

**TECHNISCHE
UNIVERSITÄT
DRESDEN**

On the Treatment of Colour-Charged Resonances in Precision Calculations of Monte Carlo Generators

Dissertation

zur Erlangung des akademischen Grads
Doctor rerum naturalium

vorgelegt von

Sebastian Liebschner

geboren am 08.05.1990 in Meerane

Institut für Kern- und Teilchenphysik

Fachrichtung Physik

Fakultät Mathematik und Naturwissenschaften

Technische Universität Dresden

2020



Eingereicht am 26. Mai 2020

1. Gutachter: Dr. Frank Siegert
2. Gutachter: Prof. Dr. Steffen Schumann
3. Gutachter: Prof. Dr. Michael Kobel

Kurzdarstellung

Diese Arbeit beschäftigt sich mit der Verbesserung von Theorievorhersagen für Teilchenkollisionen am Large Hadron Collider. Dazu werden Algorithmen für Monte-Carlo-Ereignisgeneratoren, wie SHERPA, vorgeschlagen, welche zur Simulation von Messergebnissen an solchen Beschleunigern genutzt werden. In der Berechnung von Kollisionen jenseits der führenden Ordnung in der Störungstheorie sind die Konzepte von Subtraktionsschemata und Partonshowern unverzichtbar. Allerdings weisen beide dieser Konzepte Probleme auf, wenn in dem zu behandelnden Prozess instabile Teilchen auftreten. Insbesondere bieten weder SHERPAs Subtraktionsalgorithmus noch seine Shower einen Ausweg aus dieser Problematik. In dieser Arbeit stellen wir ein neues – auf Pseudodipolen basierendes – Subtraktionsschema vor, um dieses Problem zu lösen. Darüber hinaus diskutieren wir die Konstruktion eines Showers, welcher der Anwesenheit von Resonanzen Rechnung trägt. Um unsere Ergebnisse zu validieren und zu testen, implementierten wir unsere Algorithmen in SHERPA. Diese Arbeit wird abgeschlossen durch einen detaillierten Vergleich unserer neu gefundenen Resultate mit bestehenden Simulationen.

Abstract

This thesis aims at improving theory predictions of particle collisions at the Large Hadron Collider. More specifically it introduces new algorithms for Monte-Carlo event generators, like SHERPA, which are used to simulate the measurements performed at such colliders. In calculating the process of collisions beyond the leading order in perturbation theory, the concept of subtraction schemes and parton showers, is indispensable. However, both of these concepts experience problems if the process in question features intermediate, unstable particles. In particular neither SHERPA's subtraction algorithm nor its showers provide a solution to that issue. To overcome those problems we devise a new subtraction scheme which is based on the use of so-called pseudo-dipoles. In addition we discuss the construction of a resonance-aware shower. To validate and test our findings, we have implemented the new algorithms within SHERPA. A thorough comparison of the newly found results with the established simulations concludes this thesis.

Contents

1	Introduction	1
2	Monte Carlo Event Generators	5
3	NLO QCD Computations	9
3.1	Basics for Calculating Cross-Sections	9
3.2	Extracting and Handling of Divergences	10
3.3	Catani-Seymour Dipole Subtraction	12
3.3.1	Calculation of Cross-Sections in CS Language	16
3.3.2	Differential Form	17
3.3.3	Integrated Form	23
3.4	Alternative Approaches	30
3.4.1	FKS Subtraction	30
3.4.2	Phase-Space Slicing	31
4	Resonance-Aware Subtraction with Pseudo-Dipoles	33
4.1	The Problem of Resonances for NLO Subtraction Schemes	33
4.2	Catani-Seymour Pseudo-Dipole Formalism	34
4.2.1	Differential Form	35
4.3	Using Pseudo-Dipoles for Resonance-Aware Subtraction	37
4.3.1	Rules of Application	37
4.3.2	Integrated Form	40
4.4	Resonance-Aware Subtraction of $W^+W^-b\bar{b}$ Production	46
4.4.1	Singular Limits	46
4.4.2	Physical Cross-Sections	48
4.5	Resonance-Aware Subtraction in the FKS Method	54
5	Parton Shower and Matching	57
5.1	Parton Shower	57
5.1.1	General Considerations	57
5.1.2	Outline of the Dipole-Shower	60
5.2	Matching	62
5.2.1	The Problem of Double Counting	62
5.2.2	Outline of the MC@NLO Algorithm	63
5.2.3	Subleading Colour Effects	65
6	Resonance-Aware Showering and Matching	69
6.1	Factorisation and Parametrisation	70

6.2	Ordering Variable	71
6.3	Building of Kinematics	72
6.4	Generation of Splitting Variables	74
6.4.1	Inverse Eikonal Shower IDS^{eik}	75
6.4.2	Virtuality Shower IDS^{virt}	80
6.4.3	Evaluation of α_s	81
6.5	Implementing the Algorithm and Cross-Checks	81
6.5.1	MCatNLO versus CSS	82
6.5.2	DIM versus DIRE	84
6.5.3	MCATNLO versus DIM	84
6.6	Comparison of Resonance-Aware and Non-Resonance-Aware Shower	86
6.6.1	LO + Parton Shower	87
6.6.2	NLO + Parton Shower	97
6.7	Resonances-Aware Matching in the FKS/POWHEG Framework	104
7	Conclusion and Outlook	107
	Appendices	109
A	Useful Formulae	109
B	Alternative Ansatz for Resonance-Aware Dipole-Subtraction	110
C	List of Files Affected the Most by the Implementation of the IDS	114

1 Introduction

In order to drive forward our understanding of what the smallest building blocks of our universe are and how they interact, the Large Hadron Collider (LHC) started operation in September 2008. It is one of the world’s largest machines and was mainly constructed to elicit nature’s secret of how fundamental particles acquire their mass. In connection to that, a new particle – the Higgs boson – was expected to be discovered. This particle was the last missing piece within the Standard Model of particle physics, which is the commonly accepted theory to describe almost every observation within the realm of subatomic particles. Among several matter particles, from which our world is built, it describes three of the four fundamental interactions of nature on a quantum level by means of messenger particles.¹

Since the running of the LHC a number of successes have been achieved. The most prominent amongst them is indeed the discovery of the Higgs boson in July 2012 [1, 2]² – almost half a century after its postulation in 1964 [3, 4, 5, 6]. In order to make such landmarks possible, Monte Carlo event generators are used to make accurate theory predictions that can be compared with measurements performed by detectors like ATLAS or CMS which operate at the LHC. Although the discovery of the Higgs boson completes the Standard Model of particle physics, as a successful theory of fundamental particles, there are still questions to be solved. Amongst them are “What is Dark Matter?”, “How can gravitational interactions be included within the Standard Model?” or more mathematically motivated: “Is Supersymmetry realised in nature?”. Conceivable theories providing an answer to those questions are only allowed to give very minor modifications to the predictions of measurements already performed. In order to tell whether an extended theory describes measurements better than the Standard Model, as accurate Monte Carlo predictions as possible are required for both.

One possible portal in which physics beyond the Standard Model might reveal itself is believed to be associated with processes featuring top quarks. The main reason for that lies in the top quark’s being the heaviest of all known fundamental particles. This – together with other properties – renders the top quark a preferred decay product of even heavier particles predicted by many extensions of the Standard Model. At the same time, additional theoretical uncertainties arise in predicting (differential) cross-sections for processes, which are associated with top quark production. One reason for that is that due to the complexity of those calculations, it became popular to separate the production and decay of top quarks by means of the narrow-width approximation. Its essence is to approximate the top quark propagator by a delta distribution. However, this simplification leads to less correct results, as it does

¹The gravitational interaction is suppressed by many orders of magnitude with respect to the other three ones being the electromagnetic, the strong and the weak interaction. Thus it has no measurable impact in collider experiments.

²In actuality, the community reported only the discovery of a hitherto unknown scalar particle. But since then evidence has mounted which supports the assumption that the discovered scalar particle is indeed the predicted Higgs boson.

not reproduce a Breit-Wigner distribution in the reconstructed top quark mass because off-shell effects are excluded. Furthermore, processes contributing to the same final state but no intermediate resonances as well as their interferences are not included and spin correlation effects are not correctly accounted for. At next-to-leading order (NLO) in quantum chromodynamics (QCD), an additional problem arises due to an overlap of different processes, like single top and top pair production, see e.g. [7] for a detailed explanation. To deal with this issue in a consistent way, two schemes have been proposed: diagram removal and diagram subtraction [8]. However, the prediction of those do generally not coincide thus introducing a theoretical uncertainty [9]. Despite of these drawbacks, top pair production is calculated at NLO [10, 11, 12, 13] and next-to-next-to-leading order (NNLO) [14, 15, 16] in QCD and even for combined NNLO QCD and NLO electroweak corrections [17].

To overcome the downsides of the narrow-width approximation, the production of the full final state may be calculated in one go. This has been done for top pair production at NLO QCD in [18] at the level of the $W^+W^-b\bar{b}$ final state and in [19, 20] for the $e^+\nu_e\mu^-\bar{\nu}_\mu b\bar{b}$ final state. The increased accuracy of those results has however the price of a more complex calculation. One pitfall in calculating NLO corrections for processes with intermediate resonances, i.e. unstable particles, occurs when standard subtraction schemes are used to deal with the occurring infrared (IR) divergences. As we explain later, the presence of intermediate resonances causes imperfect cancellations in the calculation of the subtracted real correction cross-section thus impairing its convergence. A solution to that problem has been proposed in the context of Frixione-Kunszt-Signer (FKS) subtraction [21] in [22, 23]. Solving this issue in Catani-Seymour (CS) dipole subtraction [24], is a main result of this thesis and also published in [7].

Building on fixed order calculations like the ones described above, Monte Carlo event generators simulate predictions, which can be compared with measured data. They do this by dividing a particle collision into separate parts. Next to the calculation of the so-called hard interaction, this includes the running of a parton shower. Again, it is this factorisation of a particle collision that causes problems for processes with intermediate resonances. The reason for that is that during a regular parton shower evolution, only individual QCD emissions are simulated, without taking into account the resonance structure of the whole process and how that is changed by the emissions and their recoil. This shows itself in distorted differential distributions and is thus a more severe problem than the one of the subtraction since it changes the physical prediction. To avoid this, adaptations of both, the shower algorithm as well as the matching framework between NLO calculation and shower, are required. The latter problem³ has first been addressed in [22, 23] and subsequently applied in [27, 28, 29] to improve predictions of top quark related processes including finite width effects. However, all this work

³The parton shower of PYTHIA [25, 26] is capable of accounting for resonances. In contrast to SHERPA's showers, it does however rely on splitting functions that do not account for the so-called soft limit of the splitting.

is based on FKS subtraction. Hence, after having devised a resonance-aware dipole subtraction scheme, it is the second aim of this thesis to construct a dipole-based resonance-aware shower along with its matching to an NLO calculation.

We start this thesis by briefly summarising the various steps of a Monte Carlo event generator to simulate particle collisions. In the rest of the thesis we focus on two of those steps in detail, namely the calculation of the hard cross-section in Chapter 3 and 4 and the simulation of the parton shower and its matching to the former in Chapter 5 and 6. Each of these two parts consists of a chapter which explains basics and introduces the established algorithm and another chapter which presents our own algorithms and results.

To set the stage, we start by reviewing some important concepts of an NLO QCD calculation in Chapter 3. This includes a brief introduction to perturbation theory, a summary of what divergences arise in NLO calculations and the presentation of CS dipole subtraction as a means to deal with part of those singularities. We close this chapter by outlining two alternatives to that algorithm. Chapter 4 is dedicated to explain and present a solution to the problems that arise when CS dipoles are used for processes with intermediate resonances. In that context, we introduce pseudo-dipoles in Section 4.2 and explain in Section 4.3 how they can be used – detached from their original use case – to achieve our aim. We verify our approach of resonance-aware dipole subtraction in Section 4.4 by showing results of an implementation of it within the public event generator SHERPA [30]. As working examples we consider the processes $e^+e^- \rightarrow W^+W^-b\bar{b}$ and $pp \rightarrow W^+W^-b\bar{b}$, which are both dominated by $t\bar{t}$ production above the threshold. This chapter ends by summarising related work in the literature. In the first chapter of the second part of this thesis we explain in Chapter 5 basic aspects of a parton shower, outline the CS dipole shower (CSS) [31] as a specific example and summarise the concept of matching a parton shower to an NLO calculation according to the MC@NLO algorithm [32]. Chapter 6 starts with our construction of a resonance-aware shower, which we dub IDS. We continue in Section 6.5 by cross-checking our implementation in SHERPA at the example of $e^+e^- \rightarrow W^+W^-b\bar{b}$. We then analyse and compare our prediction thoroughly to results obtained with the (non-resonance-aware) CSS in Section 6.6. Finally we remark upon related work in the literature before we summarise this thesis and provide an outlook in Chapter 7.

2 Monte Carlo Event Generators

Though the calculation of many processes at tree-level (see Section 3.1) are comparatively easy and possible since the early days of quantum electrodynamics (QED) or QCD, it needs more to provide a prediction of a full particle collision. This is because the so-called hard interaction is followed and accompanied by other effects which are too complex or even impossible to calculate within the framework of a diagrammatic approach (see Section 3.1). Multi-purpose Monte Carlo event generators are computer programs which are designed to model all the physics relevant to predict the experimental data measured at particle colliders.

They have established themselves as indispensable tools for making theory predictions in modern particle physics. The most frequently used Monte Carlo event generators within the ATLAS and CMS community are PYTHIA [25, 26], HERWIG [33, 34] and SHERPA [30].

Their working paradigm is to randomly generate an event such as it is happening in “real life” within a particle collider and to split its simulation into different well defined parts (see Figure 2.1), which we briefly describe in the following.

The core of almost every collision is the hard interaction being dubbed like this as the participating particles are characterised by having a relatively high energy. It is calculated from first principles and exact up to a predefined accuracy. The current standard within Monte-Carlo event generators is a fully automated computation of the hard cross-section at NLO in QCD (see Section 3.1). For a number of processes, like Higgs boson production [36, 37, 38, 39, 40, 41] as one of the first, NNLO predictions became available. They are however process-specific and not fully automated to date, which is due to technical challenges regarding IR subtraction algorithms (see Section 3.3) beyond NLO. Though the strong interaction lives up to its name, NNLO QCD corrections and NLO electroweak ones are of the same magnitude since their coupling constants fulfil $\mathcal{O}(\alpha_s^2) \approx \mathcal{O}(\alpha)$. In addition to that, differential cross-sections may experience even larger corrections as is the case in vector-boson scattering [42, 43], which has been reported by ATLAS [44, 45] and CMS [46] already at run I of the LHC. This demand triggered an automation of NLO electroweak corrections which has been implemented in SHERPA recently [47].

Following the hard interaction, a particle shower takes place which accounts for QCD and possibly QED bremsstrahlung. This part of the event generation evolves a few high energetic particles down towards many low energetic ones. The particle shower is an approximate treatment, which can – due to the many particles involved – not be computed like the hard interaction. The partons emerging the shower have energies of $\mathcal{O}(\Lambda_{\text{QCD}})$ where hadronisation occurs. To model this, so-called non-perturbative approaches are used. The final step after this is the subsequent decay of those potentially unstable hadrons into lighter stable ones which is based partially on experimental measurements and partially on approximate calculations if the former do not exist. Independent of the hard interaction with its subsequent downward evolution in energy, there is one further building block within a Monte Carlo event generator

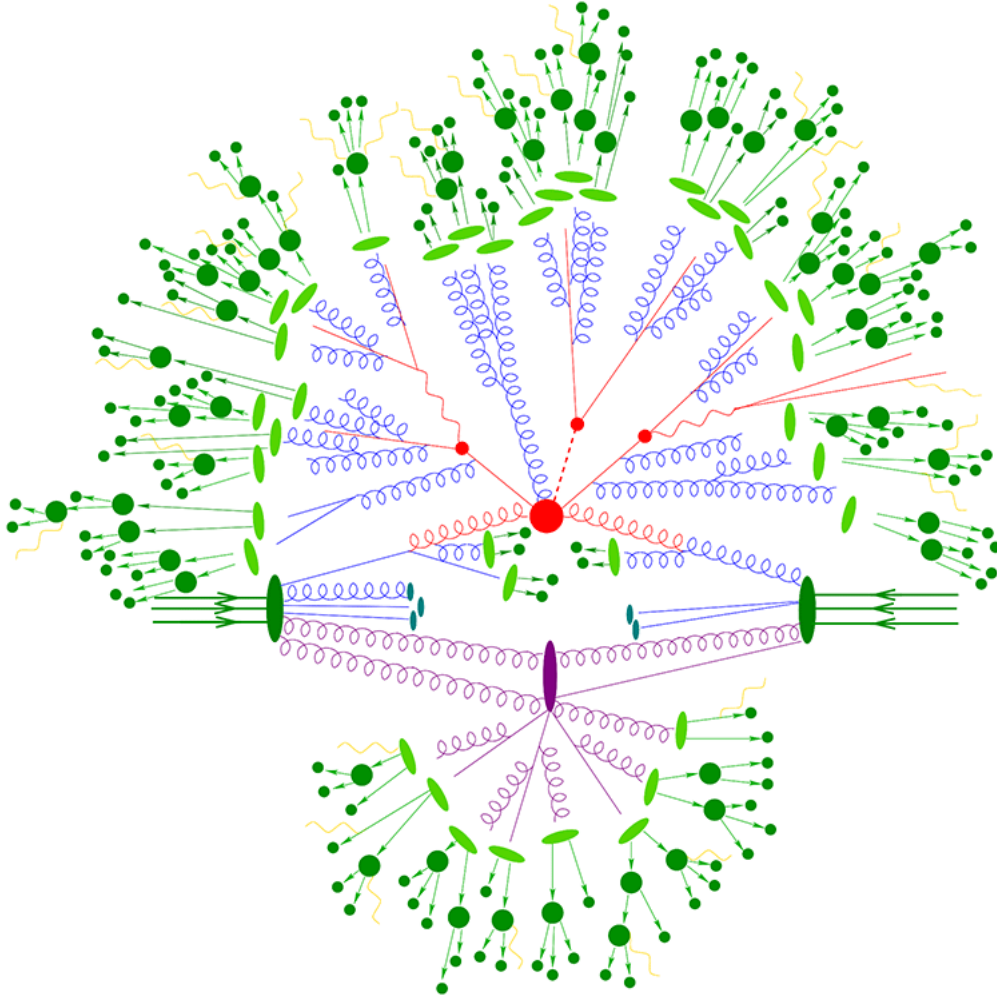


Figure 2.1: Visualisation of the various steps in a Monte Carlo simulation of a particle collision at the example of top pair production with a Higgs boson [35].

namely the modelling of the underlying event. This part takes interactions of the beam remnants in hadron collisions into account.

3 NLO QCD Computations

In this chapter we recapitulate vital concepts of perturbative QCD required for a fixed order calculation at NLO. In addition to general considerations, this includes the analytic extraction and nullification of divergences. We review CS dipole subtraction as a commonly used algorithm which allows for an automated handling of IR divergences within a Monte Carlo generator. As we finally aim to amend this subtraction, we focus on it in some detail by giving intermediate results not outlined in the original paper. This chapter closes with a short summary of alternative approaches.

3.1 Basics for Calculating Cross-Sections

The cross-sections of hard interactions within Monte Carlo generators are computed by using the concept of perturbative quantum field theory. This concept is required since the Lagrangian defining the SM is too complicated to extract exact predictions out of it. To approximate an arbitrary observable, the quantity in question is expanded in orders of a parameter which is supposed to be smaller than one, thus guaranteeing the convergence of the expansion. This parameter is taken to be the coupling constant of the various interactions. The lowest order in which a coupling constant contributes to an observable is called the leading order (LO). The next term in the expansion is then referred to as NLO and so forth. In this section we focus on the calculation of observables which are of NLO in α_s – the coupling constant of QCD.

To calculate an observable at a given order in quantum field theory, one has to sum up all quantum mechanical amplitudes (or matrix elements) and take their absolute square. It is possible to depict those amplitudes by means of drawing so called Feynman diagrams. Figure 3.1 shows four possible Feynman diagrams contributing to 2-jet production at an e^+e^- collider. The top diagram constitutes part of the LO contribution and is also called tree-level

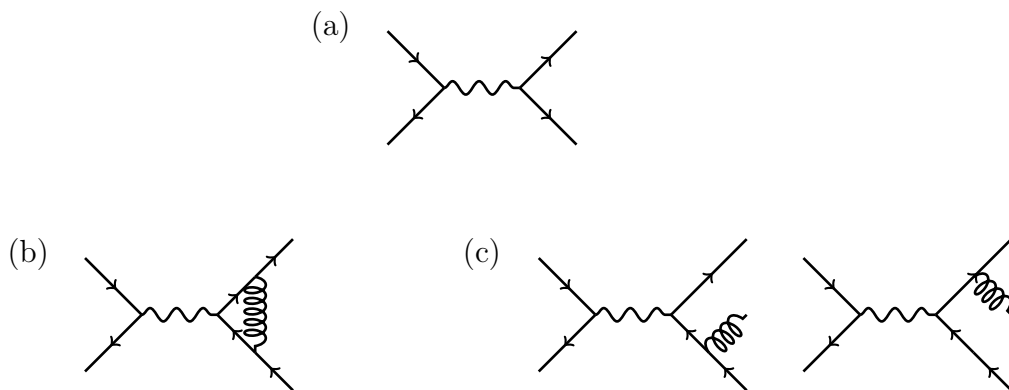


Figure 3.1: Diagrams for 2-jet production in a e^+e^- collision (a) at LO, i.e. $\mathcal{O}(\alpha_s^0)$, (b) and (c) at NLO, i.e. $\mathcal{O}(\alpha_s)$. Diagram (b) is referred to as virtual correction whereas the diagrams (c) are called real correction of the above diagram.

diagram whereas the lower two give rise to contributions of NLO in α_s .⁴ Diagram 3.1 (b) comprises an additional virtual particle compared to the LO diagram and is thus called a virtual correction. The diagrams 3.1 (c) on the other hand exhibit an additional real particle in the final state and are thus referred to as real correction diagrams. Though maybe not clear at the first glance, those kind of diagrams do give rise to 2-jet events. This is because jets and not partons are observed in the detector and if the radiated parton is sufficiently collinear to one of the other partons or its energy is sufficiently small there are only two jets. Apart from the arguments that both virtual and real corrections give rise to the same observable and are of the same order in α_s , there is yet another compelling reason to take both corrections into account. This is that both, taken separately, are infinitely large and only added up give a finite prediction. As a matter of fact the Kinoshita-Lee-Nauenberg-theorem [48, 49] states that this is always the case for so-called IR-safe observables. Such observables do not change when two collinear partons are replaced by a single one, respecting the conservation of quantum numbers and momentum, or a soft gluon is discarded in the computation of the observable. The cancellation of divergences is discussed further in Section 3.2.

As already hinted to, one motivation to calculate observables at higher orders in the coupling constant is that their result is supposed to be closer to the exact one, provided we are in the realm of applicability of perturbation theory. Another often quoted reason is to decrease the theoretical uncertainty of the calculation. There is however no commonly accepted way to reliably calculate the theoretical uncertainties of a fixed order calculation. Often a variation of a factor of two of the renormalisation and factorisation scale μ_R and μ_F (see Section 3.2 and Subsection 3.3.1) is performed, but this is not always a reliable estimate of the theoretical uncertainties. This can be seen in Figure 3.2, where the distribution of the observable thrust in e^+e^- annihilation into jets is shown for different orders in perturbation theory along with their uncertainties [50]. The uncertainties are calculated by varying μ_R by a factor of two. However, for want of a better method the variation of μ_R and μ_F by a factor of two is the standard way to estimate theoretical uncertainties of a fixed order calculation.

3.2 Extracting and Handling of Divergences

As already mentioned in the previous section, virtual and real corrections are separately divergent. In order to achieve a cancellation of divergences, those singularities need to be extracted in a well defined way, i.e. regularised. One prescription in which this is done is dimensional regularisation [51]. It means, slightly loosely speaking, to perform the calculation of an observable in D instead of four space time dimensions. This means in particular that integrals

⁴The LO diagram is of $\mathcal{O}(\alpha_s^0)$, thus its contribution to the cross-section is also of $\mathcal{O}(\alpha_s^0)$. The NLO contributions to the cross-section are of $\mathcal{O}(\alpha_s)$. To obtain this order, the loop diagram (which is of $\mathcal{O}(\alpha_s)$) has to be contracted with the LO diagram.

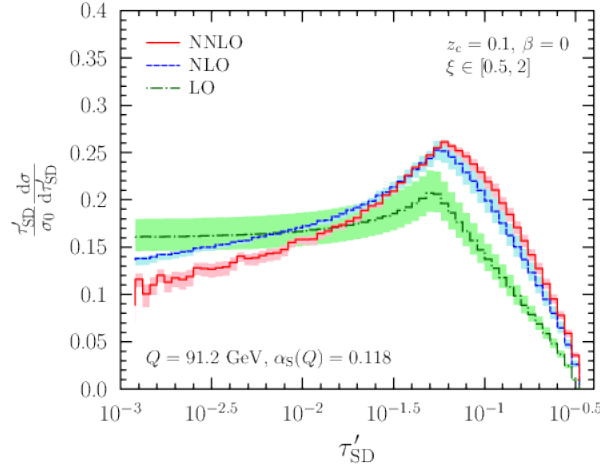


Figure 3.2: Distribution of thrust in e^+e^- annihilation into jets [50]. The center-of-mass energy $Q = 91.2 \text{ GeV}$ is taken to be the renormalisation scale μ_R . The theoretical uncertainties (coloured bands) are calculated by varying μ_R by a factor of two.

in four dimensions are promoted to D dimensions:

$$\int \frac{d^4 p}{(2\pi)^4} \rightarrow \mu_R^{4-D} \int \frac{d^D p}{(2\pi)^D}. \quad (3.1)$$

The introduction of the so called renormalisation scale μ_R is required in order to maintain the mass dimension of the integral. The introduction of a mass scale is an artefact of any regularisation procedure and thus of the perturbative expansion. This means that even though fixed order predictions in perturbation theory depend on the choice of μ_R , a hypothetical calculation which takes all orders in perturbation theory into account does not.⁵

Introducing ϵ by $D = 4 - 2\epsilon$, the divergences within the virtual and real corrections show up as poles in ϵ . In general there are two distinct kinds of divergences: ultraviolet (UV) and IR divergences.

The former ones are associated with a virtual particle in a loop whose momentum/energy tends to infinity. UV-divergences appear solely in virtual corrections and can be removed by means of renormalisation – a concept which enabled the breakthrough of quantum field theory to a vast extent: The key point of it is that the poles in ϵ , which have been extracted by means of regularisation, can be cancelled by a redefinition of the parameters of the underlying theory, i.e. coupling constant(s) and mass(es). The predictions of a renormalised calculation do no longer exhibit any UV poles in ϵ but a dependence on the energy scale μ_R , which can in principle be freely chosen. Different choices of μ_R are however related to different values of the parameters of the theory. This relation is quantitatively described by renormalisation

⁵This motivates the variation of μ_R to obtain an estimate of the theoretical uncertainty, as the dependence on μ_R should decrease for higher orders within a convergent series.

group equations and amounts to a running of the couplings and masses of the theory. It is often advantageous to choose μ_R as the typical energy scale E of the process in question since this reduces logarithmic corrections of the form $\ln \frac{E^2}{\mu_R^2}$ and powers of it, which arise at higher orders.

IR singularities on the other hand are associated with a particle whose momentum is collinear to the momentum of another one and/or a particle whose energy tends to zero. They appear in both virtual and real corrections. For the example of 2-jet production whose contributing diagrams are shown in Figure 3.1 one obtains for the total cross-section:

$$\sigma^V = \sigma^B \frac{\alpha_s}{2\pi} C_F \left(\frac{4\pi\mu_R^2}{s} \right)^\epsilon e^{-\gamma_E \epsilon} \left[-\frac{2}{\epsilon^2} - \frac{3}{\epsilon} - 8 + \frac{7}{6}\pi^2 + \mathcal{O}(\epsilon) \right], \quad (3.2)$$

$$\sigma^R = \sigma^B \frac{\alpha_s}{2\pi} C_F \left(\frac{4\pi\mu_R^2}{s} \right)^\epsilon e^{-\gamma_E \epsilon} \left[\frac{2}{\epsilon^2} + \frac{3}{\epsilon} + \frac{19}{2} - \frac{7}{6}\pi^2 + \mathcal{O}(\epsilon) \right], \quad (3.3)$$

$$\sigma^{\text{NLO}} = \sigma^B + \sigma^V + \sigma^R = \sigma^B \left(1 + \frac{\alpha_s}{\pi} \right) + \mathcal{O}(\epsilon), \quad (3.4)$$

where σ^V and σ^R are the cross-sections of the virtual and real corrections, respectively. σ^B is the Born or LO cross-section, $C_F = \frac{4}{3}$ the quadratic Casimir invariant, s the center-of-mass energy and γ_E the Euler-Mascheroni constant. The poles in Equation (3.2) and (3.3) are purely infrared ones.⁶

Poles of the virtual correction appear directly in the calculation of the loop and are therefore explicitly present at the level of the matrix element. This is not so for the real corrections where the matrix elements are finite apart from special momentum configurations. Thus the poles in the real correction occur only when integrating over the phase-space of the final-state particles.

3.3 Catani-Seymour Dipole Subtraction

As mentioned in the previous section, UV divergences are removed by means of renormalisation. IR divergences however do only drop out when virtual and real corrections are added up as exemplified above. This is impractical for Monte Carlo generators as they calculate virtual and real corrections separately and the divergences cannot be extracted in the latter part, due to the employed numerical techniques. To rectify this one employs so called subtraction schemes.

The basic idea of subtraction schemes is the addition of a “clever zero”. This is, a partonic

⁶In this specific situation the on-shell renormalisation effectively drops out, due to a Ward-identity, see [52]. This means in particular that though the virtual correction diagram is UV and IR divergent, it has the same total divergence (and finite part) as the result after renormalisation, which is only IR but not UV divergent.

cross-section is expressed at NLO by⁷

$$\sigma^{\text{NLO}} = \int_{m+1} (\text{d}\sigma^{\text{R}} - \text{d}\sigma^{\text{S}}) + \int_m (\text{d}\sigma^{\text{B}} + \text{d}\sigma^{\text{V}} + \text{d}\sigma^{\text{C}}) + \int_{m+1} \text{d}\sigma^{\text{S}} \quad (3.5)$$

$$= \int_{m+1} (\text{d}\sigma^{\text{R}} - \text{d}\sigma^{\text{S}}) + \int_m (\text{d}\sigma^{\text{B}} + \text{d}\sigma^{\text{V}} + \text{d}\sigma^{\text{I}}), \quad (3.6)$$

where $\int_m$ denotes the integral over the phase-space of m partons in the final state. The subtraction terms $\text{d}\sigma^{\text{S}}$ are constructed such that they converge to $\text{d}\sigma^{\text{R}}$ in those regions of phase-space where $\text{d}\sigma^{\text{R}}$ diverges. Thus $\text{d}\sigma^{\text{R}} - \text{d}\sigma^{\text{S}}$ is finite over the whole phase-space it is integrated over, which renders its integral finite. The second construction criterion for the subtraction terms is that they must be analytically integrable over the phase-space of the additional particle in the real correction so that

$$\int_1 \text{d}\sigma^{\text{S}} + \text{d}\sigma^{\text{C}} = \text{d}\sigma^{\text{I}} \quad (3.7)$$

can be calculated once and for all in D dimensions. The integrated subtraction terms $\text{d}\sigma^{\text{I}}$ contain then all IR divergences explicitly as poles in ϵ . Those poles cancel exactly those of the virtual corrections so that also the integrand of the second integral in Equation (3.6) is finite and computable in four space-time dimensions.

Like every subtraction scheme, CS dipole-subtraction [24] is based on the universality of divergences of the real corrections [53, 54]. Recall that IR divergences originate from two generic and well defined limits: The soft regime in which a parton's momentum tends to zero and the collinear limit in which two massless partons become collinear to each other.

The soft singularity manifests itself on the level of the absolute squared matrix element

⁷In case of initial-state partons, one has to add collinear subtraction terms $\text{d}\sigma^{\text{C}}$. For reactions with no initial-state partons, these terms vanish. We will however keep them in order to stay as generic as possible.

$|\mathcal{M}_{m+1,ab}|^2$ as

$$\begin{aligned}
|\mathcal{M}_{m+1,ab}|^2 &:= {}_{m+1,ab}\langle 1, \dots, m+1; a, b | 1, \dots, m+1; a, b \rangle_{m+1,ab} \xrightarrow{\text{soft}} -\frac{1}{\lambda^2} 8\pi\mu_R^{2\epsilon}\alpha_s \\
&\cdot \left[\sum_{i=1}^m \frac{1}{p_i q} \sum_{\substack{k=1 \\ k \neq i}}^m {}_{m,ab}\left\langle 1, \dots, m+1; a, b \left| \frac{\mathbf{T}_k \mathbf{T}_i p_k p_i}{(p_k + p_i)q} \right| 1, \dots, m+1; a, b \right\rangle_{m,ab} \right. \\
&+ \sum_{i=1}^m \frac{1}{p_i q} {}_{m,ab}\left\langle 1, \dots, m+1; a, b \left| \frac{\mathbf{T}_a \mathbf{T}_i p_a p_i}{(p_a + p_i)q} \right| 1, \dots, m+1; a, b \right\rangle_{m,ab} + (a \leftrightarrow b) \\
&+ \sum_{i=1}^m \frac{1}{p_a q} {}_{m,ab}\left\langle 1, \dots, m+1; a, b \left| \frac{\mathbf{T}_a \mathbf{T}_i p_a p_i}{(p_a + p_i)q} \right| 1, \dots, m+1; a, b \right\rangle_{m,ab} + (a \leftrightarrow b) \\
&\left. + \frac{1}{2} \frac{1}{p_a q} {}_{m,ab}\left\langle 1, \dots, m+1; a, b \left| \frac{\mathbf{T}_a \mathbf{T}_b p_a p_b}{(p_a + p_b)q} \right| 1, \dots, m+1; a, b \right\rangle_{m,ab} + (a \leftrightarrow b) \right] \quad (3.8)
\end{aligned}$$

where $p_j = \lambda q$ denotes the potentially soft gluon momentum.⁸ Here we adopted the notation of [24] where $|1, \dots, n; a, b\rangle_{m,ab}$ (${}_{m,ab}\langle 1, \dots, n; a, b|$) denotes a (complex-conjugated) matrix element with m final-state partons and two initial-state partons a and b . The colour operators $\mathbf{T}_i$ act on those matrix elements which are vectors in colour (and helicity) space. Apart from colour correlation, Equation (3.8) exhibits a full factorisation of $|\mathcal{M}_{m+1,ab}|^2$ into a sum of absolute squared m -parton matrix elements $|\mathcal{M}_{m,ab}|^2$, called underlying Born matrix elements. The sums run over all final-state partons in the underlying Born matrix elements. The underlying Born matrix elements are identical in the exact soft limit and are obtained from $\mathcal{M}_{m+1,ab}$ by simply discarding the soft gluon. The last terms in the last three lines of Equation (3.8) are a abbreviation for the previous term with swapped indices a and b . The singularity of Equation (3.8) originates from the eikonal current $\mathbf{J}^\mu$ for the emission of a soft gluon. Its contraction with itself is given by

$$\begin{aligned}
\mathbf{J}^{\mu\dagger} \mathbf{J}_\mu &= \sum_{i=1}^m \sum_{\substack{k=1 \\ k \neq i}}^m \mathbf{T}_k \mathbf{T}_i \frac{p_i p_k}{(p_i q)(p_k q)} + 2 \sum_{i=1}^m \mathbf{T}_a \mathbf{T}_i \frac{p_a p_i}{(p_a q)(p_i q)} + (a \leftrightarrow b) \\
&+ \mathbf{T}_a \mathbf{T}_b \frac{p_a p_b}{(p_a q)(p_b q)} + (a \leftrightarrow b). \quad (3.9)
\end{aligned}$$

The momentum dependence in Equation (3.8) follows from a partial fractioning in Equa-

⁸There is no “extra” singularity arising from a soft quark. This is, a real emission matrix element may diverge for an increasingly soft quark, but this singularity is counted as collinear singularity, as the transverse momentum $\vec{k}_\perp$ of the two potentially collinear partons tends to zero as well. This is different from the soft gluon scenario in which the matrix element diverges faster in a sense.

tion (3.9):

$$\frac{p_k p_i}{(p_k p_j)(p_i p_j)} = \frac{p_k p_i}{p_k p_j (p_i + p_k) p_j} + \frac{p_k p_i}{p_i p_j (p_i + p_k) p_j}. \quad (3.10)$$

The collinear limit is marked by

$$\begin{aligned} & {}_{m+1,ab} \langle 1, \dots, m+1; a, b | 1, \dots, m+1; a, b \rangle_{m+1,ab} \\ & \xrightarrow{\text{coll}} \frac{4\pi\mu_R^{2\epsilon}\alpha_s}{p_i p_j} {}_{m,ab} \langle 1, \dots, m+1; a, b | P_{(\tilde{i}j),i}(z, k_\perp) | 1, \dots, m+1; a, b \rangle_{m,ab} \end{aligned} \quad (3.11)$$

for a final-state parton splitting $\tilde{i}j \rightarrow i + j$ and by

$$\begin{aligned} & {}_{m+1,ab} \langle 1, \dots, m+1; a, b | 1, \dots, m+1; a, b \rangle_{m+1,ab} \\ & \xrightarrow{\text{coll}} \frac{4\pi\mu_R^{2\epsilon}\alpha_s}{z p_i p_a} {}_{m,ab} \langle 1, \dots, m+1; a, b | P_{a,\tilde{a}i}(z, k_\perp) | 1, \dots, m+1; a, b \rangle_{m,ab} \end{aligned} \quad (3.12)$$

for an initial-state parton splitting $a \rightarrow \tilde{a}i$, see Figure 3.3. In both cases z is the momentum

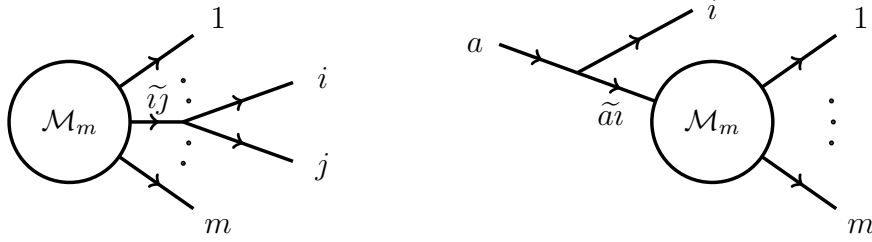


Figure 3.3: Sketch to illustrate the labelling in final-state (left) and initial-state splittings (right).

fraction of parton $i(\tilde{a}i)$ in the direction of its mother parton $\tilde{i}j(a)$ and $k_\perp$ is a momentum perpendicular to that of the mother parton, see [24]. The D -dimensional Altarelli-Parisi splitting functions $\hat{P}_{a,b}$ are identical for final- and initial-state splittings. They are matrices in helicity space, though for a splitting fermion they are proportional to the unit matrix. Their explicit form is given in Equation (4.10)-(4.14) in [24].

The singular limits in Equation (3.8), (3.11) and (3.12) suggest that the singular parts of an absolute squared real correction matrix element can be written as a sum over absolute squared matrix elements with one particle less (underlying Born matrix element) and an insertion operator which describes an $1 \rightarrow 2$ splitting. Fig 3.4 shows this with the restriction of no initial-state partons to confine to one instead of four sketches on the right hand side. The encircled $\mathcal{M}$ s together with their adjacent lines going to the left (right) stand for a (complex conjugated) matrix element and the vertical dashed line separating the two symbolises the contraction of both. The double sum runs over all possible combinations of final-state parton pairs i and j which can originate from the splitting of an underlying Born parton $\tilde{i}j$ on the

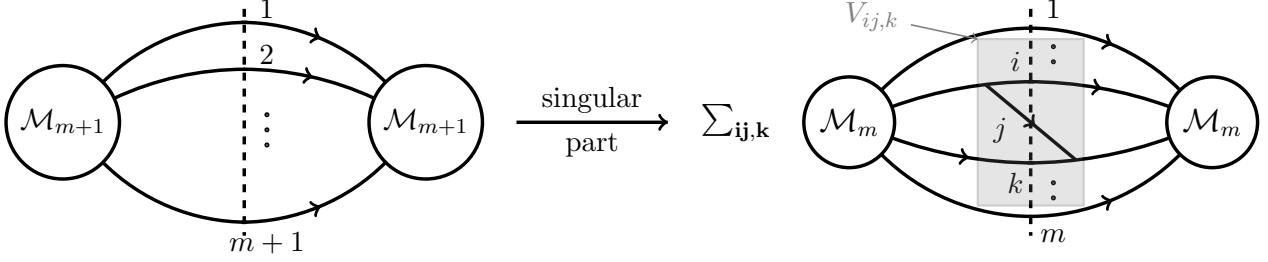


Figure 3.4: Sketch of an absolute square of real correction matrix elements (left) and its factorisation into a sum of dipoles (right). The dashed lines denote the contraction of matrix elements with their complex conjugate. The dipoles are m -parton matrix elements with an insertion operator $V_{ij,k}$. We neglect initial-state partons to keep the sketch simple.

one hand and all final-state partons $k \neq \tilde{i}j$ of the underlying Born matrix element on the other hand. The operator describing the $1 \rightarrow 2$ splitting is generic, i.e. depends only upon the momenta and quantum numbers of the emitter parton i , the emitted parton j and the spectator parton k and not on the very details of the matrix elements at hand. Since there are only two partons (emitter and spectator) of the underlying Born matrix element involved in each operator, the associated terms are referred to as dipoles.

3.3.1 Calculation of Cross-Sections in CS Language

Before we go into details of the dipoles, we like to provide some further notation in order to embed the dipole formulae into the computation of the physical cross-section.

Firstly, in case of two initial-state hadrons, one has to convolve the perturbative partonic cross-section in Equation (3.6) with non-perturbative parton distribution functions (PDFs) to arrive at a physical cross-section:

$$\sigma_{AB}^{\text{NLO}}(p_A, p_B) = \sum_{a,b} \int_0^1 d\eta_a f_{a/A}(\eta_a, \mu_F) \int_0^1 d\eta_b f_{b/B}(\eta_b, \mu_F) \sigma_{ab}^{\text{NLO}}(\eta_a p_A, \eta_b p_B, \mu_F). \quad (3.13)$$

The PDFs give the probability to find a parton a with momentum fraction η_a at energy scale μ_F within the hadron A . They can not (yet) be calculated from first principles, but once measured can be evolved to a different energy scale using the DGLAP-equations, see e.g. [55, 56].

The m -parton matrix element $\mathcal{M}_{m,ab}$ is related to the Born cross-section by

$$\begin{aligned} \int_m d\sigma_{ab}^{\text{B}}(p_a, p_b) &= \int_m \mathcal{N}_{\text{in}} \frac{1}{n_s(a)n_s(b)n_c(a)n_c(b)\Phi(p_a p_b)} \sum_{\{m\}} d\phi_m \frac{1}{S_{\{m\}}} |\mathcal{M}_{m,ab}|^2 \\ &\cdot F_J^{(m)}(p_1, \dots, p_m; p_a, p_b). \end{aligned} \quad (3.14)$$

Here $\mathcal{N}_{\text{in}}$ includes all non-QCD related factors, $n_s(a)$ ($n_c(a)$) is the number of polarisations (colours) of the initial-state parton a , $\Phi(p_a p_b)$ is the flux factor, $\sum_{\{m\}}$ indicates the sum over all

m -parton configurations and $S_{\{m\}}$ is the symmetry factor accounting for all identical partons in the final state. The jet-defining function $F_J^{(m)}$ is required to render the cross-section IR-safe, see [24].

The real correction cross-section σ^R is given by Equation (3.14) along with the replacement $m \rightarrow m + 1$. The virtual correction cross-section σ^V is also given by Equation (3.14) but with the replacement $|\mathcal{M}_{m,ab}|^2 \rightarrow 2\mathcal{R}(\mathcal{M}_{m,ab} \cdot \mathcal{M}_{m,ab}^{\text{1L ren}*})$ where $\mathcal{M}_{m,ab}^{\text{1L ren}*}$ is the complex conjugated one-loop matrix element which is already renormalised.

The collinear counterterms are given by

$$\begin{aligned} \int_m d\sigma_{ab}^C(p_a, p_b) = & -\frac{\alpha_s}{2\pi} \frac{1}{\Gamma(1-\epsilon)} \int_m \sum_{a'b'} \int_0^1 dz_a \int_0^1 dz_b d\sigma_{a'b'}^B(z_a p_a, z_b p_b) \cdot \\ & \left\{ \delta_{bb'} \delta(1-z_b) \left[-\frac{1}{\epsilon} \left(\frac{4\pi\mu_R}{\mu_F} \right)^\epsilon P^{aa'}(z_a) + K_{\text{F.S.}}^{aa'}(z_a) \right] + \right. \\ & \left. \delta_{aa'} \delta(1-z_a) \left[-\frac{1}{\epsilon} \left(\frac{4\pi\mu_R}{\mu_F} \right)^\epsilon P^{bb'}(z_b) + K_{\text{F.S.}}^{bb'}(z_b) \right] \right\}. \end{aligned} \quad (3.15)$$

in the case of two initial state hadrons. They are separately divergent for $\epsilon \rightarrow 0$ and are required since one does not integrate over the momentum of initial-state partons. Thus collinear singularities which are picked up in the virtual corrections, where the complete integral over the additional parton momentum is performed, are missing in the purely real corrections. The terms above comprise the regularised Altarelli-Parisi splitting functions $P^{aa'}(z_a)$ (see Appendix A) and factorisation scheme dependent functions $K_{\text{F.S.}}^{aa'}(z_a)$ which are zero in the $\overline{\text{MS}}$ -scheme.

The detailed formulae for the differential $d\sigma^S$ and integrated dipoles $d\sigma^I$ will be given in the following subsections.

3.3.2 Differential Form

Now we come to the explicit form of the insertion operator $\mathbf{V}_{ij,k}$ which follows from the details of the soft and collinear limit and depends on whether the emitter and spectator are initial- or final-state partons. Those four sets of insertion operators are different in the first place, as each of them is associated with a different mapping from $m+1$ to m momenta and they are very closely interwoven with the kinematic variables which are associated with those mappings.

In the most general case of two initial state partons, the singularities of the real correction absolute squared amplitude are counteracted by the following sum of dipoles:

$$\begin{aligned} &_{m+1;ab} \langle 1, \dots, m+1; a, b | 1, \dots, m+1; a, b \rangle_{m+1;ab} \rightarrow \sum_{\substack{\text{pairs} \\ i,j}} \sum_{k \neq i,j} \mathcal{D}_{ij,k} + \\ & \sum_{\substack{\text{pairs} \\ i,j}} \sum_{k \neq i,j} (\mathcal{D}_{ij}^a + (a \leftrightarrow b)) + \sum_i \sum_{k \neq i} (\mathcal{D}_k^{ai} + (a \leftrightarrow b)) + \sum_i (\mathcal{D}^{ai,b} + (a \leftrightarrow b)). \end{aligned} \quad (3.16)$$

In the following, we will review all four types of dipoles for the case of two initial-state partons by giving some details for the first type and briefly summarising the remaining three. Fig. 3.5

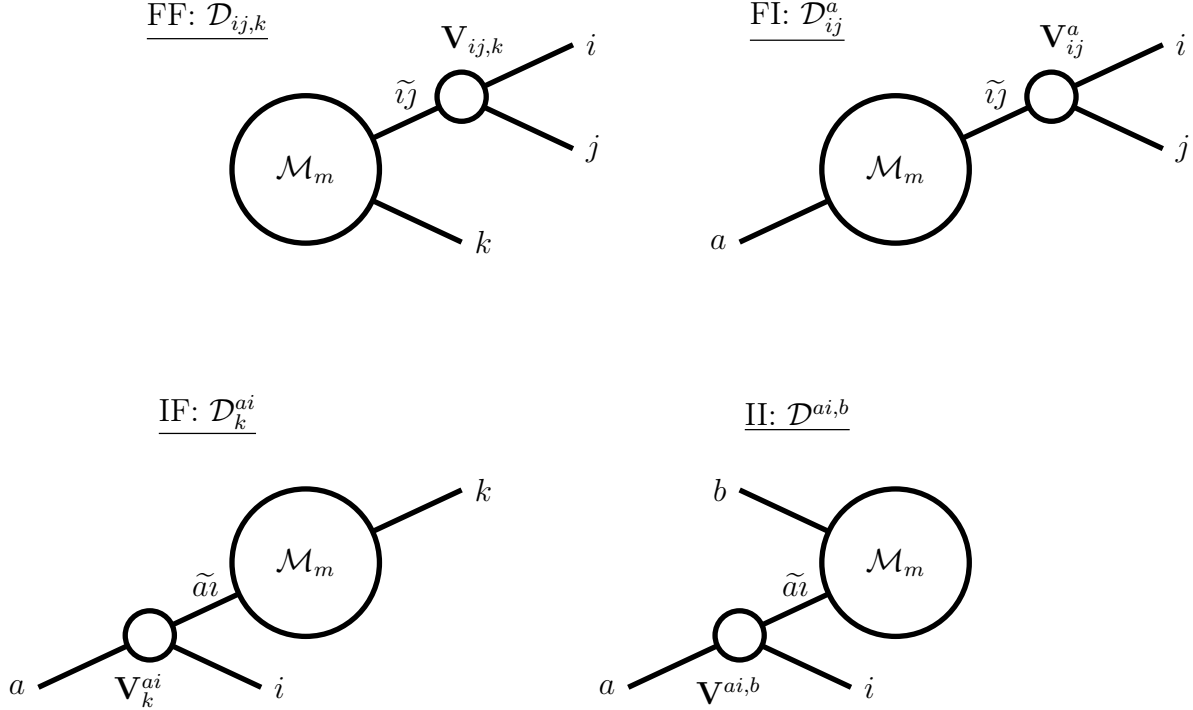


Figure 3.5: Sketch of all four dipole types to fix the labelling of emitted, emitter and spectator parton in each case.

fixes the labelling for emitted, emitter and spectator parton for all four types, which we adopted from [24].

Dipoles for Final-State Emitter and Final-State Spectator

Dipoles with both emitter and spectator being final-state partons are called FF-dipoles. They are given by

$$\mathcal{D}_{ij,k}(p_1, \dots, p_{m+1}; p_a, p_b) = -\frac{1}{2p_i p_j} \cdot_{m,ab} \left\langle 1, \dots, \tilde{i}\tilde{j}, \tilde{k}, \dots, m+1; a, b \left| \frac{\mathbf{T}_k \mathbf{T}_{ij}}{\mathbf{T}_{ij}^2} \mathbf{V}_{ij,k} \right| 1, \dots, \tilde{i}\tilde{j}, \tilde{k}, \dots, m+1; a, b \right\rangle_{m,ab} \quad (3.17)$$

where the m parton matrix element is given by the $m+1$ parton matrix element by replacing the partons i and j with the emitter parton $\tilde{i}\tilde{j}$ and k with the spectator parton $\tilde{k}$. The

corresponding mapping of momenta is given by

$$\tilde{p}_k^\mu = \frac{1}{1 - y_{ij,k}} p_k^\mu, \quad (3.18)$$

$$\tilde{p}_{ij}^\mu = p_i^\mu + p_j^\mu - \frac{y_{ik,k}}{1 - y_{ij,k}} p_k^\mu, \quad (3.19)$$

where the kinematic variable $y_{ij,k}$ is given by

$$y_{ij,k} = \frac{p_i p_j}{p_i p_j + p_i p_k + p_k p_j} = \frac{p_i p_j}{\tilde{p}_{ij} \tilde{p}_k} = \frac{p_i \tilde{p}_{ij}}{\tilde{p}_{ij} \tilde{p}_k - p_i \tilde{p}_k}. \quad (3.20)$$

The operators $\mathbf{V}_{ij,k}$ are matrices in helicity space. Depending on the flavour of the involved partons they read

$$\langle s | \mathbf{V}_{q_i g_j, k} | s' \rangle = 8\pi \mu^{2\epsilon} \alpha_s C_F \left[\frac{2}{1 - \tilde{z}_i(1 - y_{ij,k})} - (1 + \tilde{z}_i) - \epsilon(1 - \tilde{z}_i) \right] \delta_{ss'}, \quad (3.21)$$

$$\langle \mu | \mathbf{V}_{q_i \bar{q}_j, k} | \nu \rangle = 8\pi \mu^{2\epsilon} \alpha_s T_R \left[-g^{\mu\nu} - \frac{2}{p_i p_j} (\tilde{z}_i p_i^\mu - \tilde{z}_j p_j^\mu) (\tilde{z}_i p_i^\nu - \tilde{z}_j p_j^\nu) \right], \quad (3.22)$$

$$\begin{aligned} \langle \mu | \mathbf{V}_{g_i g_j, k} | \nu \rangle = 8\pi \mu^{2\epsilon} \alpha_s C_A \left[-g^{\mu\nu} \left(\frac{1}{1 - \tilde{z}_i(1 - y_{ij,k})} + \frac{1}{1 - \tilde{z}_j(1 - y_{ij,k})} - 2 \right) \right. \\ \left. + (1 - \epsilon) \frac{2}{p_i p_j} (\tilde{z}_i p_i^\mu - \tilde{z}_j p_j^\mu) (\tilde{z}_i p_i^\nu - \tilde{z}_j p_j^\nu) \right], \end{aligned} \quad (3.23)$$

where the additional kinematic variables are given by

$$\tilde{z}_i = \frac{p_i p_k}{(p_i + p_j) p_k} = \frac{p_i \tilde{p}_k}{\tilde{p}_{ij} \tilde{p}_k}, \quad \tilde{z}_j = \frac{p_j p_k}{(p_i + p_j) p_k} = \frac{p_j \tilde{p}_k}{\tilde{p}_{ij} \tilde{p}_k} = 1 - \tilde{z}_i.$$

Those splitting operators are constructed such that they reproduce the soft and collinear limits given in Equation (3.8) and (3.11). In terms of $y_{ij,k}$ and $\tilde{z}_i$, the collinear region is characterised by

$$y_{ij,k} \rightarrow 0, \quad (3.24)$$

and $\tilde{z}_i = z$ is understood. Then, $\langle s | \mathbf{V}_{ij,k} | s' \rangle \rightarrow 8\pi \mu^{2\epsilon} \alpha_s \langle s | P_{(ij),i}(z, k_\perp) | s' \rangle$ and Equation (3.17) approaches the collinear limit in Equation (3.11). The soft limit is described by $p_j^\mu \rightarrow \lambda q^\mu$ where $\lambda \rightarrow 0$ and hence

$$y_{ij,k} \rightarrow 0 \quad \text{and} \quad \tilde{z}_i \rightarrow 1. \quad (3.25)$$

Therefore there is a soft divergence in the splitting operator originating from the term

$$\frac{1}{1 - \tilde{z}_i(1 - y_{ij,k})} = \frac{p_i p_j + p_i p_k + p_j p_k}{(p_i + p_k) p_j}. \quad (3.26)$$

Again, Equation (3.17) tends to the relevant limit, i.e. Equation (3.8).

The dipoles have the advantage of smoothly interpolating between soft and collinear singularities and being analytically integrable over the phase-space of the parton i . The last property is essential to arrive at the counterterms for the virtual corrections and therefore to assure to add the same weight to them as has been subtracted from the real corrections. Note in particular that the (unintegrated) dipoles are evaluated at Born-kinematics. This means that a differential cross-section is calculated by filling the weights of dipoles according to their mapped Born kinematics into the histogram and not their real-correction kinematics. This ensures that their weight cancels with their integrated counterpart (which is discussed below) and thus “a zero” is added in each bin of the histogram.

Having introduced the explicit formulae, we write the contribution of the differential FF-subtraction terms to the cross-section as

$$\begin{aligned} \int_{m+1} d\sigma_{ab}^S(p_a, p_b) \Big|_{\text{FF}}^{\text{CS}} &= \int_{m+1} \mathcal{N}_{\text{in}} \frac{1}{n_s(a)n_s(b)\Phi(p_a p_b)} \sum_{\{m+1\}} d\phi_{m+1} \frac{1}{S_{\{m+1\}}} \\ &\cdot \sum_{\substack{\text{pairs} \\ i,j}} \sum_{\substack{k=1 \\ k \neq i,j}}^{m+1} \mathcal{D}_{ij,k}(p_1, \dots, p_{m+1}; p_a, p_b) F_J^{(m)}(p_1, \dots, \tilde{p}_{ij}, \dots, \tilde{p}_k, \dots, p_{m+1}; p_a, p_b). \end{aligned} \quad (3.27)$$

Dipoles for Final-State Emitter and Initial-State Spectator

The final-state singular limit $p_i p_j \rightarrow 0$ requires an additional so called FI-dipole:

$$\begin{aligned} \mathcal{D}_{ij}^a(p_1, \dots, p_{m+1}; p_a, p_b) &= -\frac{1}{2p_i p_j} \frac{1}{x_{ij,a}} \\ &\cdot \left\langle 1, \dots, \tilde{i}j, \dots, m+1; \tilde{a}, b \left| \frac{\mathbf{T}_a \mathbf{T}_{ij}}{\mathbf{T}_{ij}^2} \mathbf{V}_{ij}^a \right| 1, \dots, \tilde{i}j, \dots, m+1; \tilde{a}, b \right\rangle_{m,ab} \end{aligned} \quad (3.28)$$

to be counteracted. The kinematic variables are given by

$$x_{ij,a} = 1 - \frac{p_i p_j}{(p_i + p_j) p_a}, \quad \tilde{z}_i = \frac{p_i p_a}{(p_i + p_j) p_a} = 1 - \tilde{z}_j. \quad (3.29)$$

In contrast to FF-dipoles the momentum of the spectator rather than the emitter is scaled:

$$\tilde{p}_a^\mu = x_{ij,a} p_a^\mu, \quad \tilde{p}_{ij}^\mu = p_i^\mu + p_j^\mu - (1 - x_{ij,a}) p_a^\mu. \quad (3.30)$$

This is because the momenta of initial-state partons are fixed in their direction along the beam axis. The splitting operators read

$$\langle s | \mathbf{V}_{q_i g_j}^a | s' \rangle = 8\pi\mu^{2\epsilon}\alpha_s C_F \left[\frac{2}{1 - \tilde{z}_i + (1 - x_{ij,a})} - (1 + \tilde{z}_i) - \epsilon(1 - \tilde{z}_i) \right] \delta_{ss'}, \quad (3.31)$$

$$\langle \mu | \mathbf{V}_{q_i \bar{q}_j}^a | \nu \rangle = 8\pi\mu^{2\epsilon}\alpha_s T_R \left[-g^{\mu\nu} - \frac{2}{p_i p_j} (\tilde{z}_i p_i - \tilde{z}_j p_j)^\mu (\tilde{z}_i p_i - \tilde{z}_j p_j)^\nu \right], \quad (3.32)$$

$$\begin{aligned} \langle \mu | \mathbf{V}_{g_i g_j}^a | \nu \rangle = & 16\pi\mu^{2\epsilon}\alpha_s C_A \left[-g^{\mu\nu} \left(\frac{2}{1 - \tilde{z}_i + (1 - x_{ij,a})} + \frac{2}{1 - \tilde{z}_j + (1 - x_{ij,a})} - 2 \right) + \right. \\ & \left. (1 - \epsilon) \frac{1}{p_i p_j} (\tilde{z}_i p_i - \tilde{z}_j p_j)^\mu (\tilde{z}_i p_i - \tilde{z}_j p_j)^\nu \right]. \end{aligned} \quad (3.33)$$

The contribution of FI-dipoles to the cross-section is given by

$$\begin{aligned} \int_{m+1} d\sigma^S(p_a, p_b) \Big|_{\text{FI}}^{\text{CS}} = & \int_{m+1} \mathcal{N}_{\text{in}} \frac{1}{n_s(a)n_s(b)\Phi(p_a p_b)} \sum_{\{m+1\}} d\phi_{m+1} \frac{1}{S_{\{m+1\}}} \\ & \cdot \sum_{\substack{\text{pairs} \\ i,j}} \mathcal{D}_{ij}^a(p_1, \dots, p_{m+1}; p_a, p_b) F_J^{(m)}(p_1, \dots, \tilde{p}_{ij}, \dots, p_{m+1}; \tilde{p}_a, p_b) + (a \leftrightarrow b). \end{aligned} \quad (3.34)$$

Dipoles for Initial-State Emitter and Final-State Spectator

To cancel part of the initial-state singularities of the real corrections, IF-dipoles are required. The IF-dipole is given by

$$\begin{aligned} \mathcal{D}_k^{ai}(p_1, \dots, p_{m+1}; p_a, p_b) = & -\frac{1}{2p_a p_i} \frac{1}{x_{ik,a}} \\ & \cdot \left\langle 1, \dots, \tilde{k}, \dots, m+1; \tilde{a}l, b \left| \frac{\mathbf{T}_k \mathbf{T}^{ai}}{\mathbf{T}_{ai}^2} \mathbf{V}_k^{ai} \right| 1, \dots, \tilde{k}, \dots, m+1; \tilde{a}l, b \right\rangle_{m,ab}. \end{aligned} \quad (3.35)$$

The kinematic invariants corresponding to this dipole type are

$$x_{ik,a} = 1 - \frac{p_i p_k}{(p_i + p_k) p_a}, \quad u_i = \frac{p_a p_i}{(p_i + p_k) p_a} = 1 - u_k. \quad (3.36)$$

The m -parton momentum configuration is obtained by

$$\tilde{p}_{ai}^\mu = x_{ik,a} p_a^\mu, \quad \tilde{p}_k^\mu = p_k^\mu + p_i^\mu - (1 - x_{ik,a}) p_a^\mu. \quad (3.37)$$

The splitting operators read

$$\langle s | \mathbf{V}_k^{q_a g_i} | s' \rangle = 8\pi\mu^{2\epsilon}\alpha_s C_F \left[\frac{2}{1 - x_{ik,a} + u_i} - (1 + x_{ik,a}) - \epsilon(1 - x_{ik,a}) \right] \delta_{ss'}, \quad (3.38)$$

$$\langle s | \mathbf{V}_k^{g_a \bar{q}_i} | s' \rangle = 8\pi\mu^{2\epsilon}\alpha_s C_F [1 - \epsilon - 2x_{ik,a}(1 + x_{ik,a})] \delta_{ss'}, \quad (3.39)$$

$$\langle \mu | \mathbf{V}_k^{q_a g_i} | \nu \rangle = 8\pi\mu^{2\epsilon}\alpha_s T_R \left[-g^{\mu\nu} x_{ik,a} + \frac{2u_i u_k}{p_i p_k} \frac{1 - x_{ik,a}}{x_{ik,a}} \left(\frac{p_i}{u_i} - \frac{p_k}{u_k} \right)^\mu \left(\frac{p_i}{u_i} - \frac{p_k}{u_k} \right)^\nu \right], \quad (3.40)$$

$$\begin{aligned} \langle \mu | \mathbf{V}_k^{g_a g_i} | \nu \rangle = & 16\pi\mu^{2\epsilon}\alpha_s C_A \left[-g^{\mu\nu} \left(\frac{1}{1 - x_{ik,a} + u_i} - 1 + x_{ik,a}(1 - x_{ik,a}) \right) + \right. \\ & \left. \frac{2u_i u_k}{p_i p_k} \frac{1 - x_{ik,a}}{x_{ik,a}} \left(\frac{p_i}{u_i} - \frac{p_k}{u_k} \right)^\mu \left(\frac{p_i}{u_i} - \frac{p_k}{u_k} \right)^\nu \right]. \end{aligned} \quad (3.41)$$

The contribution from IF-dipoles to the cross-section reads

$$\begin{aligned} \int_{m+1} d\sigma^S(p_a, p_b) \Big|_{\text{IF}}^{\text{CS}} = & \int_{m+1} \mathcal{N}_{\text{in}} \frac{1}{n_s(a)n_s(b)\Phi(p_a p_b)} \sum_{\{m+1\}} d\phi_{m+1} \frac{1}{S_{\{m+1\}}} \\ & \cdot \sum_{i=1}^m \sum_{\substack{k=1 \\ k \neq i, j}}^m \mathcal{D}_k^{ai}(p_1, \dots, p_{m+1}; p_a, p_b) F_J^{(m)}(p_1, \dots, \tilde{p}_k, \dots, p_{m+1}; \tilde{p}_{ai}, p_b) + (a \leftrightarrow b). \end{aligned} \quad (3.42)$$

Dipoles for Initial-State Emitter and Initial-State Spectator

The dipole associated with initial state singularities with initial state spectator reads

$$\begin{aligned} \mathcal{D}_{ij}^a(p_1, \dots, p_{m+1}; p_a, p_b) = & -\frac{1}{2p_a p_i} \frac{1}{x_{i,ab}} \\ & \cdot \sum_{m,a,b} \left\langle \tilde{1}, \dots, \widetilde{m+1}; \widetilde{a\bar{l}}, b \left| \frac{\mathbf{T}_b \mathbf{T}_{ai}}{\mathbf{T}_{ai}^2} \mathbf{V}^{ai,b} \right| \tilde{1}, \dots, \widetilde{m+1}, \widetilde{a\bar{l}}, b \right\rangle_{m,a,b}. \end{aligned} \quad (3.43)$$

As the momentum of initial state partons can at most be rescaled, neither the colour spectator nor the emitting parton can take the recoil of the emitted parton. Therefore the merged parton gets rescaled

$$\tilde{p}_{ai}^\mu = x_{i,ab} p_a^\mu \quad \text{with} \quad x_{i,ab} = \frac{p_a p_b - p_i p_a - p_i p_b}{p_a p_b}, \quad (3.44)$$

the spectator parton remains the same and the recoil is distributed over all final state particles (not only partons). This is done in such a way that the mapping of these momenta can be written as a Lorentz transform

$$\tilde{k}_j^\mu = \Lambda^\mu_\nu(K, \tilde{K}) k_j^\mu \quad \text{with} \quad (3.45)$$

$$\Lambda^\mu_\nu(K, \tilde{K}) = g^\mu_\nu - \frac{2(K + \tilde{K})^\mu (K + \tilde{K})_\nu}{(K + \tilde{K})^2} + \frac{2\tilde{K}^\mu K_\nu}{K^2}, \quad (3.46)$$

where

$$\begin{aligned} K^\mu &= p_a^\mu + p_b^\mu - p_i^\mu \\ \tilde{K}^\mu &= \tilde{p}_{ai}^\mu + p_b^\mu. \end{aligned} \quad (3.47)$$

The splitting operators are given by

$$\langle s | \mathbf{V}^{q_a g_i, b} | s' \rangle = 8\pi\mu^{2\epsilon}\alpha_s C_F \left[\frac{2}{1-x_{i,ab}} - (1+x_{i,ab}) - \epsilon(1-x_{i,ab}) \right] \delta_{ss'}, \quad (3.48)$$

$$\langle s | \mathbf{V}^{g_a \bar{q}_i, b} | s' \rangle = 8\pi\mu^{2\epsilon}\alpha_s T_R [1 - \epsilon - 2x_{i,ab}(1-x_{i,ab})] \delta_{ss'}, \quad (3.49)$$

$$\langle \mu | \mathbf{V}^{q_a g_i, b} | \nu \rangle = 8\pi\mu^{2\epsilon}\alpha_s C_F \left[-g^{\mu\nu} x_{i,ab} + \frac{1-x_{i,ab}}{x_{i,ab}} \frac{2}{\tilde{v}_i p_b p_i} (p_i - \tilde{v}_i p_b)^\mu (p_i - \tilde{v}_i p_b)^\nu \right], \quad (3.50)$$

$$\begin{aligned} \langle \mu | \mathbf{V}^{g_a g_i, b} | \nu \rangle &= 16\pi\mu^{2\epsilon}\alpha_s C_A \left[-g^{\mu\nu} \left(\frac{x_{i,ab}}{1-x_{i,ab}} + x_{i,ab}(1-x_{i,ab}) \right) + \right. \\ &\quad \left. (1-\epsilon) \frac{1-x_{i,ab}}{x_{i,ab}} \frac{2}{\tilde{v}_i p_b p_i} (p_i - \tilde{v}_i p_b)^\mu (p_i - \tilde{v}_i p_b)^\nu \right]. \end{aligned} \quad (3.51)$$

Finally the contribution of II-dipoles to the cross-section is given by

$$\begin{aligned} \int_{m+1} d\sigma^S(p_a, p_b) \Big|_{\text{II}}^{\text{CS}} &= \int_{m+1} \mathcal{N}_{\text{in}} \frac{1}{n_s(a)n_s(b)\Phi(p_a p_b)} \sum_{\{m+1\}} d\phi_{m+1} \frac{1}{S_{\{m+1\}}} \\ &\cdot \sum_{i=1}^m \mathcal{D}^{ai,b}(p_1, \dots, p_{m+1}; p_a, p_b) F_J^{(m)}(\tilde{p}_1, \dots, \tilde{p}_{m+1}; \tilde{p}_{ai}, p_b) + (a \leftrightarrow b). \end{aligned} \quad (3.52)$$

3.3.3 Integrated Form

In the following we will present the integral of the above cited differential dipoles over the phase-space of the emitted parton. As for the differential dipoles, we will give some details in the calculation of FF-dipoles and will content ourselves with giving results for the remaining three types.

Dipoles for Final-State Emitter and Final-State Spectator

The mapping prescribed in Equation (3.19) and (3.18) allows to factorise the phase-space differential of parton i , j and k into a differential of the underlying Born partons $\tilde{\ell}_j$ and $\tilde{k}$ and a single-parton contribution:

$$d\phi(p_i, p_j, p_k; Q) = [dp_i(\tilde{p}_{ij}, \tilde{p}_k)] d\phi(\tilde{p}_{ij}, \tilde{p}_k; Q). \quad (3.53)$$

Here $Q = p_i + p_j + p_k$ and the one parton phase-space is given by

$$[dp_i(\tilde{p}_{ij}, \tilde{p}_k)] = \frac{d^D p_i}{(2\pi)^{D-1}} \delta_+(p_i^2) \mathcal{J}(p_i; \tilde{p}_{ij}, \tilde{p}_k). \quad (3.54)$$

The Jacobian, accounting for the transformations $p_k \rightarrow \tilde{p}_k$ and $p_j \rightarrow \tilde{p}_{ij}$ reads in terms of the variables introduced in Equation (3.20) and (3.24)⁹

$$\mathcal{J}(p_i; \tilde{p}_{ij}, \tilde{p}_k) = \Theta(1 - \tilde{z}_i) \Theta(1 - y_{ij,k}) \frac{(1 - y_{ij,k})^{D-3}}{1 - \tilde{z}_i}. \quad (3.55)$$

Transforming $|\vec{p}_i|$ and the corresponding polar angle θ to $y_{ij,k}$ and $\tilde{z}_i$ one obtains

$$[dp_i(\tilde{p}_{ij}, \tilde{p}_k)] = \frac{(2\tilde{p}_{ij}\tilde{p}_k)^{1-\epsilon}}{16\pi^2} \frac{d\Omega^{D-2}}{(2\pi)^{1-2\epsilon}} d\tilde{z}_i dy_{ij,k} \Theta(\tilde{z}_i(1 - \tilde{z}_i)) \Theta(y_{ij,k}(1 - y_{ij,k})) (\tilde{z}_i(1 - \tilde{z}_i))^{-\epsilon} (1 - y_{ij,k})^{1-2\epsilon} y_{ij,k}^{-\epsilon} \quad (3.56)$$

where $d\Omega^{D-2}$ is the differential of the solid angle perpendicular to $\tilde{p}_{ij}$ and $\tilde{p}_k$. In the sketch of three-momenta in Figure 3.6 it corresponds to the azimuthal angle ϕ . Its integral evaluates to

$$\int d\Omega^{D-2} = \frac{2\pi}{\pi^\epsilon \Gamma(1 - \epsilon)}. \quad (3.57)$$

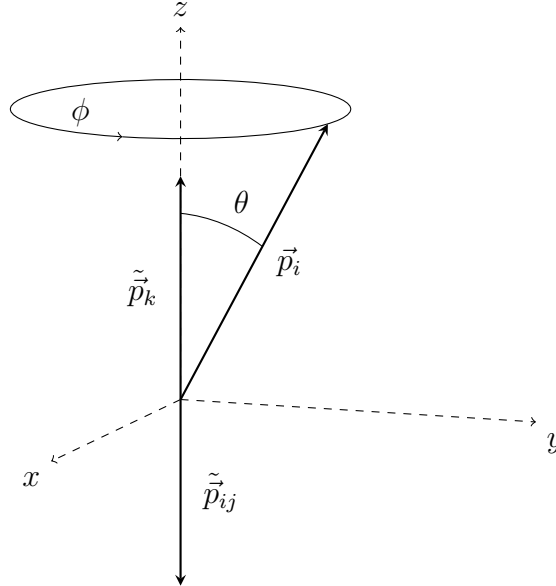


Figure 3.6: Sketch of the azimuthal angle ϕ with respect to the underlying Born momenta $\tilde{p}_{ij}$ and $\tilde{p}_k$.

⁹A factor $(1 - y_{ij,k})^{-2}$ arises from the transformation of $\delta(p_k^2)$, the denominator stems from the transformation $p_j \rightarrow \tilde{p}_{ij}$ and the rest is the result of the $p_k \rightarrow \tilde{p}_k$ transformation.

The integrated dipole reads

$$\int [dp_i(\tilde{p}_{ij}, \tilde{p}_k)] \mathcal{D}_{ij,k} = -\mathcal{V}_{ij,k} \left\langle 1, \dots, \tilde{i}j, \tilde{k}, \dots, m+1 \left| \frac{\mathbf{T}_k \mathbf{T}_{ij}}{\mathbf{T}_{ij}^2} \right| 1, \dots, \tilde{i}j, \tilde{k}, \dots, m+1 \right\rangle_m \quad (3.58)$$

with

$$\mathcal{V}_{ij,k} = \int [dp_i(\tilde{p}_{ij}, \tilde{p}_k)] \frac{1}{2p_i p_j} \langle \mathbf{V}_{ij,k} \rangle = \frac{\alpha_s}{2\pi} \frac{1}{\Gamma(1-\epsilon)} \left(\frac{4\pi\mu^2}{2\tilde{p}_{ij}\tilde{p}_k} \right)^\epsilon \mathcal{V}_{ij}(\epsilon). \quad (3.59)$$

Here $\langle \mathbf{V}_{ij,k} \rangle$ denotes the averaging of the pertaining helicity matrices in Equation (3.21) - (3.23) over the polarisation of the emitter parton, see [24], and $\mathcal{V}_{ij}(\epsilon)$ are the functions, comprising the poles in ϵ :

$$\mathcal{V}_{ij}(\epsilon) = \int_0^1 d\tilde{z}_i (\tilde{z}_i(\tilde{z}_i - 1))^{-\epsilon} \int_0^1 \frac{dy}{y} (1-y)^{1-2\epsilon} y^{-\epsilon} \frac{\langle \mathbf{V}_{ij,k} \rangle}{8\pi\alpha_s\mu^{2\epsilon}}. \quad (3.60)$$

They are evaluated by means of the Euler beta function and yield

$$\mathcal{V}_{qg}(\epsilon) = \frac{\Gamma^3(1-\epsilon)}{\Gamma(1-3\epsilon)} C_F \left[\frac{1}{\epsilon^2} + \frac{1}{\epsilon} \frac{3+\epsilon}{2(1-3\epsilon)} \right] = C_F \left[\frac{1}{\epsilon^2} + \frac{3}{2\epsilon} + 5 - \frac{\pi^2}{2} + \mathcal{O}(\epsilon) \right], \quad (3.61)$$

$$\mathcal{V}_{q\bar{q}}(\epsilon) = \frac{\Gamma^3(1-\epsilon)}{\Gamma(1-3\epsilon)} T_R \left[-\frac{1}{\epsilon} \frac{2(1-\epsilon)}{(1-3\epsilon)(3-2\epsilon)} \right] = T_R \left[-\frac{2}{3\epsilon} - \frac{16}{9} + \mathcal{O}(\epsilon) \right], \quad (3.62)$$

$$\mathcal{V}_{gg}(\epsilon) = \frac{\Gamma^3(1-\epsilon)}{\Gamma(1-3\epsilon)} 2C_A \left[\frac{1}{\epsilon^2} + \frac{1}{\epsilon} \frac{11-7\epsilon}{2(1-3\epsilon)(3-2\epsilon)} \right] = 2C_A \left[\frac{1}{\epsilon^2} + \frac{11}{6\epsilon} + \frac{50}{9} - \frac{\pi^2}{2} + \mathcal{O}(\epsilon) \right]. \quad (3.63)$$

To arrive at a formula summarising the integrated dipoles, a careful counting of symmetry factors of the m -parton configuration is required, see [24]. The contribution of the integrated subtraction terms to the cross-section, i.e. the integral of Equation (3.27), are then given by

$$\int_m d\sigma_{ab}^I(p_a, p_b) \Big|_{\text{FF}}^{\text{CS}} = \int_{m+1} d\sigma_{ab}^S(p_a, p_b) \Big|_{\text{FF}}^{\text{CS}} = \int_m d\sigma_{ab}^B(p_a, p_b) \cdot \mathbf{I}(\epsilon) \Big|_{\text{FF}}. \quad (3.64)$$

The notation $d\sigma_{ab}^B(p_a, p_b) \cdot \mathbf{I}(\epsilon) \Big|_{\text{FF}}$ stands for $d\sigma_{ab}^B(p_a, p_b)$ in which the replacement

$$\begin{aligned} |\mathcal{M}_{m,ab}|^2 &= {}_{m,ab} \langle 1, \dots, m; a, b | 1, \dots, m; a, b \rangle_{m,ab} \\ &\rightarrow {}_{m,ab} \left\langle 1, \dots, m; a, b | \mathbf{I}(\epsilon) \Big|_{\text{FF}} | 1, \dots, m; a, b \right\rangle_{m,ab} \end{aligned} \quad (3.65)$$

is made. The insertion operator in its full momentum dependence reads

$$\mathbf{I}(p_1, \dots, p_m; \epsilon) \Big|_{\text{FF}} = -\frac{\alpha_s}{2\pi} \frac{1}{\Gamma(1-\epsilon)} \sum_{i=1}^m \frac{1}{\mathbf{T}_i^2} \mathcal{V}_i(\epsilon) \sum_{\substack{k=1 \\ k \neq i}}^m \mathbf{T}_i \mathbf{T}_k \left(\frac{4\pi\mu_R}{2p_i p_k} \right)^\epsilon. \quad (3.66)$$

The singular function is given by

$$\mathcal{V}_i(\epsilon) = \begin{cases} \mathcal{V}_{qg}(\epsilon) & \text{if } i = q, \bar{q} \\ \frac{1}{2} \mathcal{V}_{gg}(\epsilon) + n_f \mathcal{V}_{q\bar{q}}(\epsilon) & \text{if } i = g \end{cases} \quad (3.67)$$

where n_f is the number of massless quarks.

Dipoles for Final-State Emitter and Initial-State Spectator

As opposed to the integration of FF-dipoles, we cannot write a factorisation of the phase-space differential but a convolution:

$$d\phi(p_i, p_j; Q + p_a) = \int_0^1 dx \, d\phi(\tilde{p}_{ij}; Q + xp_a) [dp_i(\tilde{p}_{ij}; p_a, x)] \quad (3.68)$$

where $Q = p_i + p_j - p_a$. This is because we do not integrate over initial-state parton momenta, like p_a .

Here and for the following two dipole types, we refrain from giving details of the calculation and encourage the reader to consult [24] in case of interest. The integral of the differential form of FI-dipoles, see Equation (3.34), evaluates to

$$\begin{aligned} \int_m d\sigma_{ab}^{\text{I}}(p_a, p_b) \Big|_{\text{FI}}^{\text{CS}} &= \int_{m+1} d\sigma_{ab}^{\text{S}}(p_a, p_b) \Big|_{\text{FI}}^{\text{CS}} = \int_m d\sigma_{ab}^{\text{B}}(p_a, p_b) \cdot \mathbf{I}(\epsilon) \Big|_{\text{FI}}^{\text{CS}} \\ &+ \int_0^1 dx \int_m d\sigma_{ab}^{\text{B}}(xp_a, p_b) \cdot \mathbf{K}^a(x) \Big|_{\text{FI}}^{\text{CS}} \\ &+ \int_0^1 dx \int_m d\sigma_{ab}^{\text{B}}(p_a, xp_b) \cdot \mathbf{K}^b(x) \Big|_{\text{FI}}^{\text{CS}}. \end{aligned} \quad (3.69)$$

The insertion operator containing all the poles differs from the one in Equation (3.66) only by a different sum:

$$\mathbf{I}(p_1, \dots, p_m, p_a, p_b; \epsilon) \Big|_{\text{FI}} = -\frac{\alpha_s}{2\pi} \frac{1}{\Gamma(1-\epsilon)} \sum_{i=1}^m \frac{1}{\mathbf{T}_i^2} \mathcal{V}_i(\epsilon) \mathbf{T}_i \left(\mathbf{T}_a \left(\frac{4\pi\mu_R}{2p_i p_a} \right)^\epsilon + (a \leftrightarrow b) \right). \quad (3.70)$$

The $\mathbf{K}$ -operator reads

$$\mathbf{K}^a(x) \Big|_{\text{FI}}^{\text{CS}} = -\frac{\alpha_s}{2\pi} \sum_{i=1}^m \mathbf{T}_i \mathbf{T}_a \left\{ \left(\frac{2}{1-x} \ln \frac{1}{1-x} \right)_+ + \frac{2}{1-x} \ln(2-x) - \frac{\gamma_i}{\mathbf{T}_i^2} \left[\left(\frac{1}{1-x} \right)_+ + \delta(1-x) \right] \right\}. \quad (3.71)$$

Note the presence of plus-distributions, which is necessitated by the comment above about not integrating over initial-state momenta and still being able to extract the singularities uniformly in x . The plus-distribution, avoiding a pole at $x \rightarrow 1$ is defined by its action on a test function $g(x)$ by

$$\int_0^1 dx g(x) [f(x)]_+ = \int_0^1 dx [g(x) - g(1)] f(x). \quad (3.72)$$

The constants γ_i are given by

$$\gamma_i = \begin{cases} \frac{3}{2} C_F & \text{if } i = q, \bar{q} \\ \frac{11}{6} C_A - \frac{2}{3} T_R n_f & \text{if } i = g \end{cases}. \quad (3.73)$$

Dipoles for Initial-State Emitter and Final-State Spectator

In order to cancel all divergences of the differential IF-dipoles, see Equation (3.42), we have to add collinear counterterms to their integral:

$$\begin{aligned} \int_m d\sigma_{ab}^{\text{I}}(p_a, p_b) \Big|_{\text{IF}}^{\text{CS}} &= \int_{m+1} d\sigma_{ab}^{\text{S}}(p_a, p_b) \Big|_{\text{IF}}^{\text{CS}} + \int_m d\sigma_{ab}^{\text{C}}(p_a, p_b) \Big|_{\text{IF}}^{\text{CS}} = \int_m d\sigma_{ab}^{\text{B}}(p_a, p_b) \cdot \mathbf{I}(\epsilon) \Big|_{\text{IF}}^{\text{CS}} \\ &+ \sum_{a'} \int_0^1 dx \int_m d\sigma_{a'b}^{\text{B}}(xp_a, p_b) \cdot \left(\mathbf{K}^{aa'}(x) + \mathbf{P}^{aa'}(x, \mu_F) \right) \Big|_{\text{IF}}^{\text{CS}} \\ &+ \sum_{b'} \int_0^1 dx \int_m d\sigma_{ab'}^{\text{B}}(p_a, xp_b) \cdot \left(\mathbf{K}^{bb'}(x) + \mathbf{P}^{bb'}(x, \mu_F) \right) \Big|_{\text{IF}}^{\text{CS}}. \end{aligned} \quad (3.74)$$

Note that we included only a subset of the collinear counterterms from Equation (3.15). In fact, we split them by means of colour conservation ($\mathbf{T}_{a'} + \mathbf{T}_{b'} + \sum_{k=1}^m \mathbf{T}_k = 0$):

$$d\sigma_{ab}^C(p_a, p_b) = d\sigma_{ab}^C(p_a, p_b)\Big|_{\text{IF}} + d\sigma_{ab}^C(p_a, p_b)\Big|_{\text{II}} \quad \text{with} \quad (3.75)$$

$$\begin{aligned} d\sigma_{ab}^C(p_a, p_b)\Big|_{\text{IF}} &= \frac{\alpha_s}{2\pi} \frac{1}{\Gamma(1-\epsilon)} \sum_{a'b'} \int_0^1 dz_a \int_0^1 dz_b d\sigma_{a'b'}^B(z_a p_a, z_b p_b) \cdot \\ &\quad \left\{ \delta_{bb'} \delta(1-z_b) \sum_{k=1}^m \frac{\mathbf{T}_k \mathbf{T}_{a'}}{\mathbf{T}_{a'}^2} \left[-\frac{1}{\epsilon} \left(\frac{4\pi\mu_R}{\mu_F} \right)^\epsilon P^{aa'}(z_a) + K_{\text{F.S.}}^{aa'}(z_a) \right] + \right. \\ &\quad \left. \delta_{aa'} \delta(1-z_a) \sum_{k=1}^m \frac{\mathbf{T}_k \mathbf{T}_{b'}}{\mathbf{T}_{b'}^2} \left[-\frac{1}{\epsilon} \left(\frac{4\pi\mu_R}{\mu_F} \right)^\epsilon P^{bb'}(z_b) + K_{\text{F.S.}}^{bb'}(z_b) \right] \right\}, \quad (3.76) \end{aligned}$$

$$\begin{aligned} d\sigma_{ab}^C(p_a, p_b)\Big|_{\text{II}} &= \frac{\alpha_s}{2\pi} \frac{1}{\Gamma(1-\epsilon)} \sum_{a'b'} \int_0^1 dz_a \int_0^1 dz_b d\sigma_{a'b'}^B(z_a p_a, z_b p_b) \cdot \\ &\quad \left\{ \delta_{bb'} \delta(1-z_b) \frac{\mathbf{T}_{a'} \mathbf{T}_{b'}}{\mathbf{T}_{a'}^2} \left[-\frac{1}{\epsilon} \left(\frac{4\pi\mu_R}{\mu_F} \right)^\epsilon P^{aa'}(z_a) + K_{\text{F.S.}}^{aa'}(z_a) \right] + \right. \\ &\quad \left. \delta_{aa'} \delta(1-z_a) \frac{\mathbf{T}_{a'} \mathbf{T}_{b'}}{\mathbf{T}_{b'}^2} \left[-\frac{1}{\epsilon} \left(\frac{4\pi\mu_R}{\mu_F} \right)^\epsilon P^{bb'}(z_b) + K_{\text{F.S.}}^{bb'}(z_b) \right] \right\}. \quad (3.77) \end{aligned}$$

The operator containing the singularities is again very similar to the above ones, in fact the only differences to Equation (3.70) are the subscripts of $\mathcal{V}$ and $\mathbf{T}^2$:

$$\mathbf{I}(p_1, \dots, p_m, p_a, p_b; \epsilon)\Big|_{\text{IF}} = -\frac{\alpha_s}{2\pi} \frac{1}{\Gamma(1-\epsilon)} \sum_{k=1}^m \mathbf{T}_k \left(\frac{\mathbf{T}_a}{\mathbf{T}_a^2} \mathcal{V}_a(\epsilon) \left(\frac{4\pi\mu_R}{2p_k p_a} \right)^\epsilon + (a \leftrightarrow b) \right). \quad (3.78)$$

The $\mathbf{K}$ and $\mathbf{P}$ -operators account for the splitting of an initial-state parton and are thus non-diagonal:

$$\begin{aligned} \mathbf{K}^{aa'}(x)\Big|_{\text{IF}}^{\text{CS}} &= -\frac{\alpha_s}{2\pi} \left\{ \sum_{k=1}^m \frac{\mathbf{T}_k \mathbf{T}_{a'}}{\mathbf{T}_{a'}^2} \left[\overline{K}^{aa'}(x) - \delta^{aa'} \mathbf{T}_a^2 \left[\left(\frac{2}{1-x} \ln \frac{1}{1-x} \right)_+ + \frac{2}{1-x} \ln(2-x) \right] \right. \right. \\ &\quad \left. \left. - K_{\text{F.S.}}^{aa'}(x) \right] \right\}, \quad (3.79) \end{aligned}$$

$$\mathbf{P}^{aa'}(p_1, \dots, p_m; x p_a, \mu_F)\Big|_{\text{IF}}^{\text{CS}} = \frac{\alpha_s}{2\pi} P^{aa'}(x) \sum_{k=1}^m \frac{\mathbf{T}_{a'} \mathbf{T}_k}{\mathbf{T}_{a'}^2} \ln \frac{\mu_F}{2x p_a p_k}. \quad (3.80)$$

We sum over all possible flavours a' and b' which might originate from the splitting and give a non-vanishing Born matrix element. The functions $\overline{K}^{ab}(x)$ and the regularised Altarelli-Parisi splitting functions $P^{ab}(x)$ are given in Appendix A. The functions $K_{\text{F.S.}}^{ab}(x)$ encode the factorisation scheme. They are zero in the $\overline{\text{MS}}$ -scheme.

Dipoles for Initial-State Emitter and Initial-State Spectator

We finally quote the integral of the differential II-dipoles (Equation (3.52)) along with their corresponding collinear counterterms in Equation (3.77):

$$\begin{aligned} \int_m d\sigma_{ab}^I(p_a, p_b) \Big|_{\text{II}}^{\text{CS}} &= \int_{m+1} d\sigma_{ab}^S(p_a, p_b) \Big|_{\text{II}}^{\text{CS}} + \int_m d\sigma_{ab}^C(p_a, p_b) \Big|_{\text{II}}^{\text{CS}} = \int_m d\sigma_{ab}^B(p_a, p_b) \cdot \mathbf{I}(\epsilon) \Big|_{\text{II}}^{\text{CS}} \\ &+ \sum_{a'} \int_0^1 dx \int_m d\sigma_{a'b}^B(xp_a, p_b) \cdot \left(\mathbf{K}^{aa'}(x) + \mathbf{P}^{aa'}(x, \mu_F) \right) \Big|_{\text{II}}^{\text{CS}} \\ &+ \sum_{b'} \int_0^1 dx \int_m d\sigma_{ab'}^B(p_a, xp_b) \cdot \left(\mathbf{K}^{bb'}(x) + \mathbf{P}^{bb'}(x, \mu_F) \right) \Big|_{\text{II}}^{\text{CS}}. \end{aligned} \quad (3.81)$$

The poles are contained within

$$\mathbf{I}(p_1, \dots, p_m, p_a, p_b; \epsilon) \Big|_{\text{II}} = -\frac{\alpha_s}{2\pi} \frac{1}{\Gamma(1-\epsilon)} \frac{\mathbf{T}_a \mathbf{T}_b}{\mathbf{T}_a^2} \mathcal{V}_a(\epsilon) \left(\frac{4\pi\mu_R}{2p_a p_b} \right)^\epsilon + (a \leftrightarrow b). \quad (3.82)$$

and the other two operators are given by

$$\mathbf{K}^{aa'}(x) \Big|_{\text{II}}^{\text{CS}} = -\frac{\alpha_s}{2\pi} \frac{\mathbf{T}_{a'} \mathbf{T}_b}{\mathbf{T}_{a'}^2} \left[\bar{K}^{aa'}(x) + \tilde{K}^{aa'}(x) - K_{\text{F.S.}}^{aa'}(x) \right], \quad (3.83)$$

$$\mathbf{P}^{aa'}(p_1, \dots, p_m; xp_a, \mu_F) \Big|_{\text{II}}^{\text{CS}} = \frac{\alpha_s}{2\pi} P^{aa'}(x) \frac{\mathbf{T}_{a'} \mathbf{T}_b}{\mathbf{T}_{a'}^2} \ln \frac{\mu_F}{2xp_a p_b}. \quad (3.84)$$

Also the functions $\tilde{K}^{ab}(x)$ are given in Appendix A.

Summary

We have given the integrated CS dipoles for the four types separately since it is easier this way to compare them with integrated pseudo-dipoles in the next chapter. This is particularly useful for the purpose of a step-by-step implementation of pseudo-dipoles. However, we also like to sum the four types up in order to have one succinct formula containing the final result:

$$\begin{aligned} \int_m d\sigma_{ab}^I(p_a, p_b) \Big|_{\text{II}}^{\text{CS}} &= \int_{m+1} d\sigma_{ab}^S(p_a, p_b) \Big|_{\text{II}}^{\text{CS}} + \int_m d\sigma_{ab}^C(p_a, p_b) \Big|_{\text{II}}^{\text{CS}} = \int_m d\sigma_{ab}^B(p_a, p_b) \cdot \mathbf{I}(\epsilon) \\ &+ \sum_{a'} \int_0^1 dx \int_m d\sigma_{a'b}^B(xp_a, p_b) \cdot \left(\mathbf{K}^{aa'}(x) + \mathbf{P}^{aa'}(x, \mu_F) \right) \Big|_{\text{II}}^{\text{CS}} \\ &+ \sum_{b'} \int_0^1 dx \int_m d\sigma_{ab'}^B(p_a, xp_b) \cdot \left(\mathbf{K}^{bb'}(x) + \mathbf{P}^{bb'}(x, \mu_F) \right) \Big|_{\text{II}}^{\text{CS}}. \end{aligned} \quad (3.85)$$

The three operators read

$$\begin{aligned} \mathbf{I}(p_1, \dots, p_m, p_a, p_b; \epsilon) = & -\frac{\alpha_s}{2\pi} \frac{1}{\Gamma(1-\epsilon)} \left\{ \sum_{i=1}^m \frac{1}{\mathbf{T}_i^2} \mathcal{V}_i(\epsilon) \left[\sum_{\substack{k=1 \\ k \neq i}}^m \mathbf{T}_i \mathbf{T}_k \left(\frac{4\pi\mu_R}{2p_i p_k} \right)^\epsilon + \mathbf{T}_i \mathbf{T}_a \left(\frac{4\pi\mu_R}{2p_a p_i} \right)^\epsilon \right. \right. \\ & \left. \left. + (a \leftrightarrow b) \right] + \frac{1}{\mathbf{T}_a^2} \mathcal{V}_a(\epsilon) \left[\sum_{i=1}^m \mathbf{T}_a \mathbf{T}_i \left(\frac{4\pi\mu_R}{2p_a p_i} \right)^\epsilon + \mathbf{T}_a \mathbf{T}_b \left(\frac{4\pi\mu_R}{2p_a p_b} \right)^\epsilon \right] + (a \leftrightarrow b) \right\}, \end{aligned} \quad (3.86)$$

$$\begin{aligned} \mathbf{K}^{aa'}(x) \Big|^\text{CS} = & \frac{\alpha_s}{2\pi} \left\{ \bar{K}^{aa'}(x) - K_{\text{F.S.}}^{aa'}(x) - \frac{\mathbf{T}_{a'} \mathbf{T}_b}{\mathbf{T}_{a'}^2} \tilde{K}^{aa'}(x) + \delta^{aa'} \sum_{i=1}^m \mathbf{T}_a \mathbf{T}_i \frac{\gamma_i}{\mathbf{T}_i^2} \right. \\ & \left. \cdot \left[\left(\frac{1}{1-x} \right)_+ + \delta(1-x) \right] \right\}, \end{aligned} \quad (3.87)$$

$$\mathbf{P}^{aa'}(p_1, \dots, p_m; xp_a, \mu_F) \Big|^\text{CS} = \frac{\alpha_s}{2\pi} P^{aa'}(x) \frac{1}{\mathbf{T}_{a'}^2} \left[\sum_{i=1}^m \mathbf{T}_{a'} \mathbf{T}_i \ln \frac{\mu_F}{2xp_a p_i} + \mathbf{T}_{a'} \mathbf{T}_b \ln \frac{\mu_F}{2xp_a p_b} \right]. \quad (3.88)$$

CS dipole subtraction proved itself an appropriate algorithm to automatically treat IR divergences in NLO QCD calculations. It has been implemented in Monte Carlo generators like HERWIG and SHERPA. The implementation within the latter is described in [57].

3.4 Alternative Approaches

CS dipole subtraction is not the only known way to subtract/deal with IR divergences. In this section we present two alternative approaches.

3.4.1 FKS Subtraction

There is another commonly used subtraction scheme, which is named after its inventors Frixione, Kunszt and Signer FKS subtraction [21, 58]. Like CS dipole subtraction it is based on the extraction of singularities in the real correction. To be more precise, the phase-space of the real corrections is divided into different regions and within each region there is at most one parton (pair) causing the real correction matrix element to diverge. Thus the real corrections R – being the absolute square over all amplitudes in question – can be written as

$$R = \sum_i R_i + \sum_{ij} R_{ij}. \quad (3.89)$$

The term R_i dominates when parton i becomes soft or collinear to an initial state parton and R_{ij} if the partons i and j become collinear. These contributions are projected out by a

function S whose value depends on the real correction phase-space:

$$R_i = S_i R, \quad R_{ij} = S_{ij} R \quad \text{with} \quad \sum_i S_i + \sum_{ij} S_{ij} = 1. \quad (3.90)$$

Having separated all singularities, the phase-space of those regions is parametrised in a way which allows to extract the singularities by means of analytical integration. The terms arising from that act as integrated subtraction terms and are thus added to the virtual corrections. The remainder is numerically integrable as subtracted real correction.

However, also in FKS subtraction there is a recoil associated with the mapping from real to Born kinematics, which is required for the subtraction terms. This mapping – which is not unique – is not given explicitly in the original paper [21], but one possible choice can be found in Chapter 5 of [59]: There the integrated out parton (the i th one) is parametrised (for final-state singularities) by

$$\xi_i = \frac{2p_i^0}{q^0}, \quad y_{ai} = \frac{\vec{p}_a \cdot \vec{p}_i}{|\vec{p}_a||\vec{p}_i|}, \quad \text{and} \quad \phi. \quad (3.91)$$

The energy fraction $0 \leq \xi_i \leq 1$ is a function of the center-of-mass (CMS) energy q^0 of the whole final-state, which is defined by $q = \sum_{i=1}^{m+1} p_i$ and $\vec{q} = 0$. It parametrises the soft singularity. The collinear singularity is controlled by $-1 \leq y_{ai} = \cos \theta_{ai} \leq 1$, where θ_{ai} is the angle between the potentially collinear parton pair a and i . The angle ϕ is defined as the azimuthal angle of $\vec{p}_i$ around $\vec{p}_a + \vec{p}_i$. Both angles are calculated in the CMS frame of the whole final state.

The recoil is then absorbed by all remaining final-state particles which do not take part in the splitting process, i.e. the momenta

$$\left\{ p_\beta | \beta \in \{1, \dots, m+1\}, \beta \notin \{a, i\} \right\}. \quad (3.92)$$

The Born-kinematics is thus given by

$$\tilde{p}_\beta = \mathbb{B} p_\beta, \quad \beta \in \{1, \dots, m+1\}, \beta \notin \{a, i\} \quad \text{and} \quad \tilde{p}_a = q - \mathbb{B} \sum_{\substack{\beta=1 \\ \beta \neq a, i}}^{m+1} p_i, \quad (3.93)$$

where $\mathbb{B}$ is a Lorentz boost defined in [59].

One commonly used implementation of FKS subtraction can be found in MADFKS [60] which can be interfaced to the MADGRAPH [61] matrix element generator.

3.4.2 Phase-Space Slicing

A conceptually different approach to the just outlined subtraction algorithms is the technique of phase-space slicing [52]. Here, two cutoff parameters δ_s and δ_c , one for soft and one for

collinear singularities are introduced. They act as delimiter between the soft and hard part of the cross-section on the one hand and between the hard collinear and hard non-collinear one on the other hand. In the soft and hard collinear part of the cross-section suitable approximations are performed to render those terms analytically integrable. In those approximations, terms of $\mathcal{O}(\delta)$ are neglected while a logarithmic dependence on the cutoff parameters is retained. The remaining hard non-collinear cross-section is usually integrated by means of Monte Carlo methods and also depends on δ_s and δ_c . For increasingly small values of the cutoff parameters, the dependence of the full cross-section upon them is supposed to decrease. This is often verified by producing explicit plots showing the cutoff dependence of the hard non-collinear and the remaining part of the cross-section along with their sum, see e.g. [62].

From a theoretical point of view the cutting parameters should be chosen as small as possible. On the other hand numerical issues do not allow them to be too small. This trade-off can induce large uncertainties in the integration and there is no general prescription how to deal with them. Because of this drawback, the slicing method is less popular than the aforementioned subtraction techniques.

4 Resonance-Aware Subtraction with Pseudo-Dipoles

In this chapter we explain an adaptation of the above reviewed CS dipole subtraction, which is particularly useful for the application to processes comprising intermediate resonances. We begin this chapter by illustrating the problem, which arises when using CS dipoles for processes featuring intermediate resonances, and proceed with the introduction of differential pseudo-dipoles along with their original use case. After that, we show how those can be used to render the subtraction resonance-aware. This includes a presentation of the integrated form of pseudo-dipoles. We contrast computations using pseudo-dipoles and standard CS dipoles before we conclude this chapter by discussing resonances-aware subtraction in the context of the above mentioned FKS method.

This chapter is based strongly on [7]. This means that it consists of text passages copied from this reference.¹⁰ Wherever this is not the case it follows this reference’s line of thought. Excluded from this is Section 4.5.

4.1 The Problem of Resonances for NLO Subtraction Schemes

Applying standard subtraction techniques to calculate processes with intermediate resonances at NLO results in “an undesired feature, which can most easily be explained using a concrete example, say $e^+e^- \rightarrow W^+W^-b\bar{b}$. If the center-of-mass energy is larger than the top pair threshold $\sqrt{s} \gtrsim 2m_t$, this process is dominated by on-shell $t\bar{t}$ -production and decay. One

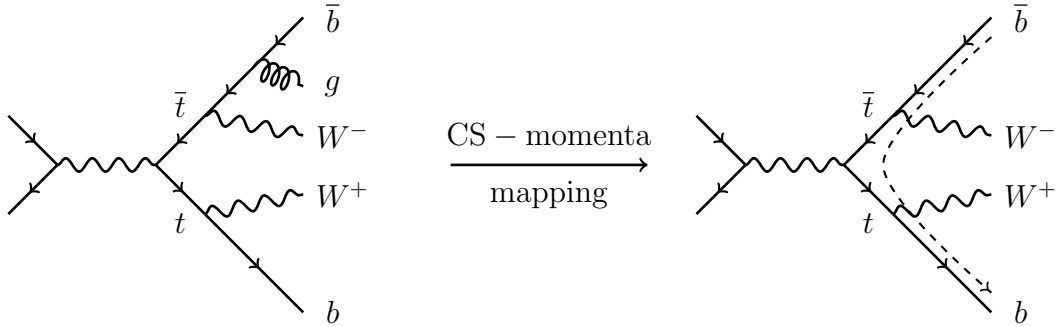


Figure 4.1: “Possible real correction configuration for $W^+W^-b\bar{b}$ production and Born configuration of associated standard CS dipole. The curved arrow on the right indicates the flow of the recoil.” [7]. This figure is taken from [7].

possible real correction to this process is depicted on the left-hand side of Figure 4.1. The subtraction term associated to the $\bar{b}g$ collinear sector is constructed from the Born diagram on the right-hand side of Figure 4.1, and its kinematics is obtained by mapping the on-shell final-state momenta of the real correction to Born kinematics using the algorithm in [24].In

¹⁰There are differences in those text passages that are due to style adjustments, change of notation and different figure numbers, etc..

the canonical method, the momenta of the emitter (the $\bar{b}$ quark) and the spectator (the b quark) are adjusted, while all other momenta remain the same. This procedure generates a recoil that is indicated by the dashed line in Figure 4.1. The recoil leads to the subtraction term being evaluated at different virtualities of the intermediate top quarks than the real correction diagrams whose divergences it counteracts. As the top quark propagator scales like $(p_t^2 - m_t^2 + im_t\Gamma_t)^{-1}$ and $\Gamma_t \ll m_t$, the change in virtuality may cause numerically large deviations between the real corrections and the corresponding subtraction terms. Though the cancellation of IR divergences still takes place, the associated large weight fluctuations may significantly affect the convergence of the Monte Carlo integration. The problem becomes manifest when interfacing the fixed order NLO calculation to a parton shower. The difference in matrix element weights arising from resonant propagators being shifted off resonance by means of adding radiation and mapping momenta from Born to real emission kinematics bears no relation with the logarithms to be resummed by the parton shower, yet its numerical impact may be similar. This motivates the usage of an improved kinematics mapping by means of pseudo-dipoles.” [7]

As an alternative, we comment on a naive approach to alter the kinematics of CS dipoles in Appendix B. We only mention this ansatz as an aside since we did – due to additional problems – not develop it as far as the one with pseudo-dipoles.

The next section, excluding its subsections, is copied from paragraphs of [7] written by the author of this thesis.

4.2 Catani-Seymour Pseudo-Dipole Formalism

The concept of pseudo-dipoles was introduced in [24] to cope with the situation where a subset of the final-state partons lead to the production of identified hadrons. In such a scenario, both emitter and spectator of a dipole may be “identified” in the sense that they fragment into identified hadrons. Because the directions of the identified hadrons are measurable, neither emitter nor spectator parton in the dipole can be allowed to absorb the recoil when mapping the momenta of the real emission final state to a Born configuration. Instead the kinematics is balanced by adjusting the momenta of all non-identified final-state particles (not just partons). This idea is reminiscent of standard CS dipoles with initial-state emitter and initial-state spectator. In fact, pseudo-dipoles may be thought of as a generalization of these configurations. In order to satisfy the constraint that both emitter and spectator retain their direction, an additional momentum must be introduced that can absorb the recoil in the momentum mapping from real emission to Born kinematics. This auxiliary momentum is defined as

$$n^\mu = p_{\text{in}}^\mu - \sum_{\alpha \in \{\text{id}\}} p_\alpha^\mu, \quad (4.1)$$

where p_{in} is the total incoming momentum in the process, and the sum runs over all outgoing

identified particles. The eventual dependence of the subtraction term on n^μ accounts for the term *pseudo*-dipole. An immediate consequence of this definition is that there are only two types of pseudo-dipoles, because the spectator momentum is always in the final state. This is in contrast to standard CS dipoles, which have four different types, corresponding to all combinations of initial-state or final-state emitter with initial-state or final-state spectator. We denote pseudo-dipoles with final-state emitter as $\mathcal{D}_{ai,b}^{(n)}$ and pseudo-dipoles with initial-state emitter as $\mathcal{D}_b^{(n)ai}$.

4.2.1 Differential Form

Figure 4.2 summarises the use case of pseudo-dipoles. In the first row, the emitter is an identified final-state parton and in the second row it is an initial-state parton. For all types, the labelling is very similar to standard II-dipoles which is due to the common features mentioned above.

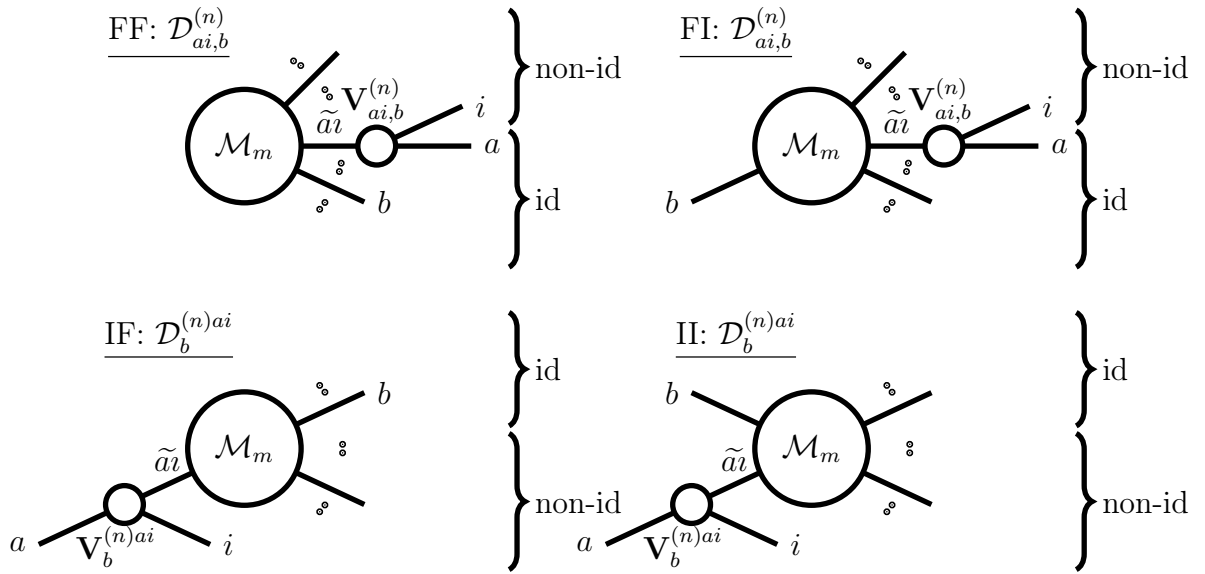


Figure 4.2: Sketch of labelling of emitter, emitted and spectator parton for pseudo-dipoles. Shown are all four possibilities which are described with two instead of four pseudo-dipole types.

Final-State Singularities

This subsection, excluding its final paragraph, is copied from text passages of [7] written by the author of this thesis.

The pseudo-dipole for splittings of final-state partons reads [24]

$$\mathcal{D}_{ai,b}^{(n)}(p_1, \dots, p_{m+1}; p_a, p_b) = -\frac{1}{2p_a p_i} \cdot_{m,a,b} \left\langle \dots, \tilde{a}l, \dots, b, \dots \left| \frac{\mathbf{T}_b \mathbf{T}_{ai}}{\mathbf{T}_{ai}^2} \mathbf{V}_{ai,b}^{(n)} \right| \dots, \tilde{a}l, \dots, b, \dots \right\rangle_{m,a,b}, \quad (4.2)$$

where a refers to an identified final-state parton (the emitter) and the color spectator b may either be another identified final-state parton or an initial-state parton. This situation is depicted in the first row of Figure 4.2. The kinematics in the correlated Born matrix element is given as follows: The momentum of the emitter is scaled as

$$\tilde{p}_{ai}^\mu = \frac{1}{z_{ain}} p_a^\mu \quad \text{where} \quad z_{ain} = \frac{p_a n}{(p_a + p_i)n}. \quad (4.3)$$

All non-identified particles (not just partons) in the final state are Lorentz transformed by

$$\tilde{k}_j^\mu = \Lambda_\nu^\mu(K, \tilde{K}) k_j^\nu \quad \text{where} \quad (4.4)$$

$$\Lambda_\nu^\mu(K, \tilde{K}) = g_\nu^\mu - \frac{2(K + \tilde{K})^\mu (K + \tilde{K})_\nu}{(K + \tilde{K})^2} + \frac{2\tilde{K}^\mu K_\nu}{K^2}. \quad (4.5)$$

The momenta K^μ and $\tilde{K}^\mu$ are given by

$$K^\mu = n^\mu - p_i^\mu, \quad (4.6)$$

$$\tilde{K}^\mu = n^\mu - (1 - x_{ain})p_a^\mu \quad \text{where,} \quad x_{ain} = \frac{(p_a - p_i)n}{p_a n}. \quad (4.7)$$

The remaining momenta, namely those of identified and initial-state particles (in particular of the color spectator: parton b) remain unchanged. The complete list of pseudo-dipole insertion operators is given in [24]. As we focus on processes with no final-state gluons at Born level, the only one relevant to our computations is the $q \rightarrow qg$ insertion operator, which reads

$$\langle s | \mathbf{V}_{qag_i,b}^{(n)} | s' \rangle = 8\pi\mu_R^{2\epsilon} \alpha_s C_F \left[2 \frac{v_{i,ab}}{z_{ain}} - (1 + z_{ain}) - \epsilon(1 - z_{ain}) \right] \delta_{ss'}, \quad (4.8)$$

where

$$v_{i,ab} = \frac{p_a p_b}{p_i(p_a + p_b)}. \quad (4.9)$$

In the soft limit $z_{ain} \rightarrow 1$ which makes it apparent that Equation (4.2) converges to Equation (3.8). To see that Equation (4.2) also converges to the collinear limit of the real correction, i.e. Equation (3.11), we substitute $p_i \rightarrow \lambda p_a$ and obtain $\langle s | \mathbf{V}_{qag_i,b}^{(n)} | s' \rangle \rightarrow 8\pi\mu_R^{2\epsilon} \alpha_s \langle s | P_{qq}(\frac{1}{1+\lambda}) | s' \rangle$. Thus $1/(1+\lambda)$ is identified with the momentum fraction z in Equation (3.11).

Initial-State Singularities

This subsection is copied from paragraphs of [7] written by the author of this thesis.

The pseudo-dipole with an initial-state emitter and identified final-state or initial-state spectator reads

$$\mathcal{D}_b^{(n)ai}(p_1, \dots, p_{m+1}; p_a, p_b) = -\frac{1}{2p_a p_i} \frac{1}{x_{ain}} \cdot \left\langle \dots, \tilde{a}l, \dots, b, \dots \left| \frac{\mathbf{T}_b \mathbf{T}_{ai}}{\mathbf{T}_{ai}^2} \mathbf{V}_b^{(n)ai} \right| \dots, \tilde{a}l, \dots, b, \dots \right\rangle_{m,a,c}. \quad (4.10)$$

The two cases are sketched in the second row of Figure 4.2. Parton c is the initial-state parton, which does not emit. The momentum mapping is chosen as follows:

$$\tilde{p}_{ai}^\mu = x_{ain} p_a^\mu, \quad \tilde{k}_j^\mu = \Lambda_\nu^\mu k_j^\nu. \quad (4.11)$$

The momenta of all identified final-state partons and the other initial-state parton are left unchanged. The Lorentz transformation matrix is the same as in Equation (4.5) and x_{ain} is defined in Equation (4.7). The splitting functions are given by

$$\begin{aligned} \langle s | \mathbf{V}_b^{(n)q_a g_i} | s' \rangle &= 8\pi \mu_R^{2\epsilon} \alpha_s C_F [2v_{i,ab} - (1 + x_{ain}) - \epsilon(1 - x_{ain})] \delta_{ss'}, \\ \langle s | \mathbf{V}_b^{(n)g_a \bar{q}_i} | s' \rangle &= 8\pi \mu_R^{2\epsilon} \alpha_s T_R [1 - \epsilon - 2x_{ain}(1 - x_{ain})] \delta_{ss'}, \\ \langle \mu | \mathbf{V}_b^{(n)q_a q_i} | \nu \rangle &= 8\pi \mu_R^{2\epsilon} \alpha_s C_F \left[-g^{\mu\nu} x_{ain} + \frac{1 - x_{ain}}{x_{ain}} \frac{4p_i p_a}{2(p_a n)(p_i n) - n^2 p_i p_a} \right. \\ &\quad \left. \left(\frac{np_a}{p_i p_a} p_i^\mu - n^\mu \right) \left(\frac{np_a}{p_i p_a} p_i^\nu - n^\nu \right) \right], \\ \langle \mu | \mathbf{V}_b^{(n)g_a g_i} | \nu \rangle &= 16\pi \mu_R^{2\epsilon} \alpha_s C_A \left[-g^{\mu\nu} (v_{i,ab} - 1 + x_{ain}(1 - x_{ain})) + (1 - \epsilon) \frac{1 - x_{ain}}{x_{ain}} \right. \\ &\quad \left. \frac{2p_i p_a}{2(p_a n)(p_i n) - n^2 p_i p_a} \left(\frac{np_a}{p_i p_a} p_i^\mu - n^\mu \right) \left(\frac{np_a}{p_i p_a} p_i^\nu - n^\nu \right) \right]. \end{aligned} \quad (4.12)$$

4.3 Using Pseudo-Dipoles for Resonance-Aware Subtraction

4.3.1 Rules of Application

“We will now explain how to apply pseudo-dipoles to resonant processes, starting with the simplest case of processes without hadronic initial states.” [7] After that we generalise our rules to processes with initial-state hadrons.

This subsection is copied from paragraphs of [7] written by the author of this thesis. Added to it are the three titles of its subsections and footnote 11.

No Initial-State Hadrons

Pseudo-dipole subtraction terms for final-state singularities that preserve the invariant mass of intermediate resonances can be constructed using the following algorithm:

1. If the emitter is the decay product of a resonance and the spectator is not a decay product of the same resonance, the dipole is replaced by a pseudo-dipole where the emitter and all particles except for the emitted particle and the remaining decay products of the resonance are identified.
2. If the emitter is not a decay product of a resonance but the spectator is, the dipole is replaced by a pseudo-dipole where the emitter and all particles, which are not decay products of the resonance to which the spectator belongs are identified.
3. If emitter and spectator are decay products of the same resonance, the standard CS subtraction formalism is used.

This technique can be used in a variety of processes, for example the highly relevant case of top quark pair production, both at lepton and at hadron colliders.¹¹ However, it does not generalize to decay chains.¹² Consider again the example $e^+e^- \rightarrow W^+W^-b\bar{b}$. If $\sqrt{s} > 2m_t$

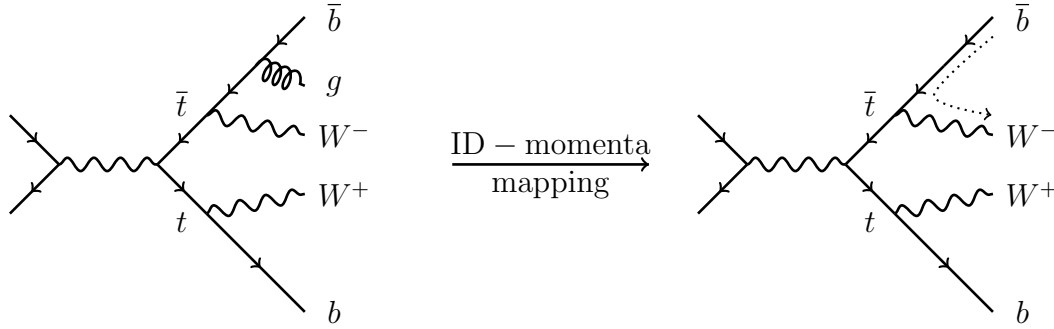


Figure 4.3: “Possible real correction configuration for $W^+W^-b\bar{b}$ production and Born configuration of associated pseudo-dipoles. The curved arrow on the right indicates the flow of the recoil.” [7] This figure is taken from [7].

the dominant contribution to the cross-section stems from diagrams like the one on the left-hand side of Figure 4.1. The standard CS dipole to cover the soft and collinear singularity associated to this diagram is constructed by using the Born level diagram on the right-hand side of Figure 4.1. In this situation the recoil from the emitter parton $\bar{b}$ to the spectator parton

¹¹Both of these processes, e.g. $e^+e^- \rightarrow W^+W^-b\bar{b}$, feature Feynman diagrams which contribute to $t\bar{t}$ -production as well as ones which do not. In this case the rules for the former diagrams take precedence, since the contribution of the latter ones are negligible with respect to them. Note that there is no harm done if standard CS dipoles are replaced by pseudo-dipoles.

¹²In particular, it would not be possible in this method to define a resonance-aware subtraction for the full six-jet (four-jet) final state in fully hadronic (semi-leptonic) $t\bar{t}$ production at hadron colliders.

b affects the potentially resonant top quark propagators. To avoid this, we replace by means of the above algorithm the standard CS dipole by a pseudo-dipole and formally “identify” particles. As the first rule takes precedence we identify $\bar{b}$, W^+ and b . In this manner, the W^- boson is the only particle left to absorb the recoil. Hence the momentum of the top quarks are unaltered and we have achieved our aim. The momentum flow corresponding to this situation is depicted in Figure 4.3. The same reasoning is applied to the pseudo-dipole in which the b quark is the emitter.

Initial-State Hadrons

When considering initial-state partons, there are in principle three more dipoles types, namely those with final-state emitter and initial-state spectator (FI), initial-state emitter and final-state spectator (IF) and finally initial-state emitter and spectator (II). As already alluded to in Section 4.2, FI-pseudo-dipoles are the same as FF-pseudo-dipoles. Hence, the rules from above apply.¹³ The case of IF-pseudo-dipoles can be generally treated by the following rule:

1. If the emitter is in the initial state and the spectator is the decay product of a resonance, the dipole is replaced by a pseudo-dipole where no particle is identified.

Thus the recoil is the same as for standard II-CS dipoles. For II-pseudo-dipoles, we choose the same recoil scheme as for IF-pseudo-dipoles. In doing so, pseudo- and standard CS dipoles of II-type are identical, which stresses the fact that standard II-CS dipoles are already resonance-aware. This is because the momentum mapping is given in the form of a Lorentz transformation, which preserves the virtuality of all final-state particles and thus all intermediate resonances, hence rendering the mapping resonance-aware. Figure 4.4 displays the recoil flow for pseudo-dipoles with initial-state singularities at the example of $gg \rightarrow W^+W^-g\bar{b}b$.

In view of our application example $pp \rightarrow W^+W^-j_bj_b$ in Section 4.4, we like to comment on the situation in which one has to deal with multiple (sub-)processes. To ensure that pseudo-dipoles are used only if potentially resonant diagrams occur, we replace standard CS dipoles with pseudo-dipoles only if both real and underlying Born configuration comprise at least one b and one $\bar{b}$ quark in the final state. In this concrete example this means that sub-processes, which do not feature a resonance, like $b\bar{b} \rightarrow W^+W^-b\bar{b}$, are treated with standard CS dipoles.

Differences to Original Use Case

We stress at this point two vital differences of the use of pseudo-dipoles for resonance-aware subtraction and their original purpose:

¹³In order to be applicable to initial-state spectators, we have to rephrase the second rule to: If the emitter is not the decay product of a resonance and the spectator is an initial-state parton, the dipole is replaced by a pseudo-dipole where the emitter and all particles, which are not decay products of any resonance are identified.

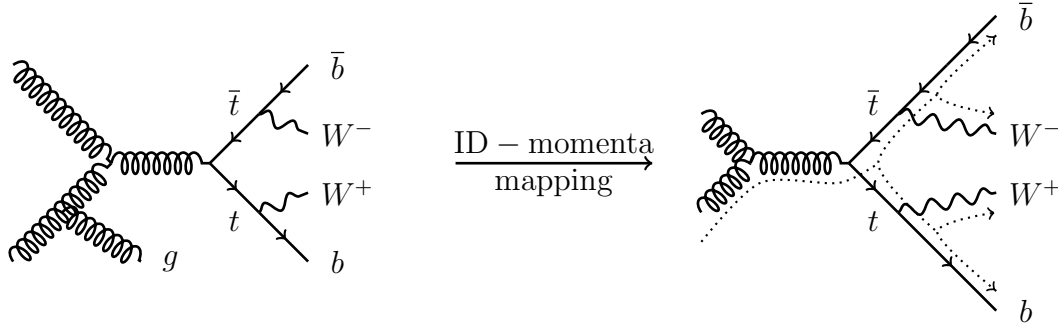


Figure 4.4: “Exemplary momentum mapping for $gg \rightarrow bW^+ \bar{b}W^-$ from a real configuration to an underlying Born configuration for an initial-state singularity. The curved arrow on the right indicates the flow of the recoil.” [7] This figure is taken from [7].

- We do not identify particles throughout the calculation, but identify different particles depending on the subtraction term.
- We integrate over the momenta of the identified partons by means of adding partonic fragmentation functions.

We will show in the following how this affects the **H**-, **K**- and **P**-operators given in [24], by focusing on the case of final-state singularities in some detail before we quote the analogous results for initial-state singularities.

4.3.2 Integrated Form

Final-State Singularities

This subsection is copied from paragraphs of [7] written by the author of this thesis. In the paragraph below Equation (4.25), the text is however slightly changed.

The integrated splitting kernel for final-state emitters is defined as

$$\frac{\alpha_s}{2\pi} \frac{1}{\Gamma(1-\epsilon)} \left(\frac{4\pi\mu^2}{2p_a p_b} \right)^\epsilon \bar{\mathcal{V}}_{ai,a} := \int [dp_i(n, p_a, z)] \frac{1}{2p_a p_i} \langle \mathbf{V}_{ai,b}^{(n)}(z_{ain}; v_{iab}) \rangle. \quad (4.13)$$

where

$$\begin{aligned} [dp_i(n, p_a, z)] &= \frac{(2p_a n)^{1-\epsilon}}{16\pi^2} \frac{d\Omega^{D-2}}{(2\pi)^{1-2\epsilon}} d\tilde{v}_i dz_{ain} \Theta(z(1-z)) \Theta(\tilde{v}_i) \Theta\left(1 - \frac{n^2 \tilde{v}_i z}{2(1-z)p_a n}\right) \\ &\quad \cdot (1-z) - 2\epsilon \delta(z - z_{ain}) \left[\frac{\tilde{v}_i z}{1-z} \left(1 - \frac{n^2 \tilde{v}_i z}{2(1-z)p_a n}\right) \right]^{-\epsilon} \end{aligned} \quad (4.14)$$

is the one-emission phase-space differential obtained by factorising the real emission phase-

space. One obtains

$$\begin{aligned} \bar{\mathcal{V}}_{q,q}(z; \epsilon; p_a, p_b, n) = & -\frac{1}{\epsilon} P^{qq}(z) + \delta(1-z) V_{qg}(\epsilon) + \tilde{K}^{qq}(z) + \bar{K}^{qq}(z) + P^{qq}(z) \ln z \\ & + \mathcal{L}^{q,q}(z; p_a, p_b, n) + \mathcal{O}(\epsilon), \end{aligned} \quad (4.15)$$

where $V_{qg}(\epsilon)$ comprises all singularities needed to cancel the poles present in the virtual corrections. It is given in Equation (3.61), and all other functions are listed in Appendix A. The single poles proportional to the Altarelli-Parisi splitting functions do not appear in the integrated standard CS dipole terms. They are cancelled by collinear mass factorisation counterterms, which – in our approach – can be viewed as the one-loop contribution to the partonic fragmentation function to be convoluted with the subtracted hard cross section.

For simplicity, we first consider a configuration with no initial-state partons and m identified final-state (anti-)quarks at Born level. In the following, the integration over non-QCD particles shall be understood whenever we write $\int_m d\phi_m$.

For now we will not integrate over the momentum of the merged parton $\tilde{a}i$. We denote this with a subscript -1 at the integral sign. Thus the incomplete integral over the pseudo-dipoles depends on the set of momenta of identified particles $\{p_a\}$ and is given by

$$\begin{aligned} \int_{m+1-1} d\sigma^S \Big|_{\text{FF}}^{\text{ID}}(\{p_a\}) &= \int_{m+1-1} \mathcal{N}_{in} \sum_{\{m+1\}} d\phi_{m+1-1} \frac{1}{S_{\{m+1\}}} \sum_{\substack{\text{pairs} \\ a,i}} \\ &\cdot \sum_{b \neq a,i} \mathcal{D}_{ai,b}^{(n)}(p_1, \dots, p_{m+1}) F_J^{(m)}(\tilde{p}_1, \dots, \tilde{p}_{ai}, \dots, \tilde{p}_{m+1}) \\ &= - \int_{m-1} \mathcal{N}_{in} \int_0^1 \frac{dz}{z^{2-2\epsilon}} \sum_{\tilde{a}i=1}^m \sum_{\{m\}} d\phi_{m-1} \frac{1}{S_{\{m\}}} F_J^{(m)} \sum_{\substack{b=1 \\ b \neq \tilde{a}i}}^m |\mathcal{M}_m^{\tilde{a}i b}|^2 \\ &\cdot \frac{\alpha_s}{2\pi} \frac{1}{\Gamma(1-\epsilon)} \left(\frac{4\pi\mu_R^2}{2p_a p_b} \right)^\epsilon \frac{1}{\mathbf{T}_{\tilde{a}i}^2} \bar{\mathcal{V}}_{\tilde{a}i,a}(z; \epsilon; p_a, p_b, n) \delta_{\tilde{a}i a}. \end{aligned} \quad (4.16)$$

Here z is used as a shorthand notation for z_{ain} , given in Equation (4.3). Again, we use the notation from [24] where $\mathcal{N}_{in}$ includes all non-QCD related factors, $\sum_{\{m+1\}}$ stands for the sum over all $m+1$ parton configurations, $S_{\{m+1\}}$ is the symmetry factor for identical partons in the final state, $F_J^{(m)}$ denotes a jet-defining function and $\mathcal{M}_m^{\tilde{a}i b}$ is a color-correlated m -parton matrix element. As we only consider $\tilde{a}i \rightarrow a+i$ as $q \rightarrow q+g$ splittings, $\tilde{a}i$ and a are always quarks. The corresponding integrated splitting function is given in Equation (4.15). Each identified final-state parton contributes a collinear mass factorisation counterterm

$$\begin{aligned} \int_{m-1} d\sigma_a^C(p_a) \Big|_{\text{FF}}^{\text{ID}} &= -\frac{\alpha_s}{2\pi} \frac{1}{\Gamma(1-\epsilon)} \int_0^1 \frac{dz}{z^{2-2\epsilon}} \delta_{\tilde{a}i a} \\ &\cdot \left[-\frac{1}{\epsilon} \left(\frac{4\pi\mu_R^2}{\mu_F^2} \right)^\epsilon P_{\tilde{a}i a}(z) + H_{\tilde{a}i a}^{F.S.}(z) \right] \int_{m-1} d\sigma_{\tilde{a}i}^B \left(\frac{p_a}{z} \right). \end{aligned} \quad (4.17)$$

where the Born cross-section is given by

$$\int_{m-1} d\sigma^B = \mathcal{N}_{in} \sum_{\{m\}} \int_{m-1} d\phi_{m-1} \frac{1}{S_{\{m\}}} F_J^{(m)} |\mathcal{M}_m|^2. \quad (4.18)$$

To avoid cluttering the notation, we drop the sub- and superscripts indicating pseudo-dipoles with final-state emitter and (color-)spectator. When we add Equation (4.16) and sum Equation (4.17) for all identified partons, we can define an insertion operator:

$$d\sigma^I(\{p_a\}) := \int_{m+1-1} d\sigma^S(\{p_a\}) + \sum_{a=1}^m \int_{m-1} d\sigma_a^C(p_a) =: \int_0^1 \frac{dz}{z^{2-2\epsilon}} \int_{m-1} d\sigma^B\left(\left\{\frac{p_a}{z}\right\}\right) \cdot \hat{\mathbf{I}}(z; \epsilon) \quad (4.19)$$

where $d\sigma^B\left(\left\{\frac{p_a}{z}\right\}\right) \cdot \hat{\mathbf{I}}(z; \epsilon)$ indicates that the squared Born matrix element $|\mathcal{M}_m|^2 = {}_m\langle p_1, \dots, p_m | p_1, \dots, p_m \rangle_m$ in Equation (4.18) is replaced by the spin- and color-correlated Born matrix element

$${}_m\left\langle p_1, \dots, \frac{p_a}{z}, \dots, p_m \left| \hat{\mathbf{I}}(z; \epsilon) \right| p_1, \dots, \frac{p_a}{z}, \dots, p_m \right\rangle_m. \quad (4.20)$$

Note that the parton $\tilde{a}i$ in this expression carries momentum $\tilde{p}_{\tilde{a}i} = p_a/z$. The insertion operator is given by

$$\begin{aligned} \hat{\mathbf{I}}(z; \epsilon) = & -\frac{\alpha_s}{2\pi} \frac{1}{\Gamma(1-\epsilon)} \sum_{\tilde{a}i=1}^m \left\{ \sum_{\substack{b=1 \\ b \neq \tilde{a}i}}^m \frac{\mathbf{T}_{\tilde{a}i} \mathbf{T}_b}{\mathbf{T}_{\tilde{a}i}^2} \left(\frac{4\pi\mu_R^2}{2p_a p_b} \right)^\epsilon \delta_{\tilde{a}i \ a} \bar{\mathcal{V}}_{q,q}(z; \epsilon; p_a, p_b, n) \right. \\ & \left. + \delta_{\tilde{a}i \ a} \left[-\frac{1}{\epsilon} \left(\frac{4\pi\mu_R^2}{\mu_F^2} \right)^\epsilon P_{\tilde{a}i \ a}(z) + H_{\tilde{a}i \ a}^{F.S.}(z) \right] \right\}. \end{aligned} \quad (4.21)$$

From this expression we extract the insertion operator $\tilde{\mathbf{I}}(\epsilon)$, which comprises all singularities

$$\tilde{\mathbf{I}}(p_1, \dots, p_a, \dots, p_m; \epsilon) = -\frac{\alpha_s}{2\pi} \frac{1}{\Gamma(1-\epsilon)} \sum_{\tilde{a}i=1}^m \delta_{\tilde{a}i \ a} \sum_{\substack{b=1 \\ b \neq \tilde{a}i}}^m \frac{\mathbf{T}_{\tilde{a}i} \mathbf{T}_b}{\mathbf{T}_{\tilde{a}i}^2} \left(\frac{4\pi\mu_R^2}{2p_a p_b} \right)^\epsilon \mathcal{V}_{qg}(\epsilon). \quad (4.22)$$

We split the remainder into **H**- and **P**-operators as

$$\hat{\mathbf{I}}(z; \epsilon) = \delta(1-z) \tilde{\mathbf{I}}(\epsilon) + \mathbf{H}(z) + \mathbf{P}(z). \quad (4.23)$$

In order to combine the μ_F -dependent terms with the collinear counterterms, we use the identity $\sum_{\substack{b=1 \\ b \neq \tilde{a}i}}^m \mathbf{T}_b = -\mathbf{T}_{\tilde{a}i}$, which arises from color conservation [24]. After a few steps, we

find up to $\mathcal{O}(\epsilon)$:

$$\mathbf{P}\left(p_1, \dots, \frac{p_a}{z}, \dots, p_m; z; \mu_F\right) = \frac{\alpha_s}{2\pi} \sum_{\tilde{a}i=1}^m \sum_{\substack{b=1 \\ b \neq \tilde{a}i}}^m \frac{\mathbf{T}_{\tilde{a}i} \mathbf{T}_b}{\mathbf{T}_{\tilde{a}i}^2} \ln \frac{z \mu_F^2}{2p_a p_b} \delta_{\tilde{a}i \ a} P_{\tilde{a}i \ a}(z), \quad (4.24)$$

$$\begin{aligned} \mathbf{H}(p_1, \dots, p_a, \dots, p_m; n; z) = & -\frac{\alpha_s}{2\pi} \sum_{\tilde{a}i=1}^m \left\{ \sum_{\substack{b=1 \\ b \neq \tilde{a}i}}^m \frac{\mathbf{T}_{\tilde{a}i} \mathbf{T}_b}{\mathbf{T}_{\tilde{a}i}^2} \delta_{\tilde{a}i \ a} \left[\bar{K}^{\tilde{a}i \ a}(z) + 2P_{\tilde{a}i \ a}(z) \ln z \right. \right. \\ & \left. \left. + \tilde{K}^{\tilde{a}i \ a}(z) + \mathcal{L}^{\tilde{a}i \ a}(z; p_a, p_b, n) \right] + \delta_{\tilde{a}i \ a} H_{\tilde{a}i \ a}^{F.S.}(z) \right\}. \end{aligned} \quad (4.25)$$

In contrast to the original pseudo-dipole formalism, we now integrate over the momentum of the “identified” partons. To evaluate the correlated Born matrix element within a Monte Carlo integration only once per given phase-space point, we replace the integration over p_a by $\tilde{p}_{ai} = p_a/z$. This renders the correlated Born matrix element z -independent – a procedure which is already used in [57] (p.24) to achieve the same purpose. The following transformation reads:

$$\int \frac{d^{D-1} p_a}{2|\vec{p}_a|} = z^{2-2\epsilon} \int \frac{d^{D-1} \tilde{p}_a}{2|\vec{\tilde{p}}_a|}. \quad (4.26)$$

The Jacobian of the transformation cancels the prefactor $1/z^{2-2\epsilon}$ in Equation (4.19), and we obtain

$$\sum_{\tilde{a}i=1}^m \int \frac{d^D p_a}{(2\pi)^{D-1}} \delta(p_a^2) \sigma^I(p_a) = \int_m d\sigma^B(p_1, \dots, p_m) \cdot \int_0^1 dz \left[\delta(1-z) \tilde{\mathbf{I}}(\epsilon) + \mathbf{H}(z) + \mathbf{P}(z) \right]. \quad (4.27)$$

The momentum of parton $\tilde{a}i$ is $\tilde{p}_{ai}$ and thus no longer z -dependent. This allows to simplify the operators:

$$\begin{aligned} \mathbf{I}(p_1, \dots, p_m; \epsilon) &= \int_0^1 dz \delta(1-z) \tilde{\mathbf{I}}(p_1, \dots, p_m; \epsilon) \\ &= -\frac{\alpha_s}{2\pi} \frac{1}{\Gamma(1-\epsilon)} \sum_{\tilde{a}i=1}^m \sum_{\substack{b=1 \\ b \neq \tilde{a}i}}^m \frac{\mathbf{T}_{\tilde{a}i} \mathbf{T}_b}{\mathbf{T}_{\tilde{a}i}^2} \left(\frac{4\pi\mu_R^2}{2\tilde{p}_{ai} p_b} \right)^\epsilon \mathcal{V}_{qg}(\epsilon), \end{aligned} \quad (4.28)$$

$$\int_0^1 dz \mathbf{P}(p_1, \dots, p_m; z; \mu_F) = \int_0^1 dz \frac{\alpha_s}{2\pi} \sum_{\tilde{a}i=1}^m \sum_{\substack{b=1 \\ b \neq \tilde{a}i}}^m \frac{\mathbf{T}_{\tilde{a}i} \mathbf{T}_b}{\mathbf{T}_{\tilde{a}i}^2} \ln \frac{\mu_F^2}{2\tilde{p}_{ai} p_b} \delta_{\tilde{a}i \ a} P_{qg}(z) = 0. \quad (4.29)$$

Note that $\int_0^1 dz \mathbf{P}(z)$ vanishes because $P_{qg}(z)$ is a pure plus-distribution. Setting $H_{qg}^{F.S.}(z) = 0$

(which corresponds to the $\overline{\text{MS}}$ -scheme), we obtain

$$\begin{aligned}
& \int_0^1 dz \mathbf{H}(p_1, \dots, p_a, \dots, p_m; n; z) \\
&= -\frac{\alpha_s}{2\pi} \sum_{\tilde{a}i=1}^m \sum_{\substack{b=1 \\ b \neq \tilde{a}i}}^m \frac{\mathbf{T}_{\tilde{a}i} \mathbf{T}_b}{\mathbf{T}_{\tilde{a}i}^2} \int_0^1 dz \left(\overline{K}^{qq}(z) + 2P_{qq}(z) \ln z + \tilde{K}^{qq}(z) + \mathcal{L}^{qq}(z; p_a, p_b, n) \right) \\
&= -\frac{\alpha_s}{2\pi} \sum_{\tilde{a}i=1}^m \sum_{\substack{b=1 \\ b \neq \tilde{a}i}}^m \mathbf{T}_{\tilde{a}i} \mathbf{T}_b \left\{ \frac{1}{4} + 2 \left[\text{Li}_2 \left(1 - \frac{1+v}{2} \frac{(\tilde{p}_{ai} + p_b)n}{\tilde{p}_{ai}n} \right) + \text{Li}_2 \left(1 - \frac{1-v}{2} \frac{(\tilde{p}_{ai} + p_b)n}{\tilde{p}_{ai}n} \right) \right] \right. \\
&\quad \left. + \int_0^1 dz (1+z) \ln \frac{n_z^2 \tilde{p}_{ai} p_b}{2z(\tilde{p}_{ai} n_z)^2} \right\}. \tag{4.30}
\end{aligned}$$

The last line of Equation (4.30) is the only z -dependent contribution which cannot be integrated analytically. Note in particular that in the last term n implicitly depends on z through Equation (4.1), where the momentum of the emitter particle is given by $p_a = z\tilde{p}_{ai}$. To make this explicit, we denote it by n_z .

We remark that the introduction of the collinear counterterms in Equation (4.17) is actually unnecessary, since they give a vanishing contribution to the cross-section. This is due to $P_{qq}(z)$ being a pure plus-distribution and the test-function with which it is convoluted not being z -dependent after we substituted $p_a = z\tilde{p}_{ai}$. This is also true for differential cross-sections, since any partonic observable can be expressed without reference to z . The vanishing effect of collinear counterterms may also be understood from another point of view: As we do not actually restrict the momenta of the “identified” partons, but integrate over them eventually, we have already collected all singularities necessary to cancel those present in the virtual corrections. Hence, no collinear mass factorisation counterterms are required.

In summary, the integrated pseudo-dipoles for final-state singularities are given by

$$\int_{m+1} d\sigma^S \Big|_{\text{FF}}^{\text{ID}} = \int_m d\sigma^B \cdot \left[\mathbf{I}(\epsilon) + \int_0^1 dz \mathbf{H}(z) \right]_{\text{FF}}^{\text{ID}}, \tag{4.31}$$

where the $\mathbf{I}$ - and $\mathbf{H}$ -operator are given in Equation (4.28) and Equation (4.30) respectively. Pseudo-dipoles describing final-state singularities with final-state and initial-state spectators are identical, apart from the replacement of b being an initial-state spectator instead of a final-state one. Hence we obtain the same formula for $\int_{m+1} d\sigma^S \Big|_{\text{FI}}^{\text{ID}}$. In contrast to standard FI-dipoles, we do not obtain a $\mathbf{K}$ -operator at this stage.

Initial-State Singularities

“In the following we will quote results of the integrated pseudo-dipoles for initial-state singularities.” [7] We follow the labelling in the second row of Figure 4.2, i.e. parton a is an initial-state emitter and b is an identified final-state spectator. The other initial state parton

is labelled with c . “The integrated splitting functions for initial-state emitters are defined by:

$$\frac{\alpha_s}{2\pi} \frac{1}{\Gamma(1-\epsilon)} \left(\frac{4\pi\mu_R^2}{2p_a p_b} \right)^\epsilon \tilde{\mathcal{V}}^{a,ai}(x; \epsilon; p_a, p_b, n) := \int [dp_i(n, p_a, x)] \frac{1}{2p_a p_i} \frac{n_s(\tilde{a}l)}{n_s(a)} \langle \mathbf{V}_b^{(n)ai}(x; v_{iab}) \rangle, \quad (4.32)$$

where $n_s(a)$ is the number of polarisations of parton a . The result is identical to the final-state case, i.e. Equation (4.15):

$$\tilde{\mathcal{V}}^{a,b}(x; \epsilon; p_a, p_b, n) = \bar{\mathcal{V}}_{a,b}(x; \epsilon; p_a, p_b, n). \quad (4.33)$$

” [7] Considering a process with m identified final-state partons, the integral over IF-pseudo-dipoles reads

$$\begin{aligned} \int_{m+1} d\sigma_{ac}^S(p_a, p_c) \Big|_{\text{IF}}^{\text{ID}} &= \int_{m+1} \mathcal{N}_{in} \frac{1}{n_s(a)n_s(c)\Phi(p_a p_c)} \sum_{\{m+1\}} d\phi_{m+1} \frac{1}{S_{\{m+1\}}} \\ &\cdot \sum_{\substack{\text{pairs} \\ a,i}} \sum_{b=1}^m \mathcal{D}_b^{(n)ai}(p_1, \dots, p_{m+1}; p_a, p_c) F_J^{(m)}(\tilde{p}_1, \dots, \tilde{p}_{m+1}; \tilde{p}_{ai}, p_c), \end{aligned} \quad (4.34)$$

“Next to the sum over all possible (a, i) -pairs the sum over b includes all identified final-state colour spectators.” [7] “As for standard dipoles we have to sum over all possible internal parton flavours a' which can be obtained in the branching $a \rightarrow a' + i$, and which lead to a non-vanishing Born matrix element. Including the collinear mass factorisation counterterms [(see Equation (3.76))], we obtain the following result:” [7]

$$\begin{aligned} \int_m d\sigma_{ac}^I(p_a, p_c) \Big|_{\text{IF}}^{\text{ID}} &= \int_{m+1} d\sigma_{ac}^S(p_a, p_c) \Big|_{\text{IF}}^{\text{ID}} + \int_m d\sigma_{ac}^C(p_a, p_c) \Big|_{\text{IF}} = \int_m d\sigma_{ac}^B(p_a, p_c) \mathbf{I}(\epsilon) \Big|_{\text{IF}} \\ &+ \sum_{a'} \int_0^1 dx \int_m d\sigma_{a'c}^B(x p_a, p_c) \left(\mathbf{K}^{a,a'}(x) + \mathbf{P}^{a,a'}(x, \mu_F) \right) \Big|_{\text{IF}}^{\text{ID}} \\ &+ \sum_{c'} \int_0^1 dx \int_m d\sigma_{ac'}^B(p_a, x p_c) \left(\mathbf{K}^{c,c'}(x) + \mathbf{P}^{c,c'}(x, \mu_F) \right) \Big|_{\text{IF}}^{\text{ID}}, \end{aligned} \quad (4.35)$$

In the following, “we refer to the color spectator as $\tilde{b}$ rather than b . This is due to our identification scheme for IF-pseudo-dipoles described in Subsection 4.3.1, where the momentum of the colour spectator is mapped from $p_b \rightarrow \tilde{p}_b$. Due to this scheme which is opposed to the original use case in Ref. [24], we are required to substitute p_b with $\tilde{p}_b$ in the differential form of the IF-pseudo-dipoles as well. Apart from the correlated Born matrix element, the momentum of parton b enters only in the kinematic variable $v_{i,ab}$ (see Equation (4.9)). We can adjust for

this by making the replacement

$$v_{i,ab} \rightarrow \tilde{v}_{i,ab} = \frac{p_a \tilde{p}_b}{p_i(p_a + \tilde{p}_b)} \quad (4.36)$$

in the splitting functions in Equation (4.12). The soft and collinear limit of the splitting function are not affected by this change.” [7]

The insertion operator $\mathbf{I}|_{\text{IF}}$ in Equation (4.35) is identical to the one in Equation (3.78) if the appropriate relabelling $k \rightarrow \tilde{b}$ and $b \rightarrow c$ is done. The $\mathbf{K}|_{\text{IF}}^{\text{ID}}$ -operator is given by

$$\begin{aligned} \mathbf{K}^{a,a'}(p_1, \dots, p_m; p_a, n, x)|_{\text{IF}}^{\text{ID}} = & -\frac{\alpha_s}{2\pi} \left\{ \sum_{\tilde{b}=1}^m \frac{\mathbf{T}_{\tilde{b}} \mathbf{T}_{a'}}{\mathbf{T}_{a'}^2} \left[\overline{K}^{a,a'}(x) + \tilde{K}^{a,a'}(x) + \mathcal{L}^{a,a'}(x; p_a, \tilde{p}_b, n) \right] \right. \\ & \left. + K_{\text{F.S.}}^{a,a'}(x) \right\}. \end{aligned} \quad (4.37)$$

The $\mathbf{P}|_{\text{IF}}$ -operator is the same as for standard dipoles and given in Equation (3.80) in which the substitution $k \rightarrow \tilde{b}$ is understood.

“For the case of initial-state spectators there is no difference to the standard dipoles.” [7]

Of course it is also possible to identified a subset of final-state partons. In this case, the sums in the $\mathbf{K}$ - and $\mathbf{H}$ -operators have to be adapted appropriately.

4.4 Resonance-Aware Subtraction of $W^+W^-b\bar{b}$ Production

This section, including its subsections, tables and figures¹⁴, is copied from content of [7] created by the author of this thesis. However, for the sake of clarity footnote 15 is added to the text. We have tested the above described resonance-aware subtraction by means of pseudo-dipoles in two reactions: $e^+e^- \rightarrow W^+W^-b\bar{b}$ and $pp \rightarrow W^+W^-j_bj_b$. In the following we are going to compare results obtained with standard CS dipoles to those obtained with pseudo-dipoles for fixed NLO QCD predictions. In Subsection 4.4.1, we first examine the cancellation of divergences between the real emission matrix elements and the different dipoles using ensembles of trajectories in phase-space, which approach the collinear and soft limits in a controlled way. Following this, we compare physical cross-sections calculated with the different subtraction techniques while paying special attention to the rate of convergence in the Monte Carlo integration.

4.4.1 Singular Limits

In this subsection we validate the implementation of the differential form of the pseudo-dipole insertion operators in Equations (4.2) and (4.10) by testing the behaviour of the subtracted

¹⁴Figure 4.9 is only based on Figure 11 of [7]. It has been updated, since we did accidentally not use the Durham jet algorithm [63] in creating the reference’s figure, but the k_t algorithm [64].

real emission corrections in their singular limits.

$$e^+e^- \rightarrow W^+W^-b\bar{b}$$

The sole real emission correction to the process $e^+e^- \rightarrow W^+W^-b\bar{b}$ at NLO is the process with an additional gluon in the final state. It develops singularities when the gluon is soft, and when it is collinear to the b (anti-)quark. To parametrise these limits we use the scaled virtualities,

$$y_{gb} = \frac{2p_g p_b}{(p_g + p_b + p_{\bar{b}})^2} \quad \text{and} \quad y_{g\bar{b}} = \frac{2p_g p_{\bar{b}}}{(p_g + p_b + p_{\bar{b}})^2}. \quad (4.38)$$

In the collinear regions, $y_{gb} \rightarrow 0$ or $y_{g\bar{b}} \rightarrow 0$, while in the soft limit $y_{gb}y_{g\bar{b}} \rightarrow 0$. We con-

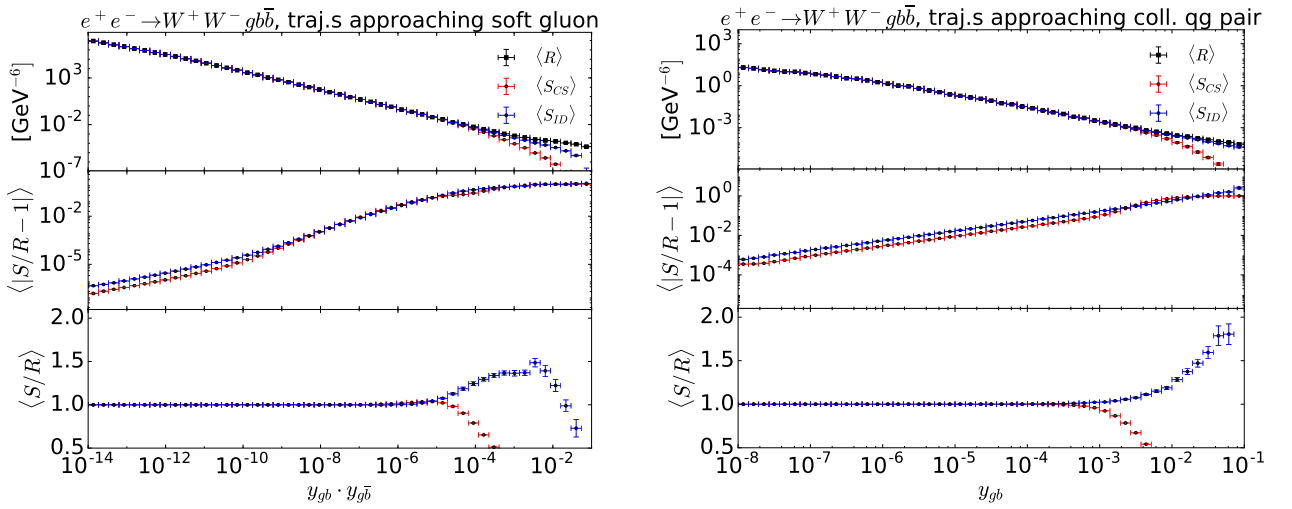


Figure 4.5: Matrix elements $R = |\mathcal{M}_R|^2$ and sum of associated dipoles $S = \sum \mathcal{D}$ (standard CS dipoles in red, pseudo-dipoles in blue) for the process $e^+e^- \rightarrow W^+W^-gbb$. Both dipole types are evaluated on the same trajectory like described in the text.

Right: Average over trajectories in phase-space with increasingly soft gluon. Left: Average over trajectories with increasingly collinear qg -pair.

struct ensembles of phase-space points that we refer to as phase-space trajectories as follows: random phase-space points are sampled according to the real emission cross-section in the narrow-width approximation, while requesting three identified jets according to the Durham jet algorithm [63] with $d_{\max} = (5 \text{ GeV})^2$. For each phase-space point, the kinematical configuration is scaled according to the algorithm described in the Appendix of [7] in order to obtain a sequence of points that approach the soft or collinear limit.

Figure 4.5 shows the values of the real emission matrix element, $R = |\mathcal{M}_R|^2$ and the sum of the associated dipoles ($S = \sum \mathcal{D}$), as well as their ratio for the soft limit (left) and the bq -collinear limit (right). We have averaged – for all sub-plots – over all entries within a bin.¹⁵ In doing

¹⁵We emphasise that we always display the arithmetic mean of a bin. This means in particular that we first calculate $|S/R - 1|$ (or S/R) for each phase-space point and then calculate the arithmetic mean in each bin.

so, the ratio plots enable us to assess the pointwise convergence of S/R best. It can be seen that the cancellation of divergences occurs in both the standard CS subtraction method and in the pseudo-dipole approach, but that the pseudo-dipoles converge faster towards the real emission matrix element, which can be seen in the lower panels of the figures.

$$pp \rightarrow W^+W^-j_bj_b$$

Next we consider the analogue to the above example at hadron colliders, namely the reaction $pp \rightarrow W^+W^-j_bj_b$, where j_b indicates a b -tagged jet. To parametrise the soft and collinear trajectories in this process, we use the following variables

$$v_i^0 = \frac{p_i p_0}{p_0 p_1} \quad \text{and} \quad v_i^1 = \frac{p_i p_1}{p_0 p_1} \quad (4.39)$$

where p_0 and p_1 are the momenta of the initial-state partons and p_i is the momentum of the additional parton in the real correction. The phase-space trajectories are again constructed by generating random phase-space points with well separated partons, which are then modified according to the algorithm in the Appendix of [7] to obtain additional phase-space points that approach the singular limits.

Figures 4.6 and 4.7 display the average values of the real emission matrix element and the corresponding dipole subtraction terms, as well as their ratio – averaged within each bin – for processes with an additional gluon (Figure 4.6) and an additional quark (Figure 4.7) in the final state. The former develop both soft and collinear singularities, shown in the left and right panels of Figure 4.6, respectively, while the latter only feature collinear singularities. Combining all tests, we validate all four initial-state splitting functions in Eq. (4.12).

It can be seen that both the standard CS as well as the pseudo-dipoles converge towards the real correction. In the soft limit, which is the numerically more important one, the pseudo-dipoles converge faster. This is also the case for the collinear limit probed in Figure 4.7. However, for the collinear limits tested on the right-hand side of Figure 4.6 this is not the case. As a reason for this we suspect that the pseudo-dipole splitting functions Equation (4.12) converge more slowly towards the associated Altarelli-Parisi functions than the standard CS ones.

4.4.2 Physical Cross-Sections

In this subsection we present first results validating the pseudo-dipole subtraction method for resonance-aware processes at the level of observable cross-sections and distributions. Results are cross-checked using two different implementations of our new algorithm within the public event generation framework Sherpa [65, 35], one using the matrix element generator AMEGIC++ [66, 57], and one using the new interface between Sherpa and OpenLoops [67]. In this interface, the color-correlated Born matrix elements are imported from OpenLoops libraries [68], while the splitting function is calculated in Sherpa and the integration is performed

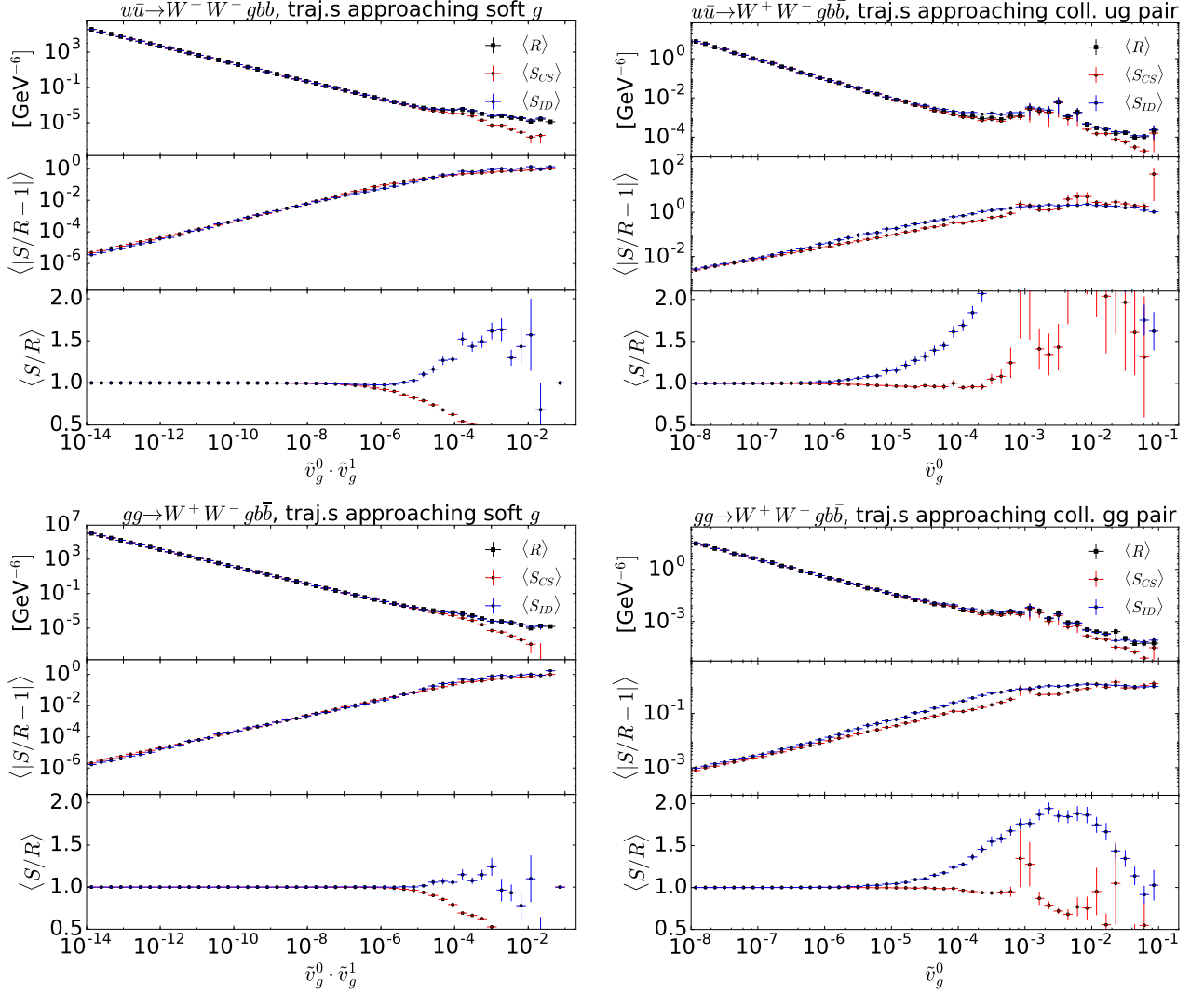


Figure 4.6: Matrix elements $R = |\mathcal{M}_R|^2$ and sum of associated dipoles $S = \sum \mathcal{D}$ (standard CS dipoles in red, pseudo-dipoles in blue) for the processes $u\bar{u} \rightarrow W^+W^-g b\bar{b}$ (top) and $gg \rightarrow W^+W^-g b\bar{b}$ (bottom). Both dipole-types are evaluated on the same trajectories like described in the text.

Left: Average over trajectories in phase-space with increasingly soft gluon. Right: Average over trajectories with increasingly collinear partons.

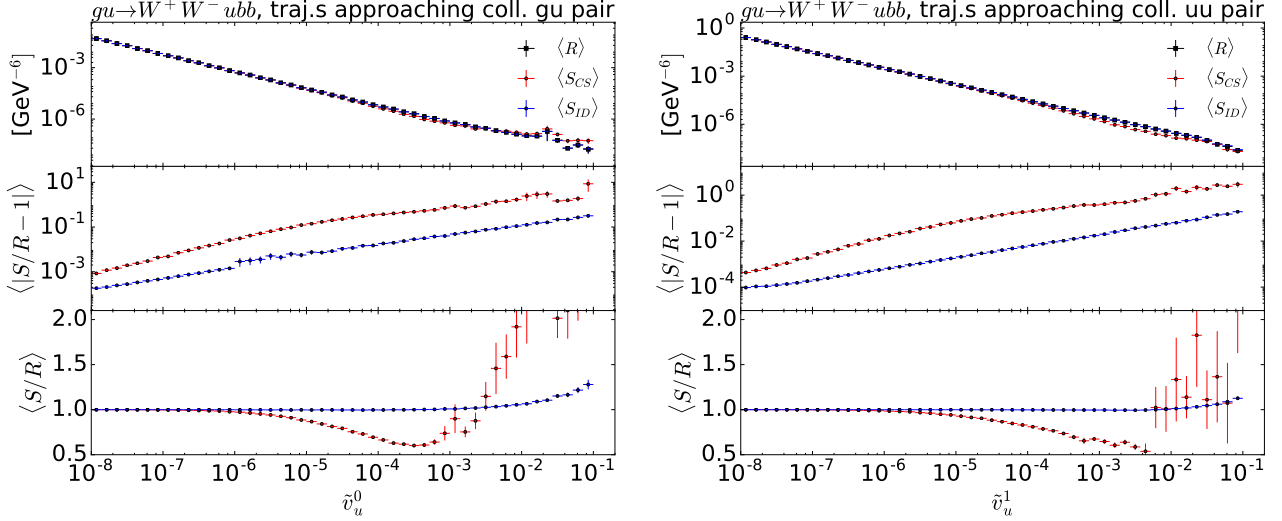


Figure 4.7: Matrix elements $R = |\mathcal{M}_R|^2$ and sum of associated dipoles $S = \sum \mathcal{D}$ (standard CS dipoles in red, pseudo-dipoles in blue) for the process $ug \rightarrow W^+W^-ub\bar{b}$. Both dipole-types are evaluated on the same trajectories, with increasingly collinear partons, like described in the text.

Left: The u -quark in the final state becomes collinear to the first initial-state parton. Right: The u -quark in the final state becomes collinear to the second initial-state parton.

using the techniques implemented in AMEGIC++ [66].

$$e^+e^- \rightarrow W^+W^-b\bar{b}$$

Again we investigate first the reaction $e^+e^- \rightarrow W^+W^-b\bar{b}$. We vary the center-of-mass energy of the collider to obtain predictions below, at and above the top-quark pair production threshold, and we do not include the effects of initial-state radiation. We require two hard jets with $d_{\max} = (5 \text{ GeV})^2$ defined according to the Durham jet algorithm [63]. The running of the strong coupling is evaluated at two loops, and the reference value is set to $\alpha_s(M_Z^2) = 0.118$, where $M_Z = 91.1876 \text{ GeV}$.

$\sigma[\text{fb}]$	$\sqrt{s} = 3m_W$		$\sqrt{s} = 2m_t$		$\sqrt{s} = 4m_t$	
	CS	ID	CS	ID	CS	ID
RS	-0.00772(6)	-0.00140(5)	-0.52(3)	-2.85(1)	-9.5(4)	-5.3(1)
BVI	0.16143(13)	0.15506(13)	148.07(9)	150.55(9)	230.0(2)	226.0(2)
Σ	0.15371(14)	0.15366(14)	147.55(9)	147.70(9)	220.5(4)	220.7(2)

Table 4.1: NLO cross-sections for $e^+e^- \rightarrow W^+W^-b\bar{b}$ at $\mu_R = m_t$ and varying center-of-mass energy, computed using standard CS subtraction terms (CS) or pseudo-dipoles (ID). The subtracted real emission contributions (RS) were calculated using 10^7 phase-space points. The Born, virtual corrections and integrated subtraction terms (BVI) were calculated using $3 \cdot 10^6$ phase-space points.

Table 4.1 shows the total cross-sections as well as the individual contributions from the sub-

tracted real emission terms (RS) as well as Born, virtual corrections and integrated subtraction terms (BVI). As expected, the RS and BVI contributions differ between the standard CS subtraction method and the pseudo-dipole approach, but their sum agrees within the statistical accuracy of the Monte Carlo integration. The cross-section is significantly enhanced at and above the production threshold for a top quark pair. For those two center-of-mass energies, we expect the pseudo-dipoles to give a more physical interpretation of the subtraction term and thus a reduced variance during the integration. This is confirmed in Figure 4.8, which shows the evolution of the Monte Carlo error during the integration. In the case of pseudo-dipole subtraction at or above threshold, the uncertainty is indeed substantially lower than for standard CS dipoles. Below threshold the performance of pseudo-dipole subtraction is similar to that of the standard technique.

Our validation for $e^+e^- \rightarrow W^+W^-b\bar{b}$ is completed by a comparison of a few selected differential cross-sections in the two subtraction schemes. Figure 4.9 displays the invariant mass of the (anti-)top quark reconstructed at the level of the $W^+W^-b\bar{b}$ final state from the W -boson and a b -jet with a matching signed flavour tag. The deviation plot shows excellent statistical compatibility between the two simulations. It also displays that the pseudo-dipole subtraction technique generates smaller statistical uncertainties in the peak region than the standard CS subtraction method.

$$pp \rightarrow W^+W^-j_bj_b$$

As a second application we consider the reaction $pp \rightarrow W^+W^-j_bj_b$, where j_b indicates a b -tagged jet with $p_T > 25$ GeV. We use the anti- k_T jet algorithm [69] with $R = 0.4$. The total cross-section and the individual contributions to the RS and the BVI cross-section for both standard CS and pseudo-dipoles are given in Table 4.2. Again it can be seen that the convergence of the Monte Carlo integration of the RS cross-section for pseudo-dipoles is significantly faster than the one for standard CS dipoles. This can also be observed in Figure 4.10, which is the analogue of Figure 4.8 for the proton-proton initial state for a center-of-mass energy of $\sqrt{s} = 13$ TeV.

$\sigma[\text{pb}]$	$\sqrt{s} = 13$ TeV	
	CS	ID
RS	-62.03(59)	-93.21(13)
BVI	360.02(39)	391.53(39)
Σ	297.99(71)	298.32(41)

Table 4.2: NLO cross-section for $pp \rightarrow W^+W^-j_bj_b$ at $\mu_R = \mu_F = m_t$ and $\sqrt{s} = 13$ TeV, computed using standard CS subtraction terms (CS) or pseudo-dipoles (ID). The subtracted real emission contributions (RS) were calculated using 10^8 phase-space points. The Born, virtual corrections and integrated subtraction terms (BVI) were calculated using $8.5 \cdot 10^6$ phase-space points.

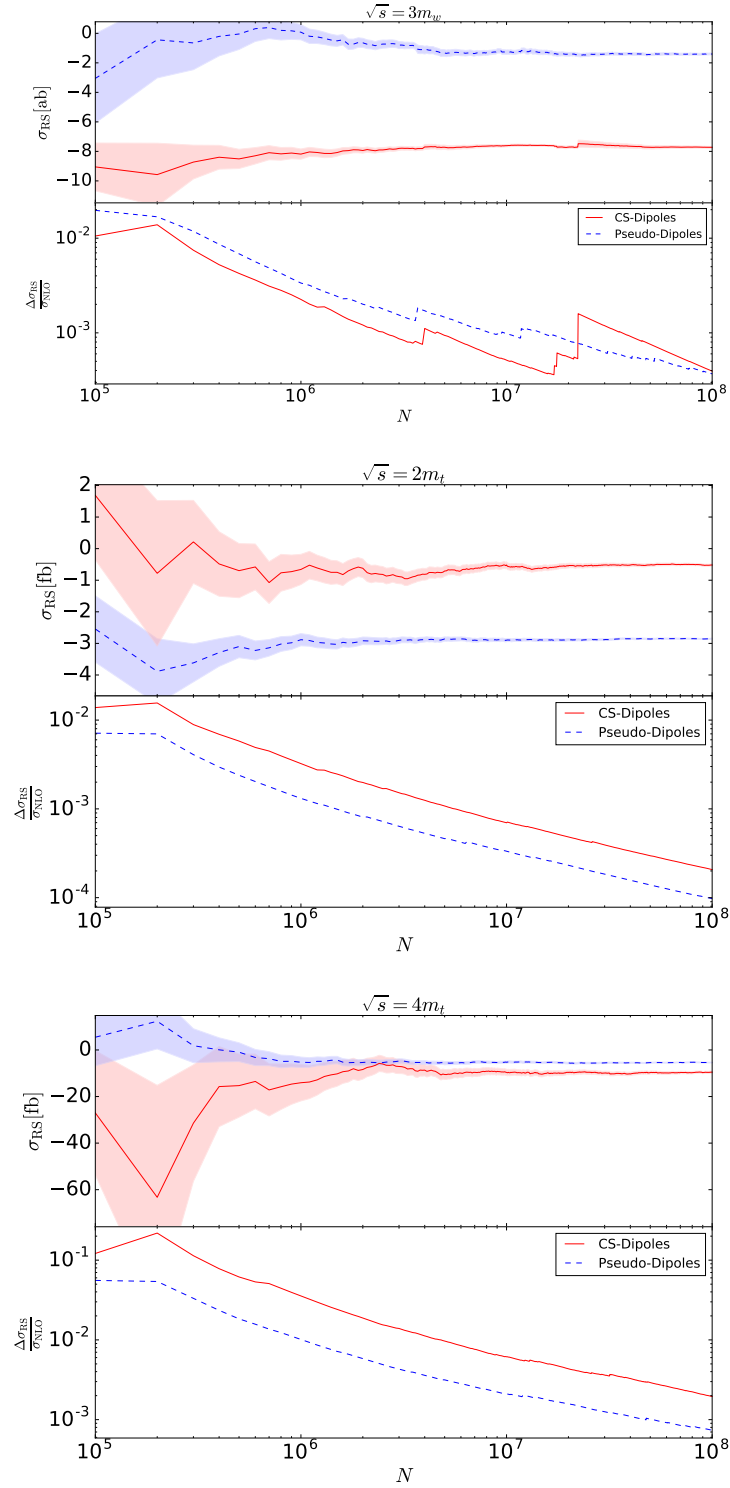


Figure 4.8: Evolution of the Monte-Carlo integration results for the subtracted real emission contribution to the total cross-section in $e^+e^- \rightarrow W^+W^-b\bar{b}$ at varying center-of-mass energy over number of sampled phase-space points N . From top to bottom: $\sqrt{s} = 3m_W$, $\sqrt{s} = 2m_t$ and $\sqrt{s} = 4m_t$. Red solid lines show results from standard CS dipoles, while blue dashed lines correspond to pseudo-dipoles. The coloured bands in the upper panels and the lines in the lower panels show the one σ statistical uncertainty of the Monte Carlo integration.

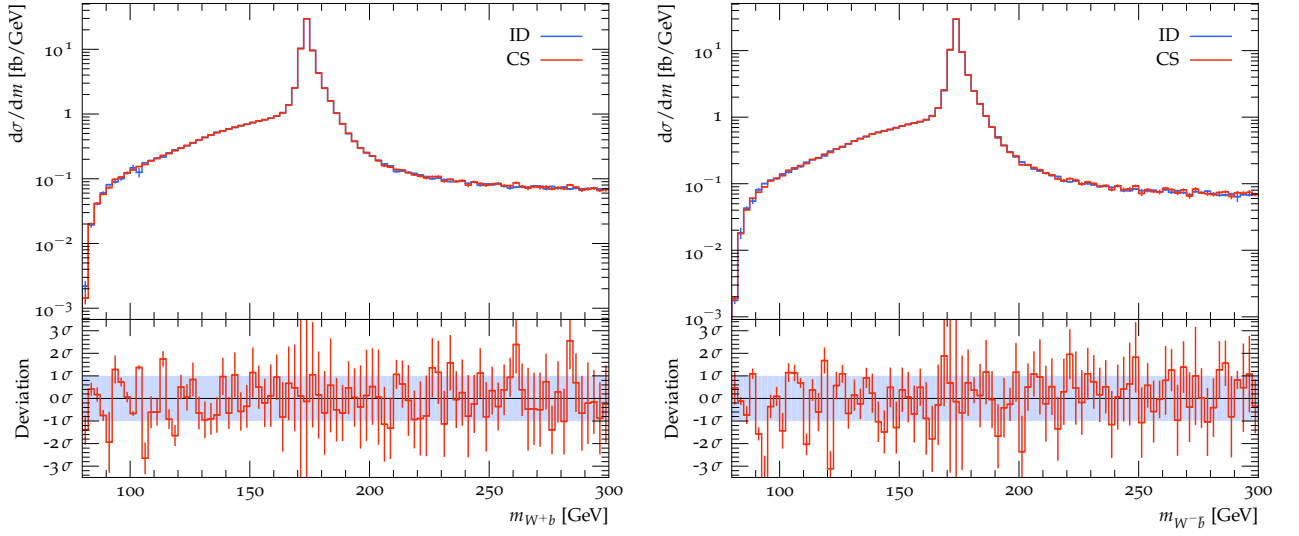


Figure 4.9: Invariant mass of the (anti-)top quark reconstructed at the level of the $W^+W^-b\bar{b}$ final state from the W -boson and a b -jet with a matching signed flavour tag.

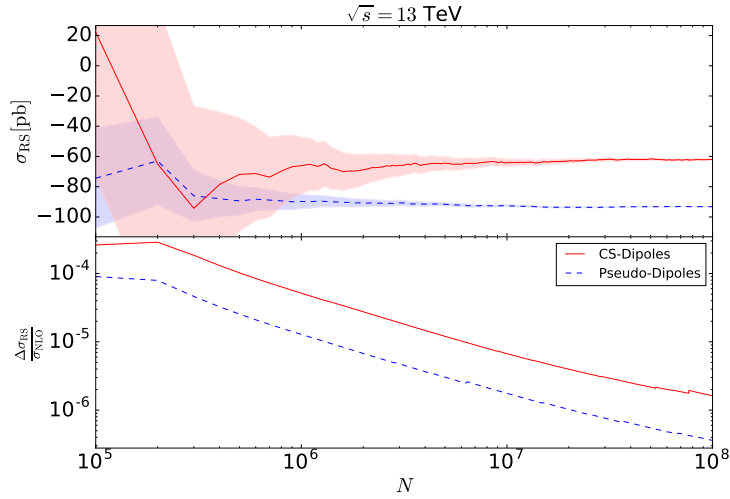


Figure 4.10: Evolution of the Monte Carlo integration results for the subtracted real emission contribution to the total cross-section in $pp \rightarrow W^+W^-j_bj_b$ at $\sqrt{s} = 13$ TeV over number of sampled phase-space points N . Red solid lines show results from standard CS-dipoles, while blue dashed lines correspond to pseudo-dipoles. The coloured bands in the upper panels and the lines in the lower panels show the one σ statistical uncertainty of the Monte Carlo integration.

Finally, in Figure 4.11 we confirm the agreement between standard CS dipoles and pseudo-dipoles for the differential cross-sections as a function of the combined W^+j_b and $W^-j_{\bar{b}}$ invariant mass. The two subtraction schemes agree within the statistical uncertainty and pseudo-dipoles exhibit a smaller statistical uncertainty.

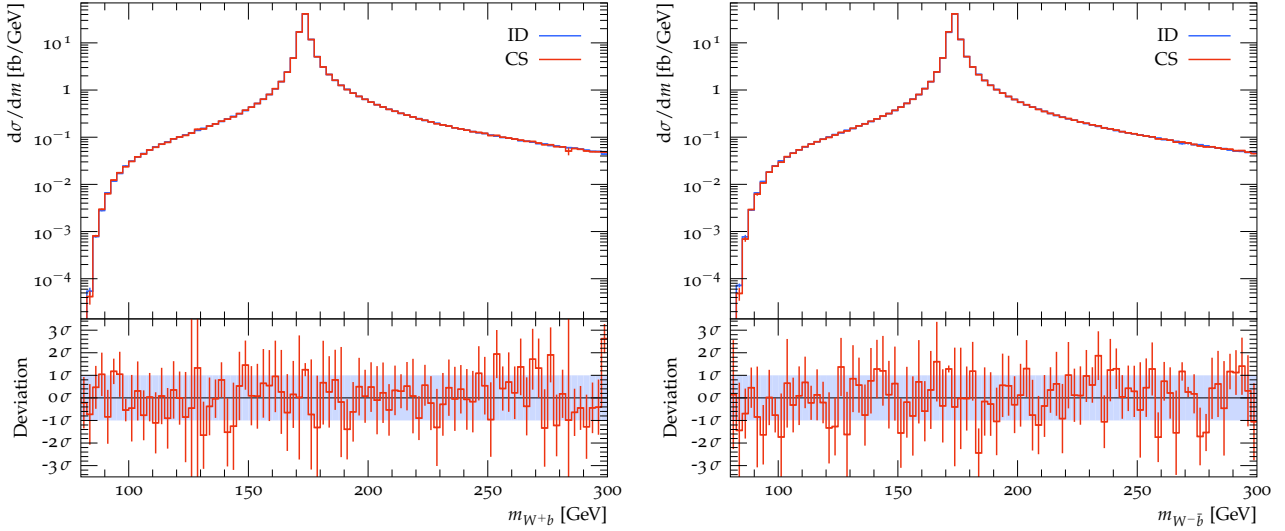


Figure 4.11: Invariant mass of the (anti-)top quark reconstructed at the level of the $W^+W^-j_bj_b$ final state from the W -boson and a b -jet with a matching signed flavour tag.

4.5 Resonance-Aware Subtraction in the FKS Method

The problem of resonances-aware subtraction has already been addressed within the context of FKS subtraction [22]. In [22] the mapping differs only from the standard one [59] if the emitter is the decay product of a resonance. In that case the recoil is absorbed by all decay products of the resonance which do not take part in the splitting, instead of all final-state particles which do not take part in the splitting. Thus the resonance’s momentum is conserved rather than the total final-state momentum. This change in parametrisation amounts to the substitution

$$q = \sum_{i=1}^{m+1} p_i \rightarrow p_{\text{res}} \quad (4.40)$$

in the calculation of ξ_i in Equation (3.91) where p_{res} is the resonance’s total momentum. All frame dependent terms in Equation (3.91) are taken in the resonance’s rest frame. For consistency, the integrated subtraction terms had to be recalculated. These results are published in [23]. The procedure of [22] is however restricted to calculations in the narrow-width-approximation (NWA).

Ref. [23] describes a resonances-aware subtraction taking finite width effects into account. A major difference of that to calculations performed in the NWA is that competing resonances

may arise. This means that for a given set of final-state particles, diagrams with different internal resonances contribute. For example, the process $u\bar{u} \rightarrow d\bar{d}u\bar{u}$ contains contributions from amplitudes with two internal Z -bosons as well as a W^+ - and a W^- -boson. The key point in treating those competing resonances is a further separation of singular regions of the real correction phase-space: Each region α_r shares a larger numerical portion of the real correction cross-section when it is close to a soft/collinear singularity *or* a resonance enhanced region of phase-space. Then, in each α_r – which is thus associated with a fixed resonance structure – the corresponding resonances-aware mapping of [22] is applied. In addition to the separation of the real corrections into different contributions, also the Born prediction is divided into different terms, each of them dominating for a fixed resonance structure. One vital requirement for the phase-space separation is that the separation in the real correction phase-space converges in the soft and collinear limit to the separation in the Born phase-space with the same resonance structure. This guarantees the proper cancellation of integrated and unintegrated subtraction terms, as they differ depending on the underlying resonance structure.

5 Parton Shower and Matching

This chapter summarises the basic concepts of a parton shower and its combination with a fixed NLO calculation, i.e. the NLO matching. We will first highlight the necessity of a parton shower and mention general properties before we review details of a specific shower, which is based on the above detailed dipole subtraction. Secondly, we explain which complications arise when combining a parton shower with a fixed NLO calculation and how these can be dealt with in a consistent way. We close this chapter by describing one of the two established methods to do so.

5.1 Parton Shower

As already stated in Chapter 2, the parton shower is responsible to describe the transition from a few high-energetic partons, whose production is modelled by fixed order calculations, to many low-energetic ones, which have typical energies to be subjected to hadronisation. From a theoretical point of view, a parton shower is not as exact as a fixed order calculation as it is based on a resummation of approximated splitting probabilities and does – a priori – not include quantum interference effects. Nonetheless, this resummation often leads to predictions which cannot be described by a pure fixed order calculation (with significantly less partons in the final state). An example of this can be seen in Figure 5.1, which we discuss in the following.

5.1.1 General Considerations

The starting point of every parton shower is the factorisation of the cross-section in the collinear limit into a cross-section of one parton less and a term describing the splitting probability:

$$d\sigma_{m+1} \approx d\sigma_m \Gamma(t, z, \phi) dt dz d\phi. \quad (5.1)$$

The variables t , z and ϕ describe the kinematics of the splitting. Equation (5.1) can be regarded as a differential equation of the form

$$\frac{d\Delta(t_{\text{res}}, t)}{dt} = \Delta(t_{\text{res}}, t) \int_{z^{\text{min}}}^{z^{\text{max}}} dz \int_0^{2\pi} d\phi \Gamma(t, z, \phi), \quad (5.2)$$

which has the solution

$$\Delta(t_{\text{res}}, t) = \exp \left(- \int_t^{t_{\text{res}}} dt' \int_{z^{\text{min}}}^{z^{\text{max}}} dz \int_0^{2\pi} d\phi \Gamma(t', z, \phi) \right). \quad (5.3)$$

This term is called Sudakov factor and can be interpreted as the non-emission probability between two phase-space points. The splitting variable t is singled out from the other ones

since it is used to order the emissions. At this point we like to make a number of comments:

- A clever choice of the explicit definition of the ordering variable t has the effect of mimicking quantum coherence effects in the shower as well as possible [70, 56].
- The splitting probability Γ is a sum over splitting probabilities into partons with different flavour. Each summand is proportional to α_s , the propagator of the splitting parton, the Jacobian J accounting for the transformation to the splitting variables and a splitting function K (which reduces to one of the regularised Altarelli-Parisi splitting functions P , see Equations (A.1) - (A.4) in the collinear limit). It can thus be written as

$$\Gamma(t, z, \phi) = \frac{\alpha_s(t)}{2\pi} \frac{1}{t} J(t, z, \phi) K(t, z, \phi). \quad (5.4)$$

- The upper bound of the ordering variable t is referred to as the squared resummation scale t_{res} . There is no general recipe to fix its numerical value. Usually it is taken to be of the order of the energy scale of the hard interaction.

In processes with initial-state hadrons the resummation scale may be set to the factorisation scale μ_F . This is because the parton shower describes an energy evolution of a parton just like the PDFs describe the energy evolution of a hadron towards a parton at energy scale μ_F . In fact, the evolution equations (derived in the collinear limit of the splitting) of parton shower and PDFs are identical. They are given by the DGLAP equations, see [55]. The only difference is that in the PDF description the additional parton in the splitting is discarded while it adds to the final state in the parton shower approach. Thus taking the scale μ_F at which the PDFs are evaluated, as the starting scale of the parton shower to perform a backward evolution unfolds the PDFs in the sense of describing partons arising from initial-state radiation.¹⁶

- The splitting probability in Equation (5.4) diverges for $t \rightarrow 0$, as this corresponds to the collinear singularity of the real correction matrix element. This motivates the introduction of a lower cutoff t_c for the evolution variable from a theoretical point of view. From the experimental point of view, this cutoff is also motivated, since two partons need to have a minimum separation in the detector in order to be resolved. Below a certain value of t this is no longer the case. A typical choice of t_c is of $\mathcal{O}(1 \text{ GeV}^2)$ [56].
- The introduction of t_c can be thought of as a phase-space separation of resolvable and unresolvable emissions. Since the no-emission probability $\Delta(t_{\text{res}}, t_c)$ is finite, one can interpret this term as corresponding to either an unresolvable emissions or a virtual correction, as both taken separately are infinite but added up yield a finite result. From

¹⁶The same logic applies for final-state radiation if a parton is to fragment into an identified final-state hadron.

this probabilistic point of view the parton shower also includes virtual corrections, which is reflected by the resummation of large logarithms of the ratio t_{res}/t_c .

- The exponent of Equation (5.3) contains potentially large logarithms which arise in the integration over Γ . According to the power with which they appear they are referred to as leading logarithms (LL), next-to-leading logarithms (NLL) and so on. In contrast to the perturbative expansion in α_s , the leading logarithm is the one with the highest power. It is those logarithms which are responsible for the so-called Sudakov suppression, which can be seen in Figure 5.1. Compared to the fixed NLO calculation (NLO) the parton shower prediction (Herwig) is suppressed by more than one order of magnitude for small values of p_T^{WW} , owing to the large scale difference in the logarithms of the Sudakov factor.
- Since the factorisation in Equation (5.1) is only valid in the strict collinear regime, the parton shower describes only collinear parton emissions correctly. Hence, the quality of modelling emissions away from the collinear limit decreases. This can also be seen in Figure 5.1, where for large values of p_T^{WW} the parton shower prediction deviates from the NLO one, which is considered to describe this region correctly, since it is dominated by a hard emission implying a sizeable recoil to the WW system.
- Since the parton shower resums potentially large corrections of successive emissions, it can be seen as a resummation technique which extends over all orders in perturbation theory and is thus complementary in its idea to fixed order calculations.

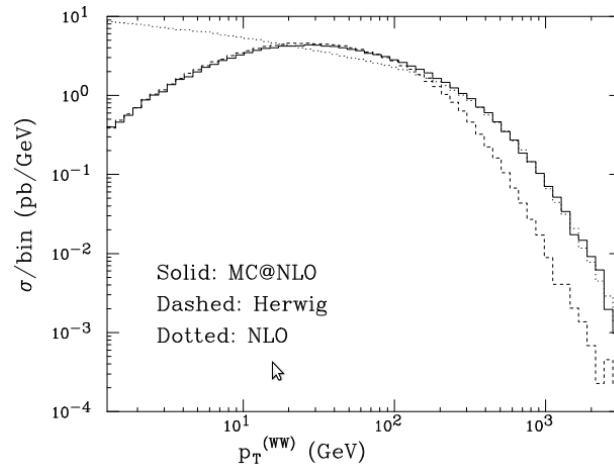


Figure 5.1: Shown is the modulus of the vector sum of the W^+ and W^- boson in W^+W^- production at the LHC as described in [32]. Compared are the predictions of a LO calculation interfaced with a parton shower (Herwig), a fixed NLO calculation and the matching of the two (MC@NLO).

5.1.2 Outline of the Dipole-Shower

In the following we review some details of the Catani-Seymour dipole shower (CSS) [31] to set the stage for the changes towards a resonance-aware dipole-shower (IDS), which we describe in Section 6.1. For simplicity's sake we focus on final-state splittings with final-state spectators with solely massless partons. From the above described subtraction formalism we know the soft and collinear limit of $|\mathcal{M}_{m+1}|^2$. We use these to approximate $|\mathcal{M}_{m+1}|^2$ by a factorisation which is only exact in the collinear limit:

$$|\mathcal{M}_{m+1}|^2 \approx |\mathcal{M}_m|^2 \sum_{\text{pairs } i,j} \sum_{k \neq i,j} \frac{1}{2p_i p_j} \frac{1}{\mathcal{N}_{ij}^{\text{spec}}} 8\pi\alpha_s \langle \mathbf{V}'_{ij,k}(y_{ij,k}, \tilde{z}_i) \rangle. \quad (5.5)$$

The factor $\mathcal{N}_{ij}^{\text{spec}}$ – which equals one for a splitting (anti-)quark and two for a splitting gluon – is the number of possible colour spectators and encodes the so-called leading colour contribution. This is, colour correlation represented by the $\mathbf{T}$ -operators (see e.g. Equation (3.17)) is approximated in the above formula and the soft limit is only correct in the limit $N_c \rightarrow \infty$ (see [31]). The spin-averaged splitting functions¹⁷ are given by

$$\langle \mathbf{V}'_{q_i g_j, k}(y_{ij,k}, \tilde{z}_i) \rangle = C_F \left[\frac{2}{1 - \tilde{z}_i(1 - y_{ij,k})} - (1 - \tilde{z}_i) \right] \quad (5.6)$$

$$\langle \mathbf{V}'_{g_i g_j, k}(y_{ij,k}, \tilde{z}_i) \rangle = 2C_A \left[\frac{2}{1 - \tilde{z}_i(1 - y_{ij,k})} + \frac{2}{1 - (1 - \tilde{z}_i)(1 - y_{ij,k})} - 2 - \tilde{z}_i(1 - \tilde{z}_i) \right] \quad (5.7)$$

$$\langle \mathbf{V}'_{q_i q_j, k}(\tilde{z}_i) \rangle = C_F \left[1 - 2\tilde{z}_i(1 - \tilde{z}_i) \right]. \quad (5.8)$$

The kinematic variables $y_{ij,k}$ and $\tilde{z}_i$ from Equation (3.20) and (3.24) are interpreted as splitting variables and used later to construct the kinematics of the emission. We adopt the factorised phase-space differential from Equation (3.56) in four dimensions omitting the integration boundaries of $y_{ij,k}$ and $\tilde{z}_i$:

$$[dp_i(\tilde{p}_{ij}, \tilde{p}_k)] = \frac{2\tilde{p}_{ij}\tilde{p}_k}{16\pi^2} (1 - y_{ij,k}) dy_{ij,k} d\tilde{z}_i \frac{d\phi}{2\pi}. \quad (5.9)$$

This leads to the factorised cross-section:

$$d\sigma_{m+1} \approx d\sigma_m \sum_{\text{pairs } i,j} \sum_{k \neq i,j} \frac{dy_{ij,k}}{y_{ij,k}} d\tilde{z}_i \frac{d\phi}{2\pi} \frac{\alpha_s}{2\pi} \frac{1}{\mathcal{N}_{ij}^{\text{spec}}} J(y_{ij,k}) \langle \mathbf{V}'_{ij,k}(y_{ij,k}, \tilde{z}_i) \rangle. \quad (5.10)$$

The Jacobian $J(y_{ij,k}) = 1 - y_{ij,k}$ accounts for the transformation of p_i , p_j and p_k to $\tilde{p}_{ij}$ and $\tilde{p}_k$ as well as for the transformation of p_i to $y_{ij,k}$, $\tilde{z}_i$ and ϕ .

¹⁷The prime as superscript is introduced here to denote the difference to the spin-averaged splitting-functions that include the factor $8\pi\mu^2\epsilon\alpha_s$.

To order emission, the CSS uses the squared transverse momentum

$$\mathbf{k}_\perp^2 = -k_\perp^2 = Q^2 y_{ij,k} \tilde{z}_i (1 - \tilde{z}_i) \quad (5.11)$$

as evolution variable t . $Q^2 = 2\tilde{p}_{ij}\tilde{p}_k$ is the invariant mass of the dipole. More precisely $k_\perp^\mu$ is the transverse momentum of the emitted parton j with respect to the momentum of its emitter i taken in the rest frame of emitter and spectator. With this choice of the evolution variable one finds

$$\frac{dy_{ij,k}}{y_{ij,k}} = \frac{d\mathbf{k}_\perp^2}{\mathbf{k}_\perp^2} \quad (5.12)$$

and can thus write the Sudakov factor for the non-splitting probability between $\mathbf{k}_{\perp,\text{high}}^2$ and a smaller $\mathbf{k}_{\perp,\text{low}}^2$ as

$$\Delta_{FF}(\mathbf{k}_{\perp,\text{high}}^2, \mathbf{k}_{\perp,\text{low}}^2) = \exp \left(- \sum_{i,j} \sum_{\text{pairs } k \neq i,j} \frac{1}{\mathcal{N}_{ij}^{\text{spec}}} \int_{\mathbf{k}_{\perp,\text{low}}^2}^{\mathbf{k}_{\perp,\text{high}}^2} \frac{d\mathbf{k}_\perp^2}{\mathbf{k}_\perp^2} \int_{\tilde{z}_i^{\text{min}}}^{\tilde{z}_i^{\text{max}}} d\tilde{z}_i \frac{\alpha_s(\mathbf{k}_\perp^2)}{2\pi} J(y_{ij,k}) \langle \mathbf{V}'_{ij,k}(y_{ij,k}, \tilde{z}_i) \rangle \right). \quad (5.13)$$

In a practical implementation the evolution variable is generated according to the Sudakov veto algorithm, which is for example described in Section 4.2 of [71]. The last paragraph of it refers to the generation of $\tilde{z}_i$ besides $\mathbf{k}_\perp^2$.

In view of the later construction of a resonance-aware shower, we quote here the overestimate of the spin-averaged splitting function in Equation (5.6):

$$C_F \frac{2}{1 - \tilde{z}_i}. \quad (5.14)$$

The integral over this overestimate constitutes part of the function $g(t)$ mentioned in [71]. However, the integral of Equation (5.14) needs regularisation, because allowing for the full range of $\tilde{z}_i$, i.e. $[0, 1]$ as indicated in Equation (3.56), it diverges. One can instead use Equation (5.11) to limit $\tilde{z}_i$ to its kinematically allowed range, which is restricted by the introduction of the shower cutoff $t_c = k_{\perp 0}^2$:

$$\tilde{z}_i^{\text{max/min}} = \frac{1}{2} \left(1 \pm \sqrt{1 - \frac{4k_{\perp 0}^2}{Q^2}} \right). \quad (5.15)$$

The variable $\tilde{z}_i$ is then generated according to its overestimate, using *inverse transform sam-*

pling:

$$\tilde{z}_i = 1 - (1 - \tilde{z}_i^{\min}) \left(\frac{1 - \tilde{z}_i^{\max}}{1 - \tilde{z}_i^{\min}} \right)^r \quad (5.16)$$

where $r \in [0, 1]$ is a uniformly distributed random number and $\phi \in [0, 2\pi]$ is generated according to a flat distribution.

Having $\mathbf{k}_\perp^2$ and $\tilde{z}_i$ at hand, one determines $y_{ij,k}$ through Equation (5.11). Then the hit-or-miss ratio, i.e. the ratio of Equation (5.6) and Equation (5.14), is calculated and the generated variables are accepted or rejected like described in [71].

Having a valid set of splitting variables $y_{ij,k}$, $\tilde{z}_i$ and ϕ at one's disposal, the momenta of the particles after the splitting can be constructed. The inverse mapping of the subtraction algorithm (see. Equation (3.18) and (3.19)) is not unique. One option is given by the Sudakov decomposition:

$$p_i = \tilde{z}_i \tilde{p}_{ij} + \frac{\mathbf{k}_\perp^2}{\tilde{z}_i Q^2} \tilde{p}_k + k_\perp, \quad (5.17)$$

$$p_j = (1 - \tilde{z}_i) \tilde{p}_{ij} + \frac{\mathbf{k}_\perp^2}{(1 - \tilde{z}_i) Q^2} \tilde{p}_k - k_\perp, \quad (5.18)$$

$$p_k = (1 - y_{ij,k}) \tilde{p}_k \quad (5.19)$$

in the rest frame of emitter $\tilde{i}j$ and spectator $\tilde{k}$. The momentum $k_\perp$ is constructed as being perpendicular to both $\tilde{p}_{ij}$ and $\tilde{p}_k$ and having a vanishing zeroth component. Its direction depends on the splitting variable ϕ , see [31] for details.

5.2 Matching

We have already discussed two complementary approaches to improve LO-predictions. The first one is extending the perturbative expansion to further orders, i.e. calculating the observable in question consistently at a fixed order. The second idea is to resum potentially large contributions to all orders in perturbation theory by means of a parton shower. The former method has the advantages of yielding a comparably accurate total cross-section and of modelling hard emissions well. The benefit of the latter approach is a treatment of *multiple* emissions, which are modelled the better the more collinear they are.

In this section, we explain how the best of those two worlds can be *matched* in a consistent way.

5.2.1 The Problem of Double Counting

When combining an fixed NLO calculation with a parton shower care has to be taken since in the most naive approach certain events will be effected by double counting [32]. Roughly

speaking, double counting occurs if there is an overlap of events from the LO + parton shower prediction and real correction from the fixed NLO calculation. A more formal definition is:

“An MC@NLO is affected by double counting if its prediction for any observable, at the first order beyond the Born approximation[...] in the expansion in the coupling constant, is not equal to the NLO prediction.” [32].

There are two established methods how this can automatically be taken care of: the MC@NLO algorithm [32] and the POWHEG algorithm [72, 59]. In the following, we explain only the MC@NLO algorithm in detail because this is the one implemented within SHERPA.

5.2.2 Outline of the MC@NLO Algorithm

Before we plunge into explaining the MC@NLO algorithm [32], we quote the formula describing the interface of an LO calculation with a parton shower at $\mathcal{O}(\alpha_s)$:

$$\sigma_{\text{PS}}^{\text{LO}} = \int_m d\sigma^{\text{B}}(\phi_m) \left[\Delta(t_{\text{res}}, t_c) + \int_1 \Gamma(\phi_1) \Delta(t_{\text{res}}, t) \right]. \quad (5.20)$$

Again $\Gamma(\phi_1)$ is the splitting probability – depending on the phase-space variables of the emitted parton – which we introduced in Section 5.1. The Sudakov factor

$$\Delta(t_{\text{res}}, t) = \exp \left(- \int_{1,t}^{t_{\text{res}}} \Gamma(\phi_1) \right) \quad (5.21)$$

and the squared resummation scale¹⁸ t_{res} have also been introduced in Section 5.1.¹⁹ The first term in the squared bracket of Equation (5.20) is the probability of having no emission between the resummation scale and the shower cutoff, whereas the second term describes the probability of having one emission at the scale t . Performing the integral in the squared bracket of Equation (5.20), which evaluates to $\Delta(t_{\text{res}}, t_{\text{res}}) - \Delta(t_c, t_{\text{res}}) = 1 - \Delta(t_{\text{res}}, t_c)$, we see that the squared bracket integrates to one, i.e. the parton shower conserves unitarity.

To extend the parton shower procedure to yield a cross-section which is correct at NLO accuracy, $d\sigma^{\text{B}}$ must be substituted. Furthermore a change in the term describing the first emission has to be done as it has to reproduce the exact real emission from the fixed NLO calculation. To achieve the latter, the approximate Γ in Equation (5.20) may be substituted with the ratio of real correction and the Born prediction. This is referred to as matrix element correction and done in the POWHEG approach [72]. A drawback of this idea is that after appropriately modifying the Sudakov factor, t_{res} has to be substituted with the hadronic center-of-mass energy in order to cover the whole phase-space for the first emission. This however implies that

¹⁸The variables t , t_{res} and t_c are given in GeV^2 . Thus they are a *squared* scale. However, in the following we discard the adjective to improve the flow of reading.

¹⁹The two notations at the integral sign $\int_{1,t}^{t_{\text{res}}}$ mean that we integrated over the one-parton phase-space and that we restrict the boundaries of the integration over t . If we do not make those boundaries explicit, the maximal boundaries t_c and t_{res} are understood.

the matrix element correction is resummed in regions in which it is not considered a good approximation. It is therefore motivated to split the real correction cross-section into a soft (divergent) and hard (finite) part: $d\sigma^R = d\sigma^{R,\text{soft}} + d\sigma^{R,\text{hard}}$. For reason that become clear in a moment, we write this separation as $d\sigma^R = d\sigma^A + d\sigma^H$. This enables us to write down the NLO analogue of Equation (5.20) – describing a matching à la MC@NLO:

$$\begin{aligned} \sigma_{\text{MC@NLO}}^{\text{NLO}} = & \int_m d\sigma^{\bar{B}}(\phi_m) \left[\Delta^A(t_{\text{res}}, t_c) + \int_1 \frac{d\sigma^A(\phi_{m+1})}{d\sigma^B(\phi_m)} \Delta^A(t_{\text{res}}, t) \right] \\ & + \int_{m+1} d\sigma^H(\phi_{m+1}). \end{aligned} \quad (5.22)$$

The reweighted Born cross-section

$$d\sigma^{\bar{B}}(\phi_m) = d\sigma^B(\phi_m) + d\sigma^V(\phi_m) + d\sigma^I(\phi_m) + \int_1 \left(d\sigma^A(\phi_{m+1}) - d\sigma^S(\phi_{m+1}) \right) \quad (5.23)$$

ensures that the total cross-section of the NLO prediction is reproduced. The Sudakov factor is given by

$$\Delta^A(t_{\text{res}}, t) = \exp \left(- \int_{1,t}^{t_{\text{res}}} \frac{d\sigma^A(\phi_{m+1})}{d\sigma^B(\phi_m)} \right) \quad (5.24)$$

Equation (5.22) suggests that there are two types of events, namely those which are described by the second line of Equation (5.22) and are generated with real correction kinematics ($\mathbb{H}$ -events) and those described by the first line of Equation (5.22) and are generated with Born kinematics ($\mathbb{S}$ -events). The latter undergo a one-step parton shower, which is indicated by the squared bracket.

The splitting of the real correction cross-section into a soft and hard one can be considered as a modified subtraction, since the term $d\sigma^A$ is subtracted from the $\mathbb{H}$ -events and added to the $\mathbb{S}$ -events.²⁰ This in turn means that $d\sigma^A$ does not have to be the *exact* soft part of $d\sigma^R$. In fact it is chosen to be an approximation of it. In the present implementation of the MC@NLO framework within SHERPA [30], those terms equal the CS subtraction terms $d\sigma^S$ up to a Heaviside-theta-function for each dipole [73]. This is, the dipoles $\mathcal{D}^A$ in $d\sigma^A$ are given by

$$\mathcal{D}^A = \mathcal{D}^S \Theta(t_{\text{res}} - t), \quad (5.25)$$

where $\mathcal{D}^S$ are the usual dipoles in $d\sigma^S$. The essence of the MC@NLO-approach is that the modified subtraction terms (in the $\mathbb{H}$ -events) are evaluated at the real correction kinematics and not the Born kinematics. In treating subtraction terms and real corrections on the same footing in that respect, the above-mentioned problem of double counting is overcome [32]. For

²⁰In actuality, the same term is *not* added and subtracted, since its interface to the parton shower is different in $\mathbb{S}$ - and $\mathbb{H}$ -events. However, this difference is of higher order in α_s . See [32] for details.

details on that point and a comparison of the POWHEG- and MC@NLO-approach see [74].

5.2.3 Subleading Colour Effects

Before we continue, we like to dwell on an important feature of the Sudakov factor Δ^A in Equation (5.24). We will come back to this in the next chapter. Equation (5.24) describes the emission probability of S-events not only up to the leading colour approximation (see beginning of Subsection 5.1.2) but takes the full colour correlation into account. However due to the presence of the colour operators in $\mathcal{D}^A$, $d\sigma^A$ can be negative. This leads to a complication as a Sudakov factor larger than unity spoils the probabilistic interpretation of this factor. A solution for that problem is provided in [74] by employing an additional veto algorithm that uses so-called analytic weights [75, 76]. In the following we summarise this algorithm [74].

The goal of the veto algorithm is to generate values of the evolution variable t according to the differential probability distribution

$$P(t_{\text{res}}, t) = f(t) \exp \left(- \int_t^{t_{\text{res}}} dt' f(t') \right). \quad (5.26)$$

The function $f(t)$ is the splitting probability, which we previously denoted as Γ , but integrated over z and ϕ . According to *inverse transform sampling*, t can be generated from a uniformly distributed random number $R \in [0, 1]$, provided $F(t) = \int_{t_c}^t dt' f(t')$ exists and is invertible:

$$t = F^{-1}(F(t_{\text{res}}) + \ln R). \quad (5.27)$$

The key point of the veto algorithm is that one can still generate t according to $P(t_{\text{res}}, t)$ if $F(t)$ is not known. In that case, one has to find an overestimate $g(t) \geq f(t)$, $\forall t$ whose integral $G(t) = \int_{t_c}^t dt' g(t')$ exists and is invertible. Then t is generated according to $g(t) \exp(-\int_t^{t_{\text{res}}} dt' g(t'))$: $t = G^{-1}(G(t_{\text{res}}) + \ln R)$ and accepted by the probability $f(t)/g(t)$. This generates values of t according to the following differential distribution:

$$P_n(t_{\text{res}}, t) = \frac{f(t)}{g(t)} g(t) \exp \left(- \int_t^{t_{\text{res}}} dt' g(t') \right) \cdot \prod_{i=1}^n \left[\int_{t_{i-1}}^{t_{i+1}} dt_i \left(1 - \frac{f(t_i)}{g(t_i)} \right) g(t_i) \exp \left(- \int_{t_i}^{t_{i+1}} dt' g(t') \right) \right]. \quad (5.28)$$

Here, $t_{n+1} = t_{\text{res}}$ and $t_0 = t$. The second line of Equation (5.28) corresponds to the generation of n values t_i that have been rejected by the probability $1 - f(t_i)/g(t_i)$. This line can be simplified to $\exp \left(\int_t^{t_{\text{res}}} dt' (g(t') - f(t')) \right)$, thus making Equation (5.28) coincide with the original differential distribution in Equation (5.26).

The idea of analytic weights is to generate a point according to the additional overestimate

$h(t)$. $h(t)$ and the ratio $f(t)/g(t)$ have to be positive definite. In the hit-or-miss ratio $f(t)$ is still compared to $g(t)$ rather than $h(t)$. This leads to the following differential distribution according to which t is generated:

$$P_n(t_{\text{res}}, t) = \frac{f(t)}{g(t)} h(t) \exp\left(-\int_t^{t_{\text{res}}} dt' h(t')\right) \cdot \prod_{i=1}^n \left[\int_{t_{i-1}}^{t_{i+1}} dt_i \left(1 - \frac{f(t_i)}{g(t_i)}\right) h(t_i) \exp\left(-\int_{t_i}^{t_{i+1}} dt' h(t')\right) \right]. \quad (5.29)$$

To account for the unchanged hit-or-miss ratio, the following weight is applied analytically rather than influencing the acceptance probability:

$$w(t, t_1, \dots, t_n) = \frac{g(t)}{h(t)} \prod_{i=1}^n \frac{g(t_i) h(t_i) - f(t_i)}{h(t_i) g(t_i) - f(t_i)}. \quad (5.30)$$

The first ratio in Equation (5.30) is due to the acceptance of the point with t and the following product accounts for all rejected points i . The weight in Equation (5.30) can be negative. Allowing for negative weights does however not mean that observables can have bins with negative value, but that bins can receive *contributions* from negative weights.

To account for subleading colour effects, the just outlined algorithm is applied in the following form *after* the successful generation of splitting variables with the standard veto algorithm.

This means that the following steps are undertaken:

1. Run the standard veto algorithm to generate a set of splitting variables.
2. Identify f with $\mathcal{D}^A$, h with the parton shower splitting kernel and g with $C \cdot f$.²¹
3. Accept the point generated by the standard veto algorithm, i.e. due to the parton shower splitting kernel, according to the hit-or-miss ratio $f/g = 1/C$.
4. In case of a rejection, calculate the term $g/h \cdot (h - f)/(g - f)$ and multiply it to the weight of the event. Then, continue with point 1.
5. If the point is accepted, compute the term g/h and multiply it to the event weight. Retain the kinematics of the event.

This reweighting algorithm is implemented in both matching modules of SHERPA, MCATNLO and DIM to account for subleading colour effects.

²¹In the current SHERPA version [30] the constant C equals 3 but it could be any number larger than one. In fact, there is a much larger freedom in choosing g . It can even be defined pointwise. This will prove useful in the following.

Analytic Weights Revisited

The concept of analytic weights can also be applied directly *within* the veto algorithm instead of *after* it.

We have just summarised the concept of analytic weights being applied after the generation of splitting variables. This algorithm can account for cases with negative splitting functions. We will however see in the next chapter that there can also be cases in which the splitting function is larger than its overestimate. In order to account for also those cases, the standard veto algorithm needs to be *replaced* with the veto algorithm featuring analytic weights.

In this case, the generation of splitting variables proceeds as follows:

1. Identify f with the parton shower splitting kernel and h with its overestimate.
2. Generate a set of splitting variables according to h .
3. Set g pointwise to $\pm h$ such that f/g is positive definite. If however $|f| > h$ set g to $C \cdot f$ ($C = 3$).
4. Calculate the acceptance probability f/g .
5. If the generated point is rejected, multiply the term $g/h \cdot (h - f)/(g - f)$ to the event weight and continue with point 2.
6. If the generated point is accepted, multiply the term g/h to the event weight and continue with those splitting variables.

This algorithm is implemented in the modules DIRE and DIM of SHERPA but not CSS and MCATNLO. Thus only the former two modules can handle the case of a splitting function being larger than its overestimate correctly.

We remark that for all “non-exotic” cases, i.e. $f(t) > 0$ and $h(t) > f(t)$, the analytic weight reduces to unity.

6 Resonance-Aware Showering and Matching

The accuracy of parton showers is often quantified by the order of logarithms, which are correctly resummed, see Subsection 5.1.1. In addition to that, it should always be stated *which* logarithm, i.e. *which* arguments, are meant by that, since their accuracy can be different [56]. Complementary to that, the recoil of a parton shower is another source of uncertainty, since different recoil schemes produce different differential distributions. In particular for processes featuring intermediate resonances, this uncertainty might be significant. The reason for that is the following. If a parton shower generates an emission, the momenta of particles become adjusted due to on-shellness requirements and momentum conservation. The weight of the matrix element is however not recalculated. This implies that the kinematical configuration of an event might not correspond to the weight of its matrix element. Thus, the differential distribution becomes distorted. Applying a resonance-aware shower instead of a non-resonance-aware one, counteracts this effect to at least some extent, since the (unchanged) virtualities of the resonances have a huge influence on the weight of the matrix element.

In this chapter, we aim to study that uncertainty by developing a resonance aware-shower based on the above discussed pseudo-dipoles and contrasting its predictions to the CSS. In analogy to the latter, we refer to it as IDS.

The labelling of involved partons in the IDS is the same as in the resonance-aware subtraction (Chapter 4) and recalled in Figure 6.1. We consider only a single emission in the process $e^+e^- \rightarrow W^+W^-b\bar{b}$. At the end of this chapter, we see that already this leads to problems. It is therefore not sensible to consider multiple emissions or more complicated processes.

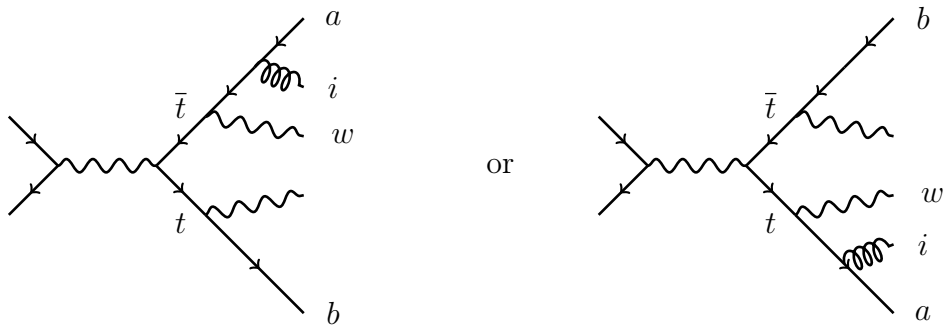


Figure 6.1: Sketch of labelling of emitter a and emitted parton i as well as kinematic spectator w and colour spectator b for the IDS in the process $e^+e^- \rightarrow W^+W^-b\bar{b}$.

6.1 Factorisation and Parametrisation

In analogy to Subsection 5.1.2, we begin by approximating $|\mathcal{M}_{m+1}|^2$ by the factorised expression

$$|\mathcal{M}_{m+1}|^2 \approx |\mathcal{M}_m|^2 \sum_{\substack{\text{pairs } b \neq a, i \\ a, i}} \frac{1}{2p_a p_i} \frac{1}{\mathcal{N}_{ai}^{\text{spec}}} 8\pi\alpha_s \langle \mathbf{V}_{ai,b}^{(n)'}(v_{i,ab}, z_{ain}) \rangle. \quad (6.1)$$

This equation resembles Equation (5.5). It differs only in the renaming of the involved partons (see Figure 6.1) and the polarisation averaged splitting function:

$$\langle \mathbf{V}_{qg}^{(n)'}(v_{i,ab}, z_{ain}) \rangle = C_F \left[2 \frac{v_{i,ab}}{z_{ain}} - (1 + z_{ain}) \right]. \quad (6.2)$$

In contrast to the splitting function of the CSS, Equation (6.2) can become negative. This spoils the probabilistic interpretation of the Sudakov factor as discussed at the end of the preceding chapter. However, this problem can be overcome, as discussed there. The factorisation of phase-space differentials is given by

$$d\phi(p_i, k_1, \dots; Q) = d\phi(\tilde{k}_1, \dots; Q) [dp_i(n, p_a, z)] \quad (6.3)$$

where the k s denote the kinematic spectators' momenta and $Q = n + p_a$ with n defined in Equation (4.1). The last term in the above formula is given by Equation (4.14). Omitting the integration boundaries of $\tilde{v}_i$ and z_{ain} and expressing everything in four dimensions, we obtain:

$$[dp_i(n, p_a, z)] = \frac{2p_a n}{16\pi^2} d\tilde{v}_i dz_{ain} \frac{d\phi}{2\pi}. \quad (6.4)$$

When we combine this with Equation (6.1), we obtain

$$d\sigma_{m+1} \approx d\sigma_m \sum_{\substack{\text{pairs } b \neq a, i \\ a, i}} \frac{d\tilde{v}_i}{\tilde{v}_i} dz_{ain} \frac{d\phi}{2\pi} \frac{\alpha_s}{2\pi} \frac{1}{\mathcal{N}_{ai}^{\text{spec}}} \langle \mathbf{V}_{qg}^{(n)'}(v_{i,ab}, z_{ain}) \rangle. \quad (6.5)$$

In comparison to Equation (5.10) the Jacobian reduces here to one. We see that the splitting in the IDS is described by the splitting variables

$$\tilde{v}_i = \frac{p_a p_i}{p_a n} \quad \text{and} \quad z_{ain} = \frac{p_a n}{(p_a + p_i)n} \quad (6.6)$$

instead of $y_{ij,k}$ and $\tilde{z}_i$ in the CSS, given in Equation (3.20) and (3.24). As for the CSS, we have to define an evolution variable t , which is required to order the emissions to mimic quantum effects as well as possible. We postpone this definition to the next section as it deserves a bit of discussion. Thus skipping the explicit form of t for the moment, we can write the Sudakov

factor for the non-splitting probability between t_{high} and t_{low} as

$$\Delta_{FF}(t_{\text{high}}, t_{\text{low}}) = \exp \left(- \sum_{\substack{\text{pairs } b \neq a, i \\ a, i}} \sum_{ai} \frac{1}{\mathcal{N}_{ai}^{\text{spec}}} \int_{t_{\text{low}}}^{t_{\text{high}}} \frac{dt}{t} \int_{z_{\text{ain}}^{\text{min}}}^{z_{\text{ain}}^{\text{max}}} dz_{\text{ain}} \frac{\alpha_s(\mathbf{p}_{i,\perp}^2)}{2\pi} J(\phi, z_{\text{ain}}, \tilde{v}_i) \langle \mathbf{V}_{qg}'^{(n)}(v_{i,ab}, z_{\text{ain}}) \rangle \right). \quad (6.7)$$

The Jacobian $J(\phi, z_{\text{ain}}, \tilde{v}_i)$ is defined by the equation

$$\frac{d\tilde{v}_i}{\tilde{v}_i} = J(\phi, z_{\text{ain}}, \tilde{v}_i) \frac{dt}{t} \quad (6.8)$$

and thus depends on the choice of the evolution variable. We stress that this Jacobian is of another origin as the one in Equation (5.10). Its analogue in the CSS equals one, see Equation (5.12).

6.2 Ordering Variable

Now we come to the point of defining the ordering or evolution variable. Typical choices are the angle between the momenta of the splitting partons, their invariant mass or (as quoted in Subsection 5.1.2) the relative transverse momentum. All of these choices are equivalent in the resummation of leading logarithms and differ only beyond it, i.e. at the level of next-to-leading logarithms. Clearly we cannot simply adopt formula (5.11), since it depends on the splitting variables $y_{ij,k}$ and $\tilde{z}_i$, which are not appropriate to parametrise a splitting on the basis of pseudo-dipoles.

We study two different choices of the evolution variable:

1. Our first choice is motivated by the evolution variable of the CSS. This can be written as

$$\mathbf{k}_{\perp}^2 = y_{ai,b} \tilde{z}_a (1 - \tilde{z}_a) Q^2 \quad (6.9)$$

$$= 2p_a p_b \frac{(p_a p_b)(p_i p_b)}{[(p_a + p_i)p_b]^2} \quad (6.10)$$

$$\xrightarrow{p_i \rightarrow 0} 2 \frac{(p_a p_i)(p_b p_i)}{p_a p_b}. \quad (6.11)$$

In the last line we have taken the soft limit. This term is proportional to the inverse of the momentum dependence of the squared eikonal current, see Equation (3.10). In order to have an evolution variable, which is as close to the one of the CSS as possible,

we define our first choice to be:²²

$$t_{\text{eik}} = \frac{(p_a p_i)(p_b p_i)}{p_a p_b}. \quad (6.12)$$

We choose t_{eik} to be proportional to the soft limit of $\mathbf{k}_\perp^2$ instead of setting it to $\mathbf{k}_\perp^2$ itself, because the scalar product $p_b p_i$ is a rather complicated function of the resonance-aware splitting variables. We will see in Section 6.4 how this complicates the calculation of $\tilde{v}_i$ in the veto algorithm.

2. To circumvent the problem in the determination of $\tilde{v}_i$, we consider a simpler definition of the evolution variable by taking it to be the invariant mass of the splitting partons (divided by two):

$$t_{\text{virt}} = p_a p_i. \quad (6.13)$$

Depending on the choice of evolution variable, we refer to those two versions of the IDS as IDS^{eik} or IDS^{virt} .

Having made two different choices for the evolution variable allows us to see which effect it has on physical predictions.

To make our line of action within the next two sections as clear as possible, we summarise the game plan of them as follows. Our aim is to generate splitting variables according to the Sudakov factor in Equation (6.7). We then use these variables to construct the kinematics after the emission. However, to achieve that, we have to proceed in reversed order. This means that we first construct the kinematics after the emission as a function of the (yet unknown) splitting variables and then generate the splitting variables. The reason for this order is that we do not yet know how the Sudakov factor in Equation (6.7) depends on the splitting variables, because we do not yet know how $v_{i,ab}$ (see Equation (4.9)) in the polarisation averaged splitting function in Equation (6.2) depends on the splitting variables. On top of that we need to express the ordering variables of this section in terms of splitting variables and Born kinematics as this is necessary for the veto algorithm.

6.3 Building of Kinematics

In this section we construct the momenta of the particles after the splitting by performing a Sudakov parametrisation. This enables us to calculate scalar products of those momenta as they occur in $v_{i,ab}$ or the definition of the evolution variables as a function of Born kinematics and the splitting variables $\tilde{v}_i$, z_{ain} and ϕ_{ib} .²³ After achieving that we can proceed to generate

²²The factor two influences at which point the shower is cut off due to t_c . We study the influence of t_c on the simulation output in Subsection 6.6.1.

²³The angle ϕ_{ib} is defined at the beginning of the next section.

the splitting variables in the Sudakov veto algorithm, which is described in Section 6.4.

The momenta which undergo a mapping are those of the emitter $\tilde{a}i$ and the kinematic spectator $\tilde{w}$ ²⁴. We thus write

$$Q_w := \tilde{p}_{ai} + \tilde{p}_w = p_a + p_i + p_w \quad (6.14)$$

and define the light-cone momenta

$$P_+ := \tilde{p}_{ai}, \quad (6.15)$$

$$P_- := \tilde{p}_w - \frac{m_w^2}{2\tilde{p}_{ai}\tilde{p}_w}\tilde{p}_{ai}. \quad (6.16)$$

Clearly, both momenta fulfil their defining property, i.e. $P_+^2 = P_-^2 = 0$. In order to coincide with the mapping of the emitter, see Equation (4.3), we write momentum conservation in P_+ -direction as

$$\left[\tilde{p}_{ai} + \tilde{p}_w\right]_{P_+} = \left(1 + \frac{m_w^2}{2\tilde{p}_{ai}\tilde{p}_w}\right)\tilde{p}_{ai} \stackrel{!}{=} z_{ain}\tilde{p}_{ai} + p_+ = \left[p_a + p_i + p_w\right]_{P_+}, \quad (6.17)$$

where p_+ is the remaining momentum in P_+ -direction not carried by p_a , but p_i and p_w and thus given by

$$p_+ = \left(1 - z_{ain} + \frac{m_w^2}{2\tilde{p}_{ai}\tilde{p}_w}\right)\tilde{p}_{ai}. \quad (6.18)$$

Analogously we find via momentum conservation in P_- -direction ($p_- := P_-$) which momentum p_i and p_w carry in that direction. Having ascertained p_+ and p_- , we write the Sudakov decomposition of p_i and p_w along with p_a and p_b as

$$p_a^\mu = z_{ain}\tilde{p}_{ai}^\mu, \quad (6.19)$$

$$p_i^\mu = xp_+^\mu - \frac{p_{\perp iw}^2}{x} \frac{1}{2p_+p_-} p_-^\mu + p_{\perp iw}^\mu, \quad (6.20)$$

$$p_w^\mu = (1-x)p_+^\mu - \frac{p_{\perp iw}^2 - m_w^2}{1-x} \frac{1}{2p_+p_-} p_-^\mu - p_{\perp iw}^\mu, \quad (6.21)$$

$$p_b^\mu = \alpha\tilde{p}_{ai}^\mu - \frac{p_{b\perp}^2}{\alpha} \frac{1}{2\tilde{p}_{ai}p_-} p_-^\mu + p_{b\perp}^\mu, \quad (6.22)$$

where $p_{\perp iw}$ is the transverse momentum between p_i and p_w and $p_{b\perp}$ is the transverse momentum of p_b with respect to $\tilde{p}_{ai}$. The transverse momenta fulfil the following orthogonality relations $p_{\perp iw}p_+ = p_{\perp iw}p_- = p_{b\perp}p_+ = p_{b\perp}p_- = 0$ and have a vanishing zeroth component in the

²⁴As before, the tilde denotes momenta of the Born configuration. The momenta without a tilde denote momenta of the real emission configuration

center-of-mass frame of P_+ and P_- . From consistency relations we obtain

$$x = \frac{1 - z_{ain}}{1 - z_{ain} + \frac{m_w^2}{Q_w'^2}} - \tilde{v}_i, \quad (6.23)$$

$$p_{\perp iw}^2 = -\tilde{v}_i Q_w'^2 \left[\tilde{v}_i \left(z_{ain} - 1 - \frac{m_w^2}{Q_w'^2} \right) + 1 - z_{ain} \right], \quad (6.24)$$

$$\alpha = \frac{p_b p_-}{\tilde{p}_{ai} p_-}, \quad (6.25)$$

$$p_{b\perp}^2 = -2\alpha \tilde{p}_{ai} p_b, \quad (6.26)$$

where $Q_w'^2 = 2\tilde{p}_{ai}\tilde{p}_w$.

Note that this mapping from Born to real kinematics, i.e. Equation (6.19)-(6.21), is related to the one in the CSS. In fact it is the same, if one

- performs the substitutions $j \rightarrow i$, $i \rightarrow w$ and $k \rightarrow a$ in the Equations (59)-(61) of [31], which are the generalisations of Equations (5.17)-(5.19) to the case with massive emitter²⁵,
- constructs the momenta in the above mentioned reference frame and
- accounts for ϕ_{ib} (see below) describing another angle than ϕ from the CSS.

We have checked explicitly that our implementations of this resonance-aware mapping reproduce the correct kinematics. We have done this by writing out the kinematics of a real correction phase-space point during the integration of the RS cross-section. For this point, we also wrote out the clustered momenta, which are used in the pseudo-dipole calculation, as well as the splitting variables calculated from the real correction momenta. We then hard-coded those Born momenta and the splitting variables and obtained the identical real correction momenta in the shower as before in the integration.

6.4 Generation of Splitting Variables

With the Sudakov parametrisation of the relevant momenta we can proceed to calculate the scalar products required for expressing the evolution variables as a function of Born momenta

²⁵As a cross-check it is interesting to note, that the term $2p_a n$ in Equation (6.4) can be rewritten as $2p_a n = z_{ain}(1 - \mu_w^2)Q_w'^2$ where $\mu_w^2 = \frac{m_w^2}{Q_w'^2}$. This in turn equals the Jacobian $\frac{(1 - \mu_i^2 - \mu_j^2 - \mu_k^2)^2}{\lambda(1, \mu_{ij}^2, \mu_k^2)}(1 - y_{ij,k})Q^2$ in the analogue of Equation (5.9) for massive partons (given in Equation (33) of [31]) with the substitutions $j \rightarrow i$, $i \rightarrow w$ and $k \rightarrow a$.

and splitting variables:

$$p_a p_b = z_{ain} \tilde{p}_{ai} p_b, \quad (6.27)$$

$$p_a p_i = \tilde{v}_i z_{ain} \frac{Q_w'^2}{2}, \quad (6.28)$$

$$p_b p_i = A + B - 2\sqrt{AB} \cos \phi_{ib}, \quad (6.29)$$

where ϕ_{ib} is the azimuthal angle between $\vec{p}_i$ and $\vec{p}_b$ in the CMS of $\tilde{p}_{ai}$ and $\vec{p}_-$. We use the following abbreviations:

$$A = \alpha \tilde{v}_i \frac{Q_w'^2}{2}, \quad (6.30)$$

$$B = \tilde{p}_{ai} p_b \left[\tilde{v}_i \left(z_{ain} - 1 - \frac{m_w^2}{Q'^2} \right) + 1 - z_{ain} \right]. \quad (6.31)$$

Now, we are in the position to explain the generation of splitting variables in the IDS. As this differs for the two evolution variables, we consider the two cases in turn.

6.4.1 Inverse Eikonal Shower IDS^{eik}

The evolution variable can be expressed by

$$\begin{aligned} t_{\text{eik}} &= \frac{(p_a p_i)(p_b p_i)}{p_a p_b} \\ &= \frac{\tilde{v}_i Q_w'^2 \left[A + B - 2\sqrt{AB} \cos \phi \right]}{2\tilde{p}_{ai} p_b}. \end{aligned} \quad (6.32)$$

In contrast to the CSS and the below described virtuality shower, the additional Jacobian defined in Equation (6.8) does not evaluate to unity. This has the consequence that it has to be multiplied to the value of the splitting function in the veto algorithm.

Generation of z_{ain}

We like to overestimate the z_{ain} dependence of the polarisation averaged splitting function from Equation (6.2). It is however not obvious how the term $v_{i,ab}$ can be overestimated in terms of z_{ain} . In want for a better choice we use the established function from Equation (5.14), i.e.

$$g_1(z_{ain}) = C_F \frac{2}{1 - z_{ain}}. \quad (6.33)$$

This function is however not for all phase-space points an overestimate. We discussed at the end of the previous chapter, how those cases can be dealt with. In Section 6.5, we return to that problem and show what quantitative influence its proper treatment has with respect to the standard one.

In order to find the correct values for $z_{ain}^{\min/\max}$, we have to find out which values of z_{ain} imply $t_{eik} = t_c$. Using Equation (6.32), we get

$$t_c = \frac{\tilde{v}_i Q_w'^2}{2\tilde{p}_{ai}p_b} \left[A + B - 2\sqrt{AB}\cos\phi_{ib} \right]. \quad (6.34)$$

The right-hand side of this equation depends on all three splitting variables. Two of them, namely ϕ_{ib} and $\tilde{v}_i$, should be chosen such that they make the right hand side of Equation (6.34) as large as possible. We can then determine the boundaries in which z_{ain} is kinematically allowed. We choose $\cos\phi_{ib} = -1$ and $\tilde{v}_i$ is set to one or zero depending where it occurs in the Equation (6.34). We therefore solve

$$t_c = \frac{Q_w'^2}{2\tilde{p}_{ai}p_b} \left[\tilde{p}_{ai}p_b(1 - z_{ain}) + 2\sqrt{\alpha\frac{Q_w'^2}{2}\tilde{p}_{ai}p_b(1 - z_{ain})} \right] \quad (6.35)$$

for z_{ain} and obtain

$$z_{ain}^{\max} = \frac{-2t_c\tilde{p}_{ai}p_b + \tilde{p}_{ai}p_bQ_w'^2 - \alpha Q_w'^4 + \sqrt{\alpha Q_w'^4(4t_c\tilde{p}_{ai}p_b + \alpha Q_w'^4)}}{\tilde{p}_{ai}p_bQ_w'^2}. \quad (6.36)$$

There is no lower boundary for z_{ain} , i.e.

$$z_{ain}^{\min} = 0. \quad (6.37)$$

Azimuthal Angle ϕ_{ib}

In order to find a ϕ -dependent²⁶ overestimate of Equation (6.2), we write

$$2\frac{v_{i,ab}}{z_{ain}} = 2\tilde{p}_{ai}p_b \left(\tilde{v}_i z_{ain} \frac{Q_w'^2}{2} + A + B \right) \frac{1}{1 - K \cos\phi} \quad (6.38)$$

with

$$K = \frac{2\sqrt{AB}}{\tilde{v}_i z_{ain} \frac{Q_w'^2}{2} + A + B}. \quad (6.39)$$

The possible values of K – as a function of $\tilde{v}_i$ – lie between zero and $K_{\max}$. The maximum of K is a local one (i.e. not at $\tilde{v}_i = 0$ or $\tilde{v}_i = \tilde{v}_i^{\max}$) and ascertained by

$$\left. \frac{\partial K}{\partial \tilde{v}_i} \right|_{\tilde{v}_i = \tilde{v}_i^{K_{\max}}} = 0, \quad \tilde{v}_i^{K_{\max}} = \frac{2\tilde{p}_{ai}p_bQ_w'^2(1 - z_{ain})}{2m_W^2\tilde{p}_{ai}p_b + 2\tilde{p}_{ai}p_bQ_w'^2(1 - z_{ain}) + Q_w'^4(\alpha + z_{ain})}, \quad (6.40)$$

$$K_{\max} = K(\tilde{v}_i = \tilde{v}_i^{K_{\max}}) = \sqrt{\frac{\alpha}{\alpha + z_{ain}}}. \quad (6.41)$$

²⁶In this subsection, we denote ϕ_{ib} with ϕ to avoid clutter.

It is not obvious how to proceed now, since $K_{\max} = 1$ requires a different procedure than $K_{\max} < 1$. Furthermore we cannot make our ϕ -overestimate dependent on z_{ain} , because its integral is required in the veto algorithm before z_{ain} is known. We thus have to choose between the two possible overestimates $g_2(\phi)$:²⁷

$$\frac{F}{1 - \cos \phi} \quad \text{and} \quad \frac{F}{1 - K \cos \phi} \quad \text{with} \quad K < 1. \quad (6.42)$$

In the following we explain both cases before we comment on the outcome of their implementation.

If we used the former one, we have to define a minimal and maximal value of ϕ in order to screen the divergences arising in that function. To find $\phi_{\min/\max}$, we have to make contact with t_c again. We thus express the evolution variable t_{eik} , see Equation (6.32), as

$$t_{\text{eik}} = \frac{\tilde{v}_i Q_w'^2}{2\tilde{p}_{ai} p_b} (A + B)(1 - \tilde{K} \cos \phi) \quad (6.43)$$

where $\tilde{K} = \frac{2\sqrt{AB}}{A+B}$. The value, which maximises $\tilde{K}$ is $\tilde{v}_i^{\tilde{K}_{\max}}$ and is defined like $\tilde{v}_i^{K_{\max}}$ above. For this value we find: $A = B$ and $\tilde{K} = 1$. We thus have to solve

$$t_c = \frac{\tilde{v}_i Q_w'^2}{2\tilde{p}_{ai} p_b} 2A(1 - \cos \phi'_{\min/\max}) \Big|_{\tilde{v}_i = \tilde{v}_i^{\tilde{K}_{\max}}} \quad (6.44)$$

and find

$$\cos \phi'_{\min/\max} = 1 - t_c \frac{[2m_W^2 \tilde{p}_{ai} p_b + Q_w'^2 (2\tilde{p}_{ai} p_b (1 - z_{ain}) + \alpha Q_w'^2)]^2}{2\tilde{p}_{ai} p_b \alpha Q_w'^8 (1 - z_{ain})^2} \quad (6.45)$$

which we underestimate with

$$\cos \phi_{\min/\max} = 1 - t_c \frac{[2m_W^2 \tilde{p}_{ai} p_b + \alpha Q_w'^4]^2}{2\tilde{p}_{ai} p_b \alpha Q_w'^8}. \quad (6.46)$$

Having ascertained $\phi_{\min}$ and $\phi_{\max} = 2\pi - \phi_{\min}$, we can calculate the regularised integral of g_2 :

$$\int_{\phi_{\min}}^{\phi_{\max}} g_2(\phi) d\phi = \frac{2F}{\tan \frac{\phi_{\min}}{2}}. \quad (6.47)$$

²⁷We have considered the overestimate functions for z_{ain} and ϕ of the splitting function separately. Thus the total overestimate function is given by $g(z_{ain}, \phi) = g_1(z_{ain}) \cdot g_2(\phi)$. The parameter F is chosen such that – for the majority of generated phase-space points – $g(z_{ain}, \phi)$ is an overestimate of the splitting function. This justifies our neglecting all prefactors in Equation (6.38). The few remaining phase-space points in which the overestimate is smaller than the splitting function are taken care of by the analytic weights procedure and the point-wise overestimate definition explained at the end of the previous chapter. In our test case of $e^+e^- \rightarrow W^+W^-b\bar{b}$, we chose $F = 1$ for t_{eik} and $F = 4$ for t_{virt} .

The normalised probability distribution is therefore given by

$$G_2(\phi) = \frac{1}{2} \tan \frac{\phi_{\min}}{2} \int_{\phi_{\min}}^{\phi} g_2(\phi') d\phi' \quad (6.48)$$

$$= \frac{1}{2} \tan \frac{\phi_{\min}}{2} \left(\frac{1}{\tan \frac{\phi_{\min}}{2}} - \frac{1}{\tan \frac{\phi}{2}} \right). \quad (6.49)$$

To generate ϕ according to $g_2(\phi)$, we use inverse transform sampling, i.e. set a uniformly distributed random number $r \in [0, 1]$ equal to $G_2(\phi)$ and find

$$\phi = 2 \arctan \left(\frac{\tan \frac{\phi_{\min}}{2}}{1 - 2r} \right). \quad (6.50)$$

Note that $\phi \in [-\pi, -\phi_{\min}] \cap [\phi_{\min}, \pi]$ according to Equation (6.50), which is equivalent to $\phi \in [\phi_{\min}, \phi_{\max}]$. This procedure has however the obvious drawback that values of ϕ larger than $\phi_{\max}$ and smaller than $\phi_{\min}$ are a priori excluded, which is only correct for a subset of phase-space points. On the other hand this overestimate has a (screened) pole which might be important for a correct generation of ϕ .

To assess which influence the choice of the overestimate has upon the simulation, we now consider the second case of Equation (6.42), namely

$$g_2(\phi) = \frac{F}{1 - K \cos \phi}. \quad (6.51)$$

The integral of that distribution is given by

$$\int_0^{2\pi} g_2(\phi) d\phi = \frac{2\pi F}{\sqrt{1 - K^2}}. \quad (6.52)$$

According to inverse transform sampling ϕ can now be calculated by

$$\phi = 2 \arctan \left(\frac{\sqrt{1 - K^2}}{1 + K} \tan(\pi r) \right) \quad (6.53)$$

where r is again a uniformly distributed random number $r \in [0, 1]$. The parameter K can be freely chosen and physical results must not depend on it. We checked that this is indeed the case, provided that K is not too close to unity, i.e. $K > 0.99999$. In those cases we suspect numerical instabilities to be the source of the arising deviations. Further, we ascertained that the numerical value of K has a minor influence on the efficiency of the algorithm.

We also compared our findings to the singular overestimate with the restricted range of ϕ and found perfect statistical agreement in the invariant mass distributions already considered in Subsection 4.4.2. Independently of that, we performed another test to assess the influence of a screened divergence in the overestimate: Observables calculated with the CSS have been

compared with a calculation in which the variable $\tilde{z}_i$ has not been generated by the overestimate in Equation (5.14) but by $C_F \frac{2}{1-K\tilde{z}_i}$, with $K = 0.9$ and $K = 0.999$. We found that all three predictions agree perfectly within their statistical uncertainty. From this we conclude that – at least for the process $e^+e^- \rightarrow W^+W^-b\bar{b}$ – it is not necessary to have a singularity in the overestimate (and screening it by restricting the range of the variable in question). Instead it is also possible to regulate the overestimate such that it does not have a singularity at all. As a side benefit of this study, we checked our implementation of the generation of ϕ . In the implementation of the IDS, we choose Equation (6.51) as our ϕ -overestimate and set $K = 0.9$.

Solving for $\tilde{v}_i$

Once we have generated z_{ain} , ϕ_{ib} and the evolution variable t_{eik} , we can solve Equation (6.32) for $\tilde{v}_i$. This step is necessary because $\tilde{v}_i$ is required for the construction of momenta after the splitting, see Section 6.3. Unfortunately this leads to a polynomial of fourth order with four lengthy complex solutions, which we will not quote here since they are not particularly illuminating.

The calculation of $\tilde{v}_{i1}$, $\tilde{v}_{i2}$, $\tilde{v}_{i3}$ and $\tilde{v}_{i4}$ for a given set of real correction momenta and its comparison with the actual $\tilde{v}_i$ from Equation (6.6) revealed that neither of the four solutions can be singled out nor discarded. That is, depending on the phase-space point, the correct $\tilde{v}_i$ is reproduced by one or more of the four solutions with no visible pattern behind it. What is more is that no correlation between the phase-space and the agreement of $\tilde{v}_i$ with one of the four solutions could be traced.

To deal with this problem, we sum over all four solutions of $\tilde{v}_i$. We do this by multiplying the integral of the overestimate function

$$g(\phi_{ib}, z_{ain}) = g_1(z_{ain})g_2(\phi_{ib}) = C_F \frac{2}{1 - z_{ain}} \frac{F}{1 - K \cos \phi_{ib}} \quad (6.54)$$

by a factor of four. This decreases the step size in which the evolution variable is decreased in the veto algorithm. At the same time we select one of the four $\tilde{v}_i$ solutions randomly. If the chosen $\tilde{v}_i$ is

- not real valued,
- its real part not between zero and $\tilde{v}_i^{\max}$ or
- it does not reproduce the correct value of t_{eik} in Equation (6.32),

the point is discarded and a new one with smaller t_{eik} is generated.

This procedure is however not ideal as it lacks understanding. It would be preferable to know which of the four solutions is/are the right one(s). The answer to that question might depend on the phase-space point. To circumvent this flaw, we consider the IDS with t_{virt} as evolution variable. In this case we do not encounter such a problem.

6.4.2 Virtuality Shower IDS^{virt}

The (scaled) virtuality can be expressed in terms of the splitting variables as

$$t_{\text{virt}} = p_a p_i \quad (6.55)$$

$$= \tilde{v}_i z_{\text{ain}} \frac{Q_w^2}{2}. \quad (6.56)$$

For this evolution variable we use the same overestimate functions as for t_{eik} , i.e. Equation (6.54), since the splitting function stays the same. We point however out that in contrast to the algorithm with t_{eik} we use $F = 4$ instead of 1.²⁸ We do this to prevent the simulation from having large fluctuations caused by the analytic weights.

We have to modify the upper limit $z_{\text{ain}}^{\text{max}}$ as this depends on the explicit definition of the evolution variable. Since Equation (6.56) does not allow to read off $z_{\text{ain}}^{\text{max}}$ right away, we substitute $\tilde{v}_i$ with its maximal value (see Equation (4.14)):

$$\tilde{v}_i^{\text{max}} = \frac{2p_a n}{n^2} \frac{1 - z_{\text{ain}}}{z_{\text{ain}}}. \quad (6.57)$$

We thus get

$$t_c = \frac{2p_a n}{n^2} (1 - z_{\text{ain}}) Q_w^2. \quad (6.58)$$

After expressing everything in terms of Born momenta, we find

$$z_{\text{ain}}^{\text{max}} = \frac{1}{2} \left(1 + \frac{t_c}{Q_w^2} \right) + \sqrt{\frac{1}{4} \left(1 + \frac{t_c}{Q_w^2} \right)^2 - \frac{t_c}{Q_w^2} \left(1 + \frac{m_w^2}{Q_w^2} \right)}. \quad (6.59)$$

This formula has however the problem of allowing for complex $z_{\text{ain}}^{\text{max}}$. This is the case if $Q_w^2 = 2\tilde{p}_{ai}\tilde{p}_w$ becomes increasingly small, i.e. emitter and kinematic spectator increasingly collinear. To overcome this problem, we omit the square root once it is not purely real. But even then, there are extremely rare cases in which $z_{\text{ain}}^{\text{max}} > 1$ for even smaller values of Q_w^2 . In want for a better method to estimate $z_{\text{ain}}^{\text{max}}$, we set its value to 0.99999 in those infrequent events.

It has been checked explicitly that no larger values of z_{ain} pass our algorithm. This means that allowing for a wider range of z_{ain} , no value above $z_{\text{ain}}^{\text{max}}$ – calculated as just described – generates a kinematically possible event. The lower boundary of z_{ain} is not important as it does not screen a singularity. We thus use $z_{\text{ain}}^{\text{min}} = 0$ again. The azimuthal angle ϕ_{ib} is generated like above, i.e. according to the distribution function in Equation (6.51). Having z_{ain} and ϕ_{ib}

²⁸Since we summed in the algorithm with t_{eik} over all four solutions of $\tilde{v}_i$ the implemented integral over the overestimate functions stays the same. The value of the unintegrated overestimate function – which enters the hit-or-miss ratio – differs however by a factor of four.

at hand, we can easily determine $\tilde{v}_i$ through Equation (6.56).

6.4.3 Evaluation of α_s

The scale at which α_s is evaluated in the CSS, is its evolution variable $\mathbf{k}_\perp^2$. This scale is chosen since it resums part of the higher order corrections to the splitting [31]. The resonance-aware shower has a different evolution variable (t_{eik} or t_{virt}), but there is no reason why the evolution variable of a shower and its scale of α_s should be identical. In fact also virtuality or angle ordered showers evaluate α_s at the transverse momentum in order to benefit from the above mentioned resummation [56]. We thus evaluate α_s at $\mathbf{p}_{i\perp}^2$, this is the transverse component of p_i with respect to its emitter a in the CMS of a , b and i .

6.5 Implementing the Algorithm and Cross-Checks

It is not possible to check the implementation of the IDS by comparing it to a reference prediction of the literature. The reason for that is of course that it constitutes a new shower, whose predictions are not expected to coincide with the ones of other showers. The best, which can be done in this case, is to validate the new algorithm by setting up at least two independent implementations of it and compare their predictions.

In this section, we cross-check the IDS implementation of a single emission in the process $e^+e^- \rightarrow W^+W^-b\bar{b}$ in not less than four modules of the public event generator SHERPA [30]. This means that we used these modules as frameworks, in which parton shower emissions are generated, and adapted their code according to our algorithm. The necessary changes can be divided into three main parts:

- the generation of splitting variables,
- the splitting functions and
- the construction of the emission kinematics.

Each of them is described in the previous sections. For readers, who are interested to see in which files the three main changes take place, we give an overview in Appendix C. The four modules are shown in Figure 6.2. The modules CSS and DIRE are the implementations of two independent parton showers [31, 77] of SHERPA. The modules MCATNLO and DIM are their respective implementations in the matching framework à la MC@NLO.

Normally it is not possible to use a shower and matching module, like CSS and MCATNLO, to cross-check a shower algorithm. But the example process $e^+e^- \rightarrow W^+W^-b\bar{b}$ is sufficiently simple to allow that. The reason for that is that the colour correlation for processes with less than four partons at tree-level factorises completely, see Appendix A of [24]. This means that

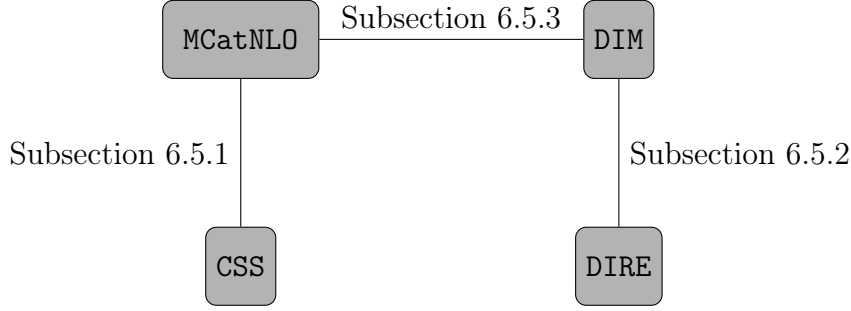


Figure 6.2: The IDS has been implemented in four modules of Sherpa: M_{CAT}NLO, CSS, DIM and DIRE. The connecting lines with their label indicate in which subsection we compare which IDS implementation.

the ratio $d\sigma^A(\phi_{m+1})/d\sigma^B(\phi_m)$ occurring in the MC@NLO formula

$$\begin{aligned} \sigma_{\text{MC@NLO}}^{\text{NLO}} = & \int_m d\sigma^{\bar{B}}(\phi_m) \left[\Delta^A(t_{\text{res}}, t_c) + \int_1 \frac{d\sigma^A(\phi_{m+1})}{d\sigma^B(\phi_m)} \Delta^A(t_{\text{res}}, t) \right] \\ & + \int_{m+1} d\sigma^H(\phi_{m+1}) \end{aligned} \quad (6.60)$$

equals the splitting kernel $\Gamma(\phi_1)$ in the LO + parton shower (PS) formula

$$\sigma_{\text{PS}}^{\text{LO}} = \int_m d\sigma^B(\phi_m) \left[\Delta(t_{\text{res}}, t_c) + \int_1 \Gamma(\phi_1) \Delta(t_{\text{res}}, t) \right]. \quad (6.61)$$

This also implies that the Sudakov factors become identical. To make the rest of the formulae coincide, we have to make two further adjustments:

- Disable the generation of $\mathbb{H}$ -events.
- Replace the weight of the $\mathbb{S}$ -events with the Born cross-section σ^B (rather than using the BVI cross-section $\sigma^{\bar{B}}$). The weight of the terms proportional to $\mathcal{D}^A - \mathcal{D}^S$ (see Equation (5.23)) is effectively set to zero by letting the resummation scale t_{res} tend to infinity.

The center-of-mass energy is set to $\sqrt{s} = 4m_t$ and we require two hard jets with $d_{\text{max}} = (10 \text{ GeV})^2$ according to the Durham jet algorithm. In the following, we compare our implementations and explain their potential differences.²⁹

6.5.1 M_{CAT}NLO versus CSS

We start by contrasting the IDS implementation in the M_{CAT}NLO module with the one in the CSS module. Like in all following comparisons we choose two representative variables. The first one is the invariant mass $m_{W-\bar{b}}$ of the W^- and the jet containing the $\bar{b}$ -quark. We refer to the latter

²⁹We restrict ourselves to show comparisons in which the IDS is run with t_{virt} as evolution variable. The agreement between the different modules has however also been checked for t_{eik} .

as $\bar{b}$ -jet This observable is clearly sensitive to the reconstruction of the resonance. Secondly we

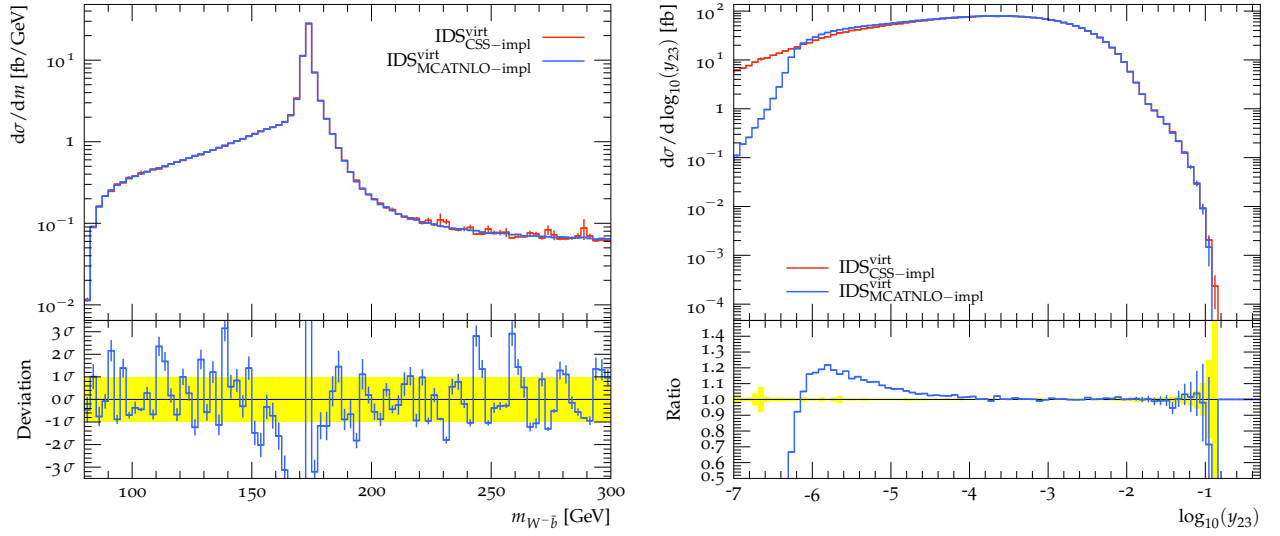


Figure 6.3: Left: invariant mass of the W^- -boson and a $\bar{b}$ -jet as described in the text, right: jet rates defined by the clustering of the Durham jet algorithm. Compared are the resonance-aware emission of the CSS and MCATNLO implementation.

show the distribution of jet rates. That is, we apply a clustering from three to two partons and histogram the smallest of all $\log_{10}(y_{ij})$ where $y_{ij} = d_{ij}/s$ and $d_{ij} = 2 \min(E_i^2, E_j^2)(1 - \cos \theta_{ij})$ is calculated according to the Durham jet algorithm [63]. This quantity is very sensitive to the emission pattern, as the smallest y_{ij} is most likely the distance d_{ij} between emitter and emitted parton.

The right-hand side plot of Figure 6.3 shows an increasing difference between both implementations for emissions with increasingly small y_{23} . The reconstructed anti-top mass does not show such a prominent difference, though a disagreement is apparent. The large deviation in the jet rates is only moderately reflected in the reconstructed anti-top mass since the jets are too broad, i.e. d_{max} is too high, to show a bigger disagreement. The reason for the incompatibility lies in the evaluation of α_s . Since we evaluated α_s at $p_{i\perp}^2$ which does not coincide with the evolution variable t_{virt} , it happens that emissions are generated whose scale of α_s is below a critical value of $\mathcal{O}(\Lambda_{\text{QCD}})$. Those cases are handled differently in both modules. It has been checked explicitly that treating those cases identically no incompatibility remains.

In Section 6.1, we commented on the possibility of having negative splitting functions. Furthermore we alluded in Section 6.4 to the fact that there are phase-space points possible in which the overestimate is smaller than the splitting function. Both cases cannot be handled appropriately in a comparison of CSS and MCATNLO.³⁰ To study the effect of those two “exotic”

³⁰The former effect can actually be taken care of in MCATNLO via a built-in reweighting, which is designed to handle subleading colour effects. We described this reweighting in Subsection 5.2.3 in the first of the two algorithms.

cases, the resonance-aware algorithm has been implemented within the framework of DIRE and DIM. Both modules have the advantage of being capable of dealing with those cases correctly by using so called analytic weights.

6.5.2 DIM versus DIRE

The Dire shower [77] employs slightly different splitting functions and a different evolution variable than the CSS [31]. Nevertheless it is possible to adapt the frameworks of DIM and DIRE to implement the resonance-aware shower algorithm. The implementations of the IDS^{virt} within both modules exhibit impeccable statistical compatibility as can be seen in Figure 6.4.

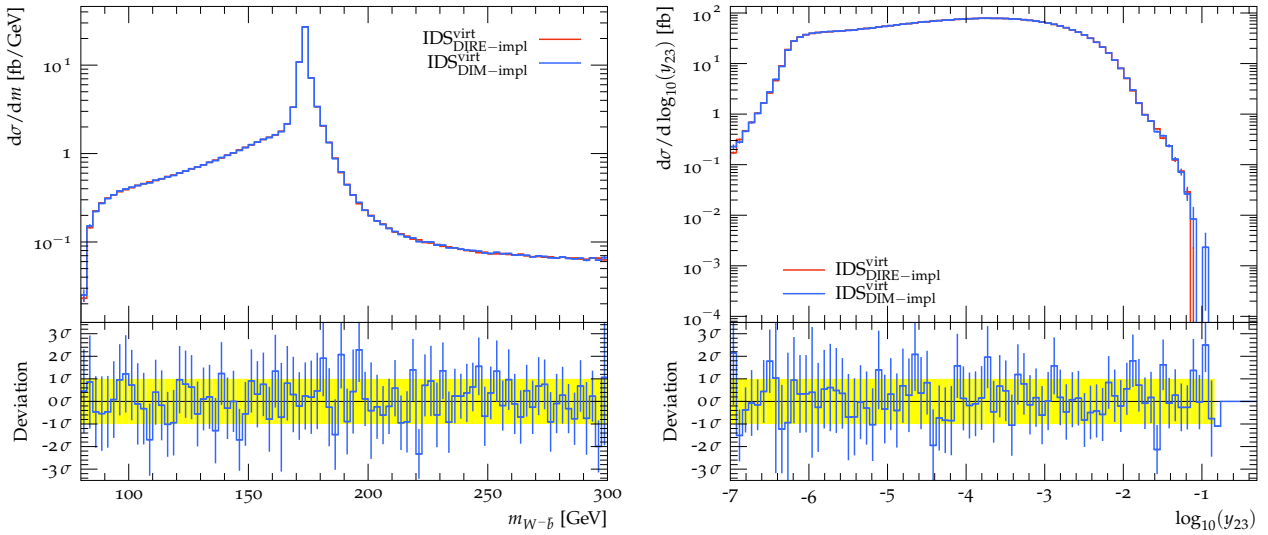


Figure 6.4: Quantities as in Figure 6.3. Compared are the DIRE and DIM implementation of the IDS^{virt} .

6.5.3 MCATNLO versus DIM

To compare those two implementations, we have to modify the code since the former does not take the two “exotic” cases into account while the latter does. For the sake of the cross-check, we simply vetoed all generated points that correspond to a negative splitting function or a splitting function being larger than its overestimate. We stress that this choice is not physically motivated.

Again both implementations show perfect statistical agreement, as can be seen in Figure 6.5. We point out that we adjusted the cutoff on the scale of α_s in both modules to be the same.³¹ Without that, both implementations exhibit a slight difference in the jet rates, but not in the reconstructed anti-top mass. This deviation has thus the same reason as the one in the

³¹Below that common cutoff of $(1\text{ GeV})^2$, α_s evaluates to zero. Thus, these points are rejected.

comparison of the MCATNLO and CSS implementation. The reason for our setting the cutoff of

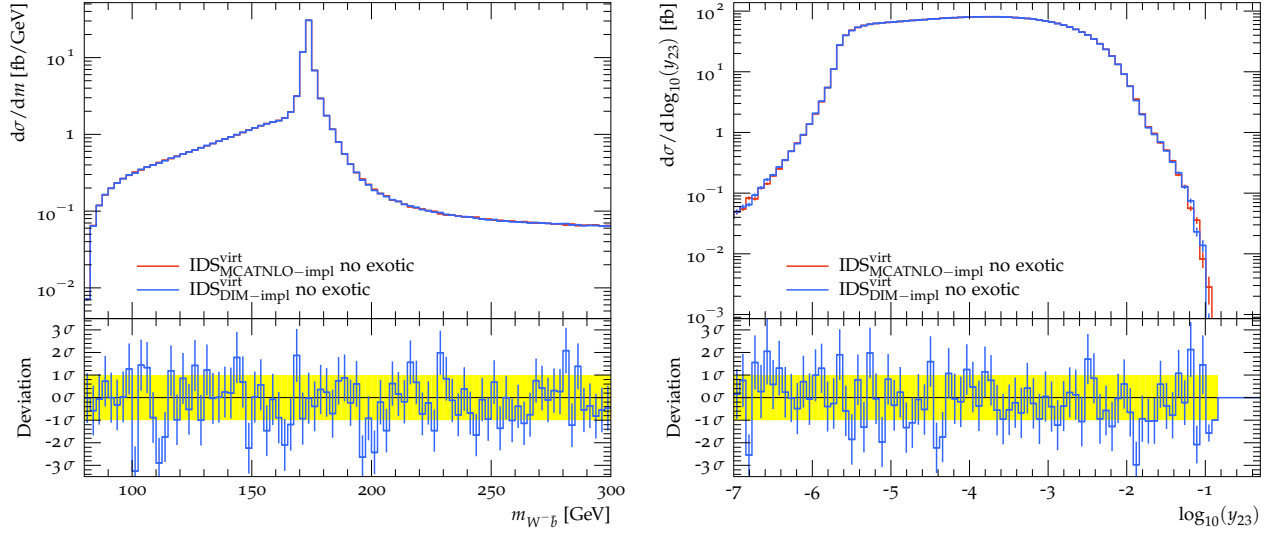


Figure 6.5: Quantities as in Figure 6.3. Compared are the resonance-aware emission of the MCATNLO and DIM implementation.

both implementations to the identical value is that we like to study the effect of the two “exotic” cases in the following. The MCATNLO and DIM implementation thus have to agree absolutely in order to attribute all arising differences to the two “exotic” cases.

Influence of Negative Splitting Functions and Imperfect Overestimate

As mentioned at the end of Subsection 6.5.1, there are two “exotic” cases, in the sense that they do not occur in the CSS: negative splitting functions and the possibility of generating points for which the splitting function is larger than its overestimate. To study their effect upon our chosen distributions, we first show the result obtained by the normal MCATNLO implementation, i.e. vetoing negative splitting functions and having the possibility of an acceptance ratio $f/g > 1$, which is not accounted for by an analytic weight. We refer to this result as “ $\text{IDS}_{\text{MCATNLO-impl}}^{\text{virt}}$ ” in Figure 6.6, as it is obtained by running MCATNLO without modifications. We contrast this with an MCATNLO run in which we changed the acceptance ratio in the *standard* veto algorithm from f/g to $|f|/g$. Thus negative splitting functions can be accepted. On top of that, we exploit the reweighting that is explained in the first algorithm in Subsection 5.2.3. There, we substitute again the splitting function with its absolute value, i.e. h with $|h|$. This takes points with negative splitting function correctly into account. We refer to that result as “ $\text{IDS}_{\text{MCATNLO-impl}}^{\text{virt}}$ with neg. f ”. Finally we compare this to the normal run of the DIM module, in which both “exotic” cases are properly accounted for by the second analytic weight algorithm in Subsection 5.2.3.

It can be seen in Figure 6.6 that the inclusion of negative splitting functions influences both

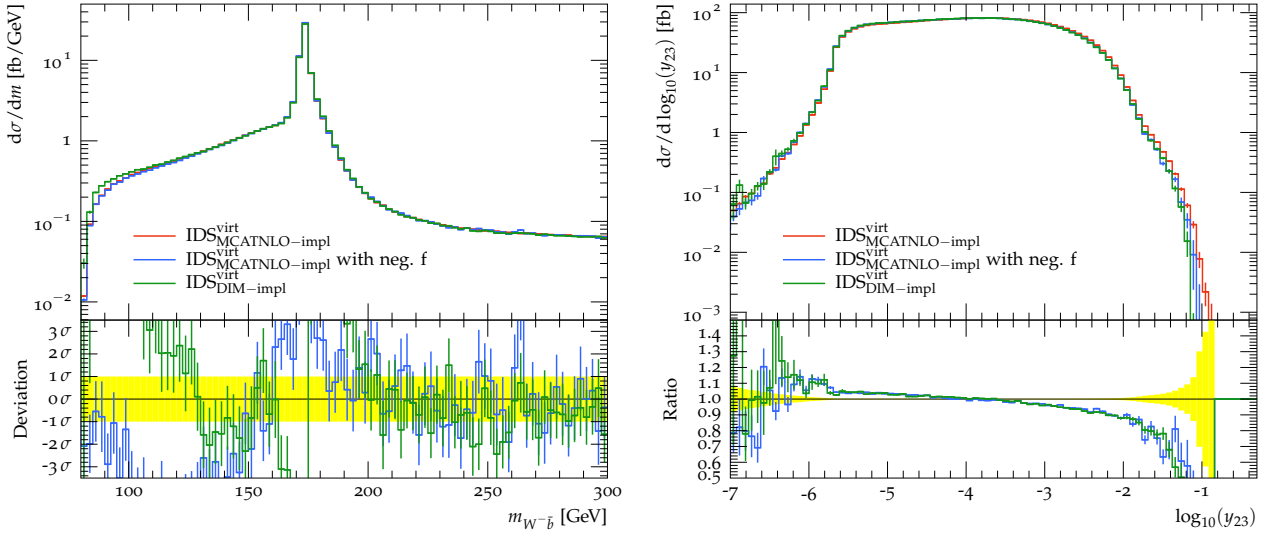


Figure 6.6: Quantities as in Figure 6.3. Compared are different treatments of the resonance-aware emission to assess the influence of the so called “exotic cases” as described in the text.

distributions. On the other hand, the $m_{W-\bar{b}}$ distribution is much more influenced by the proper treatment of the overestimate than the jet rates.

In the following, we will always refer to the DIRE (DIM) implementation of the resonance-aware shower (matching) as only this accounts for both “exotic cases”. When we refer to the CSS or a CSS matching, the CSS or MCATNLO module have been used.

6.6 Comparison of Resonance-Aware and Non-Resonance-Aware Shower

After having cross-checked our implementations of the IDS versions, we now proceed to the physically more interesting comparison between CSS and IDS versions. We do this in two steps. First, we compare the showers at LO in order to study the effect of a single parton shower emission detached from any NLO effect. In the second step, we compare CSS and IDS versions at NLO by contrasting matched calculations. It is this second step in which we find problems in the IDS versions. In order to understand their origin we extend the comparison of showers at LO beyond that what we would otherwise study.

In contrast to the above section, we now run the shower at the physically more meaningful resummation scale of the center-of-mass energy, i.e. $\sqrt{t_{\text{res}}} = \sqrt{s} = 4m_t$. This has no visible effect on the $m_{W-\bar{b}}$ distribution and only a very small one at high y_{23} in the jet rates. All other parameters are chosen like in Section 6.5.

6.6.1 LO + Parton Shower

We compare in each of the following plots the pure LO prediction without shower to a one-step IDS/CSS shower. We run the IDS with both evolution variables and refer to those two versions as IDS^{eik} and IDS^{virt} . On top of that, we perform another run with modified recoil scheme. For that we changed our prescription of “identified” particles from Subsection 4.3.1 such that, apart from the emitter, both W bosons are identified. This directs the recoil to the colour spectator as in the CSS, see Figure 4.1. Thus the particles involved in the mapping are the same as for the CSS. However, the actual mapping still differs. We refer to this version of the IDS as $\text{IDS}_{\text{CSS-rec}}^{\text{virt}}$.

We include three different versions of the IDS in our comparison in order to assess which effects are due to the recoil scheme, evolution variable and splitting function. However, as the recoil schemes of CSS and $\text{IDS}_{\text{CSS-rec}}^{\text{virt}}$ are not identical and since a change of splitting function also means changing the evolution variable, we are aware of the fact that we cannot always pin down an effect to be entirely due to – say the splitting function. Still, the three different versions of the IDS allow us to explain some characteristics.

Effect upon m_{Wb} from Emissions Solely off $b/\bar{b}$ Quark

In order to better understand the shape of distributions generated by the showers, we start with comparing the various showers in Figure 6.7 in a simplified and unphysical setup. This is, we manipulated the code such that the emitted gluon can originate exclusively from either b (upper row of Figure 6.7) or $\bar{b}$ quark (lower row of Figure 6.7). To further track down the effects of the different showers, we considered not only the invariant mass of W^- and $\bar{b}$ jet (left column of Figure 6.7), but also the invariant mass of W^- and $\bar{b}$ quark (right column of Figure 6.7).³² We refer to the latter – which is not IR-safe – as *partonic* $m_{W-\bar{b}}$.

Studying the upper left plot in Figure 6.7, we see that the distributions of LO and IDS versions (with standard recoil scheme) with only emissions off the b quark agree perfectly. This is expected since in the IDS, the invariant mass of one decay system (W^- and $\bar{b}$) is not affected by an emission off the other, i.e. the b quark. This stands in contrast to the CSS and the $\text{IDS}_{\text{CSS-rec}}^{\text{virt}}$, where due to the recoil between emitter and colour spectator the invariant mass of the “spectator decay system” is affected. More specifically, it can be seen for the CSS that the peak is slightly shifted to the left.³³ The reason for that lies in Equation (3.18) and the fact that $0 < y_{ij,k} < 1$. Thus the recoil absorbing colour spectator always *loses* momentum, which translates into a lower invariant mass after the emission. For the $\text{IDS}_{\text{CSS-rec}}^{\text{virt}}$ the situation is different, since not the spectator but the emitter momentum is rescaled. The momentum of

³²We could just as well pick m_{W+b} instead of $m_{W-\bar{b}}$. In that case the plots would be identical if one also swapped the predictions with emissions solely off the b quark with those of the $\bar{b}$.

³³By that we mean that the CSS result lies below the LO one right from the peak, whereas it is vice versa on the left-hand side.

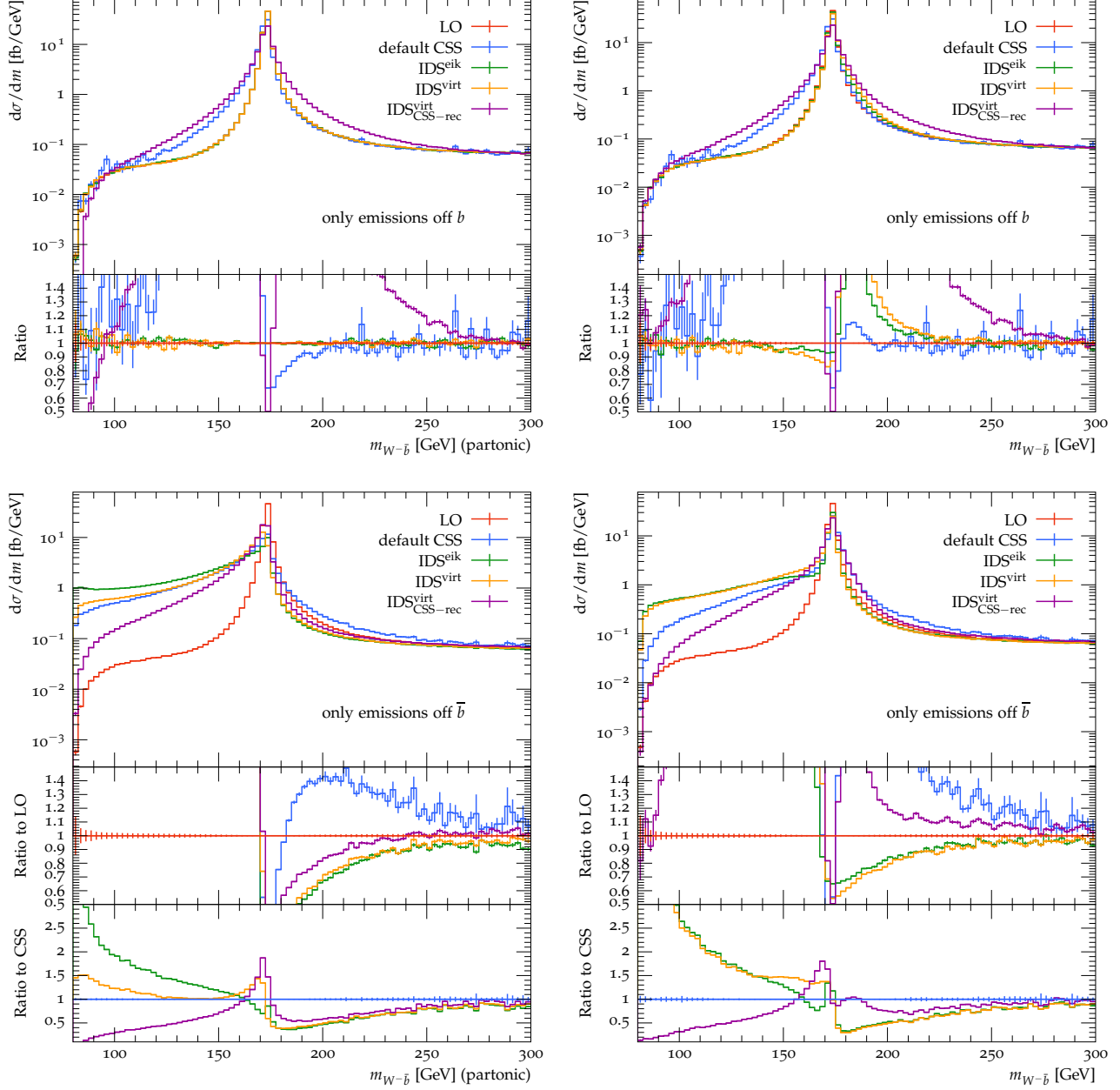


Figure 6.7: Left: invariant mass of W^- boson and $\bar{b}$ quark, right: invariant mass of W^- boson and $\bar{b}$ jet, above: results obtained by allowing solely the b quark to emit a gluon, below: results obtained by allowing solely the $\bar{b}$ quark to emit a gluon.

In each plot, we compare the distribution of the pure LO prediction with multiple one-step parton showers: the CSS, the IDS with t_{eik} as evolution variable, the IDS with t_{virt} as evolution variable and the last one with a CSS-like recoil scheme as described in the text.

the spectator is Lorentz transformed according to Equation (4.5). It is thus not obvious how the invariant mass of spectator and associated W -boson changes through the mapping. The $\text{IDS}_{\text{CSS-rec}}^{\text{virt}}$ prediction in the top left plot of Figure 6.7 suggests that it can both decrease and increase. We remark that the two left-most bins of $\text{IDS}_{\text{CSS-rec}}$ have a negative entry. It has been checked that this is due to the splitting function becoming negative, which can cause the analytic weights to be negative. We do not study this problem further.

If only the $\bar{b}$ quark can emit a gluon, the partonic $m_{W-\bar{b}}$ distributions (lower left plot of Figure 6.7) of all showers become heavily washed out to the left, since the emission of a gluon generally decreases the invariant mass of $\bar{b}$ quark and W^- . There is however a difference of how much that is the case for the different showers. The effect is less pronounced for the $\text{IDS}_{\text{CSS-rec}}^{\text{virt}}$ prediction and slightly more prominent for the IDS^{eik} and IDS^{virt} result than for the CSS one. We do not have a satisfactory explanation for this order, since it might well be a combination of multiple effects without knowing which is the dominant one. The recoil scheme might have a significant influence on it, but this conjecture is purely motivated by the lower two distributions having a non-resonance-aware recoil scheme, whereas the upper two have a resonance-aware one.

On the right hand side of the peak, it can be seen that the LO result dominates over all shower predictions with the exception of the CSS. The reason for that lies indisputably in the different recoil scheme: For all IDS versions, the $W-\bar{b}$ system always loses energy by an emission off the $\bar{b}$ quark. For the CSS the situation is different. Looking at Equation (3.19) it is not clear if $m_{W-\bar{b}}$ decreases with a (soft) emission. In other words, the spectator may donate more momentum to the emitter than the emitted gluon carries away.

We now consider the effect of replacing the $\bar{b}$ quark with a $\bar{b}$ jet in the calculation of $m_{W-\bar{b}}$. In the upper right plot of Figure 6.7, the effect of the QCD emission on the IDS versions, in which only the b quark can emit a gluon, can now clearly be seen: The LO prediction and the IDS versions do not coincide as they did for the *partonic* invariant mass. This can only be caused by events in which the emitted gluon becomes “accidentally” part of the $\bar{b}$ jet. This interpretation was checked by varying the size of the jets: The deviation to the LO result increases/decreases for larger/smaller values of d_{max} . Of course the same effect is seen for the CSS and $\text{IDS}_{\text{CSS-rec}}^{\text{virt}}$, whereas it is almost completely counteracted for the former. We can thus conclude that clustering the $\bar{b}$ to a jet washes the peak of the $m_{W-\bar{b}}$ distributions out towards higher masses, if the b emits a gluon. This effect is expected and almost independent of the recoil scheme.

The same characteristic can be seen in the lower right plot of Figure 6.7 where all distributions from a shower become washed out towards higher masses (with respect to the lower left plot). Note however that the prediction of the $\text{IDS}_{\text{CSS-rec}}^{\text{virt}}$ lies now even above the LO one right from the peak. This happens since there are events in which the emitted gluon is within the same jet as the emitting $\bar{b}$ quark and the donated momentum of the (kinematic) spectator

increases $m_{W-\bar{b}}$. This cannot happen for the IDS^{eik} and IDS^{virt} because for that recoil scheme the kinematic spectator is the W^- instead of the b . We thus conclude that also for emissions off the $\bar{b}$, the clustering to jets has the effect of blurring the peak of the $m_{W-\bar{b}}$ distributions to the right. Its strength however depends on the recoil scheme.

“Full” Comparison of CSS and IDS at LO

After discussing the effect of separate emissions off b and $\bar{b}$ quark on the (partonic) $m_{W-\bar{b}}$ distribution, we now compare the results of the various IDS versions with the CSS when the emission can originate from both partons. On top of that we contrast the jet rates, which were introduced in Section 6.5, and the gluon energy distribution of the various showers.

It can be clearly seen in Figure 6.8 that the peak of (the partonic) $m_{W-\bar{b}}$ distribution at $m_t = 173.21 \text{ GeV}$ is blurred when one of the showers is run. The actual shape depends however strongly on the shower. In the distribution of the partonic invariant mass (top left of Figure 6.8), it can be seen that the two results of the IDS (with standard mapping) drop more sharply above the peak than the CSS and $\text{IDS}_{\text{CSS-rec}}$ ones. This characteristic is entirely due to the recoil scheme as explained above. When considering this region in the (jet) invariant mass (top right of Figure 6.8), we see an increase of all shower results with respect to the partonic $m_{W-\bar{b}}$ distribution. This effect is, to some extent, recoil scheme independent and can be explained by a general shift towards higher masses due to the potential inclusion of the gluon’s momentum within the invariant mass.

Below the top mass, all shower predictions have a broader peak than the LO one. This is expected as the system of W^- and $\bar{b}$ loses energy for an emission off the latter. This observation is of course true for both, the partonic and jet $m_{W-\bar{b}}$ distribution. We stress however some interesting aspects about that:

1. The degree by which the partonic $m_{W-\bar{b}}$ distribution of the showers are increased with respect to the LO result (left from the peak) depend strongly upon the shower. As mentioned in the above subsection, it is difficult to pin down this characteristic to a certain feature of the shower. It might however be related to the recoil scheme.
2. Between $\approx 140 \text{ GeV}$ ($\approx 150 \text{ GeV}$) and the peak, the CSS result dominates over the IDS^{eik} (IDS^{virt}) one, because of recoil effects upon the $\bar{b}$ when the b quark radiates (cf. top left plot in Figure 6.7).
3. When clustering the $\bar{b}$ quark to a $\bar{b}$ jet in the $m_{W-\bar{b}}$ calculation, not every distribution changes by the same amount. The IDS^{eik} and the CSS drop the most (at the left-hand side of the peak) in that clustering process. After a first glance at the jet rates (lower left plot of Figure 6.8) this seems surprising, since for those distributions there is “less

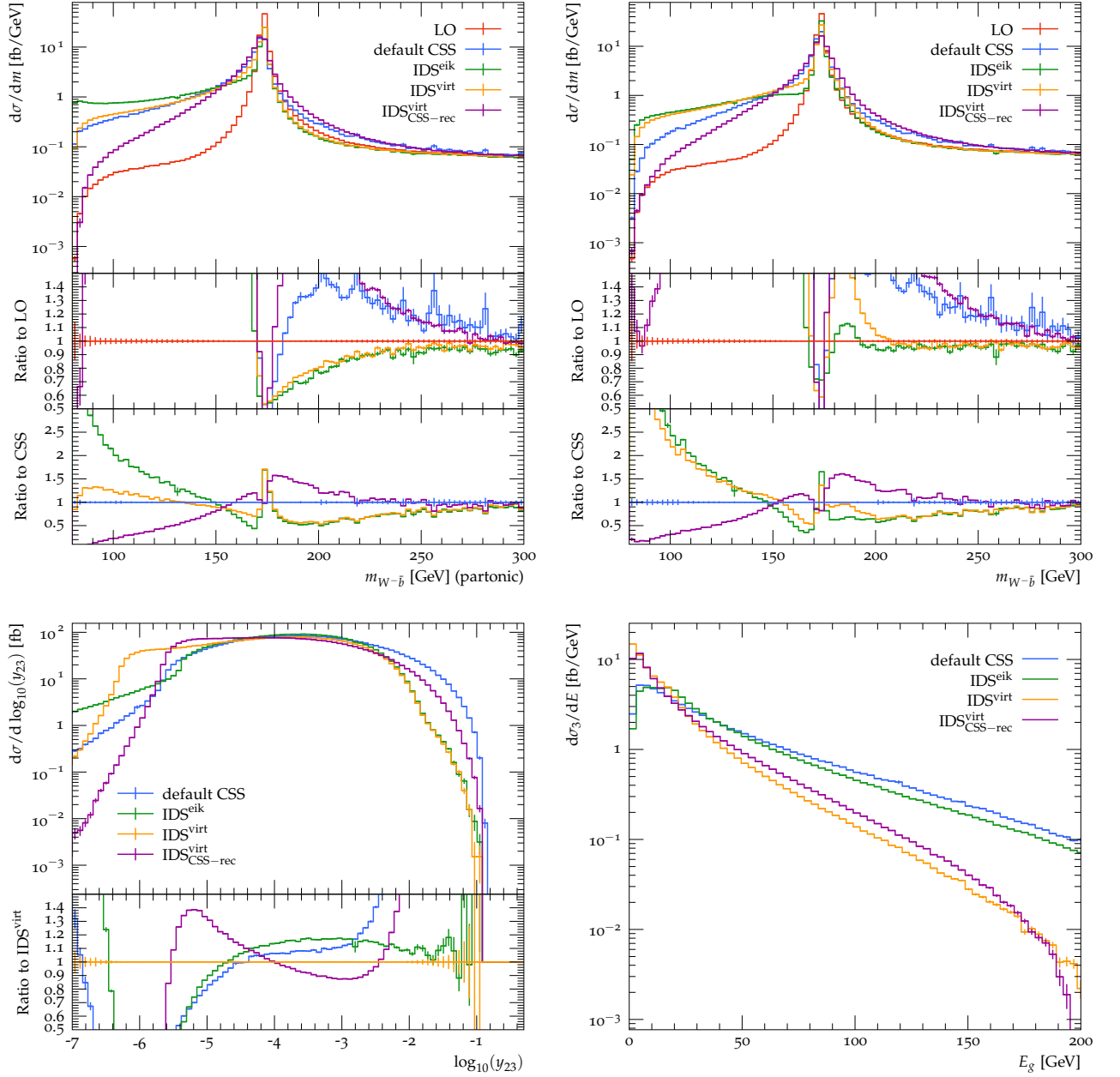


Figure 6.8: Top left: invariant mass of W^- and $\bar{b}$ quark, top right invariant mass of W^- and a $\bar{b}$ jet, bottom left: jet rates as explained in Section 6.5, bottom right: gluon energy . The compared showers are the same as in Figure 6.7.

cross-section” clustered into jets than for the IDS^{virt} and $\text{IDS}_{\text{CSS-rec}}^{\text{virt}}$.³⁴ Those events are however predominantly associated with soft emissions, which is underlined by the gluon energy distribution (lower right plot of Figure 6.8). There, it can be seen that both the IDS^{virt} and $\text{IDS}_{\text{CSS-rec}}^{\text{virt}}$ are characterised by more soft emissions than the CSS and IDS^{eik} . Events with a soft emission do not cause such a big change in the $m_{W-\bar{b}}$ distribution when clustering the partonic to the jet invariant mass, than harder emissions. We thus conclude that the low y_{23} events of the IDS^{virt} and $\text{IDS}_{\text{CSS-rec}}^{\text{virt}}$ are mainly events with soft emissions whereas the low y_{23} events of the CSS and IDS^{eik} are less dominated by those, but more by events with collinear (semi-soft) emissions.

The jet rates reveal that the IDS^{eik} and IDS^{virt} feature significantly less events in which the three partons are well separated than the other two showers. We do not see a compelling reason why this should be the case. We however suspect the recoil scheme to be of relevance, since both IDS^{eik} and IDS^{virt} lie virtually on top of each other for $10^{-2} < y_{23} < 10^{-1}$, whereas the other two showers lie distinctly above those two. In the gluon energy distribution we can see that this quantity seems to depend on the evolution variable, since t_{eik} is constructed to be as close to $\mathbf{k}_{\perp}^2$ – the evolution variable of the CSS – as possible.

As indicated at the beginning of Section 6.6, we now make some further comparisons/checks of the showers. The purpose of these is to convince ourselves that the showers behave as expected when we perform various changes. This is motivated by problems of the IDS prediction at NLO in the next subsection.

Comparison 1: Disabling the Resummation

First, we check whether the resummation encoded by the Sudakov factor hides anything unexpected.

To do this, we found a way to disable the resummation due to the Sudakov factors. We did this by setting the term $f(t_i)$ in the numerator of Equation (5.30) to zero. This effectively sets all Sudakov factors Δ to unity (see Subsection 5.2.3 for the relevant formulae). As a drawback the squared bracket in Equation (5.20), describing the emission of the extra parton, does no longer integrate to unity. In order to compare the various showers we thus have to rescale all predictions appropriately. Since the implementation of the CSS does not include analytic weights, we have to contrast the IDS to the Dire-shower rather than the CSS in order to compare to a non-resonance-aware shower.

But as we see in Figure 6.9 there are only very minor differences between the two. Actually the only significant difference can be seen in the jet rates, where the Dire-shower has more contributions at high y_{23} .

³⁴The maximal distance $d_{\text{max}} = (10\text{GeV})^2$ with which two partons are clustered to a jet translates into $\log_{10}(y_{23}^{\text{max}}) = -3.68$.

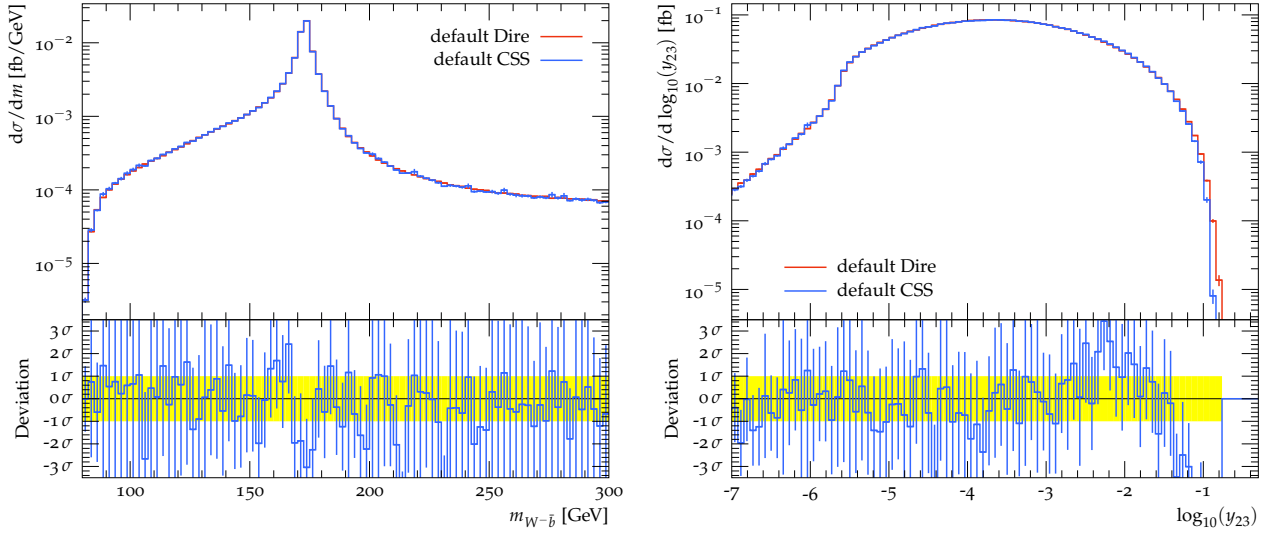


Figure 6.9: Quantities as in Figure 6.3. We compare the prediction of the CSS and the Dire-shower.

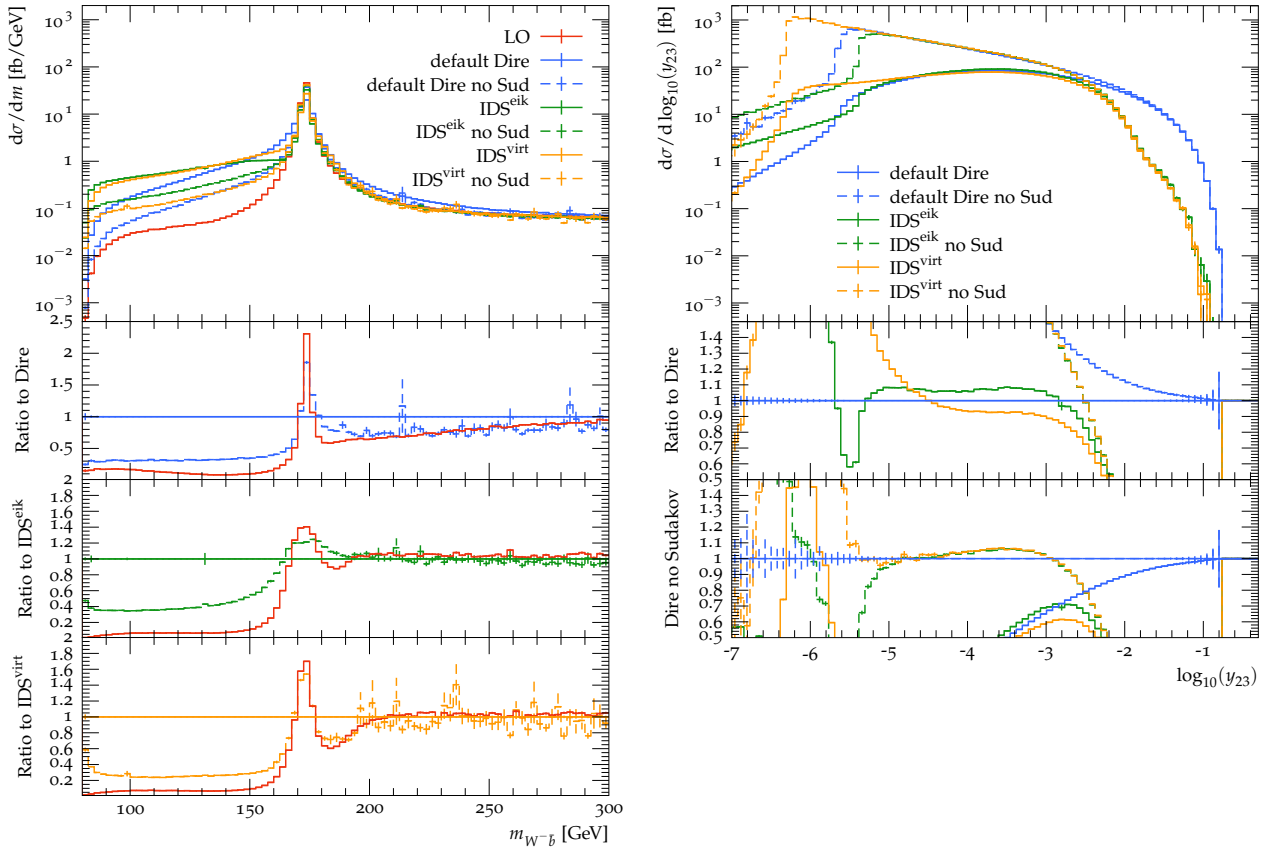


Figure 6.10: Quantities as in Figure 6.3. We compare the predictions of the Dire-shower, IDS^{eik} and IDS^{virt} . Each shower is run in its “standard” mode and a mode in which the Sudakov factors are effectively set to unity (see text).

We are now prepared to compare the “standard” Dire-shower, IDS^{eik} and IDS^{virt} with their modification in which we effectively set the Sudakov factors to unity. This can be seen in Figure 6.10. First we note that the Sudakov suppression for increasingly small y_{23} is absent for the “no Sud” prediction. Thus the result of all three showers increases for smaller values of y_{23} . The IR divergence is screened by the shower cutoff t_c , which makes the three distributions drop sharply in the range of $-6.4 < \log_{10} y_{23} < -5.2$. We note further that the predictions of those showers seem to converge before they drop. This can be regarded as yet another check of the implementation of the showers, in particular of their behaviour in the soft and/or collinear regime. Next, we see that the Dire prediction with disabled Sudakov factors agrees with the LO one above $\approx 220 \text{ GeV}$ in the invariant mass. This feature seems surprising at a first glance, but it is merely the consequence of the following effect: The disabling of Sudakov factors damps the effect of every shower in the invariant mass distribution. In other words, the shower predictions without Sudakov factors lie almost everywhere between the LO and the “standard” shower prediction. This feature can be understood by thinking of the Sudakov factor as the term incorporating the resummation (of multiple emissions). Disabling it brings the prediction closer to the LO one in which no emission effects at all are contained. This agrees with our expectation.

Comparison 2: Variation of the Shower Cutoff and Influence of Other Cuts

Second, we study the influence of various cuts in the generation of parton shower emissions upon the invariant mass distribution and the jet rates.

Since the different showers have different evolution variables, the shower cutoff t_c does not restrict emissions in the same way. This means that an emission in one shower can correspond to a value of t above t_c whereas the same emission (i.e. identical kinematics) corresponds to a value of t below t_c in another shower. A consequence of this can be seen in the right-hand plot of Figure 6.10 where the showers (without Sudakov factor) drop at different values of y_{23} , though their t_c is the same. It is thus interesting to see, how a variation of the default value $t_c = 1 \text{ GeV}^2$ influences the simulation output.

In Figure 6.11 we see that the lowering (dashed lines) and raising (dotted lines) of t_c have qualitatively the same effect for all three showers in the jet rates. This is, the higher the cutoff the higher the value of y_{23} at which the prediction falls. More concretely we can say that the variation of t_c is very similar for the Dire shower and the IDS^{eik} . This can be seen in the ratio plots of the jet rates. Also the invariant mass distribution of both showers exhibit a slightly flatter peak for $t_c = 10 \text{ GeV}^2$. This similarity is explained by the fact that both showers have the identical evolution variable. For the IDS^{virt} the situation is different. The jet rates show only a minor influence on the value of t_c and the $m_{W-\bar{b}}$ distribution does not show any visible alteration. This shows that y_{23} has a stronger correlation to the evolution variable of the Dire shower and the IDS^{eik} than to the one of the IDS^{virt} . We also point out that lowering t_c

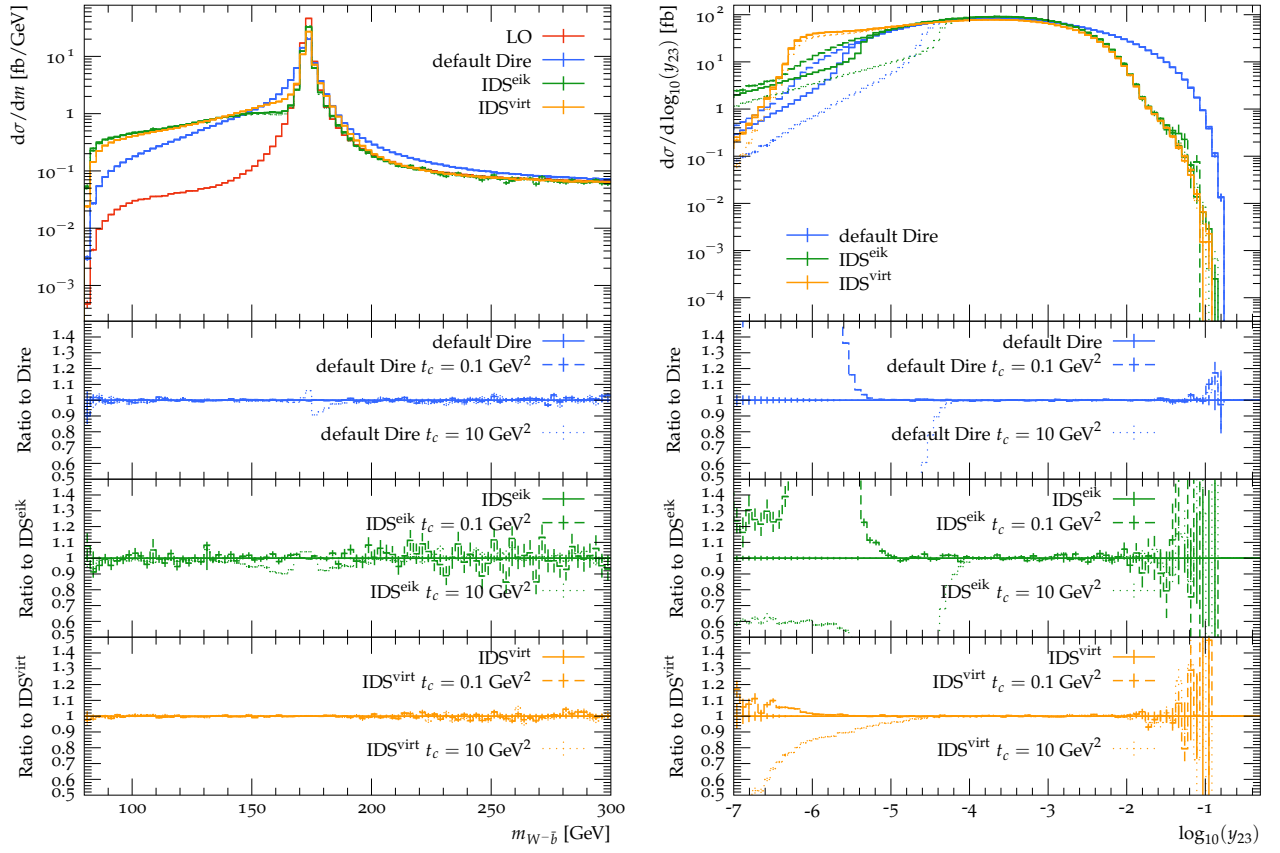


Figure 6.11: Quantities as in Figure 6.3. We compare the influence of the variation of the shower cutoff t_c for the three showers Dire, IDS^{eik} and IDS^{virt} .

below 1 GeV^2 does not effect any prediction for the invariant mass because emissions below $t = 1 \text{ GeV}^2$ are clustered anyway to the jet of the emitter parton and thus do not change the jet invariant mass.

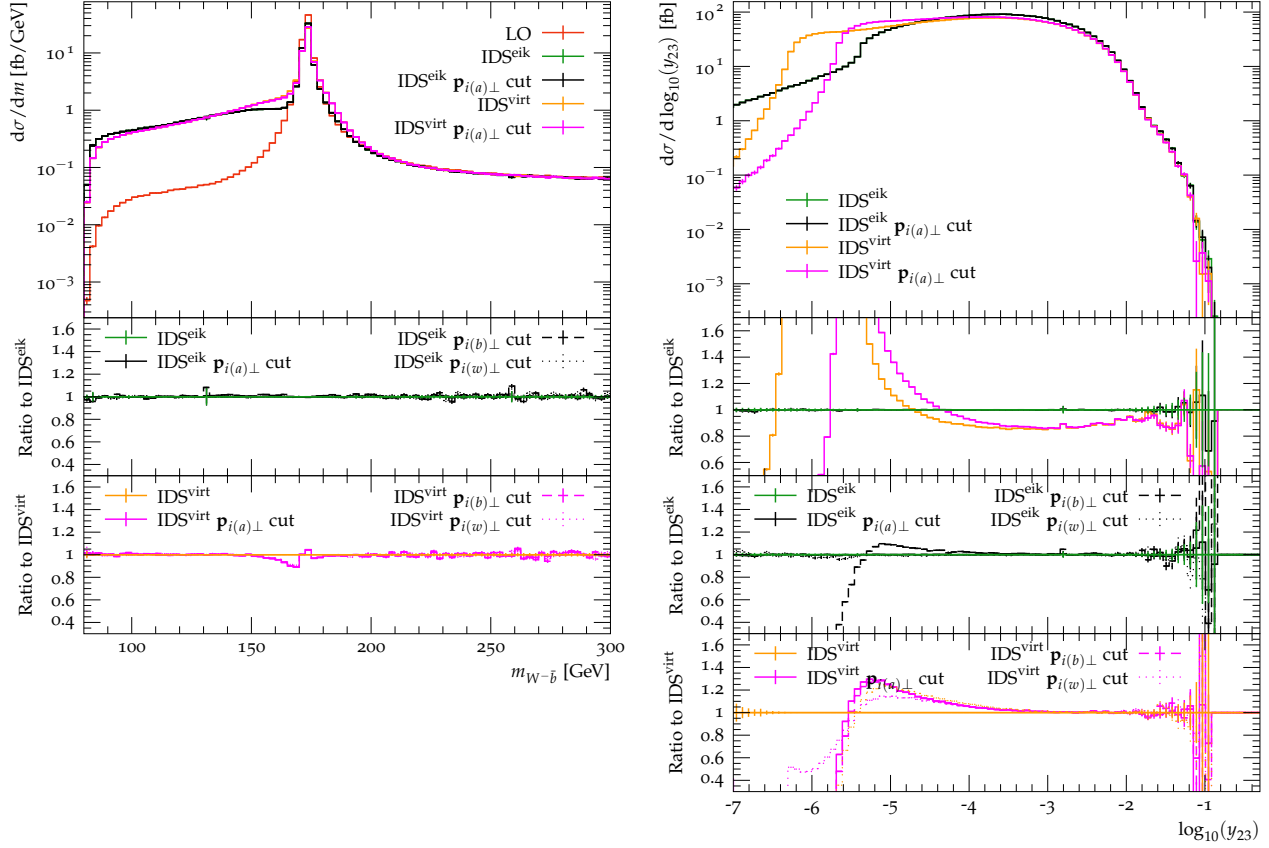


Figure 6.12: Quantities as in Figure 6.3. We compare the influence of cutoffs upon the transverse momentum of p_i with respect to p_a , p_b and p_w for the IDS^{eik} and IDS^{virt} .

After the variations of the shower cutoff, we also study the influence of another cut, namely the transverse momentum of p_i with respect to p_a ($\mathbf{p}_{i(a)\perp}$), p_b ($\mathbf{p}_{i(b)\perp}$) and p_w ($\mathbf{p}_{i(w)\perp}$) in the rest frame of the partons a , b and i . We do this because we want to minimise the possibility of having a phase-space region which causes unexpected problems. Figure 6.12 shows our findings. Those are different for the IDS^{eik} and IDS^{virt} .

The IDS^{eik} predictions with one or all three of the cuts show no difference to the uncutted IDS^{eik} in the invariant mass distribution. There is an earlier drop of the prediction with $\mathbf{p}_{i(b)\perp}$ cut in the jet rates. But since this affects only the subjet structure, it is not reflected in the invariant mass distribution.

Applying one of the three above mentioned cuts or all three of them together for the IDS^{virt} has virtually the same effect on the invariant mass, namely making the peak slightly sharper – especially on the left hand side of it. Also the influence upon the jet rates is very similar as all IDS^{virt} predictions with a cut fall at higher y_{23} . We thus conclude that the difference

between cutted and uncutted IDS^{virt} prediction is caused by the exclusion/inclusion of soft gluons, since those are effected by each cut.

We summarise that there are no surprising effects of the cuts considered.

Summary

To summarise our finding of comparing the various showers at LO, we can state that the IDS versions generally agree with our expectations in the reconstructed (anti-) top mass distribution: Most importantly they predict a sharper peak than the CSS, which is understood to be a consequence of the recoil scheme. Furthermore, both IDS versions lie below the CSS result above the peak for the same reason. In the low invariant mass region both IDS versions dominate over the CSS prediction. The shape of the IDS^{eik} is similar to the IDS^{virt} , but it has a peculiar looking dip closely below the peak of the (jet) invariant mass. The $\text{IDS}_{\text{CSS-rec}}^{\text{virt}}$ has been implemented solely for comparison reasons. It generally behaves as expected but features an incomprehensible low prediction for small invariant masses. The partonic invariant mass even drops to a negative value in the left-most bin of the upper right plot of Figure 6.8, which does not make sense from a physical point of view. In the jet rates, the IDS^{eik} and IDS^{virt} show significantly less events in which the partons are well separated than the CSS (or $\text{IDS}_{\text{CSS-rec}}^{\text{virt}}$). Our findings agree with our expectation that the recoil has an important influence on differential distributions of processes containing intermediate resonances.

6.6.2 NLO + Parton Shower

Now, we proceed to compare the IDS and CSS in an NLO-matched setup. We also add the LO and fixed NLO prediction to this comparison in order to have a reference to that. To compare the distributions of the LO and NLO calculations we have to take the overall normalisation to the total cross-section into account. We do this by rescaling the LO distributions by $\sigma_{\text{NLO}}/\sigma_{\text{LO}}$, where $\sigma_{\text{NLO}} = 220.5(3) \text{ fb}$ and $\sigma_{\text{LO}} = 237.32(8) \text{ fb}$.

We compare the calculations in the already above considered invariant mass and jet rates distribution. In doing so, we consider only the invariant mass calculated with a jet rather than a quark, because the latter is not IR safe. Figure 6.13 contains several interesting things to note. After having listed them, we turn to their explanations.

1. The first point that leaps to the eye, is that the dip of the IDS^{eik} -matched prediction in the invariant mass distribution is more pronounced as for its LO analogue in the upper right of Figure 6.8.
2. The next difference is that the CSS-matched prediction falls more sharply above the peak than the two IDS-matched ones. Furthermore, all NLO-matched predictions agree above $\approx 200 \text{ GeV}$. Both observations stand in contrast to the corresponding LO plot in Figure 6.8.

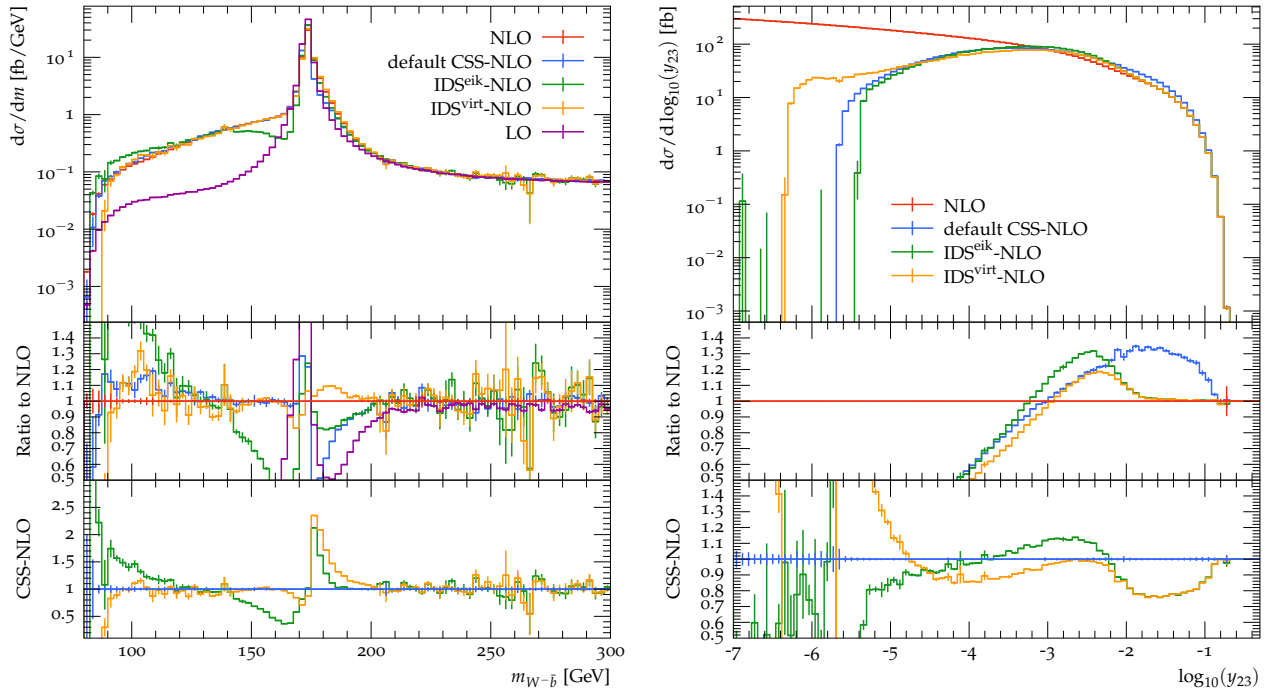


Figure 6.13: Quantities as in Figure 6.3. Compared are the resonance-aware matchings of IDS^{eik} and IDS^{virt} and the standard non-resonance-aware matching of the CSS to the NLO calculation. Those results are contrasted to the fixed NLO and LO prediction.

3. Continuing this comparison towards smaller masses, we see that the CSS-matched result dominates only over the IDS^{eik} -matched one and hardly over the IDS^{virt} -matched one between ≈ 150 GeV and the peak. In the LO analogue the CSS dominates over both IDS versions.
4. At LO, the IDS versions dominate increasingly over the CSS below ≈ 150 GeV. In the matched setups on the other hand, all predictions are comparable in size before the IDS^{eik} -matched prediction becomes dominant over the others at very small masses. The most important aspect is however that the IDS^{virt} -matched result becomes negative in the left-most bins. This is clearly unphysical and shows that this prediction cannot describe data.
5. In the jet rates, the most salient point is that the CSS-matched calculation exhibits significantly more contributions to events with three well separated partons.
6. Apart from shape differences, it is visible that the IDS-matching exhibits larger fluctuations in the m_{W-b} distribution than the CSS-matching. This is so although all matching-calculations have the same number of events, namely $1.2 \cdot 10^{10}$.

Since those two distributions are composed of $\mathbb{S}$ - and $\mathbb{H}$ -events, it makes sense to consider those contributions separately. This will help us to understand some of the above mentioned

points.

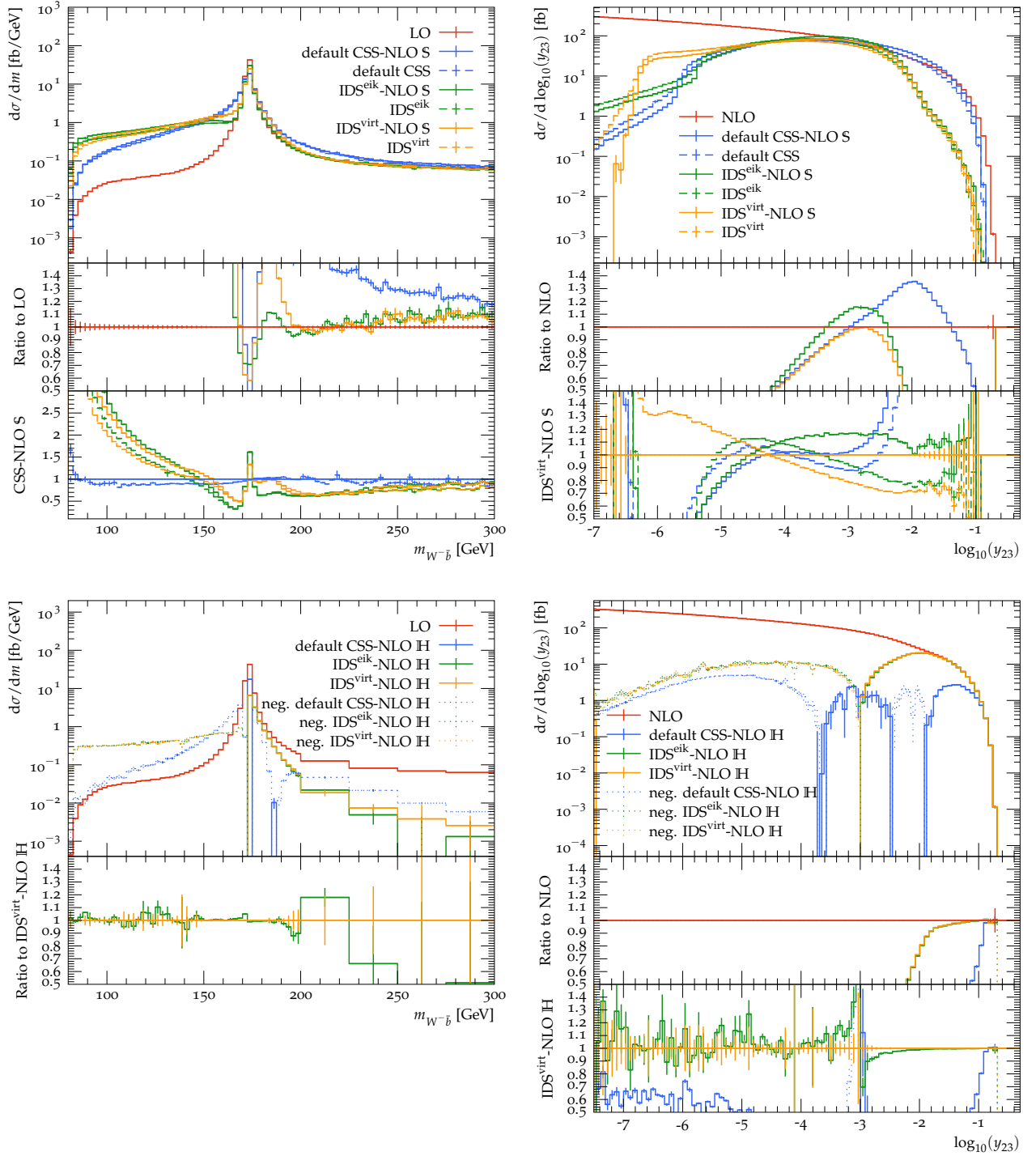


Figure 6.14: Quantities as in Figure 6.3. Compared are the contribution of $\mathbb{S}$ - (above) and $\mathbb{H}$ -events (below) between the NLO-matched results for CSS, IDS^{eik} and IDS^{virt} . Negative parts of the distributions are shown by dotted lines.

We first study the distribution of $\mathbb{S}$ -events, which is displayed in the upper plots of Fig-

ure 6.14.³⁵ Comparing the results in the lower ratio plot of the invariant mass distribution with their LO analogue in Figure 6.8, shows similar shapes. Yet there are visible differences that have the same tendency for all showers but differ in their extent: The contributions of $\mathbb{S}$ -events lie above the LO results for invariant masses above ≈ 230 GeV and more significantly below ≈ 160 GeV. In the jet rates, the difference between NLO and LO prediction is more pronounced: For all showers, the former prediction lies above the latter above $\log_{10} y_{23} \approx -4$. For values below that the situation is reversed. The cause of those differences is solely given by the substitution of the Born cross-section with the full BVI cross-section plus the terms proportional to $\mathcal{D}^A - \mathcal{D}^S$, see Equation (5.23). This substitution is different for the CSS and the IDS versions, since the former uses standard CS dipoles whereas the latter use pseudo-dipoles. But also for the two IDS versions the substitution is not identical since the term proportional to $\mathcal{D}^A - \mathcal{D}^S$ is slightly different. The reason for that is the following: For a given phase-space point the associated value of the evolution variable is – in general – different for both IDS versions. Consequently, $\mathcal{D}^A$ might equal $\mathcal{D}^S$ in one version and zero in the other.

Now we come to the studying of the $\mathbb{H}$ -events. In the lower plots of Figure 6.14 the contributions of the $\mathbb{H}$ -events of the three matched calculations are compared. Since a significant part of their contribution is negative, we plot also those parts (multiplied by a factor -1) and mark them as dotted lines. The first point we notice is that there are only negligible differences between the two IDS-matched results. This means that the above mentioned difference due to the $\mathcal{D}^A$ terms is very small. Next, we note that the contribution of $\mathbb{H}$ -events of the IDS-matched results in the invariant mass fluctuate strongly above ≈ 200 GeV and take on higher negative values than the CSS-matched $\mathbb{H}$ -events below ≈ 150 GeV. This is the reason for the huge fluctuations in the invariant mass of the IDS-matched results in Figure 6.13, see point six from above. We will dwell on that point further below. Another point of interest is that the $\mathbb{H}$ -events of the IDS-matched results get much more contributions to hard emissions ($-2 < \log_{10} y_{23} < -1$) than the CSS-matched prediction. This observation is thus essentially the opposite one than for the $\mathbb{S}$ -events, in which the CSS-matched result is clearly above the IDS-matched one. Combining $\mathbb{S}$ - and $\mathbb{H}$ -events in Figure 6.13 shows that the small contribution of the IDS-matched $\mathbb{S}$ -events to hard emissions explains point five from above. This small contribution to hard emissions is already present – and in fact stronger – in the IDS versions at LO.

In the region below ≈ 150 GeV in the invariant mass (mentioned in point four from above), both, the distribution of $\mathbb{S}$ - and $\mathbb{H}$ -events are important: That is, the contribution of $\mathbb{H}$ -events of the IDS-matched results are almost constant at a very high negative number, whereas the contribution of the CSS-matched prediction is also negative but increasingly closer to zero at small masses. In the invariant mass distribution of $\mathbb{S}$ -events we see that all three matched calculations lie above the LO+PS one. They thus partially compensate the “negativeness” of

³⁵We compare the distribution of $\mathbb{S}$ -events to the LO prediction, instead of the NLO one, since we are interested in a comparison with Figure 6.8.

$\mathbb{H}$ -events. That is in particular true for the IDS-matched results. However the compensation is not quite achieved, which results in the observation mentioned in the fourth point above. The first three points from above are mostly due to the large differences in the distribution of $\mathbb{H}$ -events between the CSS- and IDS-matched results. This motivates a cross-check of this distribution. On top of that, we perform an additional comparison of the NLO-matched calculations.

Comparison 1: RS-Events of Fixed NLO versus $\mathbb{H}$ -Events of NLO-Matched Calculation

Now we take a closer look at the distribution of $\mathbb{H}$ -events since they are the reason for significant shape differences when going from a LO+PS simulation to an NLO-matched calculation. In particular, we want to compare them to the fixed NLO RS-events.

Before we do that, we remind ourselves of the different treatment of dipoles in fixed NLO and NLO-matched calculations: In a fixed NLO calculation, the weight of each dipole is filled separately into the bins of a histogram. In other words, for one given phase-space point there are multiple – so-called NLO sub-events – filled into the histogram. The pure real correction NLO sub-event is filled in with real correction kinematics whereas each dipole is associated with its respective *Born* kinematics. In Subsection 5.2.2 we pointed out that this is not the case in an NLO-matched calculation. There, the weights of the real correction and the various dipoles are added up and filled into the histogram with the real correction kinematics.

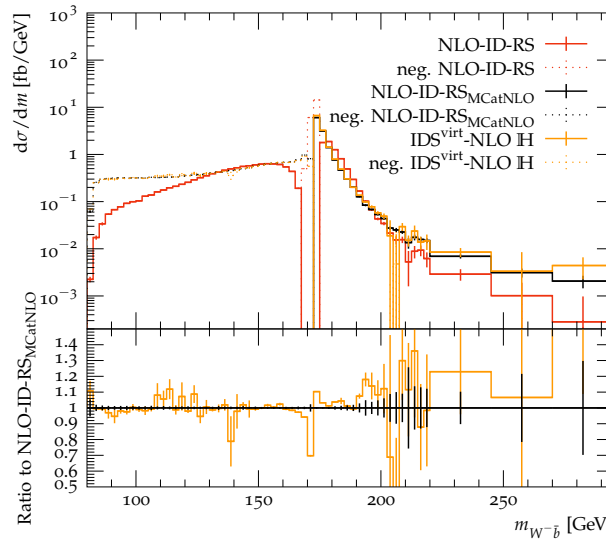


Figure 6.15: Shown is the invariant mass, like in the previous plots. We compare RS-events from the fixed NLO calculation with the $\mathbb{H}$ -events of the IDS^{virt} -matched calculation. The black lines show how the RS part of the fixed NLO calculation looks like, if it is treated like an NLO-matched calculation (see text). Negative parts of the distributions are shown by dotted lines. In all predictions we used pseudo-dipoles.

Because of this different treatment of RS- and $\mathbb{H}$ -events, we do not suspect the two to agree. In order to still check the correctness of the $\mathbb{H}$ -events³⁶, we manipulated the analysis of the fixed NLO calculation such that it treats the NLO sub-events as though they were a single NLO sub-event with real correction kinematics, thus mimicking the treatment in matched calculations.

As can be seen in Figure 6.15, the difference between RS- (red) and $\mathbb{H}$ -events (orange) is extreme at and below the peak. But it turns out that treating the RS-events like in an NLO-matched calculation (black), they have a very similar line shape, see ratio plot. The deviations may be attributed to the fact, that there is only a partial subtraction in the $\mathbb{H}$ -events, due to $\mathcal{D}^A$ being equal to zero instead of $\mathcal{D}^S$ depending on the value of t , see Equation (5.25).

The same plot as Figure 6.15 but using CS rather than pseudo-dipoles conveys the same message and is thus not shown. We remark that the distributions of RS-events of the fixed NLO calculations are very similar between the two dipole types, but that the one with pseudo-dipoles exhibits smaller statistical fluctuations. This is expected since it is a major result of chapter 4.

Comparison 2: NLO-Matching with $t_{\text{res}} = t_c$

To have another cross-check of the implementation of the resonance-aware matching, we set the resummation scale to the shower cutoff, i.e. $t_{\text{res}} = t_c$. This implies that $\mathcal{D}^A = 0$ (see Equation (5.25)) everywhere except for phase space points, which are very close to an IR singularity. Consequently, all emissions are generated by $\mathbb{H}$ -events and none by $\mathbb{S}$ -events, since the integral in the squared brackets of Equation (5.22) equals zero. We thus expect the invariant mass distributions of the various NLO-matched setups to reproduce the fixed NLO distribution. This comparison can be seen in Figure 6.16. Looking at the upper left plot of Figure 6.16 we see that this is indeed the case for the IDS^{virt} -matched result. But the IDS^{eik} -matched prediction and even the CSS-matched one deviate from the fixed NLO result. The reason for that is that emissions (from $\mathbb{H}$ -events) which are associated with an evolution variable t *smaller* than t_c have an effect upon the invariant mass distribution. This can be seen in the lower left plot of Figure 6.16 in which the IDS^{eik} - and CSS-matched setups have been rerun with $t_{\text{res}} = 0.1 \cdot t_c$ rather than t_c . The CSS-matched results exhibits statistical agreement with the fixed NLO distribution, while that is not quite the case for the IDS^{eik} -matched one, though the agreement is much better than for $t_{\text{res}} = t_c$. We stress the fact that the IDS^{eik} -matched distribution requires emissions below t_c to coincide with the fixed NLO one at the *left-hand side of the peak*. This point is so interesting because it is this region in which the IDS^{eik} -matched distribution exhibits the uncalled-for dip, see Figure 6.13. One would therefore expect that the lowering of t_c , which has been studied in Figure 6.11 would

³⁶We consider the RS-events of the fixed NLO prediction with pseudo-dipoles to be correct since they reproduce the prediction based on CS dipoles, see Chapter 4.

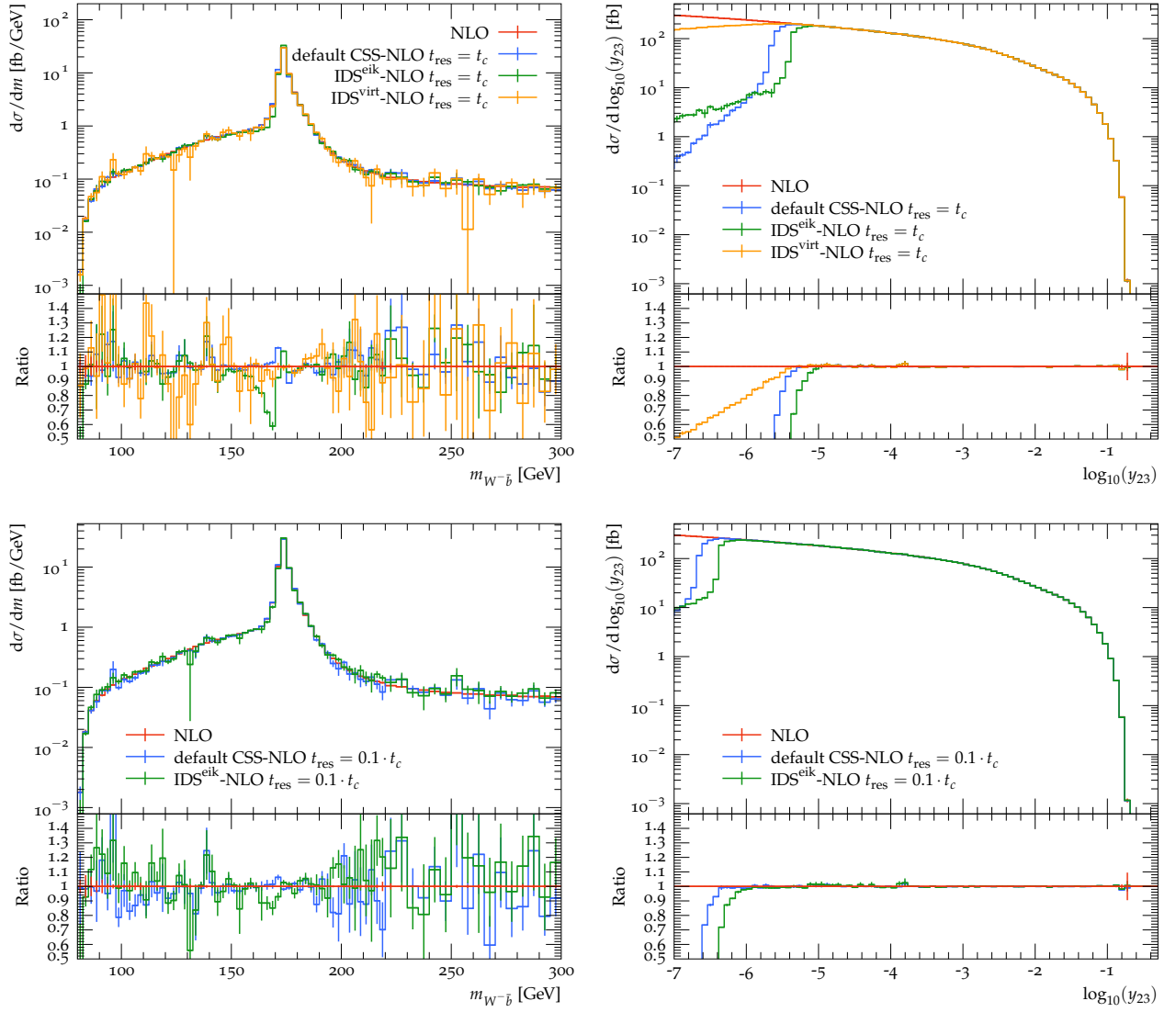


Figure 6.16: Quantities as in Figure 6.3. Compared are the matching of the three showers CSS, IDS^{eik} and IDS^{virt} with the resummation scale set to the shower cutoff t_c (above) and a tenth of this value (below).

lift the dip. But this is not the case.

Additionally we compare the jet rates of the MC@NLO runs and the fixed NLO one (see right plots of Figure 6.16). It can be clearly seen that all predictions agree for $y_{23} > 10^{-5}$ for $t_{\text{res}} = t_c$. Below that the fixed NLO prediction keeps on rising whereas the others drop. This mirrors the fact that the fixed NLO prediction is exclusively given by the real correction, whereas the matched calculations are composed of real correction *and* subtraction terms. This is a key point of the matching algorithm, which was pointed out at the end of Subsection 5.2.2.

Finally we add that the cross-sections of our various runs agree perfectly everywhere they are expected to do so.

Summary

The IDS^{virt}-matching looks promising regarding the $m_{W-\bar{b}}$ distribution, but has the flaw of having bins with negative value at the left most end of the distribution. It can thus not be seen as a meaningful result. The IDS^{eik}-matching on the other hand is throughout positive in the invariant mass distribution distribution, but can neither be a realistic prediction since it falls below the LO prediction on the left-hand side of the top-mass peak. The reason for that seems to be a lack of semi-soft/collinear emissions, as indicated in the $t = t_c$ comparison.

In both IDS versions, we expect the shower emissions, i.e. the S-events, to be the source of the incorrect NLO predictions. The reason for that is that the H-events are much more likely to be correct, since their calculation uses the same code as the fixed NLO computation, which is shown to be correct in Chapter 4. Though we have tested the shower emissions extensively in Subsection 6.6.1, we cannot be sure of their being correct since we have no reference to compare them to.

6.7 Resonances-Aware Matching in the FKS/POWHEG Framework

In Section 4.5, we have summarised the idea of a resonance-aware subtraction based upon the FKS algorithm. The papers in which this work is presented ([22] for a calculation in the NWA and [23] for a calculation including finite width effects) also report upon a resonance-aware matching. This matching is performed according to the POWHEG algorithm and implemented in the POWHEG-BOX [72, 59, 78] and referred to as POWHEG-BOX-RES. There, the extra emission is generated from the Born configuration by the inverse mapping of the employed FKS subtraction. This is, in generating this extra emission, the decomposition of phase-space into singular regions α_r – as mentioned in Section 4.5 – plays an important role. The reason for that is that thus, each emission is associated to a singular region α_r and with that to a fixed resonance structure. The resonance-aware matching described in [22, 23] is interfaced with the PYTHIA parton shower [25, 26]. This shower is capable of preserving the resonances' virtuality, if it is supplied with information about the resonance structure of the event. It does

however not describe soft emissions as well as SHERPA's showers as it is based on splitting functions that describe only the collinear regime of the splitting.

The technology of [22, 23] is applied in [27, 28, 29] to improve predictions of top quark related processes including finite width effects. In particular, $t\bar{t}$ production at the LHC is calculated in [27] at the level of the $l^+\nu_l l^-\bar{\nu}_l b\bar{b}$ final state in terms of exact matrix elements at NLO QCD matched to a parton shower. Figure 3 of [27] compares the resonance-aware and non-resonance-aware prediction of the reconstructed top mass at the level of W boson and b jet. Their findings agree with our observation of a sharper peak when the resonance-aware procedure is applied. The overall result of these works is that non-resonance-aware calculations distort the differential distributions of processes featuring resonance significantly thus emphasising the importance of a proper treatment of resonances.

7 Conclusion and Outlook

In this thesis we present a new subtraction algorithm for NLO QCD calculations and discuss how its ideas can be applied to a parton shower and the framework of NLO-matching. While the new subtraction formalism yields the desired improvements, there is still work necessary to make the resonance-aware parton shower usable.

To be more specific, this work improves NLO calculations of processes in which intermediate resonances occur. To exemplify our devised algorithms, we select the intermediate production of a top and anti-top quark at an e^+e^- collider and at the LHC as working example. In Chapter 4, we explain that established subtraction algorithms exhibit a flaw in the calculation of the subtracted real correction cross-section. Although the result is correct, the statistical uncertainties of the computation are comparatively large. The reason for that lies in an imperfect cancellations between real correction and subtraction terms due to an unsuitable recoil scheme. To improve this situation, we introduce a novel subtraction scheme which is based on the use of pseudo-dipoles. By applying this resonance-aware subtraction formalism to our example processes, a significant improvement of the convergence of the subtracted real correction cross-section is shown. These improvements do however not yet constitute a real advance in making a theory prediction more accurate, since they only decrease the integration time. In a parton shower, on the other hand, the presence of resonances are known to distort the distributions of differential cross-sections. We therefore aim at extending the idea of the resonance-aware subtraction to the parton shower. This strategy of building a parton shower from a subtraction algorithm proved already useful in constructing the Catani-Seymour shower (CSS) on the basis of Catani-Seymour dipole subtraction. In following this approach, we contrive a resonance-aware parton shower, which we dub IDS. Like the CSS, the IDS employs splitting functions and momenta mappings which are based upon or equal to their analogues in the associated subtraction method. In the choice of the evolution variable, which can not be adopted from the CSS, we are left with a certain freedom and thus consider two different evolution variables. Depending on them, we call the two versions of this shower IDS^{eik} and IDS^{virt} . We thoroughly compare the two IDS versions and the CSS at LO taking only one parton emission into account. On the whole, the differences of the IDS versions to the CSS are understood and agree with what we expect from a resonance-aware shower. Especially the narrower peak in the reconstructed top mass distribution matches our expectation of less distorted distributions. We extend this comparison to the NLO case, i.e. an NLO-matched calculation. But there we see inconsistencies of both showers which reflect themselves in either an unnatural line shape of the aforementioned invariant mass distribution or bins with negative value. Those problems make it not sensible to extend the IDS versions to describe parton emissions off gluons or initial state radiation, which would naturally be the next points to tackle.

Once the pseudo-dipole subtraction algorithm is made public in the SHERPA event generator,

it can be used by everyone to speed up the calculation of Monte Carlo predictions for data comparison. There is however still a problem to be solved in the implementation of the IDS. This thesis serves thus as a reference for theorists, who want to continue work in that direction, since it documents which steps have been undertaken to construct a resonance-aware shower. Once having a resonance-aware shower at one's disposal, a follow-up would be the consideration of competing resonances. This means a generalisation of the ideas presented in this thesis to a procedure in which the identification of particles depends on the phase-space of the event. This would allow to improve predictions for processes that receive contributions from diagrams with different resonance structure. Another possible generalisation of this work is the inclusion of finite mass effects. The work of this thesis builds on the assumption of having a massless emitter, colour spectator and emitted parton. However, to loosen this condition considerable work is thought to be necessary since it also requires to change the subtraction method along with its mappings. But once having achieved that, it does not only improve QCD predictions further, but opens up new fields of application like NLO electroweak corrections and an electroweak shower, which take resonances into account.

Appendices

A Useful Formulae

The regularised Altarelli-Parisi splitting functions are given by

$$P^{qg}(x) = P^{\bar{q}g}(x) = C_F \frac{1 + (1-x)^2}{x}, \quad (\text{A.1})$$

$$P^{gq}(x) = P^{g\bar{q}}(x) = T_R [x^2 + (1-x)^2], \quad (\text{A.2})$$

$$P^{qq}(x) = P^{q\bar{q}}(x) = C_F \left(\frac{1+x^2}{1-x} \right)_+, \quad (\text{A.3})$$

$$P^{gg}(x) = 2C_A \left[\left(\frac{1}{1-x} \right)_+ + \frac{1-x}{x} - 1 + x(1-x) \right] + \delta(1-x) \left(\frac{11}{6}C_A - \frac{2}{3}n_f T_R \right). \quad (\text{A.4})$$

In the integration of dipoles describing singularities associated with an initial-state parton or an identified final-state parton the functions

$$\bar{K}^{qg}(x) = \bar{K}^{\bar{q}g}(x) = P^{qg}(x) \ln \frac{1-x}{x} + C_F x, \quad (\text{A.5})$$

$$\bar{K}^{gq}(x) = \bar{K}^{g\bar{q}}(x) = P^{gq}(x) \ln \frac{1-x}{x} + T_R 2x(1-x), \quad (\text{A.6})$$

$$\begin{aligned} \bar{K}^{qq}(x) = \bar{K}^{q\bar{q}}(x) = C_F \left[\left(\frac{2}{1-x} \ln \frac{1-x}{x} \right)_+ - (1-x) \ln \frac{1-x}{x} + (1-x) \right] \\ - \delta(1-x)(5 - \pi^2)C_F, \end{aligned} \quad (\text{A.7})$$

$$\begin{aligned} \bar{K}^{gg}(x) = C_A \left[\left(\frac{1}{1-x} \ln \frac{1-x}{x} \right)_+ + \left(\frac{1-x}{x} - 1 + x(1-x) \right) \ln \frac{1-x}{x} \right] \\ - \delta(1-x) \left[\left(\frac{50}{9} - \pi^2 \right) C_A - \frac{16}{9} T_R n_f \right]. \end{aligned} \quad (\text{A.8})$$

occur. If in addition to that also the colour spectator is an initial-state parton or an identified final-state one, the following functions occur:

$$\tilde{K}^{ab}(x) = P_{\text{reg}}^{ab}(x) \ln(1-x) + \delta^{ab} \mathbf{T}_a^2 \left[\left(\frac{2}{1-x} \ln(1-x) \right)_+ - \frac{\pi^2}{3} \delta(1-x) \right]. \quad (\text{A.9})$$

The regular parts of the regularised Altarelli-Parisi splitting functions are given by

$$P_{\text{reg}}^{ab}(x) = P^{ab}(x) \quad \text{if } a \neq b, \quad (\text{A.10})$$

$$P_{\text{reg}}^{qq}(x) = -C_F(1+x), \quad (\text{A.11})$$

$$P_{\text{reg}}^{gg}(x) = 2C_A \left[\frac{1-x}{x} - 1 + x(1-x) \right]. \quad (\text{A.12})$$

The functions only appearing when integrating pseudo-dipoles read

$$\begin{aligned} \mathcal{L}^{a,b}(x; p_a, p_b, n) = & \delta^{ab} \delta(1-x) 2\mathbf{T}_a^2 \left[\text{Li}_2 \left(1 - \frac{1+v}{2} \frac{(p_a + p_b)n}{p_a n} \right) \right. \\ & \left. + \text{Li}_2 \left(1 - \frac{1-v}{2} \frac{(p_a + p_b)n}{p_a n} \right) \right] - P_{\text{reg}}^{ab}(x) \ln \frac{n^2(p_a p_b)}{2(p_a n)^2}, \end{aligned} \quad (\text{A.13})$$

with the dilogarithm

$$\text{Li}_2(x) = - \int_0^x \frac{dt}{t} \ln(1-t) \quad \text{and} \quad v = \sqrt{1 - \frac{n^2(p_a + p_b)^2}{[(p_a + p_b)n]^2}}. \quad (\text{A.14})$$

B Alternative Ansatz for Resonance-Aware Dipole-Subtraction

In the course of this work an alternative approach, which we call RES-dipoles, to achieve resonance-aware NLO subtraction based upon CS dipoles, has been studied. Though the divergences of the real corrections are correctly subtracted by RES-dipoles, we did not succeed in solving the integrals of the RES-dipoles and thus finding the $\mathbf{I}$ -operator in the Born-like configuration of the cross-section.

In the following, we will give a brief sketch on RES-dipoles describing final-state singularities with final-state spectators, though the idea is applicable to other kinds of dipoles. We throughout assume particles i , j , k and l as massless.

The idea of RES-dipoles is to introduce a kinematic spectator l , which is in general not the same as the colour spectator k . Consequently, we will rescale the momentum of parton l , instead of k (see Figure B.2). Therefore we redefine the well-known variables $y_{ij,k}$ and $\tilde{z}_i$ of standard FF-dipoles (see Equation (3.20) and (3.24)) by replacing p_k with p_l :

$$Y_{ij,l} = \frac{p_i p_j}{p_i p_j + p_i p_l + p_l p_j} = \frac{p_i p_j}{\tilde{p}_{ij} \tilde{p}_l} = \frac{p_i \tilde{p}_{ij}}{\tilde{p}_{ij} \tilde{p}_l - p_i \tilde{p}_l}, \quad (\text{B.1})$$

$$\tilde{Z}_i = \frac{p_i p_l}{(p_i + p_j) p_l} = \frac{p_i \tilde{p}_l}{\tilde{p}_{ij} \tilde{p}_l}, \quad (\text{B.2})$$

and the mapped momenta $\tilde{p}_{ij}$ and $\tilde{p}_l$ are given by

$$\tilde{p}_{ij}^\mu = p_i^\mu + p_j^\mu - \frac{Y_{ij,l}}{1 - Y_{ij,l}} p_l^\mu, \quad (\text{B.3})$$

$$\tilde{p}_l^\mu = \frac{1}{1 - Y_{ij,l}} p_l^\mu. \quad (\text{B.4})$$

This procedure gives us well-defined Born kinematics, which have the property that the kinematic spectator can be any particle. Now, we have to express the splitting functions $\mathbf{V}$ as

Figure B.1: From the above mentioned properties of the momenta, it follows that we work in a reference frame where $\tilde{\vec{p}}_l$ is antiparallel to $\tilde{\vec{p}}_{ij}$.

Substituting those equations into Equation (B.5), we obtain

$$S(Y_{ij,l}, \tilde{Z}_i, \phi_i) = \frac{(\tilde{p}_{ij}\tilde{p}_l + \tilde{p}_l p_k)Y_{ij,l} + \tilde{p}_{ij}p_k}{\tilde{p}_{ij}\tilde{p}_l Y_{ij,l} + \tilde{p}_l p_k Y_{ij,l} \tilde{Z}_i + \tilde{p}_{ij}p_k(1 - \tilde{Z}_i) + \sqrt{4(\tilde{p}_{ij}p_k)(\tilde{p}_l p_k)Y_{ij,l}\tilde{Z}_i(1 - \tilde{Z}_i)\cos\phi_i}}, \quad (\text{B.9})$$

where ϕ_i is the azimuthal angle between $\vec{p}_i$ and $\vec{p}_k$ in the CMS of $\tilde{p}_l$ and $\tilde{p}_{ij}$, see Figure B.1. The collinear limit is found by taking $Y_{ij,l} \rightarrow 0$, in which case we recover the well known term

$$\lim_{Y_{ij,l} \rightarrow 0} S(Y_{ij,l}, \tilde{Z}_i, \phi_i) = \frac{1}{1 - \tilde{Z}_i}. \quad (\text{B.10})$$

This motivates us to substitute $\tilde{z}_i$ with $\tilde{Z}_i$ in the remainder of the splitting functions to obtain the Altarelli-Parisi functions as correct collinear limit. In conclusion, we obtain the following resonance-aware splitting functions:

$$\frac{\langle s | \mathbf{V}_{q_i g_j, kl}^{\text{res}} | s' \rangle}{8\pi\mu^{2\epsilon}\alpha_s} = C_F \left[2S(Y_{ij,l}, \tilde{Z}_i, \phi_i) - (1 + \tilde{Z}_i) - \epsilon(1 - \tilde{Z}_i) \right] \delta_{ss'}, \quad (\text{B.11})$$

$$\frac{\langle \mu | \mathbf{V}_{q_i \bar{q}_j, kl}^{\text{res}} | \nu \rangle}{8\pi\mu^{2\epsilon}\alpha_s} = T_R \left[-g^{\mu\nu} - \frac{2}{p_i p_j} \left(\tilde{Z}_i p_i^\mu - \tilde{Z}_j p_j^\mu \right) \left(\tilde{Z}_i p_i^\nu - \tilde{Z}_j p_j^\nu \right) \right], \quad (\text{B.12})$$

$$\begin{aligned} \frac{\langle \mu | \mathbf{V}_{g_i g_j, kl}^{\text{res}} | \nu \rangle}{8\pi\mu^{2\epsilon}\alpha_s} = C_A & \left[-g^{\mu\nu} \left(S(Y_{ij,l}, \tilde{Z}_i, \phi_i) + S(Y_{ij,l}, \tilde{Z}_j, \phi_j) - 2 \right) \right. \\ & \left. + (1 - \epsilon) \frac{2}{p_i p_j} \left(\tilde{Z}_i p_i^\mu - \tilde{Z}_j p_j^\mu \right) \left(\tilde{Z}_i p_i^\nu - \tilde{Z}_j p_j^\nu \right) \right], \quad (\text{B.13}) \end{aligned}$$

where $\tilde{Z}_j = 1 - \tilde{Z}_i$ and $\phi_j = \pi - \phi_i$.

As those formulae are only applicable to massless particles i, j, k and l , we have tested them in the process $e^+e^- \rightarrow b\bar{b}j$, by choosing l as the one remaining final-state particle, which is not i, j or k (see Figure B.2).³⁷ Figure B.3 shows the convergence of the squared real emission matrix element and the sum of RES-dipoles for two trajectories in phase-space. The one in the left-hand figure is characterised by an increasingly soft gluon, the trajectory in the right figure, by two gluons, which become progressively collinear. For comparison, we also show the numerical values of standard CS dipoles and pseudo-dipoles on those trajectories. In the application of pseudo-dipoles, we have “identified” solely the emitting parton, thus the recoil is absorbed by both remaining partons. It can be seen that all dipoles describe the singularities, which are approached by the trajectories, correctly.

³⁷Of course, this process does not constitute a case, in which resonances-aware subtraction is needed, however it is a valid test-ground to check the cancellation of divergences between pure real correction and summed dipoles.

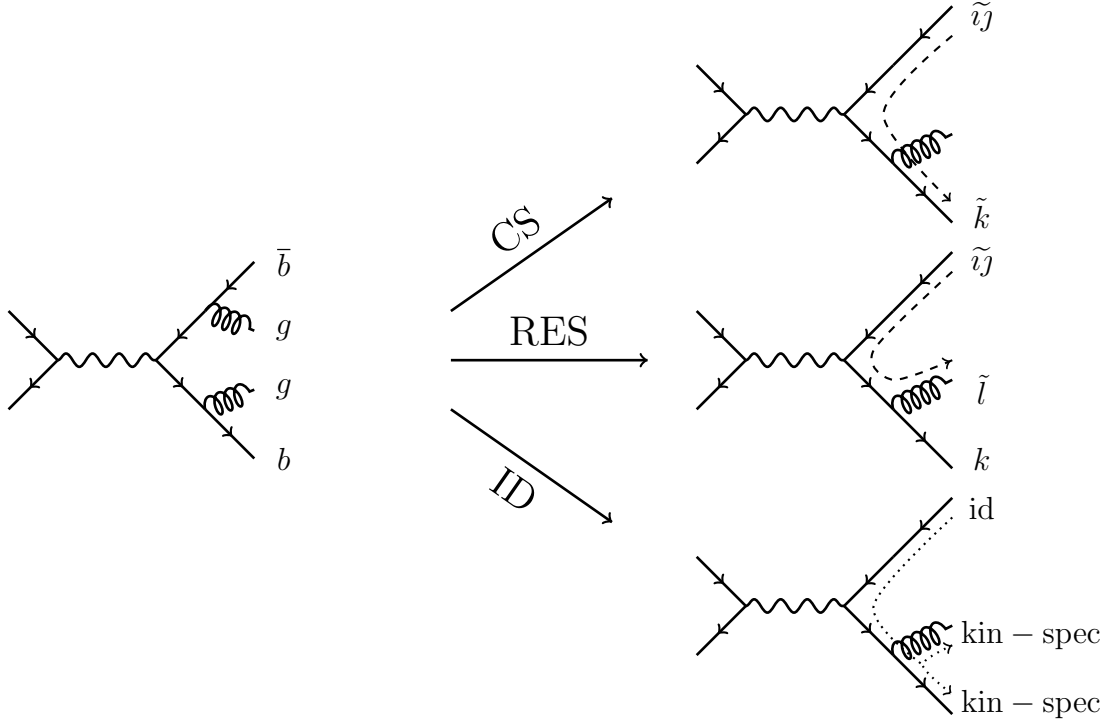


Figure B.2: One possible real correction diagram for $e^+e^- \rightarrow b\bar{b}j$ and three different mappings for three different dipoles: standard CS dipoles, RES-dipoles and pseudo-dipoles.

The labelling of momenta, used in Figure B.3 is

$$e^-(p_0) + e^+(p_1) \rightarrow j(p_2) + g(p_3) + b(p_4) + b(p_5). \quad (\text{B.14})$$

The integrated RES-dipoles read

$$\int [dp_i(\tilde{p}_{ij}, \tilde{p}_l)] \mathcal{D}_{ij,kl}^{\text{res}} = - \int [dp_i(\tilde{p}_{ij}, \tilde{p}_l)] \frac{1}{2p_i p_j} \langle \mathbf{V}_{ij,kl}^{\text{res}} \rangle_m \left\langle 1, \dots, \tilde{i}j, \tilde{l}, \dots, m+1 \left| \frac{\mathbf{T}_k \mathbf{T}_{ij}}{\mathbf{T}_{ij}^2} \right| 1, \dots, \tilde{i}j, \tilde{l}, \dots, m+1 \right\rangle_m, \quad (\text{B.15})$$

where $\langle \mathbf{V}_{ij,kl}^{\text{res}} \rangle$ are the polarisation averaged resonance-aware splitting functions. The non-trivial part of the integration is caused by the term $S(Y_{ij,l}, \tilde{Z}_i, \phi_i)$. To quote this integral, we give the parametrisation of $[dp_i(\tilde{p}_{ij}, \tilde{p}_l)]$, which is the same as in Equation (3.56), but with particle l as recoil partner and ϕ_i as explicit azimuthal angle:

$$[dp_i(\tilde{p}_{ij}, \tilde{p}_l)] = \frac{(2\tilde{p}_{ij}\tilde{p}_l)^{1-\epsilon}}{16\pi^2} \frac{d\Omega^{D-3}}{(2\pi)^{1-2\epsilon}} \sin^{-2\epsilon} \phi_i d\phi_i d\tilde{Z} dY \Theta(\tilde{Z}(1-\tilde{Z}))\Theta(Y(1-Y)) (\tilde{Z}(1-\tilde{Z}))^{-\epsilon} (1-Y)^{1-2\epsilon} Y^{-\epsilon}, \quad (\text{B.16})$$

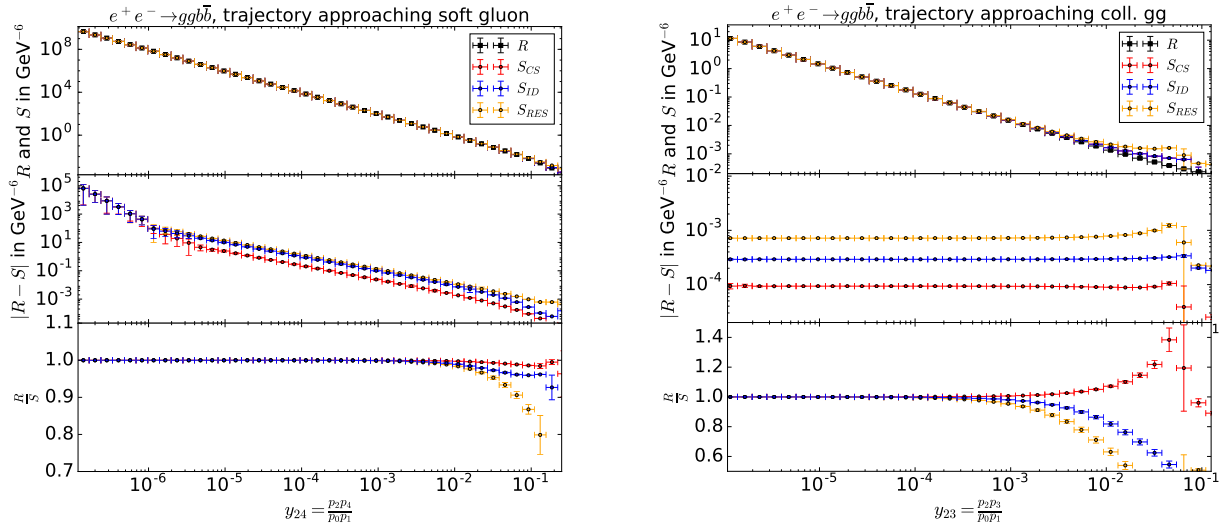


Figure B.3: Trajectories in $e^+e^- \rightarrow gg\bar{b}b$ phase-space for a soft gluon (left) and a collinear gluon-gluon-pair (right). Displayed are the values of the squared real correction matrix element $|\mathcal{M}_R|^2 = R$ along with the sum of three different dipoles $\sum_{(i,j) \in \text{pairs}} \sum_k \mathcal{D}_{ij,k} = S$: standard CS-dipoles, RES-dipoles and pseudo-dipoles.

with the surface integral over the hypersphere in $D - 3$ dimensions given by

$$\int d\Omega^{D-3} = \int d\Omega^{1-2\epsilon} = \frac{2\pi^{\frac{1}{2}-\epsilon}}{\Gamma(\frac{1}{2}-\epsilon)}. \quad (\text{B.17})$$

The integral we did not succeed in solving is

$$\int [dp_i(\tilde{p}_{ij}, \tilde{p}_l)] \frac{1}{2p_i p_j} S(Y_{ij,l}, \tilde{Z}_i, \phi_i). \quad (\text{B.18})$$

The inclusion of a finite mass for the kinematic spectator l – which is mandatory if RES-dipoles are to be applied to relevant processes like $e^+e^- \rightarrow W^+W^-\bar{b}b$ or $pp \rightarrow W^+W^-j_bj_b$ – renders the integral even more difficult. We therefore abandoned this ansatz in favour of pseudo-dipoles.

C List of Files Affected the Most by the Implementation of the IDS

As discussed in Section 6.5, there are three main alterations in the modules `CSS`, `DIRE`, `MCATNLO` and `DIM` to do in order to incorporate the IDS algorithm in them. In the following table, we list those changes and name the files in which the key points of those changes take place. We stress that the necessary changes for implementing the IDS do by no means restrict to the files listed in the table. Furthermore, there are many other changes, like the setting of the kinematic

changes	CSS and MCATNLO	DIRE and DIM
generation of splitting variables	LF_FFV.C Splitting_Function_Base.C Sudakov.C	FFV_FF.C Lorentz_FF.C Lorentz.C
splitting functions	LF_FFV.C	FFV_FF.C
construction of the emission kinematics	Kinematics_Base.C	Lorentz_FF.C

Table C.1: Listed are the three main changes to implement the IDS in the four modules of SHERPA along with the name of files in which most of these changes take place.

spectator, a potential resonance-aware clustering, adaptation of Jacobians, etc. which are not included in the three above mentioned main changes. Instead this table should be seen as a rough orientation for where to look for the key changes. Readers that are interested in the actual changes of the code can check out the development branch of the resonance-aware subtraction and matching on [gitlab.com](https://gitlab.com/sherpa-team/sherpa/-/tree/8-feature-resonance-aware-nlo-subtraction): <https://gitlab.com/sherpa-team/sherpa/-/tree/8-feature-resonance-aware-nlo-subtraction>

References

- [1] G. Aad et al., The ATLAS collaboration, *Observation of a new particle in the search for the Standard Model Higgs boson with the ATLAS detector at the LHC*, Phys. Lett. B **716** (2012), [1–29](#), [[arXiv:1207.7214](#) [hep-ex]].
- [2] S. Chatrchyan et al., The CMS collaboration, *Observation of a New Boson at a Mass of 125 GeV with the CMS Experiment at the LHC*, Phys. Lett. B **716** (2012), [30–61](#), [[arXiv:1207.7235](#) [hep-ex]].
- [3] P. W. Higgs, *Broken symmetries, massless particles and gauge fields*, Phys. Lett. **12** (1964), [132–133](#).
- [4] P. W. Higgs, *Broken Symmetries and the Masses of Gauge Bosons*, Phys. Rev. Lett. **13** (1964), [508–509](#).
- [5] F. Englert and R. Brout, *Broken Symmetry and the Mass of Gauge Vector Mesons*, Phys. Rev. Lett. **13** (1964), [321–323](#).
- [6] G. S. Guralnik, C. R. Hagen and T. W. B. Kibble, *Global Conservation Laws and Massless Particles*, Phys. Rev. Lett. **13** (1964), [585–587](#).
- [7] S. Höche, S. Liebschner and F. Siegert, *Resonance-Aware Subtraction in the Dipole Method*, Eur. Phys. J. C **79** (2019), no. 9, [728](#), [[arXiv:1807.04348](#) [hep-ph]].
- [8] S. Frixione, E. Laenen, P. Motylinski, B. R. Webber and C. D. White, *Single-top hadroproduction in association with a W boson*, JHEP **07** (2008), [029](#), [[arXiv:0805.3067](#) [hep-ph]].
- [9] M. Aaboud et al., The ATLAS collaboration, *Probing the quantum interference between singly and doubly resonant top-quark production in pp collisions at $\sqrt{s} = 13$ TeV with the ATLAS detector*, Phys. Rev. Lett. **121** (2018), no. 15, [152002](#), [[arXiv:1806.04667](#) [hep-ex]].
- [10] P. Nason, S. Dawson and R. K. Ellis, *The One Particle Inclusive Differential Cross-Section for Heavy Quark Production in Hadronic Collisions*, Nucl. Phys. **B327** (1989), [49–92](#), [Erratum: Nucl. Phys.B335,260(1990)].
- [11] W. Beenakker, W. L. van Neerven, R. Meng, G. A. Schuler and J. Smith, *QCD corrections to heavy quark production in hadron hadron collisions*, Nucl. Phys. **B351** (1991), [507–560](#).
- [12] M. L. Mangano, P. Nason and G. Ridolfi, *Heavy quark correlations in hadron collisions at next-to-leading order*, Nucl. Phys. **B373** (1992), [295–345](#).
- [13] S. Frixione, M. L. Mangano, P. Nason and G. Ridolfi, *Top quark distributions in hadronic collisions*, Phys. Lett. **B351** (1995), [555–561](#), [[arXiv:hep-ph/9503213](#) [hep-ph]].

- [14] P. Bärnreuther, M. Czakon and A. Mitov, *Percent Level Precision Physics at the Tevatron: First Genuine NNLO QCD Corrections to $q\bar{q} \rightarrow t\bar{t} + X$* , Phys. Rev. Lett. **109** (2012), [132001](#), [[arXiv:1204.5201](#) [hep-ph]].
- [15] M. Czakon and A. Mitov, *NNLO corrections to top pair production at hadron colliders: the quark-gluon reaction*, JHEP **01** (2013), [080](#), [[arXiv:1210.6832](#) [hep-ph]].
- [16] M. Czakon, P. Fiedler and A. Mitov, *Total Top-Quark Pair-Production Cross Section at Hadron Colliders Through $O(\alpha_s^4)$* , Phys. Rev. Lett. **110** (2013), [252004](#), [[arXiv:1303.6254](#) [hep-ph]].
- [17] M. Czakon, D. Heymes, A. Mitov, D. Pagani, I. Tsinikos and M. Zaro, *Top-pair production at the LHC through NNLO QCD and NLO EW*, JHEP **10** (2017), [186](#), [[arXiv:1705.04105](#) [hep-ph]].
- [18] A. Denner, S. Dittmaier, S. Kallweit and S. Pozzorini, *NLO QCD corrections to $WWbb$ production at hadron colliders*, Phys. Rev. Lett. **106** (2011), [052001](#), [[arXiv:1012.3975](#) [hep-ph]].
- [19] G. Bevilacqua, M. Czakon, A. van Hameren, C. G. Papadopoulos and M. Worek, *Complete off-shell effects in top quark pair hadroproduction with leptonic decay at next-to-leading order*, JHEP **02** (2011), [083](#), [[arXiv:1012.4230](#) [hep-ph]].
- [20] A. Denner, S. Dittmaier, S. Kallweit and S. Pozzorini, *NLO QCD corrections to off-shell top-antitop production with leptonic decays at hadron colliders*, JHEP **10** (2012), [110](#), [[arXiv:1207.5018](#) [hep-ph]].
- [21] S. Frixione, Z. Kunszt and A. Signer, *Three jet cross-sections to next-to-leading order*, Nucl. Phys. **B467** (1996), [399–442](#), [[arXiv:hep-ph/9512328](#) [hep-ph]].
- [22] J. M. Campbell, R. K. Ellis, P. Nason and E. Re, *Top-Pair Production and Decay at NLO Matched with Parton Showers*, JHEP **04** (2015), [114](#), [[arXiv:1412.1828](#) [hep-ph]].
- [23] T. Ježo and P. Nason, *On the Treatment of Resonances in Next-to-Leading Order Calculations Matched to a Parton Shower*, JHEP **12** (2015), [065](#), [[arXiv:1509.09071](#) [hep-ph]].
- [24] S. Catani and M. H. Seymour, *A General algorithm for calculating jet cross-sections in NLO QCD*, Nucl. Phys. **B485** (1997), [291–419](#), [[arXiv:hep-ph/9605323](#) [hep-ph]], [Erratum: Nucl. Phys. **B510**, 503(1998)].
- [25] T. Sjostrand, S. Mrenna and P. Z. Skands, *A Brief Introduction to PYTHIA 8.1*, Comput. Phys. Commun. **178** (2008), [852–867](#), [[arXiv:0710.3820](#) [hep-ph]].

- [26] T. Sjöstrand, S. Ask, J. R. Christiansen, R. Corke, N. Desai, P. Ilten, S. Mrenna, S. Prestel, C. O. Rasmussen and P. Z. Skands, *An Introduction to PYTHIA 8.2*, Comput. Phys. Commun. **191** (2015), 159–177, [[arXiv:1410.3012](#) [hep-ph]].
- [27] T. Sjöstrand, J. M. Lindert, P. Nason, C. Oleari and S. Pozzorini, *An NLO+PS generator for $t\bar{t}$ and Wt production and decay including non-resonant and interference effects*, Eur. Phys. J. C **76** (2016), no. 12, 691, [[arXiv:1607.04538](#) [hep-ph]].
- [28] R. Frederix, S. Frixione, A. S. Papanastasiou, S. Prestel and P. Torrielli, *Off-shell single-top production at NLO matched to parton showers*, JHEP **06** (2016), 027, [[arXiv:1603.01178](#) [hep-ph]].
- [29] S. Ferrario Ravasio, T. Sjöstrand, P. Nason and C. Oleari, *A theoretical study of top-mass measurements at the LHC using NLO+PS generators of increasing accuracy*, Eur. Phys. J. C **78** (2018), no. 6, 458, [[arXiv:1906.09166](#) [hep-ph]], [Addendum: Eur.Phys.J.C 79, 859 (2019)].
- [30] E. Bothmann et al., The Sherpa collaboration, *Event Generation with Sherpa 2.2*, SciPost Phys. **7** (2019), no. 3, 034, [[arXiv:1905.09127](#) [hep-ph]].
- [31] S. Schumann and F. Krauss, *A Parton shower algorithm based on Catani-Seymour dipole factorisation*, JHEP **03** (2008), 038, [[arXiv:0709.1027](#) [hep-ph]].
- [32] S. Frixione and B. R. Webber, *Matching NLO QCD computations and parton shower simulations*, JHEP **06** (2002), 029, [[arXiv:hep-ph/0204244](#) [hep-ph]].
- [33] M. Bahr et al., *Herwig++ Physics and Manual*, Eur. Phys. J. **C58** (2008), 639–707, [[arXiv:0803.0883](#) [hep-ph]].
- [34] J. Bellm et al., *Herwig 7.0/Herwig++ 3.0 release note*, Eur. Phys. J. **C76** (2016), no. 4, 196, [[arXiv:1512.01178](#) [hep-ph]].
- [35] T. Gleisberg, S. Hoeche, F. Krauss, M. Schonherr, S. Schumann, F. Siegert and J. Winter, *Event generation with SHERPA 1.1*, JHEP **02** (2009), 007, [[arXiv:0811.4622](#) [hep-ph]].
- [36] C. Anastasiou and K. Melnikov, *Higgs boson production at hadron colliders in NNLO QCD*, Nucl. Phys. **B646** (2002), 220–256, [[arXiv:hep-ph/0207004](#) [hep-ph]].
- [37] R. V. Harlander and W. B. Kilgore, *Next-to-next-to-leading order Higgs production at hadron colliders*, Phys. Rev. Lett. **88** (2002), 201801, [[arXiv:hep-ph/0201206](#) [hep-ph]].
- [38] S. Catani, D. de Florian and M. Grazzini, *Higgs production in hadron collisions: Soft and virtual QCD corrections at NNLO*, JHEP **05** (2001), 025, [[arXiv:hep-ph/0102227](#) [hep-ph]].

- [39] V. Ravindran, J. Smith and W. L. van Neerven, *NNLO corrections to the total cross-section for Higgs boson production in hadron hadron collisions*, Nucl. Phys. **B665** (2003), 325–366, [[arXiv:hep-ph/0302135](#) [hep-ph]].
- [40] O. Brein, A. Djouadi and R. Harlander, *NNLO QCD corrections to the Higgs-strahlung processes at hadron colliders*, Phys. Lett. **B579** (2004), 149–156, [[arXiv:hep-ph/0307206](#) [hep-ph]].
- [41] R. V. Harlander and W. B. Kilgore, *Higgs boson production in bottom quark fusion at next-to-next-to leading order*, Phys. Rev. **D68** (2003), 013001, [[arXiv:hep-ph/0304035](#) [hep-ph]].
- [42] B. Biedermann, A. Denner and M. Pellen, *Complete NLO corrections to W^+W^+ scattering and its irreducible background at the LHC*, JHEP **10** (2017), 124, [[arXiv:1708.00268](#) [hep-ph]].
- [43] B. Biedermann, A. Denner and M. Pellen, *Large electroweak corrections to vector-boson scattering at the Large Hadron Collider*, Phys. Rev. Lett. **118** (2017), no. 26, 261801, [[arXiv:1611.02951](#) [hep-ph]].
- [44] G. Aad et al., The ATLAS collaboration, *Evidence for Electroweak Production of $W^\pm W^\pm jj$ in pp Collisions at $\sqrt{s} = 8$ TeV with the ATLAS Detector*, Phys. Rev. Lett. **113** (2014), no. 14, 141803, [[arXiv:1405.6241](#) [hep-ex]].
- [45] M. Aaboud et al., The ATLAS collaboration, *Measurement of $W^\pm W^\pm$ vector-boson scattering and limits on anomalous quartic gauge couplings with the ATLAS detector*, Phys. Rev. **D96** (2017), no. 1, 012007, [[arXiv:1611.02428](#) [hep-ex]].
- [46] V. Khachatryan et al., The CMS collaboration, *Study of vector boson scattering and search for new physics in events with two same-sign leptons and two jets*, Phys. Rev. Lett. **114** (2015), no. 5, 051801, [[arXiv:1410.6315](#) [hep-ex]].
- [47] M. Schönherr, *An automated subtraction of NLO EW infrared divergences*, Eur. Phys. J. **C78** (2018), no. 2, 119, [[arXiv:1712.07975](#) [hep-ph]].
- [48] T. Kinoshita, *Mass singularities of Feynman amplitudes*, J. Math. Phys. **3** (1962), 650–677.
- [49] T. D. Lee and M. Nauenberg, *Degenerate Systems and Mass Singularities*, Phys. Rev. **133** (1964), B1549–B1562, [25(1964)].
- [50] A. Kardos, G. Somogyi and Z. Trócsányi, *Soft-drop event shapes in electron–positron annihilation at next-to-next-to-leading order accuracy*, Phys. Lett. **B786** (2018), 313–318, [[arXiv:1807.11472](#) [hep-ph]].

-
- [51] G. 't Hooft and M. J. G. Veltman, *Regularization and Renormalization of Gauge Fields*, Nucl. Phys. **B44** (1972), [189–213](#).
- [52] B. W. Harris and J. F. Owens, *The Two cutoff phase space slicing method*, Phys. Rev. **D65** (2002), [094032](#), [[arXiv:hep-ph/0102128](#) [hep-ph]].
- [53] A. Bassetto, M. Ciafaloni and G. Marchesini, *Jet Structure and Infrared Sensitive Quantities in Perturbative QCD*, Phys. Rept. **100** (1983), [201–272](#).
- [54] G. Altarelli and G. Parisi, *Asymptotic Freedom in Parton Language*, Nucl. Phys. **B126** (1977), [298–318](#).
- [55] S. Höche, *Introduction to parton-shower event generators*, Proceedings, Theoretical Advanced Study Institute in Elementary Particle Physics: Journeys Through the Precision Frontier: Amplitudes for Colliders (TASI 2014): Boulder, Colorado, June 2–27, 2014, 2015, pp. 235–295.
- [56] J. Campbell, J. Huston and F. Krauss, *The black book of quantum chromodynamics: a primer for the LHC era*, Oxford University Press, Oxford, 2018.
- [57] T. Gleisberg and F. Krauss, *Automating dipole subtraction for QCD NLO calculations*, Eur. Phys. J. **C53** (2008), [501–523](#), [[arXiv:0709.2881](#) [hep-ph]].
- [58] S. Frixione, *A General approach to jet cross-sections in QCD*, Nucl. Phys. **B507** (1997), [295–314](#), [[arXiv:hep-ph/9706545](#) [hep-ph]].
- [59] S. Frixione, P. Nason and C. Oleari, *Matching NLO QCD computations with Parton Shower simulations: the POWHEG method*, JHEP **11** (2007), [070](#), [[arXiv:0709.2092](#) [hep-ph]].
- [60] R. Frederix, S. Frixione, F. Maltoni and T. Stelzer, *Automation of next-to-leading order computations in QCD: The FKS subtraction*, JHEP **10** (2009), [003](#), [[arXiv:0908.4272](#) [hep-ph]].
- [61] J. Alwall, M. Herquet, F. Maltoni, O. Mattelaer and T. Stelzer, *MadGraph 5 : Going Beyond*, JHEP **06** (2011), [128](#), [[arXiv:1106.0522](#) [hep-ph]].
- [62] P. Diessner, W. Kotlarski, S. Liebschner and D. Stöckinger, *Squark production in R-symmetric SUSY with Dirac gluinos: NLO corrections*, JHEP **10** (2017), [142](#), [[arXiv:1707.04557](#) [hep-ph]].
- [63] S. Catani, Y. L. Dokshitzer, M. Olsson, G. Turnock and B. R. Webber, *New clustering algorithm for multijet cross sections in e^+e^- annihilation*, Phys. Lett. **B269** (1991), [432–438](#).

- [64] S. Catani, Y. L. Dokshitzer, M. Seymour and B. Webber, *Longitudinally invariant K_t clustering algorithms for hadron hadron collisions*, Nucl. Phys. B **406** (1993), [187–224](#).
- [65] T. Gleisberg, S. Höche, F. Krauss, A. Schälicke, S. Schumann and J. Winter, *Sherpa 1.0, a proof-of-concept version*, JHEP **02** (2004), [056](#), [[hep-ph/0311263](#)].
- [66] F. Krauss, R. Kuhn and G. Soff, *AMEGIC++ 1.0: A Matrix Element Generator In C++*, JHEP **02** (2002), [044](#), [[hep-ph/0109036](#)].
- [67] S. Jones and S. Kuttimalai, *Parton Shower and NLO-Matching uncertainties in Higgs Boson Pair Production*, JHEP **02** (2018), [176](#), [[arXiv:1711.03319](#) [hep-ph]].
- [68] F. Cascioli, P. Maierhofer and S. Pozzorini, *Scattering Amplitudes with Open Loops*, Phys. Rev. Lett. **108** (2012), [111601](#), [[arXiv:1111.5206](#) [hep-ph]].
- [69] M. Cacciari, G. P. Salam and G. Soyez, *The anti- k_t jet clustering algorithm*, JHEP **04** (2008), [063](#), [[arXiv:0802.1189](#) [hep-ph]].
- [70] P. Nason and B. Webber, *Next-to-Leading-Order Event Generators*, Ann. Rev. Nucl. Part. Sci. **62** (2012), [187–213](#), [[arXiv:1202.1251](#) [hep-ph]].
- [71] T. Sjostrand, S. Mrenna and P. Z. Skands, *PYTHIA 6.4 Physics and Manual*, JHEP **05** (2006), [026](#), [[arXiv:hep-ph/0603175](#) [hep-ph]].
- [72] P. Nason, *A New method for combining NLO QCD with shower Monte Carlo algorithms*, JHEP **11** (2004), [040](#), [[arXiv:hep-ph/0409146](#) [hep-ph]].
- [73] S. Hoeche and M. Schonherr, *Uncertainties in next-to-leading order plus parton shower matched simulations of inclusive jet and dijet production*, Phys. Rev. **D86** (2012), [094042](#), [[arXiv:1208.2815](#) [hep-ph]].
- [74] S. Hoeche, F. Krauss, M. Schonherr and F. Siegert, *A critical appraisal of NLO+PS matching methods*, JHEP **09** (2012), [049](#), [[arXiv:1111.1220](#) [hep-ph]].
- [75] S. Höche, S. Schumann and F. Siegert, *Hard photon production and matrix-element parton-shower merging*, Phys. Rev. **D81** (2010), [034026](#), [[arXiv:0912.3501](#) [hep-ph]].
- [76] S. Platzer and M. Sjodahl, *The Sudakov Veto Algorithm Reloaded*, Eur. Phys. J. Plus **127** (2012), [26](#), [[arXiv:1108.6180](#) [hep-ph]].
- [77] S. Höche and S. Prestel, *The midpoint between dipole and parton showers*, Eur. Phys. J. C **75** (2015), no. 9, [461](#), [[arXiv:1506.05057](#) [hep-ph]].
- [78] S. Alioli, P. Nason, C. Oleari and E. Re, *A general framework for implementing NLO calculations in shower Monte Carlo programs: the POWHEG BOX*, JHEP **06** (2010), [043](#), [[arXiv:1002.2581](#) [hep-ph]].

Acknowledgement

I like to thank Frank Siegert for his supervising this thesis, proofreading part of it and giving me the opportunity to do it in the first place. Many thanks go also to Stefan Höche for innumerable hours of discussion and many helpful advises. I am grateful to my colleagues in the Emmy Noether group and the institute for always being helpful and providing a pleasant atmosphere. I owe special thanks to my wife for continuous support in my doings.

Erklärung

Hiermit versichere ich, dass ich die vorliegende Arbeit ohne unzulässige Hilfe Dritter und ohne Benutzung anderer als der angegebenen Hilfsmittel angefertigt habe; die aus fremden Quellen direkt oder indirekt übernommenen Gedanken sind als solche kenntlich gemacht. Die Arbeit wurde bisher weder im Inland noch im Ausland in gleicher oder ähnlicher Form einer anderen Prüfungsbehörde vorgelegt.

Ich betone, dass diese Dissertation auf gemeinsamer Forschungsarbeit mit Stefan Höche und Frank Siegert basiert. Dies trifft insbesondere auf Kapitel 4 zu, welches größtenteils aus Textpassagen folgender gemeinsamer Publikation besteht:

- Stefan Höche, Sebastian Liebschner and Frank Siegert
“*Resonance-Aware Subtraction in the Dipole Method*”
Eur. Phys. J. C, vol. 79, no. 9, p. 728, 2019; archiv: 1807.04348 [hep-ph]

Ich versichere hiermit, federführend an dem Entstehen dieser Publikation gewirkt zu haben. Die Arbeit wurde unter Betreuung von Dr. Frank Siegert am Institut für Kern- und Teilchenphysik erstellt.

Es fanden keine früheren Promotionsverfahren statt. Ich erkenne die Promotionsordnung des Bereichs Mathematik und Naturwissenschaften vom 23.02.2011 an.

Sebastian Liebschner
Dresden, 26. Mai 2020