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**Infrared-Safe NLO Calculations with Massive Quarks: An Extension of
the NSC Subtraction Formalism**

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Abstract

The treatment of infrared divergences in Next-to-Leading Order (NLO) QCD calculations becomes significantly more complex when accounting for massive quarks, particularly in processes where mass effects cannot be neglected. We present a generalization of the Nested Soft-Collinear (NSC) subtraction scheme to incorporate arbitrary massive quark flavours, preserving the original framework's efficiency while systematically addressing mass-dependent divergences. By removing the need for massless approximations, this work enables precision calculations in particle-production processes where quark mass effects are theoretically or phenomenologically relevant.

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Introduction

The Standard Model of Particle Physics (SM) is, as of now, the most complete theoretical framework in subatomic physics, describing all known elementary particles and fundamental interactions [35–37], except for the very weak gravitational force. Over the last fifty years, the SM has been continuously tested via experiments, mainly in the context of particle colliders, and its validity has been confirmed by the agreement of its predictions with experimental observations, culminating in 2012 with the discovery of the Higgs boson [1, 2] at the Large Hadron Collider (LHC) at CERN.

Despite its success, there is strong evidence for the existence of Physics Beyond the SM (BSM): the most prominent indications include the existence of dark matter and dark energy, the observed matter-antimatter asymmetry and the non-vanishing neutrino masses. Contrary to earlier expectations, though, since its first run in 2009 the LHC has not yet detected any new particle, nor any confirmation of BSM physics: instead, the huge amount of data collected in its three runs (Run 3 is currently ongoing) puts increasingly stricter exclusion limits to BSM models [3–6]. As a consequence, the masses of hypothesized new particles become so large that it is unlikely that they will be produced at the LHC in sufficient numbers for detailed studies. Substantial further increase in the energy of colliding particles at the LHC (or anywhere else) is currently not feasible, hence the lack of any observation of BSM physics at the LHC has sparked a change in the research paradigm in high-energy particle physics, as it is clear that BSM physics searches based on the idea of detectable resonant-like structures on top of flat backgrounds has to be supplemented by new research strategies. Indeed, new particles can still be produced at the LHC, though in a way which does not allow for their direct detection: undetected light particles could be hidden in complex final states, while heavy particles could be virtually produced for extremely short periods of time, before disappearing back into the quantum vacuum. In the latter case, these virtual particles could affect measurable properties, prompting their indirect detection as deviations from SM predictions. [EFT ARGUMENTS] Given this shift of focus towards higher experimental precision in collider physics, it is clear that reliable theoretical predictions of hadron-collision processes are needed.

§1.1 QCD in collider physics

In general, any precision study at a hadron collider is challenging to perform, given the poorly-understood nature of the strong force which keeps hadrons together. In fact, the strong interaction is described by Quantum Chromodynamics (QCD), which has the complicated mathematical structure of a non-Abelian gauge theory (§2.1.1 for details).

Although it has not been possible, so far, to describe the properties of a single proton from first principles, in the context of hadron collisions a first-principles description is made possible for a particular class of processes: hard scattering processes, which are characterized by a large momentum transfer.

Even though hard scattering processes have a lower probability of happening, with respect e.g. to elastic scattering processes, they are of great interest to modern particle physics: in fact, these are the processes which produce electroweak (EW) bosons, the Higgs boson, new heavy particles, etc., thus allowing their detailed study. Moreover, the analysis of hard scattering processes is facilitated by a remarkable property of QCD: **asymptotic freedom**.

Asymptotic freedom is a general property of non-Abelian gauge theories. After the renormalization of a quantum field theory (QFT), the coupling constant of the interaction becomes dependent on a renormalization energy scale, a phenomenon known as the “running of the coupling” (see §2.2). The evolution of the running coupling $\alpha(\mu^2)$ as a function of the energy scale μ is described by the renormalization group equation (see e.g. Chapter 12 of [7]):

$$\mu^2 \frac{d\alpha(\mu^2)}{d\mu^2} = -2\beta(\alpha(\mu^2))\alpha(\mu^2) \quad (1.1)$$

where the Callan–Symanzik β -function has a power-series expansion like:

$$\beta(\alpha) = \sum_{n \in \mathbb{N}_0} \beta_n \left(\frac{\alpha}{4\pi} \right)^{n+1} = \beta_0 \frac{\alpha}{4\pi} + o(\alpha^2) \quad (1.2)$$

For non-Abelian gauge theories $\beta_0 > 0$ (for QCD, see [8, 9]), hence the coupling becomes small at high energies (small distances). This allows for a perturbative description of hard scattering processes: these events happen at small distances, hence the hadronic scattering can be studied through the interaction between single partons (see Fig. 1.1), i.e. the quarks and gluons which compose the hadrons.

§1.1.1 Hadronic scattering

Given the asymptotic freedom of QCD, it is clear why hard scattering processes are preferred for precision studies at hadron colliders: these scatterings are produced at high energy $Q \sim 100 \text{ GeV} - 1 \text{ TeV}$ (at the LHC), hence non-perturbative effects are suppressed by powers of Λ_{QCD}/Q , where $\Lambda_{\text{QCD}} \approx 200 \text{ MeV}$ is an energy scale describing the asymptotic freedom of QCD (see below). This is formalized by the factorization theorem [11], which states that hadronic cross-sections can be computed from partonic cross-sections as:

$$\begin{aligned} d\sigma_{h_1, h_2}(P_1, P_2) = \sum_{a, b} \int_{[0, 1]^2} d\xi_1 d\xi_2 f_a^{(h_1)}(\xi_1, \mu_F^2) f_b^{(h_2)}(\xi_2, \mu_F^2) \times \\ \times d\hat{\sigma}_{a, b}(\xi_1 P_1, \xi_2 P_2, \alpha_s, \mu_R^2, \mu_F^2) \left[1 + o\left(\frac{\Lambda_{\text{QCD}}^n}{Q^n}\right) \right] \end{aligned} \quad (1.3)$$

with $n \in \mathbb{N}$. Here, the two scattering hadrons h_1, h_2 have momenta P_1, P_2 , while the scattering partons a, b have momentum fractions $\xi_1 P_1, \xi_2 P_2$. For the rest of this work, the factorization scale μ_F is taken to be equal to the renormalization scale μ_R defined in §2.2.2. Finally, $d\hat{\sigma}_{a, b}$ is the partonic cross-section to be discussed in the next subsection.

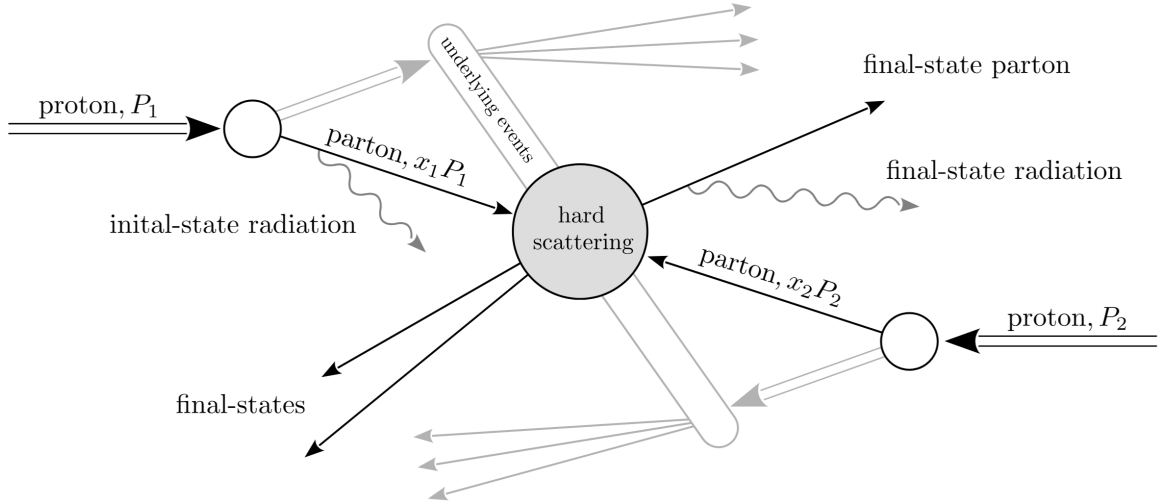


Figure 1.1: Schematics of hard hadronic scattering. Due to asymptotic freedom, individual partons can be assumed to be free particles, so that their (hard) scattering can be computed via perturbative QCD. Initial- and final-state radiation accounts for beyond-leading-order effects. Figure from [10].

The link between hadron-scale physics and parton-scale physics is given by **parton distribution functions** (PDFs): in general, $f_a^{(h)}(\xi)$ is the numerical probability of finding a parton a inside the hadron h with a definite energy fraction ξ : $p_a = \xi P_h$, where p_a and P_h are the momenta of the parton and of the hadron, respectively. A crucial property of PDFs is their universality, as they are energy-independent: this means that they can be measured in a particular process and then used in many others. However, they incapsulate non-perturbative effects which are poorly understood, thus they have not been computed from first principles so far.

Another instance of non-perturbative effects arises when considering that, after the partonic interaction, final-state partons can be clustered in the so-called jets: despite the difficulty in formally defining jets (for a review of various jet algorithms, see [12]), they can intuitively be pictured as seeds of hadronic energy flows which are barely affected by non-perturbative QCD effects. While on short time-scales QCD can be treated perturbatively, on long time-scales QCD partons (and so jets too) are subject to the phenomenon of **hadronization**. Hadronization can be explained by considering a solution to Eq. 1.1 at leading-order in α , found introducing a reference scale μ :

$$\alpha_s(\mu_R^2) = \frac{\alpha_s(\mu^2)}{1 + 2\alpha_s(\mu^2) \frac{\beta_0}{4\pi} \log \frac{\mu_R^2}{\mu^2}} \quad (1.4)$$

For example, $\alpha_s(m_Z^2) \approx 0.118$ [13]. It is customary to introduce a QCD scale Λ_{QCD} , defined as (see Chapter 2 of [14]):

$$\ln \frac{\mu_R^2}{\Lambda_{\text{QCD}}^2} \equiv \frac{1}{2} \int_{\alpha_s(\mu_R^2)}^{\infty} \frac{dx}{x\beta(x)} \quad (1.5)$$

Experimental analysis sets $\Lambda_{\text{QCD}} \approx 200$ MeV. Retaining only the β_0 term allows expressing the running coupling as:

$$\alpha_s(\mu_R^2) \equiv \frac{1}{2 \frac{\beta_0}{4\pi} \log \frac{\mu_R^2}{\Lambda_{\text{QCD}}^2}} \quad (1.6)$$

This expression shows that $\mu_R \gg \Lambda_{\text{QCD}}$ is the perturbative region, where asymptotic freedom makes α_s small enough for perturbative techniques. On the other hand, for $\mu_R \rightarrow \Lambda_{\text{QCD}}$ a Landau pole is present: this pole signals the breakdown of perturbation theory and the hadronization of partons, i.e. their confinement into bound states (hadrons).

Eq. 1.3 can be represented graphically as in Fig. 1.2. Here, the hard scattering process occurs at high energy $Q \gg \Lambda_{\text{QCD}}$, resulting in jets which are unaffected by non-perturbative QCD, since their energy is well above the QCD scale; however, this energy is radiated off in the form of parton showers, and, when the threshold energy Λ_{QCD} is reached, non-perturbative effects come into play, resulting in the hadronization of jets.

The factorization theorem also provides a numerical estimate for corrections due to non-perturbative effects. Setting the lowest energy scale of the considered scattering (e.g. a p_T -cut on a jet) to be $Q \approx 20 \text{ GeV}$ and $n = 1$ in Eq. 1.3, then non-perturbative corrections are of order $\sim 10^{-2}$, i.e. percentage-level corrections.

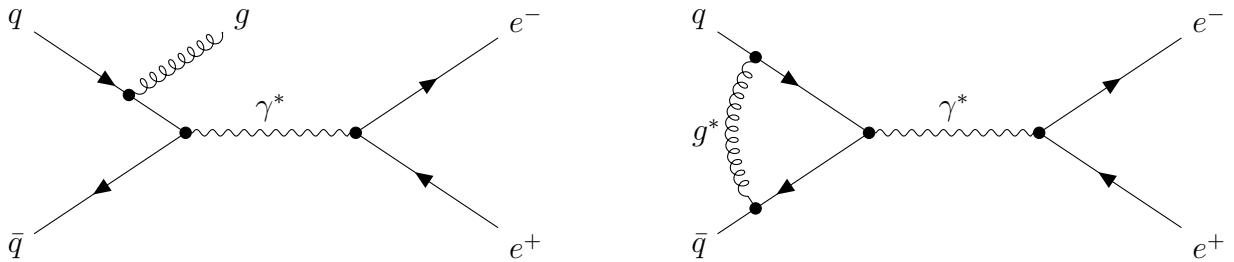
§1.1.2 Partonic scattering

For the rest of this work, the analysis is restricted to perturbative effects only. As the partonic scattering can be treated with perturbation theory, the partonic cross-section for the scattering of two partons a, b with momenta p_1, p_2 can be expressed as a power series in the running coupling:

$$d\hat{\sigma}_{a,b}(p_1, p_2) = \sum_{n \in \mathbb{N}_0} d\hat{\sigma}_{a,b}^{(n)}(p_1, p_2) \quad (1.7)$$

where each term is $d\hat{\sigma}^{(n)} \sim \alpha_s^{n_0+n}$, with $n_0 \in \mathbb{N}$ giving the dependence on $\alpha_s(\mu_R^2)$ due to the leading-order (LO) process, which is usually (but not always) a tree-level process.

The $n \geq 1$ terms form what are denoted by QCD corrections. Focusing on next-to-leading-order (NLO) corrections, they can be of two kinds: real corrections and virtual corrections. Real corrections consist in the emission of an additional parton as initial- or final-state radiation, while virtual corrections present an additional partonic loop. Examples of a real and a virtual correction to the Drell-Yan process may be:



In general, then:

$$d\hat{\sigma}_{a,b}^{(1)}(p_1, p_2) = d\hat{\sigma}_{a,b}^{\text{R}}(p_1, p_2) + d\hat{\sigma}_{a,b}^{\text{V}}(p_1, p_2) + d\hat{\sigma}_{a,b}^{\text{pdf}}(p_1, p_2) \quad (1.8)$$

where $d\hat{\sigma}_{a,b}^{\text{R}}$ and $d\hat{\sigma}_{a,b}^{\text{V}}$ are the single-real and 1-loop corrections. The additional correction $d\hat{\sigma}_{a,b}^{\text{pdf}}$ is due to the collinear renormalization of PDFs.

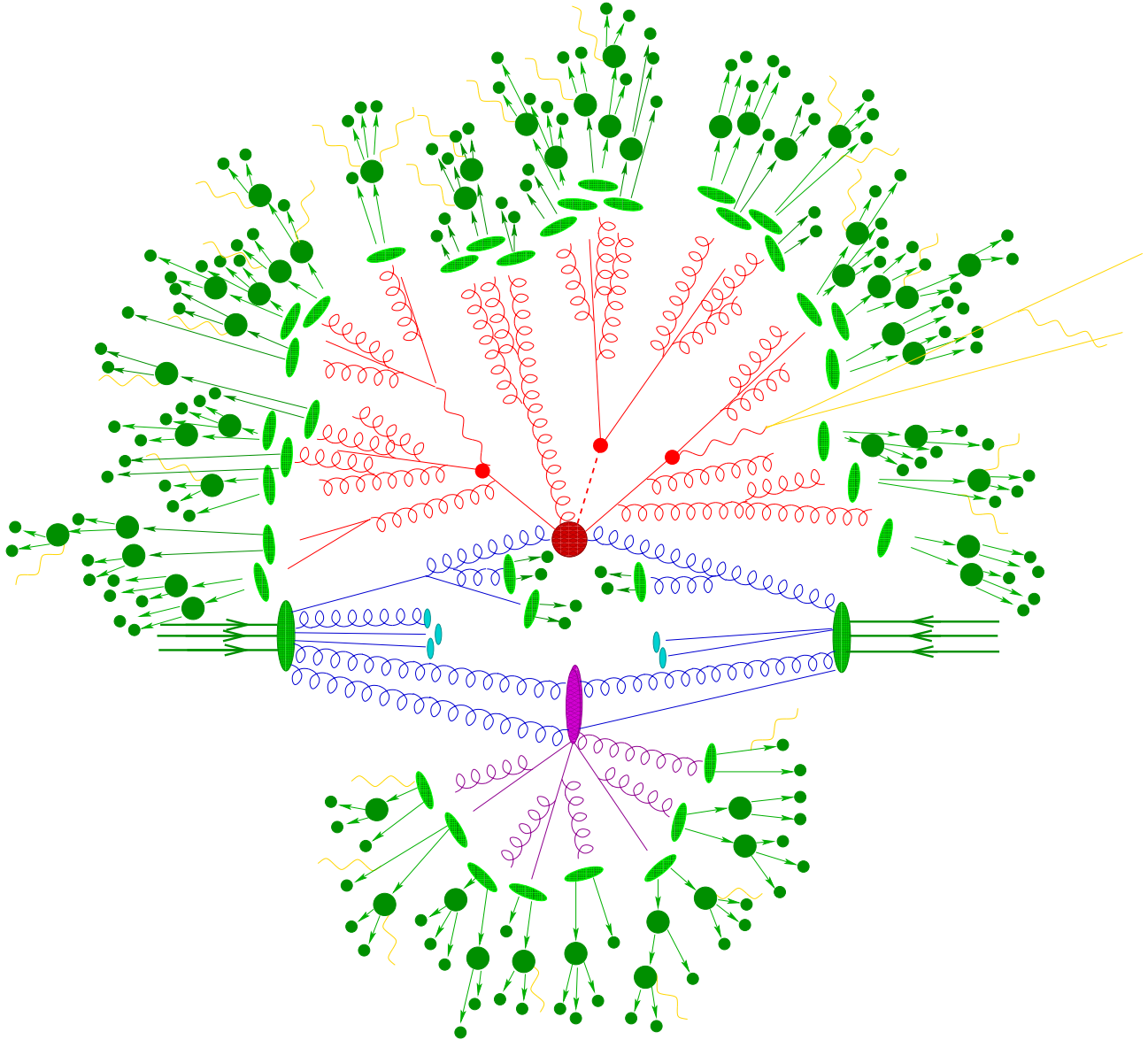


Figure 1.2: Hadronization of jets produced in a hard hadronic scattering. Incoming hadrons produce initial-state radiation (blue), which determines two hard scattering events (red and purple blobs): these scatterings give rise to partonic jets (red and purple) which undergo hadronization (light green blobs), eventually decaying into heavy hadrons (dark green blobs) and soft radiation (yellow). Figure from [15].

§1.2 Singularities in QCD amplitudes

One of the main difficulties when computing real and virtual corrections to scattering amplitudes is the presence of singularities in particular kinematic limits.

§1.2.1 Infrared poles

In the case of amplitudes with real emissions, singularities arise when the energy of a gluon vanishes (**soft singularity**) or when two massless partons are emitted in the same direction (**collinear singularity**). To illustrate why the amplitude diverges in these limits, consider a real-emission diagram like:

$$\sim \frac{1}{(p-k)^2} = \frac{1}{2E_p E_k (1 - \cos \theta)}$$

where the massless approximation¹ for the quark is employed. It is then clear that the amplitude diverges for $E_k \rightarrow 0$ and $\theta \rightarrow 0$ due to the propagator of the emitted virtual quark; note that quarks do not determine any soft singularities, as in the massless limit they provide an integrable singularity due to the structure of the Dirac propagator.

Both kinds of singularities in real emissions can be seen as one virtual massless parton going on-shell (in the above example, the virtual quark with momentum $q = p - k$ in the massless approximation), i.e. with $q^2 \rightarrow 0$, and they are collectively called infrared-collinear singularities, or simply (though less precisely) infrared (IR) singularities.

The case of virtual corrections is more complex. Indeed, virtual-correction amplitudes present an additional loop integral, which has two kinds of singularities: ultraviolet (UV) singularities and IR ones. To illustrate them, consider the following loop diagram:

$$\sim \int \frac{d^4k}{(2\pi)^4} \frac{1}{k^2} \frac{1}{(p+k)^2}$$

The UV divergence can be seen performing a Wick rotation $k^0 \mapsto ik^0$ and introducing a cutoff Λ for the Euclidean momentum's magnitude $|k_E|$: in the UV limit $k^2 \gg p^2$, so the integral is $\sim \log \Lambda$, which is clearly divergent for $\Lambda \rightarrow \infty$. However, this kind of divergences are cured through the procedure of renormalization (§2.2).

IR divergences, on the other hand, have the same origin as those in real corrections: in reality, Nature does not distinguish between “real” and “virtual” corrections, which are merely

¹In the context of collider physics, light quarks are usually approximated as massless, as they have $m_q/Q \lesssim 10^{-3}$, with $Q \sim 1$ TeV in a typical LHC process. The only exceptions are the heavy flavours: the bottom quark is sometimes treated as massive ($m_b \approx 4.18$ GeV), while the top quark is always treated as massive ($m_t \approx 172$ GeV). Data from [13].

human-made categories introduce to simplify the calculations. To confirm this, while real and virtual corrections present IR divergences when considered singularly, these poles have to cancel when the two sets of corrections are added together: this is an instance of the Kinoshita–Lee–Nauenberg theorem, which asserts that the SM is IR-finite [16, 17].

§1.2.2 Subtraction method

A problem of showing the pole cancellation is the fact that real and virtual corrections have different particle multiplicity in the phase space, so their summation is not straightforward. However, Catani’s formula [18] allows one to extract IR singularities from renormalized virtual-correction amplitudes as poles in the number of spacetime dimensions (see §2.2.1). Luckily, the same can be done with real corrections too, e.g.:

$$\int \frac{d^{d-1}k}{(2\pi)^{d-1}2E_k} \left| \text{Diagram} \right|^2 \sim \int_0^{E_{\max}} \frac{dE_k}{E_k^{5-d}} \int_0^\pi d\theta \frac{\sin^{d-3}\theta}{1-\cos\theta} \left| \text{Diagram} \right|^2$$

Integrations are trivially performed:

$$\int_0^{E_{\max}} \frac{dE_k}{E_k^{5-d}} = \frac{E_{\max}^{d-4}}{d-4} \quad \int_0^\pi d\theta \frac{\sin^{d-3}\theta}{1-\cos\theta} = \frac{2^{1-\frac{d}{2}}}{d-4}$$

Note that both integrals require $\Re d > 4$ and are divergent as $d \rightarrow 4$. It is then clear that, once the IR poles are extracted, both real and virtual corrections have the same particle multiplicity and can be safely added.

The crucial point of extracting divergences, and in particular from real corrections, is to do so without integrating over the resolved phase space, in order to obtain a fully-differential (with respect to resolved partons) cross-section which allows for the numerical evaluation of phase-space integrals for any IR-safe observable. To do so, it is necessary to introduce a subtraction method.

To illustrate the idea of a subtraction method, consider the following integral:

$$I = \int_0^1 \frac{dx}{x^{1+\epsilon}} f(x) \quad (1.9)$$

where $f(x)$ is an arbitrary integrable function regular at $x = 0$. The integrand clearly diverges at $x = 0$, and this singularity is regulated by the parameter ϵ which leads to a $\frac{1}{\epsilon}$ pole after integration. The aim of the subtraction method is to analytically extract this pole and regulate the integral, making it finite in the $\epsilon \rightarrow 0$ limit. The basic idea is to introduce a counterterm by writing $f(x) = [f(x) - f(0)] + f(0)$, so that:

$$I = \int_0^1 \frac{dx}{x^{1+\epsilon}} [f(x) - f(0)] + f(0) \int_0^1 \frac{dx}{x^{1+\epsilon}}$$

The second integral is analytically determined for $\Re \epsilon < 0$, hence:

$$I = \int_0^1 \frac{dx}{x^{1+\epsilon}} [f(x) - f(0)] - \frac{f(0)}{\epsilon} \quad (1.10)$$

The pole has successfully been isolated, and the integral is now regular at $x = 0$, allowing for its numerical integration after setting $\epsilon \rightarrow 0$.

In a similar fashion, subtraction schemes are being developed for the extraction of IR singularities from QCD corrections. The main challenge is to define $f(0)$ such that it locally removes all divergences in the first term of Eq. 1.10, while also allowing the analytic integration of the second term, in a process-independent way. At NLO this problem has been completely solved in a fully-local and analytic way with the Catani–Seymour (CS) scheme [19] and the Frixione–Kunszt–Signer (FKS) scheme [20, 21]. At NNLO a completely general, analytic and fully-local subtraction scheme has not yet been developed, but there are several candidates: in this work we consider the Nested Soft-Collinear (NSC) subtraction scheme (SS), introduced in [22].

The NSC SS can be applied to any scattering process with a generic number of final-state massless partons [23]; however, it cannot yet describe processes with final-state massive partons, e.g. top quarks. This work takes the first step in this direction, generalizing the NLO subtraction operators defined in [23–25] to account for both massless and massive final-state partons.

Preliminaries

§2.1 Quantum Chromodynamics

We consider a generalized QCD with gauge group $SU(n_c)$, with n_c colours and $n = n_f + n_F$ total quark flavours (n_f massless and n_F massive quark flavours).

§2.1.1 Yang–Mills theories

A quantum field theory can be built starting from its symmetry properties: in particular, specifying a group of local transformations, the **gauge group**, under which the theory must be invariant. Historically, the idea of gauge theories was first explored by Yang and Mills in [26], with the aim of studying isotopic gauge invariance for the nucleon, and then generalized by Utiyama in [27]. A modern treatment of gauge theories can be found in Chapter 15 of [7], which we follow for our discussion.

Consider n fermionic fields $\{\psi_k(x)\}_{k=1,\dots,n}$ and an n -spinor $\Psi(x)$ defined as:

$$\Psi(x) = \begin{pmatrix} \psi_1(x) \\ \vdots \\ \psi_n(x) \end{pmatrix} \quad (2.1)$$

As a gauge group, consider a d -dimensional Lie group G : in particular, take G to be a simply-connected, so that each element can be expressed via the exponential map, and compact, so that its representations are unitary. Then, consider $\{T^a\}_{a=1,\dots,d} \subset \mathbb{C}^{n \times n}$ a representation of the associated Lie algebra \mathfrak{g} , so that the action of G on Ψ can be expressed as:

$$\Psi(x) \mapsto V(x)\Psi(x) \quad V(x) := \exp[i\theta_a(x)T^a] \quad (2.2)$$

where the Lie parameters $\{\theta_a(x)\}_{a=1,\dots,d} \subset \mathcal{C}^\infty(\mathbb{R}^{1,3})$ define a local gauge transformation. The aim is to define a Lagrangian which is invariant under this transformation, i.e. the Lagrangian of a (local) gauge theory.

Simple terms invariant under global phase rotations, like the fermion mass term $m\bar{\Psi}\Psi$, are of course invariant under Eq. 2.2 too, but derivatives need a careful treatment: indeed, the limit-definition of a derivative involves fields at different spacetime points, which have different transformations according to Eq. 2.2. In order to define a derivative of Ψ , it is necessary to introduce a factor to subtract values of $\Psi(x)$ in a meaningful way, so consider $U(y, x) \in U(n)$: $U(x, x) = 1$ and which transforms under the action of G as:

$$U(y, x) \mapsto V(y)U(y, x)V^\dagger(x) \quad (2.3)$$

By the unitarity of the representations of G , it is clear that $U(y, x)\Psi(x)$ and $\Psi(y)$ have the same transformation law, so they can be meaningfully subtracted. Then, given $n^\mu \in \mathbb{R}^{1,3}$, the covariant derivative of a fermionic field $\Psi(x)$ along n^μ is defined as:

$$n^\mu D_\mu \Psi(x) := \lim_{\varepsilon \rightarrow 0} \frac{1}{\varepsilon} [\Psi(x + \varepsilon n) - U(x + \varepsilon n, x)\Psi(x)] \quad (2.4)$$

where $U(y, x)$ is defined through Eq. 2.3. To make this definition explicit, it is necessary to get an expression of $U(y, x)$ at infinitesimally-separated points. Given the unitarity of $U(y, x)$, it can be expressed through the generators $\{T^a\}_{a=1, \dots, d}$ as:

$$U(x + \varepsilon n, x) = I_n + ig\varepsilon n^\mu A_\mu^a(x) T_a + o(\varepsilon^2) \quad (2.5)$$

where $g \in \mathbb{R}$ is a constant. The new vector field $A_\mu^a(x)$ (actually, d different vector fields) is a **connection**, and it allows us to express the covariant derivative as (directly from Eq. 2.4):

$$D_\mu = \partial_\mu - ig A_\mu^a T_a \quad (2.6)$$

To show that $D_\mu \Psi$ transforms in the same way as Ψ , note that, from Eq. 2.3-2.5:

$$I_n + ig\varepsilon n^\mu A_\mu^a(x) T_a \mapsto I_n - \varepsilon n^\mu V(x) \partial_\mu V^\dagger(x) + V(x) (ig\varepsilon n^\mu A_\mu^a(x) T_a) V^\dagger(x) + o(\varepsilon^2)$$

Hence, the connection transforms as:

$$A_\mu^a(x) T_a \mapsto V(x) \left[A_\mu^a(x) T_a + \frac{i}{g} \partial_\mu \right] V^\dagger(x) = A_\mu^a(x) T_a - f^{abc} A_\mu^a(x) \theta^b(x) T_c + \frac{1}{g} \partial_\mu \theta^a(x) T_a + o(\theta^2)$$

The second term makes it clear that the connection transforms according to the adjoint representation. From this expression, it follows that:

$$D_\mu \Psi(x) \mapsto [I_n + i\theta^a(x) T_a + o(\theta^2)] (\partial_\mu - ig A_\mu^a(x) T_a) \Psi(x) = V(x) D_\mu \Psi(x)$$

where the relation $T_a T_b - if^{abc} T_c = T_b T_a$ of the associated Lie algebra was used.

The gauge-invariant Lagrangian can thus be built using covariant derivatives (minimal coupling prescription), but one also needs to include a kinetic term for the connection, i.e. a gauge-invariant term dependent on $A_\mu^a(x)$ only. This term can be found considering the commutator of covariant derivatives:

$$[D_\mu, D_\nu] = -ig F_{\mu\nu}^a T_a \quad (2.7)$$

with the **field-strength tensor** defined as:

$$F_{\mu\nu}^a := \partial_\mu A_\nu^a - \partial_\nu A_\mu^a + gf^{abc} A_\mu^b A_\nu^c \quad (2.8)$$

Note that the field-strength tensor is not itself a gauge-invariant quantity, as really there are d different field-strength tensors; however, it is straightforward to construct gauge-invariant combinations of $F_{\mu\nu}^a$. In fact, in general any globally-symmetric function of Ψ , $F_{\mu\nu}^a$ and their covariant derivatives is also locally-symmetric, i.e. gauge-invariant: this follows from the construction of the covariant derivative. For a complete discussion, see Chapter 15 of [7].

Usually, the following gauge-invariant term is taken as kinetic term for the gauge field (i.e. the connection $A_\mu^a(x)$):

$$\text{tr}\{(F_{\mu\nu}^a T_a)^2\} = 2F_{\mu\nu}^a F_a^{\mu\nu} \quad (2.9)$$

This allows defining the simplest non-Abelian gauge theory, **Yang–Mills theory** without fermionic species:

$$\mathcal{L}_{\text{YM}} = -\frac{1}{4}F_{\mu\nu}^a F_a^{\mu\nu} \quad (2.10)$$

To account for fermions interacting with the gauge field $A_\mu^a(x)$, the Dirac Lagrangian with minimal coupling is added (see Chapter 15 of [28]):

$$\mathcal{L} = -\frac{1}{4}F_{\mu\nu}^a F_a^{\mu\nu} + \bar{\Psi} (i\not{D} - m) \Psi \quad (2.11)$$

§2.1.2 Gauge group $\text{SU}(n_c)$

The $\text{SU}(n_c)$ group is the group of unitary transformations of n_c -dimensional complex vectors. Its (faithful) fundamental representation thus is:

$$\text{SU}(n_c) = \{U \in \mathbb{C}^{n_c \times n_c} : UU^\dagger = U^\dagger U = I_{n_c} \wedge \det U = +1\}$$

The generators of $\text{SU}(n_c)$ can be found setting $U = \exp(i\theta_a T^a) = I_{n_c} + i\theta_a T^a + o(\theta^2)$ and using $U^\dagger U = I_{n_c}$:

$$T^a = T^{a\dagger} \quad (2.12)$$

Moreover, by the Jacobi formula $(\det A(t)) \frac{d}{dt}(\det A(t)) = \text{tr}(A(t)^{-1} \frac{d}{dt} A(t))$ evaluated at $t = 0$:

$$\text{tr} T^a = 0 \quad (2.13)$$

The traceless condition can be generalized to all semi-simple Lie algebras. Therefore, the generators of $\text{SU}(n_c)$ are $\mathbb{C}^{n_c \times n_c}$ Hermitian traceless matrices: the dimension of $\mathfrak{su}(n_c)$ then is $n_c^2 - 1$.

In general, the adjoint representation of a Lie group is given by representing its generators (i.e. the basis of the Lie algebra) with the structure constants of the Lie algebra:

$$(T_{\text{ad}}^b)_{ac} \equiv \bar{T}_{ac}^b = if^{abc} \quad (2.14)$$

which, in the case of $\text{SU}(n_c)$, are $f^{abc} = \epsilon^{abc}$. Indeed, it can be shown by the Jacobi identity that the structure constants satisfy the Lie algebra:

$$f^{abd} f^{dce} - f^{acd} f^{dbe} = f^{bcd} f^{ade} \iff [[T^a, T^b], T^c] + [[T^c, T^a], T^b] + [[T^b, T^c], T^a] = 0$$

Moreover, since the structure constant are real, the adjoint representation is always a real representation: the adjoint representation of $\text{SU}(n_c)$ has degree $n_c^2 - 1$.

Representation are labelled by their Casimir operators. For any simple Lie algebra, given a representation \mathbf{r} , a Casimir operator is defined as:

$$T_{\mathbf{r}}^a T_{\mathbf{r}}^a = C_2(\mathbf{r}) I_{n_{\mathbf{r}}} \quad (2.15)$$

This is called the **quadratic Casimir operator**, as it is associated to $T^2 \equiv T^a T^a$ (a Casimir operator since $[T^b, T^2] = if^{bac} \{T^c, T^a\} = 0$ by antisymmetry). For the fundamental and the adjoint representations \mathbf{n} and \mathbf{g} of $\text{SU}(n_c)$, the quadratic Casimir operators are (§A.4):

$$C_{\mathbf{F}} \equiv C_2(\mathbf{n}) = T_{\mathbf{R}} \frac{n_c^2 - 1}{n_c} \quad C_{\mathbf{A}} \equiv C_2(\mathbf{g}) = 2T_{\mathbf{R}} n_c \quad (2.16)$$

where $T_{\mathbf{R}}$ (usually taken to be $T_{\mathbf{R}} = \frac{1}{2}$) is the trace normalization of the generators in the fundamental representation:

$$\text{tr}(T_{\mathbf{n}}^a T_{\mathbf{n}}^b) = T_{\mathbf{R}} \delta^{ab} \quad (2.17)$$

§2.1.3 Quantization

The quantization of a non-Abelian gauge theory requires careful treatment due to the presence of spurious non-physical degrees of freedom. These can be accounted for with the Faddeev–Popov method [29], i.e. imposing a gauge fixing condition and introducing non-physical ghost fields, which serve as “negative” degrees of freedom. Then, functional quantization can be performed naturally, resulting in the following Feynman rules for the Yang–Mills Lagrangian (excluding ghost fields):

$$\begin{aligned}
 & \text{Feynman rule for fermion propagator: } a \xrightarrow{p} b = \frac{i}{\not{p} - m} \delta_{ab} \quad \text{Feynman rule for gluon propagator: } \mu, a \xrightarrow{k} \nu, b = \frac{-ig_{\mu\nu}}{k^2} \delta_{ab} \\
 & \text{Feynman rule for fermion-gluon vertex: } \begin{array}{c} \mu, a \\ \text{gluon} \\ \text{fermion } b \text{ to } c \end{array} = ig\gamma^\mu T^a \delta_{bc} \quad \text{Feynman rule for three-gluon vertex: } \begin{array}{c} \mu, a \\ \text{gluon } p \\ \text{gluon } q \text{ to } \nu, b \\ \text{gluon } k \text{ to } \rho, c \end{array} = gf^{abc} [g^{\mu\nu}(p-q)^\rho + g^{\nu\rho}(q-k)^\mu + g^{\rho\mu}(k-p)^\nu] \\
 & \text{Feynman rule for four-gluon vertex: } \begin{array}{c} \mu, a \text{ gluon } \nu, b \text{ gluon} \\ \rho, c \text{ gluon } \sigma, d \text{ gluon} \end{array} = -ig^2 [f^{abe}f^{cde}(g^{\mu\rho}g^{\nu\sigma} - g^{\mu\sigma}g^{\nu\rho}) + f^{ace}f^{bde}(g^{\mu\nu}g^{\rho\sigma} - g^{\mu\sigma}g^{\nu\rho}) + f^{ade}f^{bce}(g^{\mu\nu}g^{\rho\sigma} - g^{\mu\rho}g^{\nu\sigma})]
 \end{aligned}$$

The peculiar nature of non-Abelian gauge theories is due to the possibility for gauge bosons to self-interact (last two vertices).

In the case of QCD, the quanta of the n spinor fields are the n quark flavours, while the $n_c^2 - 1$ gauge fields are gluon fields, and their colour charges are given by their respective $SU(n_c)$ representations: n_c charges for the quarks (fundamental n -dimensional representation) and $n_c^2 - 1$ charges for the gluons (adjoint representation).

§2.2 Renormalization scheme

The computation of NLO corrections to scattering processes in a generic QFT involves UV-divergent loop amplitudes. In order to obtain finite results from these divergences, a renormalization scheme must be implemented.

The generalized Catani’s formula for IR singularities in virtual corrections is provided in [30] in a charge-unrenormalized (but mass-renormalized) way, i.e. still containing UV singularities too (recall §1.2), thus it is necessary to carry out the renormalization procedure explicitly. To this end, we formally state the renormalization scheme adopted in this work.

§2.2.1 Dimensional regularization

In the evaluation of loop amplitudes, both UV- and IR-singularities are encountered. The most efficient way to simultaneously regularize both types of divergences is dimensional regularization [38].

In general, the dimensional regularization scheme consists in the analytic continuation of loop momenta to $d = 4 - 2\epsilon$ dimensions, with $\epsilon \in \mathbb{C} : \Re \epsilon < 0$ for IR divergences and $\Re \epsilon > 0$ for UV ones. This procedure turns loop integrals into meromorphic functions of $\epsilon \in \mathbb{C}$, allowing for the isolation of divergences as poles in ϵ .

The dimensional regularization prescription leaves freedom in choosing the dimensionality of external momenta, as well as the number of polarizations of both external and internal particles, thus allowing for the definition of different regularization schemes. We choose to work with **conventional dimensional regularization** (CDR), in which all momenta and polarization are analytically continued to d dimensions, as opposed to the 't Hooft–Veltman scheme (HV), in which only internal momenta and polarizations are.

When considering non-chiral gauge theories like QCD, CDR is the most natural choice, as the main difference between CDR and HV is the treatment of purely 4-dimensional objects, i.e. γ^5 and $\epsilon_{\mu\nu\sigma\rho}$. In particular, in CDR both the Dirac algebra and Lorentz indices are analytically continued to d dimensions, leading to a mathematical inconsistency stemming from the fact that, when $d \notin \mathbb{N}$, the following identities cannot hold simultaneously¹:

$$\{\gamma^5, \gamma^\mu\} = 0 \quad \forall \mu = 0, 1, \dots, d-1 \quad \text{tr}\{\gamma^5 \gamma^\mu \gamma^\nu \gamma^\rho \gamma^\sigma\} = -4i\epsilon^{\mu\nu\rho\sigma}$$

The choice of CDR over HV is then clear: in QCD, the only pathological objects are encountered when considering chiral vertices (e.g. for pseudoscalar mesons) and electroweak interactions, and both can be handled via known prescriptions, e.g. the Breitenlohner-Maison/'t Hooft-Veltman (BMHV) scheme [31] or the Larin scheme [32].

§2.2.2 Minimal subtraction

Once regularized, UV-divergences have to be removed via renormalization of fields and coupling constants. As a result of the renormalization procedure, a running coupling $\alpha_s(\mu_R^2)$ is introduced, and its definition in terms of the bare coupling $\alpha_{s,b}$ depends both on the regularization and the renormalization schemes.

In this work, we renormalize the coupling in a standard way (as in [18]) using the **modified minimal-subtraction scheme** ($\overline{\text{MS}}$), which directly subtracts UV-divergences from the coupling:

$$\alpha_{s,b} S_\epsilon = \alpha_s(\mu_R^2) \mu_R^{2\epsilon} \left[1 - \frac{\alpha_s(\mu_R^2) \beta_0}{2\pi} \frac{1}{\epsilon} + o(\alpha_s^2) \right] \quad (2.18)$$

where μ_R is an arbitrary renormalization scale, S_ϵ is the typical phase-space volume factor in dimensional regularization:

$$S_\epsilon \equiv (4\pi)^\epsilon e^{-\gamma_E \epsilon} \quad (2.19)$$

with $\gamma_E = 0.5772\dots$ the Euler-Mascheroni constant, and β_0 is the leading-order coefficient of the QCD β -function Eq. 1.2:

$$\beta_0 := \frac{11}{6} C_A - \frac{2}{3} T_R n_q \quad (2.20)$$

where n_q is the number of active quark flavours at the considered energy scale. In this work $n_q = n_f$ unless otherwise specified.

¹This inconsistency is the explicit manifestation of a more profound topological issue of analytically continuing the number of dimensions: the Levi-Civita symbol in $d = 4$ is linked to the Grassmann algebra $\bigwedge(\mathbb{R}^{1,3})$, and in particular to its top-form, but $\bigwedge^k(\mathbb{R}^d)$ is only defined for $d \in \mathbb{N}$, so the top exterior subspace $\bigwedge^d(\mathbb{R}^{1,d-1})$ is meaningless for $d \notin \mathbb{N}$ and the Levi-Civita symbol cannot be analytically continued to $d = 4 - 2\epsilon$ dimensions.

An important clarification about the dimensionality of $\alpha_{s,b}$ and α_s is needed, due to the presence of $\mu_R^{2\epsilon}$ in Eq. 2.18. In dimensional regularization, the action remains a dimensionless quantity, hence, given $\mathcal{S} = \int d^d x \mathcal{L}$ and that in natural units ($c = \hbar = 1$) all dimensions can be expressed as mass dimensions (since $[T] = [L] = [M]^{-1}$), the QCD Lagrangian Eq. 2.11 must have dimension $[\mathcal{L}] = d$, as $[d^d x] = -d$. It is now trivial to verify the following dimensions:

$$[\Psi] = \frac{d-1}{2} \quad [A_\mu^a] = \frac{d-2}{2} \quad [g] = \frac{4-d}{2} = \epsilon$$

This shows that, in dimensional regularization, $[\alpha_{s,b}] = 2\epsilon$. In order to work with dimensionless quantities, then, in Eq. 2.18 we chose to extract the mass dimension from α_s .

When dealing with scattering processes, a fundamental quantity is the amplitude of a process. In the Schrödinger picture, given a quantum system described by a Hamiltonian H and a Hilbert space \mathcal{H} , the amplitude for the process $|a\rangle \rightarrow |b\rangle$, where $|a\rangle, |b\rangle \in \mathcal{H}$ is defined as:

$$\mathcal{A} := \langle b | S(t, t_0) | a \rangle \quad (2.21)$$

where $\Delta t \equiv t - t_0$ is the time elapsed in the transition and the S -matrix is defined as:

$$S(t, t_0) := e^{-iH(t-t_0)} \quad (2.22)$$

For a $n \rightarrow m$ scattering with defined initial- and final-state momenta, the amplitude can be written in the multi-particle phase as:

$$\mathcal{A}_{n+m} := \langle \mathbf{p}_1, \dots, \mathbf{p}_n | S(+\infty, -\infty) | \mathbf{k}_1, \dots, \mathbf{k}_m \rangle \quad (2.23)$$

where $t, t_0 \rightarrow \pm\infty$ as to consider free-particle initial and final states (for a discussion on this adiabatic approximation, see Chapter 5 of [33]). The explicit expression of the amplitude can be computed from Feynman diagrams: for a complete discussion, see Chapter 4 of [7].

In general, we consider amplitudes \mathcal{A}_m involving m external QCD partons (gluons and quarks), with momenta $\{p\} \equiv \{p_1, \dots, p_m\}$, and an arbitrary number of colorless particles (photons, leptons, ...). Dependence on the momenta and quantum numbers of colorless particles is always understood and not explicitly shown. The $\overline{\text{MS}}$ -renormalized amplitude has the following perturbative expansion in α_s :

$$\mathcal{A}_m(\alpha_s(\mu_R^2), \mu_R^2; \{p\}) = \left(\frac{\alpha_s(\mu_R^2)}{2\pi} \right)^q \left[\mathcal{A}_m^{(0)}(\mu_R^2; \{p\}) + \frac{\alpha_s(\mu_R^2)}{2\pi} \mathcal{A}_m^{(1)}(\mu_R^2; \{p\}) + o(\alpha_s^2) \right] \quad (2.24)$$

where the overall power is, in general, $q \in \frac{1}{2}\mathbb{N}_0$. Note that, although UV-divergences have been removed by the renormalization procedure, these amplitudes are still IR-singular as $\epsilon \rightarrow 0$.

§2.3 Colour-space formalism

To handle the colour structure of QCD amplitudes, we adopt the colour-space formalism as in [19].

The m external partons in the amplitude \mathcal{A}_m each carry two indices: a colour index and a spin index. Colour indices are denoted by c_1, \dots, c_m : for gluons $c_i \equiv a_i \in \{1, \dots, n_c^2 - 1\}$, as the field-strength tensor Eq. 2.8 transforms according to the adjoint representation of the gauge

group, while for quarks $c_i \equiv \alpha_i \in \{1, \dots, n_c\}$, as their Dirac fields transform according to the fundamental representation of the gauge group. Spin indices, on the other hand, are denoted by s_1, \dots, s_m , and they need to take into account how helicities change in CDR: for gluons $s_i \equiv \mu_i \in \{1, \dots, d\}$, while for quarks $s_i \in \{1, 2\}$.

Consider the m -parton colour-space \mathcal{H}_c and helicity-space \mathcal{H}_s , and introduce an orthonormal basis in each:

$$\{|c_1, \dots, c_m\rangle\} \in \mathcal{H}_c \quad \{|s_1, \dots, s_m\rangle\} \in \mathcal{H}_s$$

Note that, as these are finite-dimensional Hilbert spaces, the non-canonical (basis-dependent) isomorphisms $\mathcal{H}_c \leftrightarrow \mathcal{H}_c^*$ and $\mathcal{H}_s \leftrightarrow \mathcal{H}_s^*$ are well-defined².

Then, to make the colour-helicity structure of the m -parton amplitude explicit, we define it as an abstract vector in $\mathcal{H}_c \otimes \mathcal{H}_s$, so that:

$$\mathcal{A}_m^{\{c_1, \dots, c_m\}, \{s_1, \dots, s_m\}}(\{p_1, \dots, p_m\}) \equiv \langle \{c_1, \dots, c_m\}, \{s_1, \dots, s_m\} | \mathcal{A}_m(\{p_1, \dots, p_m\}) \rangle \quad (2.25)$$

with:

$$|\{c_1, \dots, c_m\}, \{s_1, \dots, s_m\}\rangle \equiv |c_1, \dots, c_m\rangle \otimes |s_1, \dots, s_m\rangle$$

Hence, it is clear that the squared amplitude summed over colours and helicities is:

$$|\mathcal{A}_m|^2 = \langle \mathcal{A}_m | \mathcal{A}_m \rangle \quad (2.26)$$

To represent colour interactions at QCD vertices, we associate to each parton i a colour charge $\mathbf{T}_i = \{T_i^a\}_{a=1, \dots, n_c^2-1}$ related to the emission of a gluon. The action of \mathbf{T}_i onto \mathcal{H}_c is defined by:

$$\langle c_1, \dots, c_i, \dots, c_m | T_i^a | b_1, \dots, b_i, \dots, b_m \rangle = \delta_{c_1, b_1} \dots T_{c_i b_i}^a \dots \delta_{c_m, b_m} \quad (2.27)$$

So, $\{T_{c_i b_i}^a\}_{a=1, \dots, n_c^2-1}$ form a vector with respect to the colour index a of the emitted gluon, and they are matrices in different representations of $SU(n_c)$, depending on the parton i :

- if i is a gluon, then $T_{cb}^a \equiv if_{cab}$ (adjoint representation);
- if i is a final-state quark, then $T_{\alpha\beta}^a \equiv t_{\alpha\beta}^a$ (fundamental representation), while if it is a final-state antiquark $T_{\alpha\beta}^a \equiv -t_{\alpha\beta}^a$;
- if i is an initial-state quark, by crossing-symmetry $T_{\alpha\beta}^a \equiv -t_{\alpha\beta}^a$, while if it is an initial-state antiquark $T_{\alpha\beta}^a \equiv t_{\alpha\beta}^a$.

The algebra of these QCD colour-charge operators is easily determined. First of all, we set:

$$\mathbf{T}_i \cdot \mathbf{T}_j \equiv \sum_{a=1}^{n_c^2-1} T_i^a T_j^a \quad (2.28)$$

Then, by the action Eq. 2.27, it is clear that charges associated to different partons commute, i.e.:

$$\mathbf{T}_i \cdot \mathbf{T}_j = \mathbf{T}_j \cdot \mathbf{T}_i \quad \forall i \neq j \in \{1, \dots, m\} \quad (2.29)$$

²Given a finite-dimensional \mathbb{K} -vector space V and a basis $\{v_i\}_{i=1, \dots, n} \subset V$, with $n = \dim_{\mathbb{K}} V$, then a basis $\{\omega^1, \dots, \omega^n\} \subset V^*$ of $V^* := \text{Hom}(V, \mathbb{K})$ is defined by $\omega^i(v_j) = \delta_j^i$, and the function $\varphi : V \rightarrow V^* : v_i \mapsto \omega^i$ is a *non-canonical isomorphism* $V \leftrightarrow V^*$.

If V is infinite-dimensional, instead, given a basis $\{v_i\}_{i \in \mathcal{I}} \subset V$, the above construction only allows to define linearly-independent subsets of V^* , which are not granted to be bases.

Moreover, by Eq. 2.15,2.28:

$$\mathbf{T}_i^2 = C_i \text{id}_{\mathcal{H}_c} \quad (2.30)$$

with $C_i \equiv C_F$ if i is a quark/antiquark and $C_i \equiv C_A$ if it is a gluon, i.e. the quadratic Casimir operators Eq. 2.16. Finally, as each vector $|\mathcal{A}_m\rangle$ is a colour-singlet, colour conservation implies:

$$\sum_{i=1}^m \mathbf{T}_i |\mathcal{A}_m\rangle = 0 \quad (2.31)$$

This allows us to partially (or fully, if $m = 2$ or $m = 3$, as in Appendix A of [19]) factorize the colour-charge algebra in terms of quadratic Casimir operators.

NSC Subtraction Scheme

The aim of the NSC subtraction scheme (SS) is to compute integrated subtraction terms which account for QCD corrections to the inclusive¹ production of jets in a hadron collider, i.e. to the process:

$$p + p \rightarrow X + N \text{ jets} \quad (3.1)$$

Here, X is a colour-neutral system. The hadron-scale physics is known to be separated from the parton-scale physics (see Section 1.1 of [34]): this makes it possible for us to only manipulate partonic cross-sections according to Eq. 1.3, where now the sum runs over all initial-state massless partons a and b which contribute to the production of the considered final state. Moreover, for the rest of this work we set $\mu_R = \mu_F = \mu$, where μ is the typical energy scale of the considered process.

Denoting the partons' momenta as $p_i \equiv \xi_i P_i$, $i = 1, 2$, and suppressing the explicit dependence on the running coupling and the renormalization scale, it is possible to express the LO term of Eq. 1.7 as (see §A.1):

$$d\hat{\sigma}_{a,b}^{(0)}(p_1, p_2) := \sum_f \frac{\mathcal{N}}{2\hat{s}} \int d\Phi_n \left| \mathcal{A}_m^{(0)}(p_1, p_2, p_X, p_f) \right|^2 \mathcal{O}_m(p_X, p_f) \quad (3.2)$$

where $\hat{s} \equiv 2p_1 \cdot p_2$ is the partonic center-of-mass (CM) energy squared, p_f is the total final-state momentum and the normalization factor \mathcal{N} includes all necessary symmetry factors (e.g. $(N_g!)^{-1}$, with N_g number of resolved gluons in the final state), as well as averaging factors for initial-state colours and helicities. The sum runs over all possible partonic final states for the considered process (formalized in the next section).

Note that \mathcal{O}_m is an IR-finite measurement function defining the observable, which ensures that the final state contains at least N resolved jets: in particular, if the energy of a final-state gluon vanishes (soft limit), or if two partons become collinear to one another (collinear limit), then $\mathcal{O}_{m+n} \rightarrow \mathcal{O}_{m+n-1}$ for $n \in \mathbb{N}$, and $\mathcal{O}_m \rightarrow 0$.

Similarly, it is possible to write the NLO corrections in Eq. 1.7 as:

$$d\hat{\sigma}_{a,b}^R(p_1, p_2) := \sum_f \frac{\mathcal{N}_R}{2\hat{s}} \int d\Phi_{m+1} \left| \mathcal{A}_{m+1}^{(0)}(p_1, p_2, p_X, p_f) \right|^2 \mathcal{O}_{m+1}(p_X, p_f) \quad (3.3)$$

$$d\hat{\sigma}_{a,b}^V(p_1, p_2) := \sum_f \frac{\mathcal{N}_V}{2\hat{s}} \int d\Phi_m 2\Re \langle \mathcal{A}_m^{(0)} | \mathcal{A}_m^{(1)} \rangle \mathcal{O}_m(p_X, p_f) \quad (3.4)$$

¹Inclusive jet production denotes the theoretical prediction (or experimental measurement) of the cross-section for the production of jets of given kinematics, while summing/integrating over all other final-state radiation and particles.

$$d\hat{\sigma}_{a,b}^C(p_1, p_2) := \frac{\alpha_s(\mu_R^2)}{2\pi} \frac{1}{\epsilon} \sum_c \int_0^1 \frac{dz}{z} \left[\hat{P}_{c,a}^{(0)}(z) d\hat{\sigma}_{c,b}^{(0)}(zp_1, p_2) + \hat{P}_{c,b}^{(0)}(z) d\hat{\sigma}_{a,c}^{(0)}(p_1, zp_2) \right] \quad (3.5)$$

Note that in Eq. 3.3 the final state contains $m+1$ partons. The Altarelli-Parisi splitting kernels are listed in §B.2, and proof of Eq. 3.5 is provided in §3.2.2.

The rest of this chapter is devoted to the extrapolation of IR-singularities from Eq. 3.3-3.5, proving their cancellation and providing the associated integrated counterterms.

§3.1 Nested subtraction

As suggested by the name, in the NSC SS the IR-poles of real corrections are removed sequentially, starting from those arising from soft limits and then subtracting the collinear ones from the soft-regulated terms.

To show this procedure, we introduce some notation. First of all, we define the integrand function in Eq. 3.2-3.3 as:

$$\mathcal{F}_{a,b}[\mathcal{X}_m^n] \equiv \mathcal{N}_{\text{sym}} \left| \mathcal{A}_m^{(0)}(p_1, p_2, p_X, p_f) \right|^2 \mathcal{O}_m(p_X, p_f) \quad (3.6)$$

where \mathcal{X}_m^n is the set of m final-state partons and \mathcal{N}_{sym} is the relative symmetry factor. The index $n \in \mathcal{G}_m(a, b, X)$ enumerates all the possible QCD final states which may contribute to the partonic process: these include all combinations of flavours $\{f_i\}_{i=1,\dots,m}$ consistent with the initial state (a, b) and the color-singlet X . In the following, we suppress the arguments of \mathcal{G}_m . The integration on the m -parton final-state phase space is instead defined as:

$$\langle \mathcal{F}_{a,b}[\mathcal{X}_m^n] \rangle := \mathcal{N}_{\text{avg}} \int d\Phi_m \mathcal{F}_m^{a,b}[\mathcal{X}_m^n] \quad (3.7)$$

where is the appropriate initial-state averaging factor. Then, we can rewrite Eq. 3.2-3.3 as:

$$2\hat{s} d\hat{\sigma}_{a,b}^{(0)} = \sum_{n \in \mathcal{G}_m} \langle \mathcal{F}_{a,b}[\mathcal{X}_m^n] \rangle \quad 2\hat{s} d\hat{\sigma}_{a,b}^R = \sum_{n \in \mathcal{G}_{m+1}} \langle \mathcal{F}_{a,b}[\mathcal{X}_{m+1}^n] \rangle \quad (3.8)$$

Soft and collinear singularities are isolated through operators acting on \mathcal{F} functions: S_i denotes the limits in which the parton i becomes soft, while C_{ij} that in which the partons i and j become collinear to each other. In particular, these operators extract only the leading asymptotic behaviour of \mathcal{F} which is non-integrable in $d=4$ dimensions, hence, if they act on quantities without non-integrable singularities, then they identically vanish (e.g. $S_i \equiv 0$ if i is a (anti)quark).

§3.1.1 Partonic sets

A delicate step is the determination of which final-state partons can become unresolved: indeed, in fixed-order perturbative QCD, the number of final-state hard partons cannot drop below the number of jets in the LO process. This means that at NLO no more than one parton can become unresolved, and this is ensured by the \mathcal{O} operators. In order to use symmetry arguments to minimize the number of unresolved partons that need to be considered, we can partition the set of final-state partons as:

$$\mathcal{X}_m^n = \mathcal{X}_m^n(g) \cup \mathcal{X}_m^n(q) \cup \mathcal{X}_m^n(\bar{q}) \cup \mathcal{X}_m^n(w) \cup \mathcal{X}_m^n(\bar{w})$$

which are respectively the subsets of final-state gluons, massless quarks, massless antiquarks, massive quarks and massive antiquarks. It is also useful to define the set of all massless partons:

$$\mathcal{H}_{m,0}^n \equiv \{a, b\} \cup \mathcal{X}_m^n(g) \cup \mathcal{X}_m^n(q) \cup \mathcal{X}_m^n(\bar{q}) \equiv \{a, b\} \cup \mathcal{H}_m^n$$

as we only consider massless initial-state partons. Note that $\mathcal{X}_m^n(q)$ and $\mathcal{X}_m^n(\bar{q})$ can be further partitioned into sets of definite massless quark flavours, and the same can be done with $\mathcal{X}_m^n(w)$ and $\mathcal{X}_m^n(\bar{w})$ with massive quark flavours.

For NLO real emissions we consider an additional parton, i.e. a final state \mathcal{X}_{m+1}^n with $n \in \mathcal{G}_{m+1}$. To extract soft singularities from Eq. 3.8, we first consider a partition of unity such that:

$$\sum_{i \in \mathcal{H}_{m+1}^n} \Delta^i = 1 \quad : \quad S_i \Delta^j = \delta_i^j \quad \wedge \quad C_{ij} \Delta^k = \begin{cases} 0 & i, j \neq k \\ 1 & i = k, j \in \{a, b\} \\ z_{k,j} & i = k, j \in \mathcal{H}_{m+1}^n - \{i\} \end{cases} \quad (3.9)$$

with $z_{k,j} \equiv E_k/(E_k + E_j)$. An explicit construction of these damping factors is given in §A.3. It is clear that a term multiplied by Δ^i vanishes if any parton other than i becomes unresolved, thus this partition allows for the extraction of single unresolved partons:

$$2\hat{s} d\hat{\sigma}_{a,b}^R = \sum_{n \in \mathcal{G}_{m+1}} \sum_{i \in \mathcal{H}_{m+1}^n} \langle \Delta^i \mathcal{F}_{ab}[\mathcal{X}_{m+1}^n] \rangle$$

We can relabel the potentially-unresolved parton i in each term as \mathbf{m}_f : then, for each allowed massless² flavour f , there are N_f equal terms, where N_f is the number of final-state partons of flavour f . We can account for the cancellation of these factors with symmetry factors defining $\mathcal{X}_m^n(\mathbf{m}_f) \equiv \mathcal{X}_{m+1}^n - \{\mathbf{m}_f\}$, thus imposing that the symmetry factors of $\mathcal{F}_{a,b}[\mathcal{X}_m^n(\mathbf{m}_f)]$ are determined ignoring \mathbf{m}_f (i.e. implicitly multiplying by N_f), but with the convention that the amplitude in $\mathcal{F}_{a,b}[\mathcal{X}_m^n(\mathbf{m}_f)]$ still contains the potentially-unresolved parton \mathbf{m}_f . Therefore:

$$\begin{aligned} 2\hat{s} d\hat{\sigma}_{a,b}^R = & \sum_{n \in \mathcal{G}_{m+1}(g)} \langle \Delta^{\mathbf{m}} \mathcal{F}_{a,b}[\mathcal{X}_m^n(\mathbf{m}_g)] \rangle + \sum_{\rho=1}^{n_f} \sum_{n \in \mathcal{G}_{m+1}(q_\rho)} \langle \Delta^{\mathbf{m}} \mathcal{F}_{a,b}[\mathcal{X}_m^n(\mathbf{m}_{q_\rho})] \rangle \\ & + \sum_{\rho=1}^{n_f} \sum_{n \in \mathcal{G}_{m+1}(\bar{q}_\rho)} \langle \Delta^{\mathbf{m}} \mathcal{F}_{a,b}[\mathcal{X}_m^n(\mathbf{m}_{\bar{q}_\rho})] \rangle \end{aligned} \quad (3.10)$$

where $\mathcal{G}_m(f) \subset \mathcal{G}_m : N_f \geq 1$ denotes the subset of possible final states with at least one parton of flavour f .

Now, the nested subtraction procedure introduced in [22] can be applied. In particular, for each term we rewrite the identity operator as:

$$\text{id} = S_{\mathbf{m}} + \sum_{i \in \mathcal{H}_{m,0}^n(\mathbf{m})} \bar{S}_{\mathbf{m}} C_{i\mathbf{m}} + \mathcal{O}_{\text{NLO}}^{\mathbf{m}} \quad \mathcal{O}_{\text{NLO}}^{\mathbf{m}} := \sum_{i \in \mathcal{H}_{m,0}^n(\mathbf{m})} \bar{S}_{\mathbf{m}} \bar{C}_{i\mathbf{m}} \omega^{\mathbf{m}i} \quad (3.11)$$

where we defined the notation for generic operators $\bar{\mathcal{O}} \equiv \text{id} - \mathcal{O}$ and introduced an angular partition of unity (see §A.3):

$$\sum_{i \in \mathcal{H}_{m,0}^n(\mathbf{m})} \omega^{\mathbf{m}i} = 1 \quad : \quad C_{j\mathbf{m}} \omega^{\mathbf{m}i} = \delta_j^i \quad (3.12)$$

There now remains to understand how the operators in Eq. 3.11 act on the \mathcal{F} functions and how the a parton set $\mathcal{X}_m^n(\mathbf{m})$ changes when \mathbf{m} effectively becomes unresolved.

²Massive partons cannot go unresolved, as they do not determine neither soft nor collinear singularities.

§3.1.2 Soft limits

§3.1.3 Collinear limits

§3.1.3.1 Soft-collinear limits

§3.1.4 Real operators

§3.2 Non-real corrections

§3.2.1 Virtual corrections

§3.2.2 Collinear renormalization

§3.3 Integrated counterterms

NSC SS with Massive Quarks

Appendices

Appendix A

Mathematical reference

§A.1 Phase-space parametrization

In dimensional regularization with $d = 4 - 2\epsilon$, we define the measure on the phase space of a parton i to be:

$$[dp_i] \equiv \frac{d^{d-1}p_i}{(2\pi)^{d-1}2E_i} \theta(E_{\max} - E_i) \quad (\text{A.1})$$

Note that E_{\max} is an upper bound on the energies of individual partons: it is an arbitrary parameter to be taken sufficiently large as to be greater or equal to the maximal energy that a final-state parton can reach.

This measure can be cast in a more useful form introducing a suitable parametrization of the phase space: in particular, given that $\mathbb{R}^n - \{\mathbf{0}\} \cong \mathbb{R}^+ \times \mathbb{S}^{n-1}$, it is convenient to introduce hyperspherical coordinates on the \mathbb{S}^{d-2} component of the phase space. In general, the **hyper-spherical measure** on \mathbb{S}^n is recursively defined as:

$$d\Omega_n = \sin^{n-1} \varphi \, d\varphi \, d\Omega_{n-1} \quad (\text{A.2})$$

Using Eq. A.2 (with $\sin \varphi \, d\varphi = d \cos \varphi$), we can express the measure $d^{d-1}p_i$ as:

$$d^{d-1}p_i = |\mathbf{p}_i|^{d-2} \, d|\mathbf{p}_i| \, \sin^{d-4} \varphi \, d \cos \varphi \, d\Omega_{d-2} \quad (\text{A.3})$$

As we are only interested in integrations on phase spaces of real unresolved partons, which can only be massless, we can use the on-shell condition $p_i^2 = 0$ to express $|\mathbf{p}_i| = E_i$, so that the phase-space measure becomes:

$$[dp_i] = \theta(E_{\max} - E_i) E_i^{d-3} dE_i \, \sin^{d-4} \varphi \, d \cos \varphi \, \frac{d\Omega_{d-2}}{2(2\pi)^{d-1}} \quad (\text{A.4})$$

with $E_i \in \mathbb{R}^+$ and $\varphi \in [0, \pi]$.

§A.1.1 Multi-particle phase space

When considering scattering processes, in general the final state is a multi-particle state, hence the measure on the final-state phase space must account for energy conservation too.

Given a $2 \rightarrow m$ scattering process with well-defined initial momenta p_A and p_B , then the differential cross-section is (see Chapter 4 of [7]):

$$d\sigma = \frac{1}{2E_a 2E_b |\mathbf{v}_a - \mathbf{v}_b|} \prod_{k=1}^m \int \frac{d^3p_k}{(2\pi)^3 2E_k} |\mathcal{A}(ab \rightarrow \mathcal{H})|^2 (2\pi)^4 \delta^{(4)}(p_a + p_b - \sum_{i=1}^m p_i) \quad (\text{A.5})$$

where $\mathcal{A}(ab \rightarrow \mathcal{H})$ is the amplitude of the scattering process and $\mathbf{v}_k \equiv \frac{\mathbf{p}_k}{E_k}$ is the velocity of the k^{th} particle.

As we are only interested in massless initial-state partons, in the center-of-mass (CM) frame $p_{a,b} = (E, \pm \mathbf{p})$, hence it is trivial to see that the flux factor in Eq. A.5 is just $2\hat{s} := 2(p_a + p_b)^2$. The differential cross-section can then be rewritten as:

$$d\sigma = \frac{1}{2\hat{s}} \int d\Phi_m |\mathcal{M}(ab \rightarrow \mathcal{H})|^2 \quad (\text{A.6})$$

where the **invariant m -body phase space measure** is defined as:

$$d\Phi_m \equiv \prod_{k=1}^m [dp_k] (2\pi)^4 \delta^{(4)}(p_a + p_b - \sum_{i=1}^m p_i) \quad (\text{A.7})$$

§A.2 Angular integrals

§A.3 Partitions of unity

To define a partition of unity such as Eq. 3.9, define $\mathcal{H}^i \equiv \mathcal{H}_{m+1}^n - \{i\}$ and introduce the function:

$$d^i \equiv \prod_{k \in \mathcal{H}^i} p_{k,\perp} \prod_{l < m \in \mathcal{H}^i} \rho_{lm} \quad (\text{A.8})$$

where $p_{k,\perp}$ is the transverse momentum of the parton k . Then, the partition is found as:

$$\Delta^i := \frac{d^i}{\sum_{j \in \mathcal{H}_{m+1}^n} d^j} \quad (\text{A.9})$$

These clearly provide a \mathcal{H}_{m+1}^n -partition of unity. To prove its properties, note that:

$$S_i d^j = \lim_{E_i \rightarrow 0} \prod_{k \in \mathcal{H}^i} p_{k,\perp} \prod_{l < m \in \mathcal{H}^i} \rho_{lm} = \begin{cases} 0 & i \neq j \\ d_j & i = j \end{cases}$$

Thus trivially $S_i \Delta^j = \delta_i^j$. The collinear limit is slightly more complex:

$$C_{ij} d^k = \lim_{\rho_{ij} \rightarrow 0} \prod_{s \in \mathcal{H}^i} p_{s,\perp} \prod_{l < m \in \mathcal{H}^i} \rho_{lm} = \begin{cases} 0 & i, j \neq k \\ d^k & i = k \neq j \end{cases}$$

The latter case has two possibilities: either $j \in \{a, b\}$ or $j \in \mathcal{H}^i$. Then, clearly $C_{ia} d^i = C_{ib} d^i = 1$, while if $j \in \mathcal{H}^i$:

$$C_{ij} \Delta^i = \frac{d^i}{d^i + d^j} = \left[1 + \frac{d^j}{d^i} \right]^{-1}$$

With explicit calculation:

$$\frac{d^j}{d^i} = \frac{p_{i,\perp}}{p_{j,\perp}} \frac{\rho_{1,j} \cdots \rho_{i-1,j} \rho_{i+1,j} \cdots \rho_{j-1,j} \rho_{j,j+1} \cdots \rho_{j,m+1}}{\rho_{1,i} \cdots \rho_{i-1,i} \rho_{i,i+1} \cdots \rho_{i,j-1} \rho_{i,j+1} \cdots \rho_{i,m+1}} = \frac{p_{i,\perp}}{p_{j,\perp}} = \frac{E_i}{E_j}$$

where we have used the fact that $\rho_{ik} \rightarrow \rho_{jk} \forall k \neq i, j$ as $\rho_{ij} \rightarrow 0$. This completes the proof. To construct the angular partition of unity in Eq. 3.12, we set $g_{kl} \equiv \rho_{kl}^{-1}$ and define the angular factors:

$$\omega^{mi} := \frac{g_{im}}{\sum_{j \in \mathcal{H}_{m,0}^n(\mathbf{m})} g_{jm}} \quad (\text{A.10})$$

These clearly provide a $\mathcal{H}_{m,0}^n(\mathbf{m})$ -partition of unity. Moreover:

$$C_{jm} \omega^{mi} = \lim_{\rho_{jm} \rightarrow 0} \frac{g_{im}}{\sum_{k \in \mathcal{H}_{m,0}^n(\mathbf{m})} g_{km}} = \left[\lim_{\rho_{jm} \rightarrow 0} \sum_{k \in \mathcal{H}_{m,0}^n(\mathbf{m})} \frac{\rho_{im}}{\rho_{km}} \right]^{-1} = \begin{cases} 1^{-1} & j = i \\ \infty^{-1} & j \neq i \end{cases} = \delta_j^i$$

where we made an abuse of notation. This completes the proof.

§A.4 Quadratic Casimir operators of $\text{SU}(n_c)$

To prove Eq. 2.16, first consider the fundamental representation \mathbf{n} of $\text{SU}(n_c)$. Then, contracting Eq. 2.15 with δ^{ab} (with $a, b = 1, \dots, n^2 - 1$, as they label the basis of $\mathfrak{su}(n_c)$):

$$C_2(\mathbf{n})n_c = \frac{1}{2}(n_c^2 - 1)$$

To compute the Casimir operator for the adjoint representation \mathbf{g} , consider the decomposition of the direct product of two representations:

$$\mathbf{r}_1 \otimes \mathbf{r}_2 = \bigoplus_i \mathbf{r}_i$$

In this representation $T_{\mathbf{r}_1 \otimes \mathbf{r}_2}^a = T_{\mathbf{r}_1}^a \otimes \text{id}_{\mathbf{r}_2} + \text{id}_{\mathbf{r}_1} \otimes T_{\mathbf{r}_2}^a$, and it acts on tensor objects Ξ_{pq} whose first index transforms according to \mathbf{r}_1 and the second index according to \mathbf{r}_2 . Recalling that $\text{tr } T^a = 0$:

$$\begin{aligned} \text{tr}(T_{\mathbf{r}_1 \otimes \mathbf{r}_2}^a)^2 &= \text{tr}((T_{\mathbf{r}_1}^a)^2 \otimes \text{id}_{\mathbf{r}_2} + 2T_{\mathbf{r}_1}^a \otimes T_{\mathbf{r}_2}^a + \text{id}_{\mathbf{r}_1} \otimes (T_{\mathbf{r}_2}^a)^2) \\ &= \text{tr}(C_2(\mathbf{r}_1) \text{id}_{\mathbf{r}_1} \otimes \text{id}_{\mathbf{r}_2}) + \text{tr}(C_2(\mathbf{r}_2) \text{id}_{\mathbf{r}_1} \otimes \text{id}_{\mathbf{r}_2}) = (C_2(\mathbf{r}_1) + C_2(\mathbf{r}_2))n_{\mathbf{r}_1}n_{\mathbf{r}_2} \end{aligned}$$

However, by the decomposition above:

$$\text{tr}(T_{\mathbf{r}_1 \otimes \mathbf{r}_2}^a)^2 = \sum_i C_2(\mathbf{r}_i)n_{\mathbf{r}_i}$$

Consider $\mathbf{n} \otimes \mathbf{n}^*$, where \mathbf{n}^* is the complex conjugate of the fundamental representation (for complex representations, \mathbf{r} and \mathbf{r}^* are generally inequivalent representations): then Ξ_{pq} contains a term proportional to the invariant δ_{pq} , while the other $n_c^2 - 1$ independent components transform as a general $n_c \times n_c$ traceless tensor, i.e. under the adjoint representation of $\text{SU}(n_c)$ (as of Eq. 2.12-2.13), thus $\mathbf{n} \otimes \mathbf{n}^* = \mathbf{1} \oplus \mathbf{g}$ and the above identity becomes:

$$(C_2(\mathbf{1}) + C_2(\mathbf{g}))(n_c^2 - 1) = (C_2(\mathbf{n}) + C_2(\mathbf{n}^*))n_c^2$$

Using $C_2(\mathbf{1}) = 0$ (as all generators are trivially zero) and $C_2(\mathbf{n}^*) = C_2(\mathbf{n})$:

$$C_2(\mathbf{g})(n_c^2 - 1) = \frac{n_c^2 - 1}{n_c} n_c^2$$

which completes the proof.

Appendix B

Collection of relevant equations

In this Appendix, we provide definitions of relevant objects used in this work. To simply various formulas, we use a notation analogous to [25]:

$$\begin{aligned} \bar{z} &\equiv 1 - z & \mathcal{D}_n(z) &\equiv \left[\frac{\log^n(1 - z)}{1 - z} \right]_+ \\ L_i &\equiv \log \frac{E_{\max}}{E_i} & \mathcal{L}_i &\equiv \log \frac{2E_i}{\mu_R} & L_{\max} &\equiv \log \frac{2E_{\max}}{\mu_R} \end{aligned} \quad (\text{B.1})$$

§B.1 Useful constants

Denoting the colour-charge operators \mathbf{T}_i , with the conventional normalization $T_R = \frac{1}{2}$ for $\text{SU}(n_c)$, the squares of these operators are the quadratic Casimir operators of the corresponding representations:

$$\mathbf{T}_q^2 = \mathbf{T}_{\bar{q}}^2 = C_F = \frac{n_c^2 - 1}{2n_c} \quad \mathbf{T}_g^2 = C_A = n_c \quad (\text{B.2})$$

The quark and gluon anomalous dimensions are:

$$\gamma_q = \frac{3}{2}C_F \quad \gamma_g = \frac{11}{6}C_A - \frac{2}{3}T_R n_q \quad (\text{B.3})$$

where n_q is the number of active flavours.

The strong coupling is renormalized in the $\overline{\text{MS}}$ scheme, so that the bare and running couplings are related by:

$$\alpha_{s,b} S_\epsilon = \alpha_s(\mu_R^2) \mu_R^{2\epsilon} \left[1 - \frac{\alpha_s(\mu_R^2)}{2\pi} \frac{\beta_0}{\epsilon} + o(\alpha_s^2) \right] \quad (\text{B.4})$$

where $S_\epsilon \equiv (4\pi)^\epsilon e^{-\gamma_E \epsilon}$ and:

$$\beta_0 = \frac{11}{6}C_A - \frac{2}{3}T_R n_q = \gamma_g \quad (\text{B.5})$$

It is convenient to define a quantity related to the running coupling:

$$[\alpha_s] \equiv \frac{\alpha_s(\mu_R^2)}{2\pi} \frac{e^{\gamma_E \epsilon}}{\Gamma(1 - \epsilon)} \quad (\text{B.6})$$

§B.2 Splitting functions

THIS TO BE PARTIALLY MOVED TO SECTION ON COLLINEAR SINGULARITIES

Consider the final-state splitting process $[i\mathbf{m}]^* \rightarrow i(z) + \mathbf{m}(1-z)$, where i and \mathbf{m} are two partons of flavours f_i and $f_{\mathbf{m}}$ and $[i\mathbf{m}]$ is the corresponding clustered parton of flavour $f_{[i\mathbf{m}]}$. Recall that, given the interaction vertices determined by the QCD Lagrangian Eq. 2.11 (see FIGURE), a gluon clustered with any type of parton preserves the latter's flavours, while a quark clustered with an antiquark gives a gluon.

The energy fraction carried by the parton i is defined as $z \equiv 1 - E_{\mathbf{m}}/E_{[i\mathbf{m}]}$. As a consequence, the parton \mathbf{m} carries an energy fraction $1 - z$. Denoting the spin-averaged final-state splitting functions as $P_{f_{[i\mathbf{m}]}f_i}(z)$, they read:

$$P_{qq}(z) = C_F \left[\frac{1+z^2}{1-z} - \epsilon(1-z) \right] \quad (\text{B.7})$$

$$P_{qg}(z) = C_F \left[\frac{1-(1-z)^2}{z} - \epsilon z \right] \equiv P_{qg}(1-z) \quad (\text{B.8})$$

$$P_{gq}(z) = T_R \left[1 - \frac{2z(1-z)}{1-\epsilon} \right] \quad (\text{B.9})$$

$$P_{gg}(z) = 2C_A \left[\frac{z}{1-z} + \frac{1-z}{z} + z(1-z) \right] \quad (\text{B.10})$$

Now, consider instead the initial-state splitting process $i \rightarrow [i\mathbf{m}]^* + \mathbf{m}$, where i and \mathbf{m} are respectively an ingoing and outgoing parton, while the clustered parton $[i\mathbf{m}]^*$ enters the hard scattering process. In this case, we define the z variable as $z \equiv 1 - E_{\mathbf{m}}/E_i$. The spin- and color-averaged initial-state splitting functions, denoted as $P_{f_{[i\mathbf{m}]}f_i,i}(z)$, are:

$$P_{qq,i} = -zP_{qq}(1/z) \equiv P_{qq}(z) \quad (\text{B.11})$$

$$P_{qg,i} = \left[\frac{2n_c}{2(1-\epsilon)(n_c^2-1)} \right] zP_{qg}(1/z) \equiv P_{qg}(z) \quad (\text{B.12})$$

$$P_{gq,i} = \left[\frac{2(1-\epsilon)(n_c^2-1)}{2n_c} \right] zP_{gq}(1/z) \equiv P_{gq}(z) \quad (\text{B.13})$$

$$P_{gg,i} = -zP_{gg}(1/z) \equiv P_{gg}(z) \quad (\text{B.14})$$

Finally, the LO Altarelli-Parisi splitting kernels are:

$$\hat{P}_{qq}^{(0)}(z) = C_F \left[2\mathcal{D}_0(z) - (1+z) + \frac{3}{2}\delta(1-z) \right] \quad (\text{B.15})$$

$$\hat{P}_{qg}^{(0)}(z) = T_R \left[(1-z)^2 + z^2 \right] \quad (\text{B.16})$$

$$\hat{P}_{gq}^{(0)}(z) = C_F \left[\frac{1+(1-z)^2}{z} \right] \quad (\text{B.17})$$

$$\hat{P}_{gg}^{(0)}(z) = 2C_A \left[\mathcal{D}_0(z) + z(1-z) + \frac{1}{z} - 2 \right] + \beta_0\delta(1-z) \quad (\text{B.18})$$

All these splitting functions and kernels can be found in [14].

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