



UNIVERSITÀ DEGLI STUDI DI MILANO
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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 [26–28], 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: on the contrary, 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, although still not excluded, their frequent production at the LHC is hardly possible. The lack of any observation of BSM physics at the LHC has sparked a change in the research paradigm in High-Energy Particle Physics. Substantial further increase in the energy of colliding particles at the LHC (or anywhere else) is currently not feasible, hence 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.

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

Systematic searches for BSM physics through precision studies at hadron colliders are difficult 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 (§2.2.1 for details).

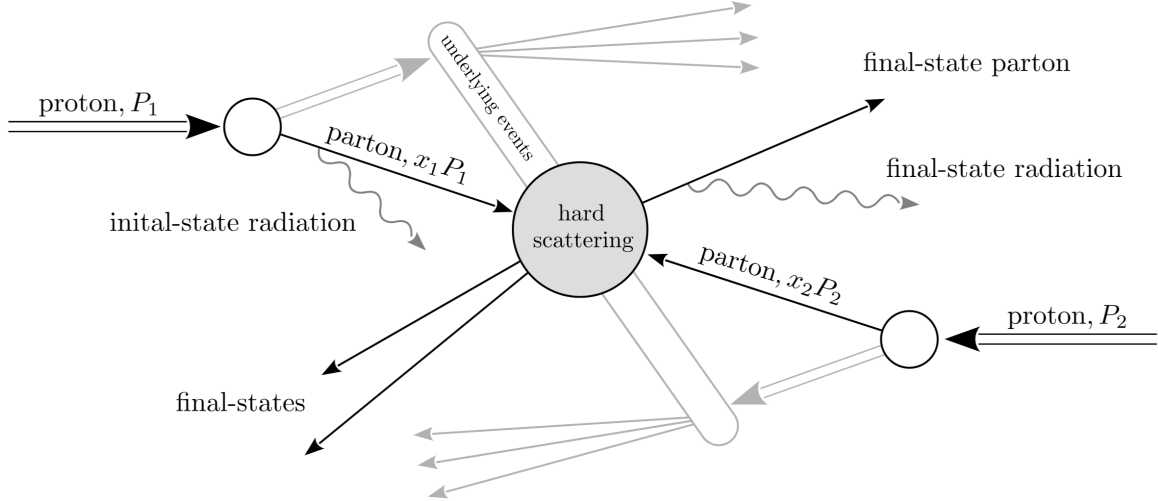


Figure 1.1: Schematics of hard hadronic scattering. Due to asymptotic freedom, individual partons can be assumed to be free particles, so that their (hard) scattering can be computed via perturbative QCD. Initial- and final-state radiation accounts for beyond-leading-order effects. Figure from [10].

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-principle description is made possible for a particular class of processes: hard scattering processes.

Even though hard scattering processes have a lower probability of happening, with respect, for example, to elastic scattering processes, they are of great interest to modern particle physics. To understand why, a remarkable property of non-Abelian gauge theory needs to be stated: **asymptotic freedom**. The evolution of the coupling $\alpha(\mu^2)$ of a quantum field theory 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 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, which are characterized by a large momentum transfer: this kind of 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

Theoretical predictions for hard hadronic scattering are based on the factorization theorem [11], which states that hadronic cross-sections can be computed from partonic cross-sections as:

$$d\sigma_{h_1, h_2}(P_1, P_2) = \sum_{a, b} \int_{[0,1]^2} d\xi_1 d\xi_2 f_a^{(h_1)}(\xi_1, \mu_F^2) f_b^{(h_2)}(\xi_2, \mu_F^2) d\hat{\sigma}_{a, b}(\xi_1 P_1, \xi_2 P_2, \alpha_s, \mu^2, \mu_F^2) \quad (1.3)$$

Here, the two scattering hadrons h_1, h_2 have momenta P_1, P_2 , while the scattering partons a, b have momentum fractions $x_1 P_1, x_2 P_2$. The factorization scale μ_F is taken to be equal to the renormalization scale μ for the rest of this work.

The link between hadron-scale physics and parton-scale physics is given by **parton distribution functions** (PDFs): in general, $f_a^{(h)}(x)$ is the numerical probability of finding a parton a inside the hadron h with a definite energy fraction $x : p_a = x P_h$, 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 encapsulate 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 flow 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, found introducing a reference scale Q :

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

For e.g. $\alpha_s(m_Z^2) \approx 0.118$ [14]. It is customary to introduce a QCD scale $\Lambda_{\text{QCD}} \approx 300 \text{ MeV}$, so that:

$$\alpha_s(\mu^2) = \frac{1}{2\frac{\beta_0}{4\pi} \log \frac{\mu^2}{\Lambda_{\text{QCD}}^2}} \quad (1.5)$$

This expression shows that $\mu \gg \Lambda_{\text{QCD}}$ is the perturbative region, where asymptotic freedom makes α_s small enough for perturbative techniques. On the other hand, for $\mu \rightarrow \Lambda_{\text{QCD}}$ 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).

As illustrated in Fig. 1.2, the hard scattering process occurs at high energy $Q \gg \Lambda_{\text{QCD}}$ (typically $Q \sim 1 \text{ TeV}$ at the LHC), resulting in jets which are unaffected by non-perturbative QCD, as 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.

§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:

$$d\hat{\sigma}_{a,b}(p_1, p_2) = \sum_{n \in \mathbb{N}_0} d\hat{\sigma}_{a,b}^{(n)}(p_1, p_2) \quad (1.6)$$

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

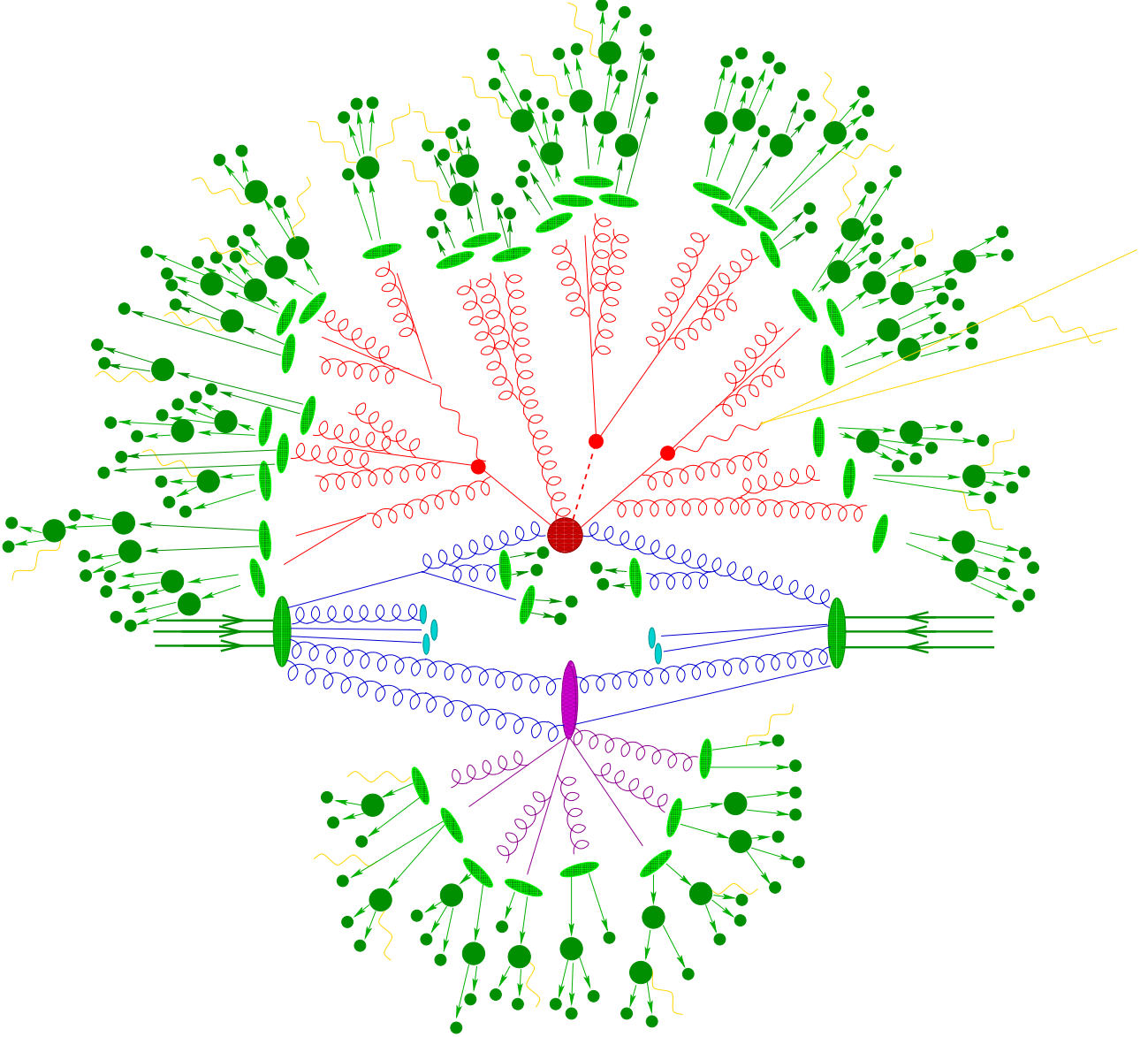
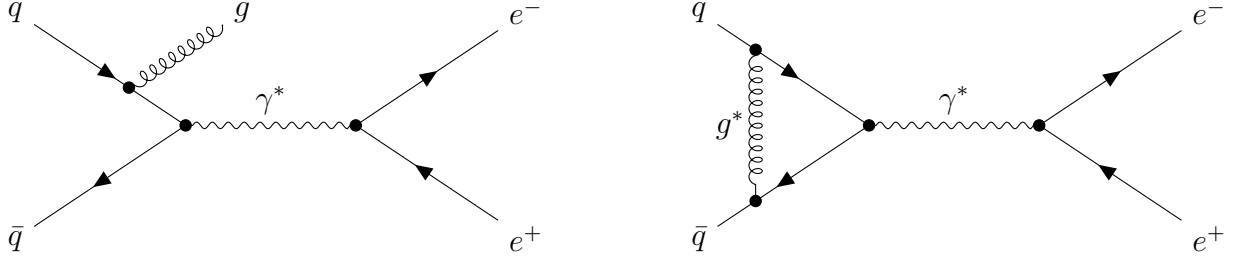


Figure 1.2: Hadronization of jets produced in a hard hadronic scattering. Incoming hadrons produce initial-state radiation (blue), which determines two hard scattering events (red and purple blobs): these scatterings give rise to partonic jets (red and purple) which undergo hadronization (light green blobs), eventually decaying into heavy hadrons (dark green blobs) and soft radiation (yellow). Figure from [13].

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:

$$d\hat{\sigma}_{a,b}^{(1)}(p_1, p_2) = d\hat{\sigma}_{a,b}^R(p_1, p_2) + d\hat{\sigma}_{a,b}^V(p_1, p_2) + d\hat{\sigma}_{a,b}^{\text{pdf}}(p_1, p_2) \quad (1.7)$$

where $d\hat{\sigma}_{a,b}^R$ and $d\hat{\sigma}_{a,b}^V$ 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.

§1.2 Singularities in QCD amplitudes

show how divergences arise in the soft and collinear limits for the real case

cite UV-singularities for the virtual case (link to section about renormalization), then say that IR-singularities cancel when combined with real ones due to the kinoshita-lee-nauenberg theorem

prove the general form of collinear pdf renormalization counterterms

Preliminaries

§2.1 Renormalization scheme

The computation of NLO corrections to scattering processes often involves diverging loop amplitudes. In order to obtain finite results from these divergences, a renormalization scheme must be implemented.

As the generalized Catani's formula for virtual corrections is provided in [15] in a charge-unrenormalized (but mass-renormalized) way, it is necessary to carry out the renormalization procedure explicitly. To this end, we formally state the renormalization scheme adopted in this work.

§2.1.1 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, a regularization scheme first introduced by 't Hooft and Veltman in [16].

In general, the dimensional regularization scheme consists in the analytic continuation of loop momenta to $d = 4 - 2\epsilon$ dimensions, with $\epsilon \in \mathbb{C} : \Re \epsilon < 0$. This procedure turns loop integrals into meromorphic¹ 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 when $d \notin \mathbb{N}$.

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 outlined in [17].

¹Given an open set $D \subset \mathbb{C}$, then $f : D \rightarrow \mathbb{C}$ is *meromorphic* if it is holomorphic on $D - P$, where $P \subset D$ is a set of isolated points called *poles*. Recall that a function $f : D \rightarrow \mathbb{C}$ is *holomorphic* on D if it is complex differentiable at every point in D .

§2.1.2 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 $\alpha_s(\mu^2)$ 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:

$$\alpha_{s,b} S_\epsilon = \alpha_s(\mu^2) \mu^{2\epsilon} \left[1 - \frac{\alpha_s(\mu^2)}{2\pi} \frac{\beta_0}{\epsilon} + o(\alpha_s^2) \right] \quad (2.1)$$

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

$$S_\epsilon \equiv (4\pi)^\epsilon e^{-\gamma_E \epsilon} \quad (2.2)$$

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

$$\beta_0 := \frac{11}{6} C_A - \frac{2}{3} T_R n_q \quad (2.3)$$

where C_A and T_R are linked to the gauge group $\text{SU}(n_c)$ (see §2.2) and n_q is the number of active quark flavours at the considered energy scale².

An important clarification about the dimensionality of $\alpha_{s,b}$ and α_s is needed, due to the presence of $\mu^{2\epsilon}$ in Eq. 2.1. Consider the QCD Lagrangian, i.e. a Yang-Mills Lagrangian with gauge group $\text{SU}(n_c)$ and n quark species (see e.g. Chapter 15 of [19], or §2.2.1):

$$\mathcal{L} = -\frac{1}{4} F_{\mu\nu}^a F_a^{\mu\nu} + \bar{\Psi} (i \not{D} - m) \Psi \quad (2.4)$$

with covariant derivative and field-strength tensor defined as:

$$D_\mu := \partial_\mu - ig A_\mu^a T_a \quad F_{\mu\nu}^a := \partial_\mu A_\nu^a - \partial_\nu A_\mu^a + g f^{abc} A_\mu^b A_\nu^c \quad (2.5)$$

where $\{T_a\}_{a=1,\dots,n_c^2-1} \subset \mathbb{C}^{n \times n}$ is a Hermitian representation of $\mathfrak{su}(n_c)$ and Ψ is a n -spinor. Recall that the structure constants $f^{abc} \in \mathbb{R}$ of $\mathfrak{su}(n_c)$ are $f^{abc} = \epsilon^{abc}$.

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 Lagrangian 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. 2.1 we chose to extract the mass dimension from α_s .

In general, we consider amplitudes \mathcal{M}_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

²Out of $n = n_f + n_F$ total quark flavours (n_f massless and n_F massive quark flavours), we generally consider an energy scale such that $n_q = n_f$, unless otherwise specified.

understood and not explicitly shown. The $\overline{\text{MS}}$ -renormalized amplitude has the following perturbative expansion in α_s :

$$\mathcal{M}_m(\alpha_s(\mu^2), \mu^2; \{p\}) = \left(\frac{\alpha_s(\mu^2)}{2\pi} \right)^q \left[\mathcal{M}_m^{(0)}(\mu^2; \{p\}) + \frac{\alpha_s(\mu^2)}{2\pi} \mathcal{M}_m^{(1)}(\mu^2; \{p\}) + o(\alpha_s^2) \right] \quad (2.6)$$

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

§2.2 Colour-space formalism

We consider a generalized QCD with gauge group $\text{SU}(n_c)$, with n_c colours and $n = n_f + n_F$ quark flavours (see footnote 2). To handle the colour structure of QCD amplitudes, we adopt the colour-space formalism as in [20].

§2.2.1 Gauge theories

In order to better understand the colour-space formalism, it is useful to state how a general gauge theory is defined, and then analyze the specific case of a $\text{SU}(n_c)$ gauge theory.

§2.2.1.1 Yang-Mills Lagrangian

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 [21], with the aim of studying isotopic gauge invariance for the nucleon, and then generalized by Utiyama in [22]. 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:

$$\Psi(x) = \begin{pmatrix} \psi_1(x) \\ \vdots \\ \psi_n(x) \end{pmatrix} \quad (2.7)$$

As a gauge group, consider a d -dimensional Lie group G : in particular, take G to be a simply-connected Lie group, so that each element can be expressed via the exponential map, and compact too, 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:

$$\Psi(x) \mapsto V(x)\Psi(x) \quad V(x) := \exp[i\theta_a(x)T^a] \quad (2.8)$$

where the Lie parameters $\{\theta_a(x)\}_{a=1,\dots,d} \subset \mathcal{C}^\infty(\mathbb{R}^{1,3})$ so 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. 2.8 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. 2.8. 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:

$$U(y, x) \mapsto V(y)U(y, x)V^\dagger(x) \quad (2.9)$$

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:

$$n^\mu D_\mu \Psi(x) := \lim_{\varepsilon \rightarrow 0} \frac{1}{\varepsilon} [\Psi(x + \varepsilon n) - U(x + \varepsilon n, x)\Psi(x)] \quad (2.10)$$

where $U(y, x)$ is defined in Eq. 2.9. 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:

$$U(x + \varepsilon n, x) = I_n + ig\varepsilon n^\mu A_\mu^a(x)T_a + o(\varepsilon^2) \quad (2.11)$$

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 to express the covariant derivative as (directly from Eq. 2.10):

$$D_\mu = \partial_\mu - igA_\mu^a T_a \quad (2.12)$$

It is straightforward to show that $D_\mu \Psi$ transforms in the same way as Ψ .

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

$$[D_\mu, D_\nu] = -igF_{\mu\nu}^a T_a \quad (2.13)$$

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

$$F_{\mu\nu}^a := \partial_\mu A_\nu^a - \partial_\nu A_\mu^a + gf^{abc}A_\mu^b A_\nu^c \quad (2.14)$$

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 the following theorem holds: any globally-symmetric function of Ψ , $F_{\mu\nu}^a$ and their covariant derivatives is also locally-symmetric, i.e. gauge-invariant (see Chapter 15 of [7]).

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

$$\text{tr}\{(F_{\mu\nu}^a T_a)^2\} = 2F_{\mu\nu}^a F_a^{\mu\nu} \quad (2.15)$$

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

$$\mathcal{L}_{\text{YM}} = -\frac{1}{4}F_{\mu\nu}^a F_a^{\mu\nu} \quad (2.16)$$

To account for fermions interacting with the gauge field (i.e. the connection $A_\mu^a(x)$), the Dirac Lagrangian with minimal coupling is added:

$$\mathcal{L} = -\frac{1}{4}F_{\mu\nu}^a F_a^{\mu\nu} + \bar{\Psi} (i\not{D} - m) \Psi \quad (2.17)$$

§2.2.1.2 Gauge group $SU(n)$

The $SU(n)$ group is the group of unitary transformations of n -dimensional complex vectors. Its (faithful) fundamental representation thus is:

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

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

$$T^a = T^{a\dagger} \quad (2.18)$$

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 $t = 0$:

$$\text{tr} T^a = 0 \quad (2.19)$$

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

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:

$$(T_{\text{ad}}^b)_{ac} \equiv \bar{T}_{ac}^b = i f^{abc} \quad (2.20)$$

which, in the case of $SU(n)$, are $f^{abc} = \epsilon^{abc}$. Indeed, it can be shown by the Jacobi identity that the structure constants satisfy the Lie algebra. Moreover, since the structure constants are real, the adjoint representation is always a real representation: the adjoint representation of $SU(n)$ has degree $n^2 - 1$.

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

$$T_{\mathbf{r}}^a T_{\mathbf{r}}^a = C_2(\mathbf{r}) I_{n_{\mathbf{r}}} \quad (2.21)$$

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

$$C_{\mathbf{F}} \equiv C_2(\mathbf{n}) = T_{\mathbf{R}} \frac{n^2 - 1}{n} \quad C_{\mathbf{A}} \equiv C_2(\mathbf{g}) = 2T_{\mathbf{R}} n \quad (2.22)$$

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:

$$\text{tr}(T_{\mathbf{n}}^a T_{\mathbf{n}}^b) = T_{\mathbf{R}} \delta^{ab} \quad (2.23)$$

§2.2.2 QCD amplitudes

The m external partons in the amplitude \mathcal{M}_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. 2.5 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, being these 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-defined³.

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

$$\mathcal{M}_m^{\{c_1, \dots, c_m\}, \{s_1, \dots, s_m\}}(\{p_1, \dots, p_m\}) \equiv \langle \{c_1, \dots, c_m\}, \{s_1, \dots, s_m\} | \mathcal{M}_m(\{p_1, \dots, p_m\}) \rangle \quad (2.24)$$

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:

$$|\mathcal{M}_m|^2 = \langle \mathcal{M}_m | \mathcal{M}_m \rangle \quad (2.25)$$

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:

$$\langle c_1, \dots, c_i, \dots, c_m | T_i^a | b_1, \dots, b_i, \dots, b_m \rangle = \delta_{c_1, b_1} \dots T_{c_i b_i}^a \dots \delta_{c_m, b_m} \quad (2.26)$$

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 colour-charge operators is easily determined. First of all, we set:

$$\mathbf{T}_i \cdot \mathbf{T}_j \equiv \sum_{a=1}^{n_c^2-1} T_i^a T_j^a \quad (2.27)$$

Then, by the action Eq. 2.26, it is clear that charges associated to different partons commute, i.e.:

$$\mathbf{T}_i \cdot \mathbf{T}_j = \mathbf{T}_j \cdot \mathbf{T}_i \quad \forall i \neq j \in \{1, \dots, m\} \quad (2.28)$$

³Given two \mathbb{K} -vector spaces V, W , the set of all \mathbb{K} -linear functions $V \rightarrow W$ is denoted by $\text{Hom}(V, W)$; for finite-dimensional spaces $\dim_{\mathbb{K}} \text{Hom}(V, W) = \dim_{\mathbb{K}} V \cdot \dim_{\mathbb{K}} W$. The *dual space* is defined as $V^* := \text{Hom}(V, \mathbb{K})$. If V is finite-dimensional, given a basis $\{v_i\}_{i=1, \dots, n} \subset V$, with $n = \dim_{\mathbb{K}} V$, then a basis $\{\omega^1, \dots, \omega^n\} \subset V^*$ 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. 2.21,2.27:

$$\mathbf{T}_i^2 = C_i \text{id}_{\mathcal{H}_c} \quad (2.29)$$

with $C_i \equiv C_F$ if i is a quark/antiquark and $C_i \equiv C_A$ if it is a gluon. Finally, as each vector $|\mathcal{M}_m\rangle$ is a colour-singlet, colour conservation implies:

$$\sum_{i=1}^m \mathbf{T}_i |\mathcal{M}_m\rangle = 0 \quad (2.30)$$

This allows to partially (or fully, if $m = 2$ or $m = 3$, as in Appendix A of [20]) factorize the colour-charge algebra in terms of quadratic Casimir operators.

Chapter 3

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 [23]): this makes it possible for us to only manipulate partonic cross-sections, as the hadronic cross-section for the considered process can be factorized in terms of partonic cross-sections via the parton distribution functions (PDFs):

$$d\sigma(P_1, P_2) = \sum_{a,b} \int_{[0,1]^2} d\xi_1 d\xi_2 f_a(\xi_1, \mu_F^2) f_b(\xi_2, \mu_F^2) d\hat{\sigma}_{a,b}(\xi_1 P_1, \xi_2 P_2, \alpha_s(\mu^2), \mu^2, \mu_F^2) \quad (3.2)$$

where μ is the renormalization scale, μ_F is the factorization scale (which is set to $\mu_F = \mu$ from now on) and the sum runs over all initial-state massless partons a and b which contribute to the production of the considered final state.

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 expand the partonic cross-section as a power series in $\alpha_s(\mu^2)$:

$$d\hat{\sigma}_{a,b}(p_1, p_2) = \sum_{n \in \mathbb{N}_0} d\hat{\sigma}_{a,b}^{(n)}(p_1, p_2) \quad (3.3)$$

where each term is $d\hat{\sigma}^{(n)} \sim \alpha_s^{n_0+n}$, with $n_0 \in \mathbb{N}$ giving the LO-dependence on $\alpha_s(\mu^2)$. Each term of this expansion will have a different multiplicity of the final state, due to the increasing number of corrections and their different nature. At leading-order (see §A.1.1):

$$d\hat{\sigma}_{a,b}^{(0)}(p_1, p_2) := \frac{\mathcal{N}}{2\hat{s}} \int d\Phi_n |\mathcal{M}_m^{(0)}(p_1, p_2, p_X, p_{\mathcal{H}})|^2 \mathcal{O}_m(p_{\mathcal{H}}, p_X) \quad (3.4)$$

where $\hat{s} \equiv 2p_1 \cdot p_2$ is the partonic CM energy squared, \mathcal{H} is the set of all final-state partons (with $p_{\mathcal{H}}$ its total 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.

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.

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 parton 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 $\mathcal{O}_m \rightarrow 0$.

Non-trivial combinations of different-multiplicity final states emerges already at next-to-leading order:

$$d\hat{\sigma}_{a,b}^{(1)}(p_1, p_2) = d\hat{\sigma}_{a,b}^R(p_1, p_2) + d\hat{\sigma}_{a,b}^V(p_1, p_2) + d\hat{\sigma}_{a,b}^C(p_1, p_2) \quad (3.5)$$

where:

$$d\hat{\sigma}_{a,b}^R(p_1, p_2) := \frac{\mathcal{N}}{2\hat{s}} \int d\Phi_{m+1} \left| \mathcal{M}_{m+1}^{(0)}(p_1, p_2, p_X, p_{\mathcal{H}}) \right|^2 \mathcal{O}_{m+1}(p_{\mathcal{H}}, p_X) \quad (3.6)$$

$$d\hat{\sigma}_{a,b}^V(p_1, p_2) := \frac{\mathcal{N}}{2\hat{s}} \int d\Phi_m 2\Re \langle \mathcal{M}_m^{(0)} | \mathcal{M}_m^{(1)} \rangle \mathcal{O}_m(p_{\mathcal{H}}, p_X) \quad (3.7)$$

$$d\hat{\sigma}_{a,b}^C(p_1, p_2) := \frac{\alpha_s(\mu^2)}{2\pi} \frac{1}{\epsilon} \sum_c \int_0^1 \frac{dz}{z} \left[\hat{P}_{c,a}^{(0)}(z) d\hat{\sigma}_{c,b}^{(0)}(zp_1, p_2) + \hat{P}_{c,b}^{(0)}(z) d\hat{\sigma}_{a,c}^{(0)}(p_1, zp_2) \right] \quad (3.8)$$

In Eq. 3.6 \mathcal{H} contains $m+1$ partons, while in Eq. 3.7 it only contains m partons. The Altarelli-Parisi splitting kernels are listed in §B.2, and proof of Eq. 3.8 is provided in SECTION.

The rest of this chapter is devoted to the extrapolation of IR-singularities from Eq. 3.6-3.8, proving their cancellation and providing the associated 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.

Observation A.1.1 (Hyperspherical coordinates)

In general, \mathbb{S}^n can be described as a surface embedded in \mathbb{R}^{n+1} , defined by:

$$\sum_{i=1}^{n+1} x_i^2 = 1 \quad (\text{A.2})$$

Therefore, \mathbb{S}^n can be parametrized by **hyperspherical coordinates** $\{\varphi_1, \dots, \varphi_{n-1}, \varphi_n\} \subset [0, \pi]^{n-1} \times [0, 2\pi)$ as:

$$\begin{aligned} x_1 &= \cos \varphi_1 \\ x_2 &= \sin \varphi_1 \cos \varphi_2 \\ x_3 &= \sin \varphi_1 \sin \varphi_2 \cos \varphi_3 \\ &\vdots \\ x_{n-1} &= \sin \varphi_1 \dots \sin \varphi_{n-2} \cos \varphi_{n-1} \\ x_n &= \sin \varphi_1 \dots \sin \varphi_{n-2} \sin \varphi_{n-1} \cos \varphi_n \\ x_{n+1} &= \sin \varphi_1 \dots \sin \varphi_{n-2} \sin \varphi_{n-1} \sin \varphi_n \end{aligned} \quad (\text{A.3})$$

It is then possible to define the hyperspherical measure on \mathbb{S}^n :

$$d\Omega_n \equiv \sin^{n-1} \varphi_1 \sin^{n-2} \varphi_2 \dots \sin^2 \varphi_{n-2} \sin \varphi_{n-1} d\varphi_1 d\varphi_2 \dots d\varphi_{n-2} d\varphi_{n-1} d\varphi_n \quad (\text{A.4})$$

It is clear that this is a recursive relation, as:

$$d\Omega_n = \sin^{n-1} \varphi \, d\varphi \, d\Omega_{n-1} \quad (\text{A.5})$$

Using Eq. A.5 (with $\sin \varphi \, d\varphi = d \cos \varphi$), we can express the measure $d^{d-1}p_i$ as:

$$d^{d-1}p_i = |\mathbf{p}_i|^{d-2} \, d|\mathbf{p}_i| \, \sin^{d-4} \varphi \, d \cos \varphi \, d\Omega_{d-2} \quad (\text{A.6})$$

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:

$$[dp_i] = \theta(E_{\max} - E_i) E_i^{d-3} dE_i \, \sin^{d-4} \varphi \, d \cos \varphi \, \frac{d\Omega_{d-2}}{2(2\pi)^{d-1}} \quad (\text{A.7})$$

with $E_i \in \mathbb{R}_0^+$ 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.

Theorem A.1.1 (Scattering cross-section)

Given a $2 \rightarrow m$ scattering process with well-defined initial momenta $p_{\mathcal{A}}$ and $p_{\mathcal{B}}$, then the **differential cross-section** is:

$$d\sigma = \frac{1}{2E_{\mathcal{A}}2E_{\mathcal{B}} |\mathbf{v}_{\mathcal{A}} - \mathbf{v}_{\mathcal{B}}|} \prod_{k=1}^m \int \frac{d^3p_k}{(2\pi)^3 2E_k} |\mathcal{M}(\mathcal{AB} \rightarrow \{f\})|^2 (2\pi)^4 \delta^{(4)}(p_{\mathcal{A}} + p_{\mathcal{B}} - \sum_{i=1}^m p_i) \quad (\text{A.8})$$

where $\mathcal{M}(\mathcal{AB} \rightarrow \{f\})$ is the matrix element of the scattering process and $\mathbf{v}_k \equiv \frac{\mathbf{p}_k}{E_k}$ is the velocity of the k^{th} particle.

Proof. See Chapter 4 of [7]. □

As we are only interested in massless initial-state partons, in the center-of-mass (CM) frame $p_{\mathcal{A},\mathcal{B}} = (E, \pm \mathbf{p})$, hence it is trivial to see that the flux factor in Eq. A.8 is just $2\hat{s} := 2(p_{\mathcal{A}} + p_{\mathcal{B}})^2$. The differential cross-section can then be rewritten as:

$$d\sigma = \frac{1}{2\hat{s}} \int d\Phi_m |\mathcal{M}(\mathcal{AB} \rightarrow \{f\})|^2 \quad (\text{A.9})$$

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

$$d\Phi_m \equiv \prod_{k=1}^m [dp_k] (2\pi)^4 \delta^{(4)}(p_{\mathcal{A}} + p_{\mathcal{P}} - \sum_{i=1}^m p_i) \quad (\text{A.10})$$

§A.2 Angular integrals

Appendix B

Collection of relevant equations

In this Appendix, we provide definitions of relevant objects used in this work. To simplify various formulas, we use a notation analogous to [24]:

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

§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:

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

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 coupling constant:

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

§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. 2.17 (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 [25].

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