Coulomb potential

The coefficient $V_C(\alpha_s)$ encodes the quantum corrections to the Coulomb potential, which are needed up to the three-loop order. The insertions of Coulomb potentials are finite, so we do not need the $d$-dimensional expression of the potential, as long as only Coulomb potential insertions are considered. This reflects the fact that the Schrödinger equation with the $1/r$ potential is non-singular and could be solved exactly, without referring to PNRQCD perturbation theory, as was done, for instance in [43]. However, in the third-order computation of the top anti-top production cross section also the double insertion

\footnote{Note that in [48] it was incorrectly stated that this term should be subtracted from the potential (rather than added to it).}
of the NLO Coulomb potential together with the singular insertion of a NNLO non-Coulomb potential has to be taken into account; hence the order $\epsilon$ part of the one-loop Coulomb potential multiplies a divergent quantity and contributes to the final result. The coefficient $\gamma^{(1)}_C$ is therefore given with the full $\epsilon$ dependence.

The first four terms in the expansion of the Coulomb potential can be represented in the form

$$\gamma^{(0)}_C = 1,$$

$$\gamma^{(1)}_C = \left[ \left( \frac{\mu^2}{q^2} \right)^\epsilon - 1 \right] \frac{\beta_0}{\epsilon} + \left( \frac{\mu^2}{q^2} \right)^\epsilon a_1(\epsilon),$$

$$\gamma^{(2)}_C = a_2 + (2a_1\beta_0 + \beta_1) \ln \frac{\mu^2}{q^2} + \beta_0^2 \ln^2 \frac{\mu^2}{q^2},$$

$$\gamma^{(3)}_C = a_3 + (2a_1\beta_1 + \beta_2 + 3a_2\beta_0 + 8\pi^2 C_A^3) \ln \frac{\mu^2}{q^2} + \left( \frac{5}{2} \beta_0 \beta_1 + 3a_1\beta_0^2 \right) \ln^2 \frac{\mu^2}{q^2} + \beta_0^3 \ln^3 \frac{\mu^2}{q^2},$$

with

$$a_1(\epsilon) = \left( C_A [11 - 8\epsilon] - 4TFn_f \right) e^{\gamma_E\epsilon} \frac{\Gamma(1 - \epsilon) \Gamma(2 - \epsilon) \Gamma(\epsilon)}{(3 - 2\epsilon) \Gamma(2 - 2\epsilon)} - \frac{\beta_0}{\epsilon},$$

$$a_2 = \left( \frac{4343}{162} + 4\pi - \frac{\pi^2}{4} + \frac{22}{3} \zeta_3 \right) C_A^2 - \left( \frac{1798}{81} + \frac{56}{3} \zeta_3 \right) C_A TFn_f$$

$$- \left( \frac{55}{3} - 16\zeta_3 \right) C_F TFn_f + \frac{400}{81} (TFn_f)^2.$$
The numerical coefficients are quoted from [56,111], and the color factors $d_{X}^{abcd}$ and $d_{Y}^{abcd}$ for $SU(N_c)$ are given by

$$
\frac{d_{F}^{abcd}d_{F}^{abcd}}{2N_{A}T_{F}} = \frac{N_{c}^{4} - 6N_{c}^{2} + 18}{96N_{c}^{2}}, \quad \frac{d_{A}^{abcd}d_{F}^{abcd}}{2N_{A}T_{F}} = \frac{N_{c}(N_{c}^{2} + 6)}{48}.
$$

(4.68)

Parts of the NNNNLO Coulomb potential are also known [112], but not needed for the third-order cross section calculation.

The third-order Coulomb potential has an IR divergence [34,104], which cancels against a divergence in the calculation of the NNNLO ultrasoft calculation. The corresponding $1/\epsilon$ pole is subtracted and therefore does not appear in (4.64), but the logarithmic part multiplied by $C_{A}^{3}$ in this equation comes from this divergence. Note that the coefficient of this logarithm agrees with [41], but is three times larger than the one in [34]. The reason for this is that here as in [41] all three loops are computed in $d$ dimensions not just the divergent one, as is required for consistency with the ultrasoft calculation. Hence the divergence related to the Coulomb potential in (4.59) is multiplied by $(\mu^{2}/q^{2})^{3\epsilon}$ rather than $(\mu^{2}/q^{2})^{\epsilon}$.

### 4.4.2 The $1/m$ potential

The coefficient of the $O(1/m^{1})$ potential is generated first at the one-loop order, where it is suppressed by $\alpha_{s}\nu$ relative to the leading Coulomb potential. Hence the two-loop coefficient is required for the NNNLO calculation of the cross section. The insertions of this potential cause ultraviolet divergences such that we need the one-loop coefficient to $O(\epsilon^{2})$ and the two-loop one to $O(\epsilon)$. Up to the two-loop order we can represent the $O(1/m)$ potential in the form}

\[ V_{1/m}(0) = 0, \]

\[ V_{1/m}^{(1)} = \left( \frac{\mu^{2}}{q^{2}} \right)^{\epsilon} b_{1}(\epsilon), \]

\[ V_{1/m}^{(2)} = \left[ \left( \frac{\mu^{2}}{q^{2}} \right)^{2\epsilon} - 1 \right] \left( -\frac{8}{3\epsilon} \right) \left( 2C_{F}C_{A} + C_{A}^{2} \right), \]
+ \left[ \left( \frac{\mu^2}{q^2} \right)^2 - \left( \frac{\mu^2}{q^2} \right) \right] \frac{2\beta_0}{\epsilon} b_1(\epsilon) + \left( \frac{\mu^2}{q^2} \right)^2 4b_2(\epsilon), \quad (4.71)

with

\begin{align*}
b_1(\epsilon) &= \left( \frac{C_F}{2} [1 - 2\epsilon] - C_A \right) \frac{\epsilon \gamma \epsilon \Gamma \left( \frac{1}{2} - \epsilon \right)^2}{\pi^{3/2} \Gamma \left( 1 - 2\epsilon \right)} \Gamma \left( \frac{1}{2} + \epsilon \right), \quad (4.72) \\
b_2(\epsilon) &= \left[ \frac{65}{18} - \frac{8}{3} \ln 2 \right] C_A C_F - \left[ \frac{101}{36} + \frac{4}{3} \ln 2 \right] C_A^2 \\
&\quad + \left[ \frac{49}{36} C_A - \frac{2}{9} C_F \right] T_F n_f + \epsilon b_2^{(\epsilon)} + O(\epsilon^2). \quad (4.73)
\end{align*}

Once again we subtracted the $1/\epsilon$ IR pole that remains after charge renormalization by adding the relevant part of $\delta V_{c.t.}$ from [59]. Hence (4.71) is finite; however, the expansion in $\epsilon$ must be performed only after the computation of the potential insertion.

The one-loop expression $b_1(\epsilon)$ has been computed in $d$ dimensions [24], and the four-dimensional value $b_2(\epsilon = 0)$ of the two-loop coefficient is quoted from [40]. The $O(\epsilon)$ term of $b_2(\epsilon)$ has been parameterized above by $b_2^{(\epsilon)}$. While known, it has not yet been published [113]. In the numerical results in part II of the paper we use the estimate $b_2^{(\epsilon)} = -300$, which is significantly larger but more realistic than our previous estimate $b_2^{(\epsilon)} = 0 \pm 2b_2(0) = 0 \pm 34$ ($n_f = 5$) [48].

4.4.3 The $1/m^2$ potential

The coefficients of the $O(1/m^2)$ potentials are generated at tree level, where they are suppressed by $v^2$ relative to the leading Coulomb potential. Hence the one-loop coefficients are required for the NNNLO calculation of the cross section. The tree-level coefficients are:

\begin{align*}
\mathcal{V}_\delta^{(0)} &= 1, \quad \mathcal{V}_p^{(0)} = 1, \quad \mathcal{V}_{so}^{(0)} = 1, \quad \mathcal{V}_{k_f}^{(0)} = 1, \quad \mathcal{V}_s^{(0)} = 0. \quad (4.74)
\end{align*}

As can be seen from (4.57), spin-dependence arises first within the $O(1/m^2)$ potentials. The insertions of these potentials are again ultraviolet divergent. We therefore need the $O(\epsilon)$ term of the one-loop coefficients. These are available only from [59]. We computed the $d$-dimensional expressions and confirmed the previous result. The spin-projected expression has already been given in our previous work [48].

The complete one-loop coefficients consist of two different contributions. The first arises from the one-loop correction to the NRQCD couplings $d_i$, already discussed in the previous section. We call this the “hard” contribution. It can be extracted from the tree diagrams in figure 8 with one-loop corrected NRQCD vertices. The second contribution arises from explicitly integrating out soft loops. The corresponding one-loop NRQCD

\footnote{And, in general, the part of potential loops not reproduced by the PNRQCD interactions of lower}
Figure 8: NRQCD tree level diagrams of order $1/m^2$. Dashed (curly) lines denote the $A^0$ ($A^i$) gluon field. The number $i$ at the vertex refers to the NRQCD interaction with coefficient function $d_i$; see also figure 4 and (3.8), (3.11), (3.12). Symmetric diagrams are not shown.

diagrams are shown in figure 9. These contributions will be called “soft”. The total potential including tree and one-loop correction is then $V_X(\alpha_s) = V_X^{(\text{hard})}(\alpha_s) + V_X^{(\text{soft})}(\alpha_s)$.

The hard one-loop contributions can be easily calculated with the Feynman rules presented in figure 4, since all required $d$-dimensional NRQCD matching coefficients are already known at one-loop order from the previous section. The result reads:

$$V_\delta^{(\text{hard})}(\alpha_s) = \frac{1}{2}(1 + d_2 - 16d_5) + \frac{1}{2\pi C_F \alpha_s}(d_{ss} + C_F d_{os}) + O(\alpha_s^2)$$

$$= 1 + \frac{\alpha_s}{\pi} \left( \frac{\mu^2}{m^2} e^{\gamma_E} \right)^\epsilon \Gamma(\epsilon) \left[ C_A \frac{12\epsilon^3 - 44\epsilon^2 + 21\epsilon - 13}{-96\epsilon^2 + 24} + C_F \frac{12\epsilon^4 - 32\epsilon^3 - 63\epsilon^2 - 4\epsilon + 3}{6(2\epsilon - 1)(2\epsilon + 1)(2\epsilon + 3)} \right] + O(\alpha_s^2),$$

$$V_p^{(\text{hard})}(\alpha_s) = 1 + O(\alpha_s^2),$$

$$V_{so}^{(\text{hard})}(\alpha_s) = \frac{1}{3}(2d_1 + d_3) + O(\alpha_s^2)$$

$$= 1 + \frac{\alpha_s}{\pi} \left( \frac{\mu^2}{m^2} e^{\gamma_E} \right)^\epsilon \Gamma(\epsilon) \left[ C_A(2\epsilon^2 - 1) - 2C_F\epsilon(2\epsilon + 1) \right] + O(\alpha_s^2),$$

$$V_{hf}^{(\text{hard})}(\alpha_s) = d_1^2 + O(\alpha_s^2)$$

$$= 1 + \frac{\alpha_s}{\pi} \left( \frac{\mu^2}{m^2} e^{\gamma_E} \right)^\epsilon \Gamma(\epsilon) \left[ C_A(2\epsilon^2 - 1) - 2C_F\epsilon(2\epsilon + 1) \right] + O(\alpha_s^2),$$

order. This happens for the $1/m$ potential as discussed in section 4.3 below. However, there is no such contribution to the $1/m^2$ potentials at one loop. The reason for this is that in the case of the $1/m$ potential the relevant contribution arises from the box integral with all vertices of the leading-order $\psi^\dagger \psi A^0$ type, expanded to subleading order in the potential region. The next correction is always suppressed by two powers of $v$ (for instance, from replacing one of the vertices by a $O(v^2)$ vertex from the NRQCD Lagrangian), and hence can contribute only at order $1/m^3$. 

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In this notation the tree-level value of the potential coefficient is included and assigned to the hard contribution.

The soft contributions come from diagrams of order 1/$m^2$ shown in figure 9 from diagrams of order 1/$m^0$, where the denominator of a propagator has been expanded to higher orders as appropriate to the soft region, from soft self-energy insertions containing gluons and light quarks into the tree diagrams, and from charge renormalization counterterms. The final result is:

$$\mathcal{V}_s^{(soft)}(\alpha_s) = \frac{\alpha_s}{4\pi} \left( \frac{\mu^2}{q^2} \right)^\epsilon \frac{\epsilon \Gamma(-\epsilon)^2 \Gamma(\epsilon) e^{\gamma_E \epsilon}}{12(4\epsilon^2 - 8\epsilon + 3)\Gamma(-2\epsilon)} \left( C_A (48\epsilon^3 - 230\epsilon^2 + 328\epsilon - 138) 
- 3d_1^2(4\epsilon^2 - 9\epsilon + 5) - 4C_F(\epsilon - 1)(16\epsilon^2 - 38\epsilon + 21) \right)$$
Here the coefficients, but we obtain (4.80) to (4.84) with that with the second method we cannot get the result in terms of the hard matching has also been performed and we checked that the results are exactly the same. Note than in the NRQCD calculation (but more terms from the expansion). This calculation the soft region directly from the QCD diagrams. In this way, there are fewer diagrams of order $\alpha_s^2$ divergences. It is instructive to separate the two: contribution is infrared, while the soft contribution contains both infrared and ultraviolet counterterm (4.59), so the expressions given are still divergent. The $1/\epsilon$ coefficients. We first note that we did not yet add the relevant contribution from the $V^\alpha\beta\gamma\epsilon\epsilon_\alpha\beta\gamma\epsilon_\epsilon\alpha\beta\gamma\epsilon_\epsilon\alpha\beta\gamma\epsilon_\epsilon$ potential

\[ V_\beta(\alpha_s) = 1 + \frac{\alpha_s}{4\pi\epsilon} \left\{ \left( \frac{\mu^2}{m^2} \right)^\epsilon \left[ \frac{13}{6} C_A - \frac{2}{3} C_F \right] \right\}_{\text{IR}} + \left( \frac{\mu^2}{q^2} \right)^\epsilon \left[ \frac{13}{6} C_A + \frac{2}{3} C_F \right]_{\text{UV}} + \left[ \frac{8}{3} C_A - \frac{16}{3} C_F \right]_{\text{IR}} \right\} + O(\alpha_s^2), \]  

(4.85)  

Here the $d_i$ can be set to their tree-level value 1, since the entire expressions are already of order $\alpha_s$. An alternative method of calculating the soft contribution is to extract the soft region directly from the QCD diagrams. In this way, there are fewer diagrams than in the NRQCD calculation (but more terms from the expansion). This calculation has also been performed and we checked that the results are exactly the same. Note that with the second method we cannot get the result in terms of the hard matching coefficients, but we obtain (4.81) to (4.84) with $d_i = 1$.

Some remarks are in order on the pole structure of the hard and soft $1/m^2$ potential coefficients. We first note that we did not yet add the relevant contribution from the counterterm (4.59), so the expressions given are still divergent. The $1/\epsilon$ pole in the hard contribution is infrared, while the soft contribution contains both infrared and ultraviolet divergences. It is instructive to separate the two:
\[ V_p(\alpha_s) = 1 + \frac{\alpha_s}{4\pi\epsilon} \left( \frac{\mu^2}{q^2} \right)^\epsilon \left[ \frac{8}{3} C_A \right]_{\text{IR}} + O(\alpha_s^2), \]  

(4.86)

\[ V_{so}(\alpha_s) = 1 + \frac{\alpha_s}{4\pi\epsilon} \left\{ \left( \frac{\mu^2}{m^2} \right)^\epsilon \left[ \frac{4}{3} C_A \right]_{\text{IR}} + \left( \frac{\mu^2}{q^2} \right)^\epsilon \left[ \frac{4}{3} C_A \right]_{\text{UV}} \right\} + O(\alpha_s^2), \]  

(4.87)

\[ V_{hf}(\alpha_s) = 1 + \frac{\alpha_s}{4\pi\epsilon} \left\{ \left( \frac{\mu^2}{m^2} \right)^\epsilon \left[ \frac{2}{2} C_A \right]_{\text{IR}} + \left( \frac{\mu^2}{q^2} \right)^\epsilon \left[ -2 C_A \right]_{\text{UV}} \right\} + O(\alpha_s^2), \]  

(4.88)

\[ V_s(\alpha_s) = \frac{\alpha_s}{4\pi\epsilon} \left\{ \left( \frac{\mu^2}{m^2} \right)^\epsilon \left[ \tau \left( \sigma_i^a \sigma_i^b \right) \right]_{\text{IR}} \right. + \left( \frac{\mu^2}{q^2} \right)^\epsilon \left[ \tau \left( \sigma_i^a \sigma_i^b \right) \right]_{\text{UV}} \} + O(\alpha_s^2). \]  

(4.89)

A term \( \beta_0 \left( \frac{\mu^2}{q^2} \right)^\epsilon - 1 \) that was included in (4.80) to (4.84), which is related to the logarithms from charge renormalization, has been omitted from the expression in curly brackets for all potentials except the last one, which has no tree-level term. We see that the IR poles from the hard region cancel the UV poles from the soft region, as it should be, since these singularities arise from hard-soft factorization. The remaining IR singularities in the soft contribution appear only in the spin-independent potentials \( V_s, V_p \). They are precisely of the form of the remaining terms in the subtraction term (4.59) and therefore cancel with UV divergences in the ultrasoft calculation. Again, the structure of divergences is as required by consistency, since the ultrasoft contribution is spin-independent at NNNLO.

### 4.5 The spin-projected colour-singlet potential

Since the spin-dependent potentials appear first at NNLO, their double insertion is of higher order than NNNLO. Hence, when one computes the correlation function of the spin-triplet current (4.3), or the corresponding spin-singlet one, the spin-algebra can effectively be performed before the computation by working with spin-projected potentials. Given a potential with spin-dependence \( a \otimes b \), where \( a \) (or) refers to the spin-matrix on the quark (anti-quark) line, we replace

- **spin-triplet:** \( a \otimes b \rightarrow \frac{\text{tr} \left( \sigma^i a \sigma^j b \right)}{\text{tr} \left( \sigma^i \sigma^j \right)} \ 1 \otimes 1 = \frac{\text{tr} \left( \sigma^i a \sigma^j b \right)}{2(d - 1)} 1 \otimes 1 \)  

(4.90)

- **spin-singlet:** \( a \otimes b \rightarrow \frac{\text{tr} (ab)}{\text{tr} 1} \ 1 \otimes 1 = \frac{\text{tr} (ab)}{2} 1 \otimes 1 \)  

(4.91)

Note that the traces must be performed in \( d - 1 \) space dimensions. Only the spin-triplet projection is relevant to the third-order top production cross section in \( e^+ e^- \) collisions. For the three spin-dependent terms in the general potential (4.57), the projections result in

\[ [\sigma_i, \sigma_j] q_i p_j \otimes 1 \otimes 1 \rightarrow [\sigma_i, \sigma_j] q_i p_j \rightarrow 0, \]  

(4.92)

\[ [\sigma_i, \sigma_j] q_j \otimes [\sigma_i, \sigma_k] q_k \rightarrow \frac{10 - 7d + d^2}{1 - d} 4q^2, \]  

(4.93)
\[
[\sigma_i, \sigma_j] \otimes [\sigma_i, \sigma_j] \to (-4)(10 - 7d + d^2), \tag{4.94}
\]
where we have omitted the trivial \(1 \otimes 1\) dependence as done earlier.

After the projection the four potentials \(\mathcal{V}_\delta, \mathcal{V}_{so}, \mathcal{V}_{hf}, \mathcal{V}_s\) in (4.57) can be merged into a single expression \(\mathcal{V}_{1/m^2}\), and we arrive at the spin-triplet, colour-singlet potential already presented in [48]:

\[
\mathcal{V}(\mathbf{p}, \mathbf{p}') = -\frac{4\pi\alpha_s C_F}{q^2} \left[ \mathcal{V}_C - \mathcal{V}_{1/m} \frac{\pi^2 |q|}{m} + \mathcal{V}_{1/m^2} \frac{q^2}{m^2} + \mathcal{V}_p \frac{p^2 + p'^2}{2m^2} \right]. \tag{4.95}
\]

The Coulomb and \(1/m\) potentials are as given earlier. The two \(1/m^2\) terms read, up to the one-loop order:

\[
\mathcal{V}_p^{(0)} = 1, \tag{4.96}
\]
\[
\mathcal{V}_p^{(1)} = \left[ \left( \frac{\mu^2}{q^2} \right)^\epsilon - 1 \right] \frac{1}{\epsilon} \left( \frac{8}{3} C_A + \beta_0 \right) + \left( \frac{\mu^2}{q^2} \right)^\epsilon \mathcal{V}_p^{(1)}(\epsilon), \tag{4.97}
\]
\[
\mathcal{V}_{1/m^2}^{(0)} = \mathcal{V}_0(\epsilon) = -\frac{4 - \epsilon - 2\epsilon^2}{6 - 4\epsilon}, \tag{4.98}
\]
\[
\mathcal{V}_{1/m^2}^{(1)} = \left[ \left( \frac{\mu^2}{m^2} \right)^\epsilon - 1 \right] \frac{1}{\epsilon} \left( \frac{7}{3} C_F - \frac{11}{6} C_A + \beta_0 \mathcal{V}(\epsilon) \right) + \left[ \left( \frac{\mu^2}{m^2} \right)^\epsilon - 1 \right] \frac{1}{\epsilon} \left( \frac{C_F}{3} + \frac{C_A}{2} \right) + \left( \frac{\mu^2}{q^2} \right)^\epsilon \mathcal{V}_q^{(1)}(\epsilon) + \left( \frac{\mu^2}{m^2} \right)^\epsilon \mathcal{V}_m^{(1)}(\epsilon). \tag{4.99}
\]

The one-loop coefficients (expanded up to \(O(\epsilon)\)) are given by

\[
\mathcal{V}_p^{(1)}(\epsilon) = \frac{31}{9} C_A - \frac{20}{9} T_F n_f + \epsilon \left\{ \left( \frac{188}{27} - \frac{19\pi^2}{36} \right) C_A + \left( - \frac{112}{27} + \frac{\pi^2}{9} \right) T_F n_f \right\} + O(\epsilon^2), \tag{4.100}
\]
\[
\mathcal{V}_q^{(1)}(\epsilon) = -\frac{C_F}{3} - \frac{11}{27} C_A + \frac{40}{27} T_F n_f + \epsilon \left\{ \left( - \frac{419}{81} + \frac{77\pi^2}{216} \right) C_A + \left( \frac{274}{81} - \frac{2\pi^2}{27} \right) T_F n_f \right\} + O(\epsilon^2), \tag{4.101}
\]
\[
\mathcal{V}_m^{(1)}(\epsilon) = -\frac{C_F}{3} - \frac{29}{9} C_A + \frac{4}{15} T_F + \epsilon \left\{ \left( \frac{379}{54} + \frac{\pi^2}{24} \right) C_A + \left( - 10 + \frac{\pi^2}{36} \right) C_F \right\} + O(\epsilon^2), \tag{4.102}
\]

where now the \(1/m^2\) pieces of the subtraction term (4.59) have been added so that there are no \(1/\epsilon\) poles. The four-dimensional expressions \(v_i^{(1)}(\epsilon = 0)\) for \(i = \{q, m, p\}\) agree with those obtained from [41][52], and the \(O(\epsilon)\) term agrees with [52].
4.6 Matching of the NRQCD vector current

Having determined the matching coefficients of the PNRQCD Lagrangian we now return to the question whether the NRQCD spin-triplet current is renormalized when it is matched to PNRQCD. In general, we may write, in analogy with (3.1),

\[
\psi^\dagger \sigma^i \chi|_{\text{NRQCD}} = \tilde{c}_v \psi^\dagger \sigma^i \chi|_{\text{PNRQCD}} + \frac{\tilde{d}_{v1}}{6m^2} \psi^\dagger \sigma^i D^2 \chi|_{\text{PNRQCD}} + \ldots,
\]

(4.103)

\[
\psi^\dagger \sigma^i D^2 \chi|_{\text{NRQCD}} = \tilde{d}_{v2} \psi^\dagger \sigma^i D^2 \chi|_{\text{PNRQCD}} + \ldots.
\]

(4.104)

Non-trivial (\(\tilde{c}_v, \tilde{d}_{v2} \neq 1, \tilde{d}_{v1} \neq 0\)) PNRQCD matching coefficients of the currents can arise from three sources: (1) Soft loops not accounted in the matching of the Lagrangian. This implies that the soft loop momentum must flow through the external current vertex. (2) Off-shell effects. Since the PNRQCD Lagrangian is matched on-shell, off-shell effects that are not reproduced by the Lagrangian interactions must be absorbed into a renormalization of the external currents. (3) \(O(\epsilon)\) terms of soft loops contributing to the matching of the Lagrangian that multiply \(1/\epsilon\) poles of PNRQCD loops are local and must be absorbed into a renormalization of the external currents, when the PNRQCD matching coefficients (the potentials) are defined in four dimensions. As discussed before, we choose to work with \(d\)-dimensional potentials, hence these contributions are included in the PNRQCD calculation without a modification of the external current. We shall now prove that there is also no further renormalization of the currents from (1) and (2), that is, \(\tilde{c}_v = 1\) to three loops, and \(\tilde{d}_{v1} = 0, \tilde{d}_{v2} = 1\) at one loop.\(^{17}\)

We first consider the issue (1) of soft renormalization of the NRQCD currents. The relevant vertex diagram at the one-loop order is shown in figure\(^{10}\) with external momenta \(q = (2m + E, 0), p_1 = \frac{q}{2} + p = (m + E/2, p)\) and \(p_2 = \frac{q}{2} - p = (m + E/2, -p)\), and \(p_1^2 = p_2^2 = m^2\). The NRQCD expression is

\[
A_{\text{NRQCD}} = (ig_s)^2 C_F \mu^{-2\epsilon} \int \frac{d^d k}{(2\pi)^d} \frac{i}{k^2 + k^0 - \frac{(p+k)^2}{2m}} \times \text{poly}(p, k),
\]

(4.105)

\(^{17}\)The arguments presented make it clear that this should remain true to any order in perturbation theory.
where the $+i\epsilon$ prescription for the propagators is left implicit. The unspecified polynomial factor arises from derivatives in the subleading NRQCD interactions or from the subleading external current.

Power-counting for soft loop momentum $k^0 \sim k \sim mv$ shows that this integral gives rise to a $O(\alpha_s)$ correction to $\tilde{c}_v, \tilde{d}_{v1}, \tilde{d}_{v2}$. However, in the soft region we pick the pole at $k^0 = -|k| + i\epsilon$ of the gluon propagator and expand the two quark propagators in $E^2 + (p + k)^2 / (2m)$. The resulting integral $\int d^{d-1}k / |k|^3 \times \text{poly}(p, k)$ is scaleless and vanishes in dimensional regularization. This holds to any order in the expansion in the soft region [14], hence there is no soft one-loop correction to the matching of the PNRQCD currents.

Moving to the two-loop level, we consider as an example the planar vertex diagram in figure 11. The momentum regions of interest are s-s and s-p, where the first letter refers to the inner vertex subgraph and loop momentum $l$, the second to the box subgraph and loop momentum $k$. The p-s combination is not relevant, since the soft loop does not flow through the external vertex. Such contributions are included in the one-loop potentials. The inner vertex subdiagram in the s-s and s-p regions is an expression similar to (4.105) with $k \rightarrow k + l$ in the quark propagator and $k^2 \rightarrow l^2$ in the gluon propagator. Picking up the gluon propagator pole results in

$$\int \frac{d^{d-1}l}{(2\pi)^{d-1}|l|} \frac{1}{(k^0 - |l|)^2}$$

for the inner integral. Now, in the s-p region $k$ is potential, and $k^0 \sim mv^2 \ll |l|$ must be expanded, in which case the integral is scaleless as before. If, as in the s-s region, $k$ is also soft, then the $k^0$-integration picks up the pole of the second gluon propagator at $k^0 = -|k| + i\epsilon$ and the entire 2-loop integral is scaleless. This discussion evidently applies to all 2-loop vertex diagrams. Since the vanishing of the integrals is due to the analytic structure of the propagator denominators, it generalizes to higher orders in the velocity expansion, which contains higher powers of the same propagators and numerator polynomials. Hence, we conclude that there are no s-p and s-s contributions to two-loop vertex diagrams in any order in the threshold expansion, in accordance with the results of [14], and hence no soft renormalization of the currents at two loops.

The structure of the analysis extends to higher loop orders. Either one of the inner sub-graphs is scaleless, because an outer loop momentum is potential. Or the entire
diagram is soft and scaleless, because the external quark momenta are potential. We therefore conclude that there is no contribution to the matching of the NRQCD currents to PNRQCD from soft loops (item (1)).

We now turn to the discussion of off-shell effects, item (2), and start again with the one-loop diagram shown in figure 10. Now, however, the loop momentum is potential, and we have to compare the NRQCD potential contribution contained in (4.105) with the PNRQCD expression

\[ A_{\text{PNRQCD}} = (ig_s)^2 C_F \tilde{\mu}^{2\epsilon} \int \frac{d^{d-1}k}{(2\pi)^{d-1}} \frac{1}{k^2} \frac{1}{E - \frac{(p+k)^2}{m}} \times \text{poly}'(p, k), \]  

(4.107)

which arises from the single insertion of the tree-level PNRQCD potential and the \( O(\alpha_s) \) term of the Coulomb Green function. The factor \( 1/k^2 \) corresponds to the Coulomb potential insertion, while higher-order potentials as well as derivative factors from the external current are contained in the unspecified polynomial. The potential contribution in NRQCD is defined as the contribution from the quark-propagator pole at \( k^0 = E/2 - (p+k)^2/(2m) + i\epsilon \) in (4.105).

The difference \( \Delta A \) between \( A_{\text{NRQCD}} \) and \( A_{\text{PNRQCD}} \) contributes to the matching of the external current and arises as follows: when the tree-level PNRQCD potential is derived from the one-gluon exchange diagram, the external quark lines are assumed on-shell, which implies \( p^2 = (p+k)^2 \) and \( E_{p+k} - E_p = k^0 = 0 \) with the momentum assignment as in figure 10. However, no such restrictions are imposed on the loop momentum \( k \) in the calculation of the NRQCD diagram, figure 10. Thus the difference between \( A_{\text{NRQCD}} \) and \( A_{\text{PNRQCD}} \) comes from the expansion of the gluon propagator in the potential region

\[ \frac{1}{k^2} - \frac{1}{-k^2} = -\frac{[k^0]^2}{k^2} + O(v^2), \]

(4.108)

and the difference of polynomial factors, which after a short computation can be determined to be

\[ \text{poly}(p, k) - \text{poly}'(p, k) = \frac{p^2}{2m^2} - \frac{(p+k)^2}{2m^2} + O(v^4). \]

(4.109)

Note that the leading contribution to \( A_{\text{NRQCD}} \) and \( A_{\text{PNRQCD}} \) is of order \( \alpha_s/v \). The terms neglected in (4.108) and (4.109) are therefore of order \( \alpha_s v^3 \). These are fourth-order corrections to the cross section beyond the accuracy we aim at. In total, we arrive at

\[ \Delta A = (ig_s)^2 C_F \tilde{\mu}^{2\epsilon} \int \frac{d^{d-1}k}{(2\pi)^{d-1}} \frac{1}{k^2} \frac{1}{E - \frac{(p+k)^2}{m}} \times \left\{ \frac{p^2}{2m^2} - \frac{(p+k)^2}{2m^2} - \frac{[k^0]^2}{k^2} \right\} \bigg| \begin{array}{c} k^0 = \frac{E}{2} - \frac{(p+k)^2}{2m} \\ k^0 = \frac{E}{2} \end{array} \]

\[ = (ig_s)^2 C_F \tilde{\mu}^{2\epsilon} \int \frac{d^{d-1}k}{(2\pi)^{d-1}} \frac{1}{k^2} \frac{1}{2k^0} \times \left\{ \frac{k^0}{m} - \frac{[k^0]^2}{k^2} \right\} \bigg| \begin{array}{c} k^0 = \frac{E}{2} - \frac{(p+k)^2}{2m} \\ k^0 = \frac{E}{2} \end{array} \].

(4.110)

To arrive at the second line we used that the on-shell condition implies \( E = E_p + E_{-p} = p^2/m \). The two terms in curly brackets each cancel the heavy-quark propagator denominator \( 1/(2k^0) \), after which the integral is scaleless and vanishes. This must be so,
Figure 12: One-loop box diagram, whose potential region is not completely reproduced by PNRQCD with potentials matched at tree-level.

Since a non-zero contribution to $\Delta A$ at this order would have scaled as $\alpha_s v$, but there is no $O(v)$ production current.

That off-shell effects from the potential region are relevant in general can be seen from the calculation of the $1/m$-potential at $O(\alpha_s^2)$. The potential region of the one-loop box diagram shown in figure 12 is not completely reproduced by PNRQCD. The difference is a contribution to the $1/m$ potential, that is, a PNRQCD matching coefficient, which is crucial to obtain the gauge-invariant result given in [24] and (4.72). The difference between the box and the vertex diagram discussed above is that the box loop integral is not scaleless after the cancellation of the quark propagator by the off-shell terms, since there is a second gluon propagator $1/(k + p - p')^2$.

Returning to the vertex diagrams, we now consider the planar two-loop diagram of figure 11 in the $p-p$ and $p-s$ region, where the first letter refers again to the inner vertex subgraph. The corresponding PNRQCD diagrams are the two-loop vertex diagram with tree-level potentials and a one-loop vertex diagram with insertion of a one-loop potential, respectively. The off-shell terms of the NRQCD diagram in the $p-p$ region are precisely the ones that contribute to the $1/m$ potential discussed in the previous paragraph; they are correctly reproduced by the PNRQCD diagram with the insertion of the $1/m$ potential. The off-shell terms in the $p-s$ region have a similar origin as in the one-loop vertex diagram. The soft box graph gives rise to a one-loop potential, but since the potentials are matched on-shell, the soft box graph is not completely reproduced when it appears as a subgraph in a larger diagram. Since the leading $p-s$ region is $O(\alpha_s^2/v)$, if all the off-shell corrections were of order $v^2$ relative to the leading term as in (4.108), (4.109), we could immediately dismiss them, since there is no $O(\alpha_s^2 v)$ hard vertex correction into which it could be absorbed. This is indeed true for the planar diagram but not in general.

As an example, we consider the non-planar NRQCD two-loop diagram shown in figure 13 which (neglecting constant factors) is given by the expression

$$
\int \frac{d^d k}{(2\pi)^d} \frac{d^d l}{(2\pi)^d} \frac{i}{E^2 + k^0 - (p+k)^2/2m} \frac{-i}{E^2 + k^0 - (p+k)^2/2m} \times \frac{i}{E^2 + l^0 - (p+l)^2/2m} \frac{-i}{E^2 + l^0 - (p+l)^2/2m} \times \frac{1}{l^2 - (l-k)^2}.
$$

In the $p-s$ region$^{18}$ the $l$-integral for the soft crossed-box subdiagram is exactly the same

$^{18}$The $p-p$ region is zero for the non-planar diagram.
that appears in the computation of the one-loop Coulomb and $1/m$ potentials except for the additional $k^0$ in the last quark propagator that is absent when the quark lines of the inner vertex subgraph are on-shell (see discussion above). Since $k$ is potential, $k^0 \sim mv^2$ must be expanded relative to $l^0 \sim mv$, which results in a series of corrections beginning at $O(v)$. If this off-shell correction were non-zero, it would result in a NNLO $O(\alpha_s^2)$ contribution to the coefficient function $\tilde{c}_v$. However, as $k$ is potential, the $k^0$-integral is the contribution from the pole of the quark propagator in the first line of (4.111). Thus, in complete analogy with the discussion of the one-loop vertex diagram, the expansion in $k^0$ cancels the remaining quark propagator and renders the $k$-integral scaleless. This cancellation is generic for all two-loop vertex diagrams in the p-s region.

The structure of the argument extends to the 3-loop order. The possible off-shell terms are either already accounted in the matching of subleading potentials; or an inner vertex subgraph becomes scaleless due to a cancellation of the remaining quark-propagator of a potential loop. Hence, we conclude that there is no contribution to the matching of the NRQCD currents to PNRQCD from off-shell terms (item (2)), at least up to the NNNLO order.

### 4.7 Equation of motion identities for current and potential insertions

The integrals for PNRQCD diagrams with insertions of potentials or external currents such as (4.10) can sometimes be simplified by the equation of motion for the PNRQCD quark-antiquark propagator. We will make use of this to reduce the number of independent insertions that need to be calculated (in part II of the paper), and provide the relevant identities here.

In the present context the equation of motion is the Lippmann-Schwinger equation (4.5) for the colour-singlet Coulomb Green function written in the form

$$\frac{p_1^2}{m} G_0(p_1, p_2; E) = E G_0(p_1, p_2; E) + (2\pi)^{d-1} \delta^{(d-1)}(p_1 - p_2)$$

$$+ 4\pi \alpha_s C_F \bar{\mu}^{2\epsilon} \int \frac{d^{d-1}k}{(2\pi)^{d-1}} \frac{1}{(k - p_2)^2} G_0(p_1, k; E). \quad (4.112)$$
In the remainder of this subsection we drop the energy argument of the Green function, which is always $E$, and set $\mu = 1$ to simplify the notation.

As our first example we consider the insertion of the subleading derivative current (3.44) into one of the vertices. The relevant integral is

$$\int \prod_{i=1}^{2} \frac{d^{d-1}p_i}{(2\pi)^{d-1}} G_0(p_1, p_2) \frac{p_2^2}{m^2} = \frac{E}{m} \int \prod_{i=1}^{2} \frac{d^{d-1}p_i}{(2\pi)^{d-1}} G_0(p_1, p_2) + \frac{1}{m} \int \frac{d^{d-1}p_1}{(2\pi)^{d-1}}$$

+ \frac{4\pi \alpha_s C_F}{m} \int \prod_{i=1}^{2} \frac{d^{d-1}p_i}{(2\pi)^{d-1}} \frac{d^{d-1}k}{(2\pi)^{d-1}} \frac{1}{(k - p_2)^2} G_0(p_1, k). \quad (4.113)

The second term on the right-hand side is a scaleless integral. The third one is seen to contain $\int d^{d-1}p_2/p_2^2 = 0$ after shifting $p_2 \rightarrow p_2 + k$. Hence, the insertion of $p_2^2/m^2$ can be replaced by the factor $E/m$. This holds true in expressions of the form

$$\int \left[ \prod_{i} \frac{d^{d-1}p_i}{(2\pi)^{d-1}} \right] \frac{p_1^2}{m^2} G_0(p_1, p_2) iG_0(p_1, p_2) iG_0(p_1, p_2) iG_0(p_1, p_2) \ldots$$

that contain multiple potential insertions. This shows that the unrenormalized, dimensionally regulated matrix element of the subleading external current operator $\psi^\dagger \sigma_i D^2 \chi$ is $-mE$ times the unrenormalized matrix element of the leading-order current $\psi^\dagger \sigma_i \chi$, which has been used in (12).

As our second example we consider the insertion of the $p^2/(m^2 q^2)$ potential. With $q = p_3 - p_2$ we find

$$\int \prod_{i=1}^{4} \frac{d^{d-1}p_i}{(2\pi)^{d-1}} G_0(p_1, p_2) \frac{p_2^2}{m^2 q^2} G_0(p_3, p_4)$$

$$= \frac{E}{m} \int \prod_{i=1}^{4} \frac{d^{d-1}p_i}{(2\pi)^{d-1}} G_0(p_1, p_2) \frac{1}{q^2} G_0(p_3, p_4) + \frac{1}{m} \int \prod_{i=1,3,4} \frac{d^{d-1}p_i}{(2\pi)^{d-1}} \frac{G_0(p_1, p_4)}{(p_1 - p_3)^2}$$

+ \frac{4\pi \alpha_s C_F}{m} \int \prod_{i=1}^{4} \frac{d^{d-1}p_i}{(2\pi)^{d-1}} \frac{d^{d-1}k}{(2\pi)^{d-1}} \frac{1}{G_0(p_1, k)} \frac{1}{(k - p_2)^2} \frac{1}{(p_2 - p_3)^2} G_0(p_3, p_4)

$$= \int \prod_{i=1}^{4} \frac{d^{d-1}p_i}{(2\pi)^{d-1}} G_0(p_1, p_2) \left[ \frac{E}{m} \frac{1}{q^2} + \frac{\pi \alpha_s C_F}{2m} \frac{k(0)}{[q^2]^{\frac{d}{2}+\epsilon}} \right] G_0(p_3, p_4). \quad (4.115)

The final expression follows, since the second term on the left-hand side of the first equation contains the scaleless $p_1$-integral, while in the third term the integration over $p_2$ can be performed with the help of the integral

$$\bar{\mu}^{2\epsilon} \int \frac{d^{d-1}k}{(2\pi)^{d-1}} \frac{1}{[k^2]^{1+\epsilon}} \frac{1}{(q - k)^2} \equiv \frac{1}{[q^2]^{\frac{d}{2}+\epsilon}} \frac{k(u)}{8} \quad (4.116)$$
with
\[ k(u) = \mu^2 e \frac{e^{\rho e \epsilon}}{\Gamma(1 + u + \epsilon) \Gamma(1 - u - \epsilon)} \frac{\Gamma(1 + u) \Gamma(1 - u - 2\epsilon)}{\Gamma(1 + u - 2\epsilon)}, \]

(4.117)

whose general form for \( u \neq 0 \) will be needed below. This shows that the insertion of the \( p^2/(m^2 q^2) \) potential can be eliminated in favour of the insertion of the Coulomb and the \( d \)-dimensional \( 1/(m|q|) \) potential.

In the general case, after applying the spin projection, only six different types of insertions are needed for the NNNLO calculation:
\[ \frac{1}{q^2} \left( \frac{\mu^2}{q^2} \right)^{a \epsilon} G_0(p_1, p_2)(2\pi)^{d-1} \delta^{(d-1)}(q) \]
\[ \frac{1}{q^2} \left( \frac{\mu^2}{q^2} \right)^{a \epsilon} \frac{p^2}{2q^2} \left( \frac{\mu^2}{q^2} \right)^{a \epsilon} \delta^{(d-1)}(q), \]
\[ \frac{1}{q^2} \left( \frac{\mu^2}{q^2} \right)^{a \epsilon} \delta^{(d-1)}(q), \]
\[ \frac{1}{q^2} \left( \frac{\mu^2}{q^2} \right)^{a \epsilon} \delta^{(d-1)}(q). \]

(4.118)

The first four come from the potentials in (4.95), the fifth is the kinetic energy correction and the last might be used for the conversion of the pole scheme to threshold mass scheme as discussed in paper II. The identities given below show that the last three types of insertions can be reduced by using the equation of motion to the first three and the delta-function potential \( \delta^{(d-1)}(q) \) without factors of \( p^2 \). At third order, both, single insertions and double insertions with an additional Coulomb potential insertion have to be considered. For the single insertions, the equation of motion relations read:

\[ \delta^{(d-1)}(q) \frac{P_2^2}{m^2} : \int \prod_{i=1}^{4} \frac{d^{d-1}p_i}{(2\pi)^{d-1}} G_0(p_1, p_2)(2\pi)^{d-1} \delta^{(d-1)}(q) \]
\[ \frac{P_2^2}{m} G_0(p_3, p_4) \]
\[ = E \int \prod_{i=1}^{3} \frac{d^{d-1}p_i}{(2\pi)^{d-1}} G_0(p_1, p_2) G_0(p_2, p_3) + \int \prod_{i=1}^{2} \frac{d^{d-1}p_i}{(2\pi)^{d-1}} G_0(p_1, p_2) \]
\[ + 4\pi C_F \alpha_s \int \prod_{i=1}^{4} \frac{d^{d-1}p_i}{(2\pi)^{d-1}} G_0(p_1, p_2) \frac{1}{q^2} G_0(p_3, p_4), \]
\[ (4.119) \]

\[ \delta^{(d-1)}(q) \frac{P_4^2}{m^3} : \int \prod_{i=1}^{4} \frac{d^{d-1}p_i}{(2\pi)^{d-1}} G_0(p_1, p_2)(2\pi)^{d-1} \delta^{(d-1)}(q) \frac{P_4^2}{m^3} G_0(p_3, p_4) \]
\[ = \frac{E^2}{m} \int \prod_{i=1}^{3} \frac{d^{d-1}p_i}{(2\pi)^{d-1}} G_0(p_1, p_2) G_0(p_2, p_3) + \frac{2E}{m} \int \prod_{i=1}^{2} \frac{d^{d-1}p_i}{(2\pi)^{d-1}} G_0(p_1, p_2) \]
\[ + \frac{8\pi C_F \alpha_s E}{m} \int \prod_{i=1}^{4} \frac{d^{d-1}p_i}{(2\pi)^{d-1}} G_0(p_1, p_2) \frac{1}{q^2} G_0(p_3, p_4) \]
\[ + \frac{(4\pi C_F \alpha_s)^2}{m} \int \prod_{i=1}^{4} \frac{d^{d-1}p_i}{(2\pi)^{d-1}} G_0(p_1, p_2) \frac{1}{[q^2]^{2+\epsilon}} \frac{k(0)}{8} G_0(p_3, p_4), \]
\[ (4.120) \]

\[^{19}\text{As a matter of fact, the implementation will be done in a different way, and the result is given here only for completeness.}\]
\[
\frac{p_2^2 + p_3^2}{2m^2q^2} = \int \prod_{i=1}^{4} \frac{d^{d-1}p_i}{(2\pi)^{d-1}} G_0(p_1, p_2) \frac{p_2^2 + p_3^2}{2m^2q^2} G_0(p_3, p_4)
= \int \prod_{i=1}^{4} \frac{d^{d-1}p_i}{(2\pi)^{d-1}} G_0(p_1, p_2) \left[ \frac{E}{mq^2} + \frac{\pi C_F \alpha_s}{2m} \frac{k(0)}{[q^2]^{\frac{1}{2}+\epsilon}} \right] G_0(p_3, p_4).
\]

The delta-function potential \(\delta^{(d-1)}(q)\) appears implicitly in the first two relations in integrands of the form \(G_0(p_1, p_2)G_0(p_2, p_3)\), where the delta-function has been eliminated to set two arguments equal. The equation of motion identities for the double insertions with a Coulomb potential (with \(q_1 = p_3 - p_2\) and \(q_2 = p_5 - p_4\)) read:

\[
\delta^{(d-1)}(q_1) \frac{p_2^2}{m} = \int \prod_{i=1}^{6} \frac{d^{d-1}p_i}{(2\pi)^{d-1}} G_0(p_1, p_2) (2\pi)^{-d-1} \delta^{(d-1)}(q_1) \frac{p_2^2 G_0(p_3, p_4) G_0(p_5, p_6)}{[q_2^2]^{1+u}}
= E \int \prod_{i=1,3-6} \frac{d^{d-1}p_i}{(2\pi)^{d-1}} G_0(p_1, p_3) \frac{G_0(p_3, p_4) G_0(p_5, p_6)}{[q_2^2]^{1+u}}
+ \int \prod_{i=1}^{4} \frac{d^{d-1}p_i}{(2\pi)^{d-1}} G_0(p_1, p_2) G_0(p_3, p_4)
+ 4\pi C_F \alpha_s \int \prod_{i=1}^{6} \frac{d^{d-1}p_i}{(2\pi)^{d-1}} G_0(p_1, p_2) \frac{1}{q_1^2} G_0(p_3, p_4) G_0(p_5, p_6),
\]

\[
\delta^{(d-1)}(q_1) \frac{p_4^2}{m^3} = \int \prod_{i=1}^{6} \frac{d^{d-1}p_i}{(2\pi)^{d-1}} G_0(p_1, p_2) (2\pi)^{-d-1} \delta^{(d-1)}(q_1) \frac{p_4^2 G_0(p_3, p_4) G_0(p_5, p_6)}{[q_2^2]^{1+u}}
= \frac{E^2}{m} \int \prod_{i=1,3-6} \frac{d^{d-1}p_i}{(2\pi)^{d-1}} G_0(p_1, p_3) \frac{G_0(p_3, p_4) G_0(p_5, p_6)}{[q_2^2]^{1+u}}
+ \int \prod_{i=1}^{4} \frac{d^{d-1}p_i}{(2\pi)^{d-1}} G_0(p_1, p_2) \left[ \frac{2E}{m} \frac{1}{[q_1^2]^{1+u}} + \frac{\pi C_F \alpha_s}{2m} \frac{k(u)}{[q_1^2]^{\frac{1}{2}+\epsilon}} \right] G_0(p_3, p_4)
+ 4\pi C_F \alpha_s \int \prod_{i=1}^{6} \frac{d^{d-1}p_i}{(2\pi)^{d-1}} G_0(p_1, p_2) \left[ \frac{2E}{m} \frac{1}{q_1^2} + \frac{\pi C_F \alpha_s}{2m} \frac{k(0)}{[q_1^2]^{\frac{1}{2}+\epsilon}} \right] G_0(p_3, p_4) \times \frac{G_0(p_3, p_4) G_0(p_5, p_6)}{[q_2^2]^{1+u}},
\]

\[
\frac{p_2^2 + p_3^2}{2m^2q_1^2} = \int \prod_{i=1}^{6} \frac{d^{d-1}p_i}{(2\pi)^{d-1}} G_0(p_1, p_2) \frac{p_2^2 + p_3^2}{2m^2q_1^2} G_0(p_3, p_4) G_0(p_5, p_6)
= \int \prod_{i=1}^{6} \frac{d^{d-1}p_i}{(2\pi)^{d-1}} G_0(p_1, p_2) \left[ \frac{E}{mq_1^2} + \frac{\pi C_F \alpha_s}{2m} \frac{k(0)}{[q_1^2]^{\frac{1}{2}+\epsilon}} \right] G_0(p_3, p_4) G_0(p_5, p_6).
\]
We note that we have kept the insertion of the Coulomb potential in the more general form $1/|q_2^{2}|^{1+u}$, since in the double insertions we may also need the $d$-dimensional Coulomb potential, implying $u = \epsilon$.

### 4.8 Ultrasoft interaction

At third order there is for the first time a contribution from an ultrasoft loop momentum region. The ultrasoft correction to the heavy-quark correlation function has been computed separately in [52] and will be incorporated in the results shown in paper II. Here we provide a short overview of the ultrasoft calculation and discuss some issues of the factorization, which are important to understand the splitting of various divergent parts.

The relevant ultrasoft interaction terms in the PNRQCD Lagrangian (4.1) are given by

$$g\,\bar{\psi}(x)[A_0(t, 0) - x \cdot E(t, 0)]\,\psi(x) + g\,\bar{\chi}(x)[A_0(t, 0) - x \cdot E(t, 0)]\,\chi(x).$$

(4.125)

The derivation of the chromoelectric dipole interaction from the multipole expansion of the NRQCD Lagrangian can be found in [95]. The interaction with $A_0(t, 0)$ can be removed by a field redefinition involving a time-like Wilson line. This modifies the external current that creates the heavy-quark pair, as discussed in [97]. In the present case of colour-singlet production in $e^+e^-$ collisions the Wilson lines cancel, and the $A_0(t, 0)$ terms in (4.125) can be dropped. With $x \sim 1/v$, and $g_s E \sim v^{9/2}$ for ultrasoft gluon fields, it follows that the chromoelectric dipole interaction is suppressed by $v^{3/2}$ relative to the kinetic term in the action. Two ultrasoft interaction vertices are required to form a loop, from which it follows that the leading ultrasoft contribution arises first at the third order.

The ultrasoft correction can be expressed in the form

$$\delta^{\text{us}} G(E) = ig_s^2 C_F \int d^3 r \, d^3 r' \int \frac{d^4 k}{(2\pi)^4} \left[ \frac{k_0^2 \cdot r - (r \cdot k)(r' \cdot k)}{k^2 + i\epsilon} \right] \times G_0^{(1)}(0, r; E) G_0^{(8)}(r, r'; E - k_0) G_0^{(1)}(r', 0; E),$$

(4.126)

with the understanding that one picks up only the pole at $k_0 = |k| - i\epsilon$ in the gluon propagator. Here $G_0^{(1)}$ is the colour-singlet and $G_0^{(8)}$ the colour-octet Coulomb Green function (4.15). However, as explained in [49], this expression cannot be used in practice, because it is ultraviolet (UV) divergent. The regularization and subtraction of divergences must be done consistently with the calculation of potential insertions and hard
matching coefficients, which have been done in dimensional regularization. In order to 
apply dimensional regularization to the ultrasoft contribution, (4.126) is transformed 
to momentum space. It also turns out to be convenient to revert the derivation of the 
PNRQCD ultrasoft interaction (4.125) and to instead use the NRQCD vertices. The 
reason for this is that the derivation of (4.125) uses the PNRQCD equation of motion, 
which reshuffles the loop expansion, and employs four-dimensional identities [95]. The 
correspondence between UV divergences in the ultrasoft calculation and IR divergences 
in the potential and hard matching calculations is more directly seen at the level of 
NRQCD diagrams, and the correct evaluation of the finite terms requires the consistent 
use of dimensional regularization in every loop order.

The UV divergences arise from the integral over the three-momentum $k$ of the 
ultrasoft gluon, and from the subsequent potential loop integrations. The former divergence 
is related to the factorization of the ultrasoft scale from the other scales, and cancels 
when all pieces of the calculation are added. The UV-divergent part of the ultrasoft 
integral has the form of a single insertion of a third-order potential and of a one-loop 
correction to the coefficient $d_v$ of the derivative current in (3.45). We therefore define the 
ultrasoft correction by adding counterterms that cancel these ultrasoft subdivergences. 
With these subtractions, the ultrasoft correction reads [49]

$$
\delta_{us} G(E) = \left[\tilde{\mu}^{2n}\right]^2 \int \frac{d^{d-1} \ell}{(2\pi)^{d-1}} \frac{d^{d-1} \ell'}{(2\pi)^{d-1}} \left\{ \delta \delta_{d_v}^{\text{div}} (-1) \frac{\ell^2 + \ell'^2}{6m^2} G_0^{(1)}(\ell, \ell'; E) + \left[\tilde{\mu}^{2n}\right]^2 \int \frac{d^{d-1} p}{(2\pi)^{d-1}} \frac{d^{d-1} p'}{(2\pi)^{d-1}} G_0^{(1)}(\ell, p; E) i \left[\delta U - \delta V_{c.t.}\right] i G_0^{(1)}(p', \ell'; E) \right\}. 
$$

(4.127)

Here $\delta V_{c.t.}$ represents the potential subtraction (4.59), and $\delta U$ is the ultrasoft insertion (containing the octet Green function) [20]. The first line of (4.127) is related to the 
renormalization of the $1/m^2$ suppressed vector current $j_{1/m^2} = \psi^{\dagger} \sigma^i D^2 \chi$. If $[j_{1/m^2}]_{\text{ren}} = Z_{1/m^2}[j_{1/m^2}]_{\text{bare}}$, the one-loop counterterm $Z_{1/m^2} - 1$ equals the infrared divergence $\delta d_v^{\text{div}}$ 
that was subtracted to obtain the finite expression (3.45). The explicit expression is

$$
\delta d_v^{\text{div}} = Z_{1/m^2} - 1 = -\frac{\alpha_s}{4\pi} \frac{16C_F}{\epsilon}. 
$$

(4.128)

The remaining divergences are associated with the three-loop hard matching coefficient

$\delta U$ with an opposite sign compared to [49].
The subtracted expression is then simplified and reduced to a number of integrations that can mostly be done only numerically. The code that computes the ultrasoft correction was developed in conjunction with \cite{52}, and is implemented in our program for the third-order cross section.

5 Master formula for the third-order cross section

We have now collected all prerequisites to write down the expansion of the non-relativistic correlation function

$$G(E) = \frac{\hat{G}_0(E)}{2N_c(d-1)} \int d^d x \ e^{iEx_0} \langle 0 | T(\chi^\dagger \sigma^j \psi)(x) [\psi^\dagger \sigma^j \chi](0) ) | 0 \rangle|_{\text{PNRQCD}}$$

(see (3.3)) to third order in non-relativistic (PNRQCD) perturbation theory. Adopting the operator notation from section 4.2.2, the expansion is given by

$$G(E) = G_0(E) + \delta_1 G(E) + \delta_2 G(E) + \delta_3 G(E) + \ldots$$

(5.2)

with $G_0(E) = \langle 0 | \hat{G}_0(E) | 0 \rangle = G_0(0, 0; E)$ as given in (4.53), and

$$\delta_1 G(E) = \langle 0 | \hat{G}_0(E) i \delta V_1 \hat{G}_0(E) | 0 \rangle,$$

(5.3)

$$\delta_2 G(E) = \langle 0 | \hat{G}_0(E) i \delta V_1 \hat{G}_0(E) i \delta V_1 \hat{G}_0(E) | 0 \rangle + \langle 0 | \hat{G}_0(E) i \delta V_2 \hat{G}_0(E) | 0 \rangle,$$

(5.4)

$$\delta_3 G(E) = \langle 0 | \hat{G}_0(E) i \delta V_1 \hat{G}_0(E) i \delta V_1 \hat{G}_0(E) i \delta V_1 \hat{G}_0(E) | 0 \rangle$$

$$+ 2 \langle 0 | \hat{G}_0(E) i \delta V_2 \hat{G}_0(E) i \delta V_2 \hat{G}_0(E) | 0 \rangle + \langle 0 | \hat{G}_0(E) i \delta V_3 \hat{G}_0(E) | 0 \rangle$$

$$+ \delta_{us} G(E).$$

(5.5)

In momentum space these expressions are of the form of single and multiple insertions of potentials as defined in (4.10) plus the ultrasoft correction. $\delta V_n$ denotes a potential correction of order $n$. The first-order potential consists only of the one-loop correction to the Coulomb potential:

$$\delta V_1 = -\frac{4\pi\alpha_s C_F}{q^2} \hat{V}_C^{(1)}.$$ 

(5.6)

At second order, we have the two-loop Coulomb potential, the one-loop $1/(m|q|)$ potential and the $v^2$-suppressed potentials at tree-level. Together with the kinetic-energy correction, we obtain

$$\delta V_2 = \left[ \hat{V}_C^{(2)} - \hat{V}_1^{(1)} \frac{\pi^2}{m} \frac{|q|}{m^2} \frac{q^2}{m^2} + \hat{V}_p^{(0)} \frac{p^2 + p'^2}{2m^2} \right]$$

$$- 2 \left( \frac{P^4}{8m^3} \right) (2\pi)^{d-1} \delta^{(d-1)}(q).$$

(5.7)
The notation for the potentials is defined in (4.95), where also the explicit expressions are given. Note that different from (4.58) the $n$-loop potential $\hat{V}_X^{(n)}$ includes the coupling constant factor, i.e. $\hat{V}_X^{(n)} = \left(\frac{\alpha_s}{4\pi}\right)^n V_X^{(n)}$. There are no new potentials appearing at third order, hence

$$\delta V_3 = -\frac{4\pi\alpha_s C_F}{q^2} \left[ \hat{V}_C^{(3)} - \hat{V}_1^{(2)} \frac{\pi^2 |q|}{m} + \hat{V}_1^{(1)} \frac{q^2}{m^2} + \hat{V}_p^{(1)} \frac{p^2 + p'^2}{2m^2} \right]. \quad (5.8)$$

Note that there is no kinetic-energy term in $\delta V_3$, because the kinetic energy term in the Lagrangian is not renormalized.

These potentials appear as single insertions in $\delta G(E)$. In addition, $\delta G(E)$ receives contributions from multiple insertions of the lower-order potentials. To complete the perturbative expansion of the third-order cross section, the expansion (5.2) of the Green function is inserted into (1.2),

$$R = 12\pi e_i^2 \text{Im} \left[ \frac{N_c}{2m^2} \left( c_v - \frac{E}{m} \left( c_v + \frac{d_v}{3} \right) \right) G(E) + \ldots \right]. \quad (5.9)$$

The coefficient functions $c_v$ and $d_v$ are likewise expanded, and product terms of order higher than three in non-relativistic perturbation theory are dropped. Note that $E/m \sim v^2$ counts as second order in this expansion.

This work concerns the third-order correction $\delta_3 G(E)$. The triple insertion of the first-order Coulomb potential is algebraically complicated but has no UV or IR divergences and can therefore be computed numerically as done in [15]. The ultra soft correction was obtained in [52]. In part II of the present work we will give the details of the calculation of the remaining single and double insertions in the second line of (5.5) in dimensional regularization as is necessary for a consistent combination with the matching calculations performed and summarized in part I. A more precise master formula for the third-order correction to the Green function that accounts for the pole structure of the $d$-dimensional potentials will be given in part II.

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