PHYSICAL REVIEW D **76,** 094003 (2007)

Parton showers from the dipole formalism

Michael Dinsdale, Marko Ternick, and Stefan Weinzierl

Institut für Physik, Universität Mainz, D-55099 Mainz, Germany

(Received 11 September 2007; published 2 November 2007)

We present an implementation of a parton shower algorithm for hadron colliders and electron-positron colliders based on the dipole factorization formulas. The algorithm treats initial-state partons on equal footing with final-state partons. We implemented the algorithm for massless and massive partons.

DOI: 10.1103/PhysRevD.76.094003 PACS numbers: 13.85.Hd, 13.66.Bc

I. INTRODUCTION

Event generators like Pythia [1,2], Herwig [3,4] or Sherpa [5] are a standard tool in high energy particle physics. In these tools the physics of particle collisions is modeled by a simulation with different stages—hard scattering, parton showering, hadronization—to name the most important ones. The hard scattering process is calculable in perturbation theory. The same holds—in theory at least—for the parton showering process, the relevant scales are still large enough for perturbation theory to be applicable. In practice, however, one is forced into approximations due to the large parton multiplicities. These approximations are derived from the behavior of the matrix elements in singular regions. The matrix elements become singular in phase space regions corresponding to the emission of collinear or soft particles. The first showering algorithms started from the collinear factorization of the matrix elements and approximated color interference effects through angular ordering [6,7]. An exception is the algorithm implemented in Ariadne [8–12], which is based on a dipole cascade picture. Most shower algorithms are in the collinear limit accurate to the leading-logarithmic approximation. Extensions to the next-to-leading logarithmic approximation have been studied in [13–16].

Recent years have witnessed significant developments related to shower algorithms, including procedures to match parton showers to fixed-order tree-level matrix elements [17–21] and methods to combine parton showers with next-to-leading-order (NLO) matrix elements [22–45]. The shower algorithms in Pythia, Herwig, and Ariadne have been improved [46–48] and new programs like the shower module Apacic ++ [49,50] of Sherpa have become available. Other improvements include the study of uncertainties in parton showers [51–53], as well as showers in the context of the soft-collinear effective theory [54].

Of particular importance is the matching of parton showers with next-to-leading-order matrix elements. The pioneering project MC@NLO [31,55–58] used an existing shower program (Herwig) and adapted the NLO calculation to the shower algorithm, at the expense of sacrificing the correctness in certain soft limits. It is clear that a better but more labor-intensive approach would adapt the shower algorithm to NLO calculations. Nowadays in NLO computations the dipole subtraction method [59–63] is widely used. Nagy and Soper [35,36] proposed to build a shower algorithm from the dipole subtraction terms.

In this paper we report on an implementation of a shower algorithm based on the dipole formalism as suggested by Nagy and Soper. We take the dipole splitting functions as the splitting functions which generate the parton shower. In the dipole formalism, a dipole consists of an emitter-spectator pair, which emits a third particle, soft or collinear to the emitter. The formalism treats initial- and final-state partons on the same footing. In contrast to other shower algorithms, no distinction is made between final- and initial-state showers. The only difference between initial- and final-state particles occurs in the kinematics. In the implementation we have the four cases final-final, final-initial, initial-final, and initial-initial corresponding to the possibilities of the particles of the emitter-spectator pair to be in the initial or final state. All four cases are included; therefore, the shower can be used for hadron colliders and electron-positron colliders. We implemented the shower for massless and massive partons. Initial-state partons are, however, always assumed to be massless. We use spin-averaged dipole splitting functions. The shower algorithm is correct in the leading-color approximation. As the evolution variable we use the transverse momentum in the massless case, and a variable suggested in [47,64] for the massive case. The variable for the massive case reduces to the transverse momentum in the massless limit. Schumann and Krauss report on a similar but separate implementation of a parton shower algorithm based on the dipole formalism [65].

This paper is organized as follows: In Sec. II we review basic facts about the color decomposition of QCD amplitudes and the dipole formalism. In Sec. III we discuss the shower algorithm. In Sec. IV we present numerical results from the parton shower simulation program. Finally, Sec. V contains the summary. Technical details can be found in the appendices. Appendix A discusses the case of a massless final-state emitter and a massless final-state spectator in detail. Appendix B describes the construction of the four-momenta of the $(n + 1)$-particle state in all cases. This appendix is also useful in the context of a phase space generator for the real emission part of NLO computations.

II. QCD AMPLITUDES AND THE DIPOLE FORMALISM

In this section we briefly review the color decomposition of QCD amplitudes and the dipole formalism.

A. Color decomposition

In this paper we use the normalization

$$\mathrm{Tr}\, T^a T^b = \tfrac{1}{2}\delta^{ab} \tag{1}$$

for the color matrices. Amplitudes in QCD may be decomposed into group-theoretical factors (carrying the color structures) multiplied by kinematic functions called partial amplitudes [66–70]. The partial amplitudes are gauge-invariant objects. In the pure gluonic case tree-level amplitudes with n external gluons may be written in the form

$$\mathcal{A}_n(1, 2, \ldots, n) = \left(\frac{g}{\sqrt{2}}\right)^{n-2} \sum_{\sigma\in S_n/Z_n} \delta_{i_{\sigma_1} j_{\sigma_2}} \delta_{i_{\sigma_2} j_{\sigma_3}} \ldots \delta_{i_{\sigma_n} j_{\sigma_1}} \times A_n(\sigma_1, \ldots, \sigma_n), \tag{2}$$

where the sum is over all noncyclic permutations of the external gluon legs. The quantities $A_n(\sigma_1, \ldots, \sigma_n)$, called the partial amplitudes, contain the kinematic information. They are color-ordered, e.g. only diagrams with a particular cyclic ordering of the gluons contribute. The choice of the basis for the color structures is not unique, and several proposals for bases can be found in the literature [71,72]. Here we use the "color-flow decomposition" [72,73]. This basis is obtained by replacing every contraction over an index in the adjoint representation by two contractions over indices i and j in the fundamental representation:

$$\begin{aligned} V^a E^a &= V^a \delta^{ab} E^b = V^a (2T^a_{ij} T^b_{ji}) E^b \\ &= (\sqrt{2} T^a_{ij} V^a)(\sqrt{2} T^b_{ji} E^b). \end{aligned} \tag{3}$$

As a further example we give the color decomposition for a tree amplitude with a pair of quarks:

$$\mathcal{A}_{n+2}(q, 1, 2, \ldots, n, \bar{q}) = \left(\frac{g}{\sqrt{2}}\right)^{n} \sum_{S_n} \delta_{i_q j_{\sigma_1}} \delta_{i_{\sigma_1} j_{\sigma_2}} \ldots \delta_{i_{\sigma_n} j_{\bar{q}}} \times A_{n+2}(q, \sigma_1, \sigma_2, \ldots, \sigma_n, \bar{q}), \tag{4}$$

where the sum is over all permutations of the gluon legs. The tree amplitude with a pair of quarks, n gluons and an additional lepton pair has the same color structure as in Eq. (4). In squaring these amplitudes a color projector

$$\delta_{\bar{i}i}\delta_{j\bar{j}} - \frac{1}{N_c}\delta_{\bar{i}\bar{j}}\delta_{ji} \tag{5}$$

has to be applied to each gluon. In these examples we have two basic color structures, a color cluster described by the "closed string"

$$\delta_{i_{\sigma_1} j_{\sigma_2}} \delta_{i_{\sigma_2} j_{\sigma_3}} \ldots \delta_{i_{\sigma_n} j_{\sigma_1}} \tag{6}$$

and a color cluster corresponding to the "open string"

$$\delta_{i_q j_{\sigma_1}} \delta_{i_{\sigma_1} j_{\sigma_2}} \ldots \delta_{i_{\sigma_n} j_{\bar{q}}}. \tag{7}$$

Born amplitudes with additional pairs of quarks have a decomposition in color factors, which are products of the two basic color clusters above. The color factors in Eqs. (2) and (4) are orthogonal to leading order in $1/N_c$.

B. The dipole formalism

The starting point for the calculation of an observable O in hadron-hadron collisions in perturbation theory is the following formula:

$$\begin{aligned} \langle O \rangle = &\int dx_1 f(x_1) \int dx_2 f(x_2) \frac{1}{2K(\hat{s})} \frac{1}{(2J_1+1)} \frac{1}{(2J_2+1)} \\ &\times \frac{1}{n_1 n_2} \int d\phi_n(p_1, p_2; p_3, \ldots, p_{n+2}) \\ &\times O(p_1, \ldots, p_{n+2}) |\mathcal{A}_{n+2}|^2. \end{aligned} \tag{8}$$

This equation gives the contribution from the n-parton final state. The two incoming particles are labeled p_1 and p_2, while p_3 to p_{n+2} denote the final-state particles. $f(x)$ gives the probability of finding a parton a with momentum fraction x inside the parent hadron h. A sum over all possible partons a is understood implicitly. $2K(s)$ is the flux factor, $1/(2J_1 + 1)$ and $1/(2J_2 + 1)$ correspond to an averaging over the initial helicities and n_1 and n_2 are the number of color degrees of the initial-state particles. $d\phi_n$ is the phase space measure for n final-state particles, including (if appropriate) the identical particle factors. The matrix element $|\mathcal{A}_{n+2}|^2$ is calculated perturbatively. At leading and next-to-leading order one has the following contributions:

$$\begin{aligned} \langle O \rangle^{LO} &= \int_n O_n d\sigma^B, \\ \langle O \rangle^{NLO} &= \int_{n+1} O_{n+1} d\sigma^R + \int_n O_n d\sigma^V + \int_n O_n d\sigma^C. \end{aligned} \tag{9}$$

Here we used a rather condensed notation. $d\sigma^B$ denotes the Born contribution, while $d\sigma^R$ denotes the real emission contribution, whose matrix element is given by the square of the Born amplitudes with $(n + 3)$ partons $|\mathcal{A}^{(0)}_{n+3}|^2$. $d\sigma^V$ gives the virtual contribution, whose matrix element is given by the interference term of the one-loop amplitude $\mathcal{A}^{(1)}_{n+2}$ with $(n + 2)$ partons with the corresponding Born amplitude $\mathcal{A}^{(0)}_{n+2}$. $d\sigma^C$ denotes a collinear subtraction term, which subtracts the initial-state collinear singularities. Within the subtraction method one constructs an approximation term $d\sigma^A$ with the same singularity structure as $d\sigma^R$. The NLO contribution is rewritten as

$$\langle O\rangle^{NLO} = \int_{n+1}(O_{n+1}d\sigma^R - O_n d\sigma^A) + \int_n\left(O_n d\sigma^V + O_n d\sigma^C + \int_1 O_n d\sigma^A\right), \quad (10)$$

such that the terms inside the two brackets are separately finite. The matrix element corresponding to the approximation term $d\sigma^A$ is given as a sum over dipoles [59–63]:

$$\sum_{\text{pairs } i,j}\sum_{k\neq i,j}\mathcal{D}_{ij,k} + \left[\sum_{\text{pairs } i,j}\mathcal{D}^a_{ij} + \sum_j\sum_{k\neq j}\mathcal{D}^{aj}_k + \sum_j \mathcal{D}^{aj,b} + (a \leftrightarrow b)\right]. \quad (11)$$

In Eq. (11) the labels i, j, and k denote final-state particles, while a and b denote initial-state particles. The first term describes dipoles where both the emitter and the spectator are in the final state. $\mathcal{D}^a_{ij}$ denotes a dipole where the emitter is in the final state, while the spectator is in the initial state. The reverse situation is denoted by $\mathcal{D}^{aj}_k$: Here the emitter is in the initial state and the spectator is in the final state. Finally, $\mathcal{D}^{aj,b}$ denotes a dipole where both the emitter and the spectator are in the initial state. The full complexity is only needed for hadron colliders; for electron-positron annihilation the subtraction terms inside the square bracket are absent. The dipole subtraction terms for a final-state emitter-spectator pair have the following form:

$$\mathcal{D}_{ij,k} = \mathcal{A}^{(0)*}_{n+2}(p_1, \ldots, \tilde{p}_{(ij)}, \ldots, \tilde{p}_k, \ldots)\frac{(-\mathbf{T}_k\cdot\mathbf{T}_{ij})}{\mathbf{T}^2_{ij}} \times \frac{V_{ij,k}}{2p_i\cdot p_j}\mathcal{A}^{(0)}_{n+2}(p_1, \ldots, \tilde{p}_{(ij)}, \ldots, \tilde{p}_k, \ldots). \quad (12)$$

The structure of the dipole subtraction terms with initial-state partons is similar. Here $\mathbf{T}_i$ denotes the color charge operator for parton i and $V_{ij,k}$ is a matrix in the spin space of the emitter parton (ij). In general, the operators $\mathbf{T}_i$ lead to color correlations, while the $V_{ij,k}$'s lead to spin correlations. The color charge operators $\mathbf{T}_i$ for a quark, gluon, and antiquark in the final state are

$$\begin{aligned} &\text{quark}: \ \mathcal{A}^*(\ldots q_i\ldots)(T^a_{ij})\mathcal{A}(\ldots q_j\ldots),\\ &\text{gluon}: \ \mathcal{A}^*(\ldots g^c\ldots)(if^{cab})\mathcal{A}(\ldots g^b\ldots),\\ &\text{antiquark}: \ \mathcal{A}^*(\ldots \bar{q}_i\ldots)(-T^a_{ji})\mathcal{A}(\ldots \bar{q}_j\ldots).\end{aligned} \quad (13)$$

The corresponding color charge operators for a quark, gluon, and antiquark in the initial state are

$$\begin{aligned} &\text{quark}: \ \mathcal{A}^*(\ldots \bar{q}_i\ldots)(-T^a_{ji})\mathcal{A}(\ldots \bar{q}_j\ldots),\\ &\text{gluon}: \ \mathcal{A}^*(\ldots g^c\ldots)(if^{cab})\mathcal{A}(\ldots g^b\ldots),\\ &\text{antiquark}: \ \mathcal{A}^*(\ldots q_i\ldots)(T^a_{ij})\mathcal{A}(\ldots q_j\ldots).\end{aligned} \quad (14)$$

In the amplitude an incoming quark is denoted as an outgoing antiquark and vice versa.

In this paper we neglect spin correlations and work to leading order in $1/N_c$. Therefore we replace the splitting functions $V_{ij,k}$ by the spin-averaged splitting functions:

$$V_{ij,k} \to \langle V_{ij,k}\rangle. \quad (15)$$

In the leading-color approximation we only have to take into account emitter-spectator pairs, which are adjacent inside a color cluster. For those pairs we obtain for the color charge operators

$$\frac{(-\mathbf{T}_k\cdot\mathbf{T}_{ij})}{\mathbf{T}^2_{ij}} = \begin{cases} 1/2 & \text{emitter } (ij) \text{ is a gluon,}\\ 1 & \text{emitter } (ij) \text{ is a quark or antiquark.}\end{cases} \quad (16)$$

We introduce the notation

$$\begin{aligned} \mathcal{P}_{ij,k} &= \frac{\langle V_{ij,k}\rangle}{(p_i+p_j)^2 - m^2_{ij}}\cdot\theta(\langle V_{ij,k}\rangle),\\ \mathcal{P}_{ij,a} &= \frac{\langle V^a_{ij}\rangle}{(p_i+p_j)^2 - m^2_{ij}}\cdot\frac{1}{x}\cdot\theta(\langle V^a_{ij}\rangle),\\ \mathcal{P}_{aj,k} &= \frac{\langle V^{aj}_k\rangle}{|2p_a\cdot p_j|}\cdot\frac{1}{x}\cdot\theta(\langle V^{aj}_k\rangle),\\ \mathcal{P}_{aj,b} &= \frac{\langle V^{aj,b}\rangle}{|2p_a\cdot p_j|}\cdot\frac{1}{x}\cdot\theta(\langle V^{aj,b}\rangle).\end{aligned} \quad (17)$$

The functions $\mathcal{P}$ will govern the emission of additional particles in the shower algorithm. The spin-averaged dipole splitting functions $\langle V\rangle$ can be found in [59,63]. The Heaviside theta functions ensure that the functions $\mathcal{P}$ will be nonnegative. They are needed for splittings between an initial- and a final-state particle, since the dipole splitting functions $\langle V^a_{ij}\rangle$ and $\langle V^{aj}_k\rangle$ may take negative values in certain regions of phase space. In addition, the spin-averaged dipole splitting functions for massive partons are slightly modified: Terms related to the soft singularity are rearranged between the two dipoles forming an antenna, in order to ensure positivity of the individual dipole splitting functions in the singular limit.

III. THE SHOWER ALGORITHM

In this section we describe the shower algorithm. We first discuss the color treatment in Sec. III A. The shower algorithm for massless final-state partons is discussed in Sec. III B. The necessary modifications for initial-state partons are discussed in Sec. III C. Finally, massive partons are discussed in Sec. III D.

A. Color treatment

Before starting the parton showers, the partons from the hard matrix element have to be assigned to color clusters. For the simplest matrix elements, like $e^+e^- \to q\bar{q}$, the choice is unique: The quark-antiquark pair forms a color cluster. For the parton shower we work in the leading-color approximation. In the leading-color approximation we have to take into account only emitter-spectator pairs, which are adjacent inside a color cluster. We have implemented two options: In the first one, which we call the "strict leading-color approximation," we take exactly the terms which are leading in an expansion in $1/N_c$ and only those. As a consequence, all splittings $g \to q\bar{q}$ are ignored, as they are color-suppressed compared to $g \to gg$. In this approximation C_F is replaced by

$$C_F \to \tfrac{3}{2}. \tag{18}$$

For the second option, which we call the "modified leading-color approximation," we include the splitting $g \to q\bar{q}$ and keep C_F as $(N_c^2 - 1)/2/N_c$. In this case, if a gluon in a closed string splits into a quark-antiquark pair, the closed string becomes an open string. If a gluon in an open string splits into a quark-antiquark pair, the open string splits into two open strings.

B. The shower algorithm for massless final-state partons

We first describe the shower algorithm for electron-positron annihilation. The extension to initial-state partons is treated in Sec. III C. For the shower algorithm we use as an evolution variable

$$t = \ln \frac{-k_\perp^2}{Q^2}, \tag{19}$$

where Q^2 is a fixed reference scale and $k_\perp$ is the transverse momentum of a splitting. During the shower evolution we move towards smaller (more negative) values of t. We start from a given n-parton configuration. In the dipole formalism, emission of additional partons is described by an emitter-spectator pair. In the leading-color approximation emitter and spectator are always adjacent in the cyclic order. The probability to evolve from t_1 to t_2 (with $t_1 > t_2$) without any resolvable branching is given by the Sudakov factor. For the algorithm considered here, the Sudakov factor is given as a product of factors corresponding to the no-emission probabilities for individual dipoles' emissions:

$$\Delta(t_1, t_2) = \prod_{\tilde{i},\tilde{k}} \Delta_{\tilde{i},\tilde{k}}(t_1, t_2). \tag{20}$$

If parton $\tilde{i}$ can emit different partons, $\Delta_{\tilde{i},\tilde{k}}(t_1, t_2)$ factorizes in turn into different contributions:

$$\Delta_{\tilde{i},\tilde{k}}(t_1, t_2) = \prod_j \Delta_{ij,k}(t_1, t_2). \tag{21}$$

An example is the possibility of a gluon to split either into two gluons or into a $\bar{q}q$ pair. We denote the emitter before the splitting by $\tilde{i}$, while the emitter after a splitting is denoted by i. This notation takes into account that the emitter might change its "flavour" due to a splitting, like in the case of a $g \to \bar{q}q$ splitting. $\Delta_{ij,k}(t_1, t_2)$ is the probability that the dipole formed by the emitter $\tilde{i}$ and spectator $\tilde{k}$ does not emit a parton j. It is given by

$$\Delta_{ij,k}(t_1, t_2) = \exp\left(-\int_{t_2}^{t_1} dt \mathcal{C}_{\tilde{i},\tilde{k}} \times \int d\phi_{\text{unres}} \delta(t - T_{\tilde{i},\tilde{k}}) \mathcal{P}_{ij,k}\right), \tag{22}$$

where $\mathcal{C}_{\tilde{i},\tilde{k}}$ is a color factor. In the leading color approximation this factor is nonzero only if $\tilde{i}$ and $\tilde{k}$ are adjacent in a color cluster. Then $\mathcal{C}_{\tilde{i},\tilde{k}}$ is obtained from Eq. (16) and given by

$$C_{\tilde{i},\tilde{k}} = \begin{cases} \frac{1}{2} & \text{for } \tilde{i} = g, \\ 1 & \text{for } \tilde{i} = q, \bar{q}. \end{cases} \tag{23}$$

The dipole phase space is given by

$$\int d\phi_{\text{unres}} = \frac{(p_{\tilde{i}} + p_{\tilde{k}})^2}{16\pi^2} \int_0^1 d\kappa \int_{z_-(\kappa)}^{z_+(\kappa)} dz \frac{1}{4z(1-z)} \times \left(1 - \frac{\kappa}{4z(1-z)}\right), \tag{24}$$

with

$$z_\pm(\kappa) = \tfrac{1}{2}(1 \pm \sqrt{1-\kappa}). \tag{25}$$

The variable κ is proportional to the transverse momentum of the splitting

$$\kappa = 4 \frac{(-k_\perp^2)}{(p_{\tilde{i}} + p_{\tilde{k}})^2}. \tag{26}$$

$T_{\tilde{i},\tilde{k}}$ depends on the dipole invariant mass $(p_{\tilde{i}} + p_{\tilde{k}})^2$ and the phase space variable κ for the emission of an additional particle and is given by

$$T_{\tilde{i},\tilde{k}} = \ln \frac{\kappa}{4} \frac{(p_{\tilde{i}} + p_{\tilde{k}})^2}{Q^2}. \tag{27}$$

With the help of the delta-function we may perform the integration over κ, while keeping the integration over t and z. Then

$$\kappa(t) = \frac{4Q^2 e^t}{(p_{\tilde{i}} + p_{\tilde{k}})^2}. \tag{28}$$

$\mathcal{P}_{ij,k}$ is the dipole splitting function. As an example we quote the splitting function for the $q \to qg$ splitting:

$$\mathcal{P}_{q\to qg} = C_F \frac{8\pi\alpha_s(\mu^2)}{(p_{\tilde{i}} + p_{\tilde{k}})^2} \frac{1}{y} \left[\frac{2}{1 - z(1-y)} - (1+z)\right], \quad y = \frac{\kappa(t)}{4z(1-z)}. \tag{29}$$

α_s is evaluated at the scale $\mu^2 = -k_\perp^2 = \frac{\kappa}{4}(p_{\tilde{i}} + p_{\tilde{k}})^2$. The probability that a branching occurs at t_2 is given by

$$\sum_{\tilde{i},\tilde{k}} \sum_{j} \mathcal{C}_{\tilde{i},\tilde{k}} \int d\phi_{\text{unres}} \delta(t_2 - T_{\tilde{i},\tilde{k}}) \mathcal{P}_{ij,k} \Delta(t_1, t_2). \quad (30)$$

We can now state the shower algorithm. Starting from an initial evolution scale t_1 we proceed as follows:

(1) Select the next dipole to branch and the scale t_2 at which this occurs. This is done as follows: For each dipole we generate the scale $t_{2,ij,k}$ of the next splitting for this dipole from a uniformly distributed number $r_{1,ij,k}$ in [0, 1] by solving (numerically) the equation

$$\Delta_{ij,k}(t_1, t_{2,ij,k}) = r_{1,ij,k}. \quad (31)$$

We then set

$$t_2 = \max(t_{2,ij,k}). \quad (32)$$

The dipole which has the maximal value of $t_{2,ij,k}$ is the one which radiates off an additional particle.

(2) If t_2 is smaller than a cutoff scale $t_{\min}$, the shower algorithm terminates.

(3) Next we have to generate the value of z. Again, using a uniformly distributed random number r_2 in [0, 1] we solve

$$\int_{z_-(t_2)}^{z} dz' J(t_2, z') \mathcal{P}_{ij,k} = r_2 \int_{z_-(t_2)}^{z_+(t_2)} dz' J(t_2, z') \mathcal{P}_{ij,k}, \quad (33)$$

where the Jacobian factor $J(t_2, z)$ is given by

$$J(t_2, z) = \frac{\kappa(t_2)}{4z(1-z)} \left(1 - \frac{\kappa(t_2)}{4z(1-z)}\right). \quad (34)$$

(4) Select the azimuthal angle ϕ. Finally we generate the azimuthal angle from a uniformly distributed number r_3 in [0, 1] as follows:

$$\phi = 2\pi r_3. \quad (35)$$

(5) With the three kinematical variables t_2, z, and ϕ and the information, that parton $\tilde{i}$ emits a parton j, with parton $\tilde{k}$ being the spectator, we insert the new parton j. The momenta $p_{\tilde{i}}$ and $p_{\tilde{k}}$ of the emitter and the spectator are replaced by new momenta p_i and p_k. The details of how the momenta p_i, p_j, and p_k are constructed are given in Appendix B.

(6) Set $t_1 = t_2$ and go to step 1.

Remark: Step 1 of the algorithm is equivalent to first generating the point t_2 from a uniformly distributed number r_1 in [0, 1] by solving (numerically) the equation for the full Sudakov factor

$$\Delta(t_1, t_2) = r_1, \quad (36)$$

and then selecting an individual dipole with emitter $\tilde{i}$, emitted particle j, and spectator k with probability [74]

$$P_{ij,k} = \frac{\mathcal{C}_{\tilde{i},\tilde{k}} \int d\phi_{\text{unres}} \delta(t_2 - T_{\tilde{i},\tilde{k}}) \mathcal{P}_{ij,k}}{\sum_{\tilde{l},\tilde{n}} \sum_{m} \mathcal{C}_{\tilde{l},\tilde{n}} \int d\phi_{\text{unres}} \delta(t_2 - T_{\tilde{l},\tilde{n}}) \mathcal{P}_{lm,n}}. \quad (37)$$

C. The shower algorithm with initial-state partons

In this subsection we discuss the necessary modifications for the inclusion of initial-state partons. In the presence of initial-state partons there is no separation into final-state showers and initial-state showers. Initial-state radiation is treated on the same footing as final-state radiation. The algorithm generates initial-state radiation through backward evolution, starting from a hard scale and moving towards softer scales. Therefore the shower evolves in all cases from a hard scale towards lower scales.

1. Final-state emitter and initial-state spectator

For an initial-state spectator we modify the Sudakov factor in Eq. (22) to

$$\Delta_{ij,a}(t_1, t_2) = \exp\left(-\int_{t_2}^{t_1} dt \mathcal{C}_{\tilde{i},\tilde{a}} \int d\phi_{\text{unres}} \delta(t - T_{\tilde{i},\tilde{a}}) \times \frac{x_a f(x_a, t)}{x_{\tilde{a}} f(x_{\tilde{a}}, t)} \mathcal{P}_{ij,a}\right), \quad (38)$$

where $x_{\tilde{a}}$ is the momentum fraction of the initial hadron carried by $\tilde{a}$, while x_a is the momentum fraction carried by a. The initial parton of the n-particle state is denoted by $\tilde{a}$, while the initial parton of the $(n+1)$-particle state is denoted by a. We set

$$x = \frac{x_{\tilde{a}}}{x_a}. \quad (39)$$

The unresolved phase space is given by

$$\int d\phi_{\text{unres}} = \frac{|2p_{\tilde{i}} p_{\tilde{a}}|}{16\pi^2} \int_{x_{\tilde{a}}}^{1} \frac{dx}{x} \int_0^1 dz. \quad (40)$$

The transverse momentum between i and j is expressed as

$$-k_\perp^2 = \frac{(1-x)}{x} z(1-z)(-2p_{\tilde{i}} p_{\tilde{a}}) \quad (41)$$

and $T_{\tilde{i},\tilde{a}}$ is therefore given by

$$T_{\tilde{i},\tilde{a}} = \ln \frac{-k_\perp^2}{Q^2} = \ln \frac{(-2p_{\tilde{i}} p_{\tilde{a}})(1-x)z(1-z)}{xQ^2}. \quad (42)$$

A subtlety occurs for the emission between a final-state spectator and an initial-state emitter. We discuss this for the splitting $q \to qg$. The spin-averaged splitting function for the $q \to qg$ splitting is given by

$$\langle V^k_{qg} \rangle = 8\pi\alpha_s C_F \left[\frac{2}{1-z+(1-x)} - (1+z) \right]. \tag{43}$$

In contrast to the final-final case this function is not a positive function on the complete phase space. It can take negative values in certain (nonsingular) regions of phase space. This is no problem for its use as a subtraction terms in NLO calculations, but prohibits a straightforward interpretation as a splitting probability for a shower algorithm. However, since negative values occur only in nonsingular regions, we can ensure positiveness by modifying the splitting functions through nonsingular terms. The simplest choice is to set

$$\mathcal{P}_{ij,a} = \frac{\langle V^a_{ij} \rangle}{(p_i + p_j)^2} \cdot \frac{1}{x} \cdot \theta(\langle V^a_{ij} \rangle). \tag{44}$$

For a final-state emitter we eliminate the x-integration with the help of the delta function:

$$\int_{x_{\tilde{a}}}^1 \frac{dx}{x} \delta(t - T_{\tilde{i},\tilde{a}}) = \frac{1}{1 + \frac{4z(1-z)}{\kappa(t)}}, \qquad x = \frac{1}{1 + \frac{\kappa(t)}{4z(1-z)}}, \qquad \kappa(t) = \frac{4Q^2 e^t}{(-2p_{\tilde{i}} p_{\tilde{a}})}. \tag{45}$$

For the boundaries we obtain

$$\kappa(t) < \frac{1 - x_{\tilde{a}}}{x_{\tilde{a}}}, \qquad z_-(t) < z < z_+(t), \qquad z_\pm(t) = \frac{1}{2}\left(1 \pm \sqrt{1 - \kappa(t)\frac{x_{\tilde{a}}}{1 - x_{\tilde{a}}}}\right). \tag{46}$$

The modifications to the shower algorithm are as follows: The dipoles for the emission from a final-state emitter with an initial-state spectator are included in the Sudakov factor in Eq. (20). With this modification steps 1 and 2 are as above. Let us define

$$f_{lm,n} = \begin{cases} 1, & \text{if } l \text{ and } n \text{ are final-state particles,} \\ \frac{x_a f(x_a,t)}{x_{\tilde{a}} f(x_{\tilde{a}},t)}, & \text{if } l = a \text{ is an initial-state particle,} \\ \frac{x_b f(x_b,t)}{x_{\tilde{b}} f(x_{\tilde{b}},t)}, & \text{if } n = b \text{ is an initial-state particle and } l \text{ is a final-state particle.} \end{cases} \tag{47}$$

In step 3 we replace formula (33) by

$$\int_{z_-(t_2)}^{z} dz' J(t_2, z') f_{ij,a} \mathcal{P}_{ij,a} = r_2 \int_{z_-(t_2)}^{z_+(t_2)} dz' J(t_2, z') f_{ij,a} \mathcal{P}_{ij,a}, \tag{48}$$

with the Jacobian

$$J(t,z) = \frac{1}{1 + \frac{4z(1-z)}{\kappa(t)}}. \tag{49}$$

Steps 4 to 6 proceed as in the case described above.

2. Initial-state emitter and final-state spectator

For an initial-state emitter $\tilde{a}$ with a final-state spectator $\tilde{i}$ the Sudakov factor is given by

$$\Delta_{aj,i}(t_1, t_2) = \exp\left(- \int_{t_2}^{t_1} dt \mathcal{C}_{\tilde{a},\tilde{i}} \int d\phi_{\text{unres}} \delta(t - T_{\tilde{a},\tilde{i}}) \times \frac{x_a f(x_a, t)}{x_{\tilde{a}} f(x_{\tilde{a}}, t)} \mathcal{P}_{aj,i} \right). \tag{50}$$

The unresolved phase space is again given by Eq. (40). The transverse momentum between a and j is given by

$$-k_\perp^2 = \frac{(1-x)}{x}(1-z)(-2p_{\tilde{i}} p_{\tilde{a}}) \tag{51}$$

and $T_{\tilde{a},\tilde{i}}$ is given by

$$T_{\tilde{a},\tilde{i}} = \ln \frac{(-2p_{\tilde{i}} p_{\tilde{a}})(1-x)(1-z)}{xQ^2}. \tag{52}$$

For an initial-state emitter we eliminate the z-integration with the help of the delta function:

$$\int_0^1 dz \delta(t - T_{\tilde{a},\tilde{i}}) = \frac{\kappa(t)}{4} \frac{x}{(1-x)}, \qquad z = 1 - \frac{\kappa(t)}{4} \frac{x}{(1-x)}, \qquad \kappa(t) = \frac{4Q^2 e^t}{(-2p_{\tilde{i}} p_{\tilde{a}})}. \tag{53}$$

For the boundaries we obtain

$$\kappa(t) < 4\frac{1 - x_{\tilde{a}}}{x_{\tilde{a}}}, \qquad x < x_+(t), \qquad x_+(t) = \frac{1}{1 + \frac{\kappa(t)}{4}}. \tag{54}$$

There are no new modifications to the shower algorithms compared to the case for a final-state emitter and an initial-state spectator, except that in step 3 we now generate the value of x according to

$$\int_{x_{\tilde{a}}}^{x} dx' J(t_2, x') f_{aj,i} \mathcal{P}_{aj,i} = r_2 \int_{x_{\tilde{a}}}^{x_+(t_2)} dx' J(t_2, x') f_{aj,i} \mathcal{P}_{aj,i}, \tag{55}$$

with the Jacobian

$$J(t,x) = \frac{\kappa(t)}{4(1-x)}. \tag{56}$$

3. Initial-state emitter and initial-state spectator

For an initial-state emitter $\tilde{a}$ with an initial-state spectator $\tilde{b}$ the Sudakov factor is given by

$$\Delta_{aj,b}(t_1,t_2) = \exp\left(-\int_{t_2}^{t_1} dt \mathcal{C}_{\tilde{a},\tilde{b}} \int d\phi_{\text{unres}} \delta(t - T_{\tilde{a},\tilde{b}}) \times \frac{x_a f(x_a,t)}{x_{\tilde{a}} f(x_{\tilde{a}},t)} \mathcal{P}_{aj,b}\right). \tag{57}$$

In this case we do not rescale the momentum of the spectator, but transform all final-state momenta. Therefore no factor

$$\frac{x_b f(x_b,t)}{x_{\tilde{b}} f(x_{\tilde{b}},t)} \tag{58}$$

appears in the Sudakov factor. The unresolved phase space is given by

$$\int d\phi_{\text{unres}} = \frac{|2p_{\tilde{a}}p_{\tilde{b}}|}{16\pi^2} \int_{x_{\tilde{a}}}^1 \frac{dx}{x} \int_0^{1-x} dv. \tag{59}$$

The transverse momentum between a and j is given by

$$-k_\perp^2 = \frac{(1-x)}{x} v(2p_{\tilde{a}}p_{\tilde{b}}) \tag{60}$$

and $T_{\tilde{a},\tilde{b}}$ is given by

$$T_{\tilde{a},\tilde{b}} = \ln \frac{(2p_{\tilde{a}}p_{\tilde{b}})(1-x)v}{xQ^2}. \tag{61}$$

We integrate over v with the help of the delta-function:

$$\begin{gathered} \int_0^{1-x} dv \delta(t - T_{\tilde{a},\tilde{b}}) = \frac{\kappa(t)}{4} \frac{x}{(1-x)}, \\ v = \frac{\kappa(t)}{4} \frac{x}{(1-x)}, \qquad \kappa(t) = \frac{4Q^2 e^t}{(2p_{\tilde{a}}p_{\tilde{b}})}. \end{gathered} \tag{62}$$

For the boundaries we obtain

$$\begin{gathered} \kappa(t) < 4\frac{(1-x_{\tilde{a}})^2}{x_{\tilde{a}}}, \qquad x < x_+(t), \\ x_+(t) = \frac{1}{2}\left(2 + \frac{\kappa(t)}{4} - \sqrt{\kappa(t) + \frac{\kappa(t)^2}{16}}\right). \end{gathered} \tag{63}$$

In step 3 of the shower algorithm we again select x according to

$$\int_{x_{\tilde{a}}}^{x} dx' J(t_2,x') f_{aj,b} \mathcal{P}_{aj,b} = r_2 \int_{x_{\tilde{a}}}^{x_+(t_2)} dx' J(t_2,x') f_{aj,b} \mathcal{P}_{aj,b}, \tag{64}$$

with the Jacobian

$$J(t,x) = \frac{\kappa(t)}{4(1-x)}. \tag{65}$$

D. The shower algorithm for massive partons

In this subsection we discuss the modifications of the shower algorithms due to the presence of massive partons. We first address the issue of a splitting of a gluon into a heavy quark pair. This mainly concerns the splitting of a gluon into b-quarks. We will always require that initial-state particles are massless. Therefore for processes with initial-state hadrons we do not consider $g \to Q\bar{Q}$ splittings. Calculations for initial-state hadrons should be done in the approximation of a massless b-quark. In the case of electron-positron annihilation the parton shower affects only the final state. Here we can consistently allow splittings of a gluon into a pair of massive quarks. As an evolution variable we use in the massive case

$$t = \ln \frac{-k_\perp^2 + (1-z)^2 m_i^2 + z^2 m_j^2}{Q^2}. \tag{66}$$

This choice reduces to Eq. (19) in the massless limit and is suggested by dispersion relations for the running coupling [47,64].

1. Final-state emitter and final-state spectator

The unresolved phase space is given by

$$\int d\phi_{\text{unres}} = \frac{(p_{\tilde{i}} + p_{\tilde{k}})^2}{16\pi^2}(1-\mu_i^2-\mu_j^2-\mu_k^2)^2 \times [\lambda(1,\mu_{ij}^2,\mu_k^2)]^{-(1/2)} \int_{y_-}^{y_+} dy(1-y) \times \int_{z_-(y)}^{z_+(y)} dz, \tag{67}$$

where the reduced masses μ_l and the boundaries on the integrations are defined in Appendix B in Eqs. (B18)–(B21). $T_{\tilde{i},\tilde{k}}$ is given by

$$T_{\tilde{i},\tilde{k}} = \ln \frac{((p_{\tilde{i}} + p_{\tilde{k}})^2 - m_i^2 - m_j^2 - m_k^2) yz(1-z)}{Q^2}. \tag{68}$$

Again, we have to ensure that the splitting functions are positive. The original spin-averaged dipole splitting functions can take negative values in certain regions of phase space. In the massive case the negative region can extend into the singular region. The problem is related to the soft behavior of the dipole splitting functions. Since a squared Born matrix element is positive in the soft gluon limit, the negative contribution from a particular dipole is compensated by the contribution from the dipole, where emitter and spectator are exchanged. The sum of the two contributions is positive in the singular region. Therefore we can cut out the negative region from the first dipole and add it to the second dipole. The second dipole will stay positive.

As in the massless case we eliminate the y-integration:

$$\int_{y_-}^{y_+} dy(1-y)\int_{z_-(y)}^{z_+(y)} dz\delta(t - T_{\tilde{i},\tilde{k}}) = \int_{z_{\min}}^{z_{\max}} dzy(1-y),$$
$$y = \frac{\kappa(t)}{4z(1-z)}, \qquad \kappa(t) = \frac{4Q^2 e^t}{(p_{\tilde{i}} + p_{\tilde{k}})^2 - m_i^2 - m_j^2 - m_k^2}. \tag{69}$$

The physical region is defined by

$$\left(1 - \frac{\kappa}{4z(1-z)}\right)^2\left[\frac{\kappa}{4} - (1-z)^2\bar{m}_i^2 - z^2\bar{m}_j^2\right] - \left(\frac{\kappa}{4z(1-z)}\right)^2\bar{m}_k^2 + 4\bar{m}_i^2\bar{m}_j^2\bar{m}_k^2 \geq 0, \tag{70}$$

with

$$\bar{m}_l^2 = \frac{m_l^2}{(p_{\tilde{i}} + p_{\tilde{k}})^2 - m_i^2 - m_j^2 - m_k^2} \quad \text{for } l \in \{i, j, k\}. \tag{71}$$

This equation is solved numerically for $z_{\min}$ and $z_{\max}$. Then z is generated according to

$$\int_{z_{\min}(t_2)}^{z} dz' J(t_2, z')\mathcal{P}_{ij,k} = r_2 \int_{z_{\min}(t_2)}^{z_{\max}(t_2)} dz' J(t_2, z')\mathcal{P}_{ij,k}, \tag{72}$$

with the Jacobian

$$J(t,z) = (1 - \mu_i^2 - \mu_j^2 - \mu_k^2)^2[\lambda(1, \mu_{ij}^2, \mu_k^2)]^{-(1/2)} \times \frac{\kappa(t)}{4z(1-z)}\left(1 - \frac{\kappa(t)}{4z(1-z)}\right). \tag{73}$$

2. Final-state emitter and initial-state spectator

The unresolved phase space is given by

$$\int d\phi_{\text{unres}} = \frac{|2p_{\tilde{i}}p_{\tilde{a}}|}{16\pi^2}\int_{x_{\tilde{a}}}^{1}\frac{dx}{x}\int_{z_-(x)}^{1} dz = \frac{|2p_{\tilde{i}}p_{\tilde{a}}|}{16\pi^2}\int_{z_-(x_{\tilde{a}})}^{1} dz \int_{x_{\tilde{a}}}^{x_+(z)}\frac{dx}{x}. \tag{74}$$

The integration boundary is given by

$$z_-(x) = \frac{x\tilde{\mu}^2}{1 - x(1-\tilde{\mu}^2)}, \qquad x_+(z) = \frac{z}{\tilde{\mu}^2 + z(1-\tilde{\mu}^2)}, \qquad \tilde{\mu}^2 = \frac{m_i^2}{|2p_{\tilde{i}}p_{\tilde{a}}|}. \tag{75}$$

$T_{\tilde{i},\tilde{a}}$ is given by

$$T_{\tilde{i},\tilde{a}} = \ln\frac{-k_\perp^2 + (1-z)^2 m_i^2}{Q^2} = \ln\frac{(-2p_{\tilde{i}}p_{\tilde{a}})(1-x)z(1-z)}{xQ^2}. \tag{76}$$

For a final-state emitter we eliminate the x-integration with the help of the delta function:

$$\int_{x_{\tilde{a}}}^{1}\frac{dx}{x}\delta(t - T_{\tilde{i},\tilde{a}}) = \frac{1}{1 + \frac{4z(1-z)}{\kappa(t)}},$$
$$x = \frac{1}{1 + \frac{\kappa(t)}{4z(1-z)}}, \qquad \kappa(t) = \frac{4Q^2 e^t}{(-2p_{\tilde{i}}p_{\tilde{a}})}. \tag{77}$$

For the boundaries we obtain

$$z_+(t) = \frac{1}{2}\left(1 + \sqrt{1 - \kappa(t)\frac{x_{\tilde{a}}}{1 - x_{\tilde{a}}}}\right),$$
$$z_-(t) = \max\left(\frac{x_{\tilde{a}}\tilde{\mu}^2}{1 - x_{\tilde{a}}(1-\tilde{\mu}^2)}, \frac{1}{2}\left(1 - \sqrt{1 - \kappa(t)\frac{x_{\tilde{a}}}{1 - x_{\tilde{a}}}}\right), 1 - \sqrt{\frac{\kappa(t)}{4\tilde{\mu}^2}}\right). \tag{78}$$

The boundary on $\kappa(t)$ is given for $\tilde{\mu}^2 < (1 - x_{\tilde{a}})/x_{\tilde{a}}$ by

$$\kappa(t) < \frac{1 - x_{\tilde{a}}}{x_{\tilde{a}}}. \tag{79}$$

For $(1 - x_{\tilde{a}})/x_{\tilde{a}} < \tilde{\mu}^2$ we have

$$\kappa(t) < \frac{1 - x_{\tilde{a}}}{x_{\tilde{a}}}\left[1 - \left(\frac{1 - \frac{1 - x_{\tilde{a}}}{x_{\tilde{a}}\tilde{\mu}^2}}{1 + \frac{1 - x_{\tilde{a}}}{x_{\tilde{a}}\tilde{\mu}^2}}\right)^2\right] = \frac{4\tilde{\mu}^2}{(1 + \frac{x_{\tilde{a}}\tilde{\mu}^2}{1 - x_{\tilde{a}}})^2}. \tag{80}$$

z is generated according to

$$\int_{z_-(t_2)}^{z} dz' J(t_2, z') f_{ij,a}\mathcal{P}_{ij,a} = r_2 \int_{z_-(t_2)}^{z_+(t_2)} dz' J(t_2, z') f_{ij,a}\mathcal{P}_{ij,a}, \tag{81}$$

with the Jacobian

$$J(t,z) = \frac{1}{1 + \frac{4z(1-z)}{\kappa(t)}}. \tag{82}$$

3. Initial-state emitter and final-state spectator

$T_{\tilde{a},\tilde{i}}$ is given by

$$T_{\tilde{a},\tilde{i}} = \ln\frac{(-2p_{\tilde{i}}p_{\tilde{a}})(1-x)(1-z)}{xQ^2}. \tag{83}$$

For an initial-state emitter we eliminate the z-integration with the help of the delta function:

$$\int_{z_-(x)}^{1} dz \delta(t - T_{\tilde{a},\tilde{i}}) = \frac{\kappa(t)}{4} \frac{x}{(1-x)},$$
$$z = 1 - \frac{\kappa(t)}{4} \frac{x}{(1-x)}, \qquad \kappa(t) = \frac{4Q^2 e^t}{(-2p_{\tilde{i}} p_{\tilde{a}})}. \tag{84}$$

For the boundaries we obtain

$$\kappa(t) < \frac{4(1-x_{\tilde{a}})^2}{x_{\tilde{a}}[1 - x_{\tilde{a}}(1-\tilde{\mu}^2)]}, \qquad x < x_+(t),$$
$$x_+(t) = \frac{2 + \frac{\kappa(t)}{4} - \sqrt{\frac{\kappa(t)^2}{16} + \tilde{\mu}^2 \kappa(t)}}{2(1 + \frac{\kappa(t)}{4}(1-\tilde{\mu}^2))}. \tag{85}$$

The value of x is generated according to

$$\int_{x_{\tilde{a}}}^{x} dx' J(t_2, x') f_{aj,i} \mathcal{P}_{aj,i} = r_2 \int_{x_{\tilde{a}}}^{x_+(t_2)} dx' J(t_2, x') f_{aj,i} \mathcal{P}_{aj,i}, \tag{86}$$

with the Jacobian

$$J(t, x) = \frac{\kappa(t)}{4(1-x)}. \tag{87}$$

IV. NUMERICAL RESULTS

In this section we show numerical results obtained from the parton shower. We first discuss in Sec. IV A observables related to electron-positron annihilation and then in Sec. IV B the shower in hadron collisions. The shower algorithm depends on two parameters, the strong coupling α_s and the scale $Q_{\min}$. For the strong coupling we use the leading-order formula

$$\alpha_s(\mu) = \frac{4\pi}{\beta_0 \ln\frac{\mu^2}{\Lambda^2}}, \qquad \beta_0 = 11 - \frac{2}{3}N_f. \tag{88}$$

The cutoff scale $Q_{\min}$ gives the scale at which the shower terminates. As our shower is correct in the leading-color approximation, we also study the effects of different treatments of subleading color contributions. As described in Sec. III A we have implemented two options: The strict leading-color approximation and the modified leading-color approximation. Numerical differences from these two options will give an estimate of uncertainties due to subleading-color effects.

A. Electron-positron annihilation

For electron-positron annihilation we use $\alpha_s(m_Z) = 0.118$ corresponding to $\Lambda_5 = 88$ MeV. We start the shower from the $2 \to 2$ hard matrix element $e^+e^- \to q\bar{q}$. We first study the event shape variables thrust, the C-parameter and the D-parameter. The distributions of the first moments of these observables are shown in Fig. 1 for two choices of the cutoff parameter: $Q_{\min} = 1$ GeV and $Q_{\min} = 2$ GeV. The distributions are normalized to unity. The different prescriptions for the color-treatment do not change the distributions significantly. In Fig. 2 we show the distributions for the four-jet angles. Again we start from the $2 \to 2$ hard matrix element. The particles in an event are first clustered into jets, defined according to the Durham algorithm [75] with $y_{\mathrm{cut}} = 0.008$ and the E-scheme for the recombination. Then events with exactly four jets are selected. We consider the modified Nachtmann-Reiter angle [76], the Körner-Schierholz-Willrodt angle [77], the Bengtsson-Zerwas angle [78],

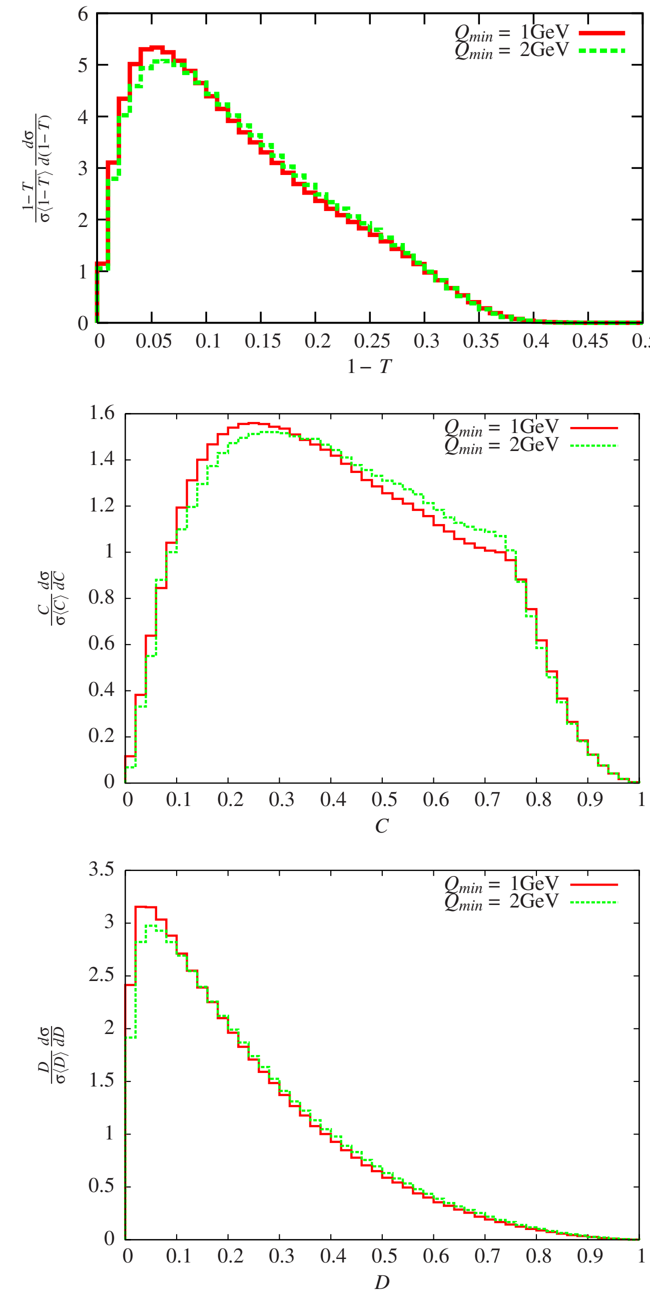

FIG. 1 (color online). The first moments of the thrust distribution, the C-parameter distribution and the D-parameter distribution. The results are from the parton shower for two different values of the cutoff scale $Q_{\min}$.

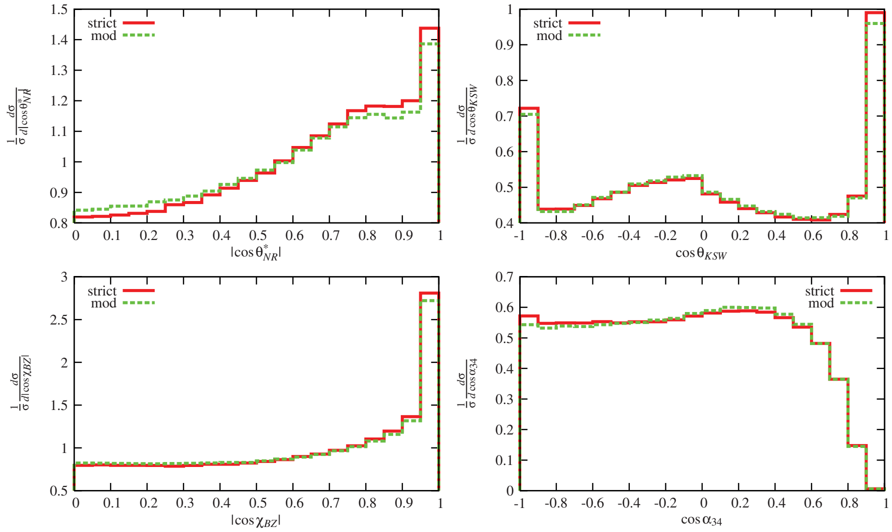

FIG. 2 (color online). The distributions for the four-jet angles. From top left to bottom right: The modified Nachtmann-Reiter angle, the Körner-Schierholz-Willrodt angle, the Bengtsson-Zerwas angle, and the angle α_{34} between the smallest energy jets. As cutoff parameter $Q_{\min} = 1$ GeV is used. Shown are the result from the "strict leading-color approximation" and the "modified leading-color approximation."

and the angle α_{34} between the jets with the smallest energy [79]. In the plots we show the results from the different options for the color treatment for $Q_{\min} = 1$ GeV. A variation of the cutoff scale does not change the distributions significantly.

B. Hadron colliders

For the Tevatron and the LHC we study Z/γ^*-production. We start from the $2 \to 2$ hard matrix element $q\bar{q} \to Z/\gamma^* \to l^+l^-$. As parton distribution functions we use the CTEQ 6L1 set [80,81]. For consistency we

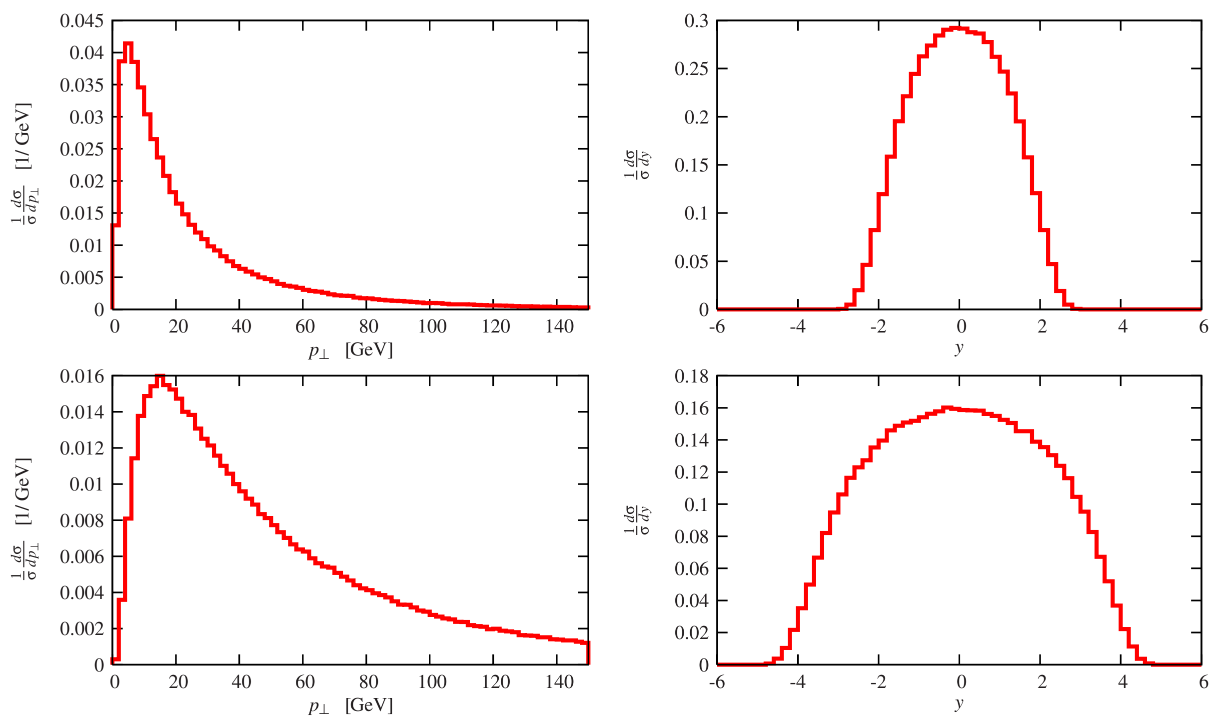

FIG. 3 (color online). The transverse momentum distribution and the rapidity distribution of the lepton pair for Z/γ^*-production for the Tevatron and the LHC. As cutoff parameter $Q_{\min} = 1$ GeV is used.

use here $\alpha_s(m_Z) = 0.130$ corresponding to $\Lambda_5 = 165$ MeV. The center-of-mass energy we set to $\sqrt{s} = 1.96$ TeV for the Tevatron and to $\sqrt{s} = 14$ TeV for the LHC. We require a cut on the invariant mass of the lepton pair of

$$m_{l^+l^-} > 80 \text{ GeV}. \tag{89}$$

As cutoff parameter for the parton shower we use $Q_{\min} = 1$ GeV. In Fig. 3 we show the transverse momentum distribution and the rapidity distribution of the lepton pair for the Tevatron and the LHC.

V. SUMMARY

In this paper we presented an implementation of a shower algorithm based on the dipole formalism. The formalism treats initial- and final-state partons on the same footing. The shower can be used for hadron colliders and electron-positron colliders. We also included in the shower algorithm massive partons in the final state. We studied numerical results for electron-positron annihilation, the Tevatron and the LHC.

ACKNOWLEDGMENTS

We would like to thank Zoltan Nagy for discussions and useful comments on the manuscript.

APPENDIX A: SUDAKOV FACTORS FOR MASSLESS FINAL-STATE PARTONS

In this appendix we discuss in more detail the Sudakov factors for massless final-state partons. This case is simple enough that one integration can be done analytically. The spin-averaged dipole subtraction terms in four dimensions are

$$\begin{aligned}
\mathcal{P}_{q\to qg} &= C_F \frac{8\pi\alpha_s(\mu^2)}{s_{ijk}} \frac{1}{y}\left[\frac{2}{1-z(1-y)} - (1+z)\right],\\
\mathcal{P}_{g\to gg} &= C_A \frac{8\pi\alpha_s(\mu^2)}{s_{ijk}} \frac{1}{y}\left[\frac{2}{1-z(1-y)} \right.\\
&\quad \left. + \frac{2}{1-(1-z)(1-y)} - 4 + 2z(1-z)\right],\\
\mathcal{P}_{g\to q\bar{q}} &= T_R \frac{8\pi\alpha_s(\mu^2)}{s_{ijk}} \frac{1}{y}[1-2z(1-z)],
\end{aligned} \tag{A1}$$

with

$$s_{ijk} = (p_i + p_j + p_k)^2 = (p_{\tilde{i}} + p_{\tilde{k}})^2. \tag{A2}$$

The dipole phase space measure is

$$\int d\phi_{\text{unres}} = \frac{s_{ijk}}{16\pi^2}\int_0^1 d\kappa \int_{z_-(\kappa)}^{z_+(\kappa)} dz \frac{1}{4z(1-z)} \times \left(1 - \frac{\kappa}{4z(1-z)}\right), \tag{A3}$$

with

$$z_\pm(\kappa) = \tfrac{1}{2}(1 \pm \sqrt{1-\kappa}). \tag{A4}$$

The strong coupling is evaluated at the scale $\mu^2 = -k_\perp^2$:

$$\alpha_s(\mu^2) = \alpha_s\left(\frac{1}{4}\kappa s_{ijk}\right). \tag{A5}$$

The Sudakov factor is given by

$$\Delta_{ij,k}(t_1, t_2) = \exp\left(-\int_{t_2}^{t_1} dt \mathcal{C}_{\tilde{i},\tilde{k}} \int d\phi_{\text{unres}} \times \delta(t - T_{\tilde{i},\tilde{k}})\mathcal{P}_{ij,k}\right). \tag{A6}$$

For the splitting $q \to qg$ we obtain

$$\Delta_{ij,k}(t_1, t_2) = \exp\left\{-\mathcal{C}_{\tilde{i},\tilde{k}} C_F \int_{\kappa_-}^{\kappa_+} \frac{d\kappa}{\kappa}\frac{\alpha_s(\mu^2)}{2\pi}\int_{z_-(\kappa)}^{z_+(\kappa)} dz \times (1-y)\left[\frac{2}{1-z(1-y)} - (1+z)\right]\right\}, \tag{A7}$$

with

$$\begin{aligned}
\kappa_- &= 4\frac{Q^2}{s_{ijk}}e^{t_2}, \qquad \kappa_+ = \min\left(1, 4\frac{Q^2}{s_{ijk}}e^{t_1}\right),\\
y &= \frac{\kappa}{4z(1-z)}, \qquad \mu^2 = \frac{1}{4}\kappa s_{ijk}.
\end{aligned} \tag{A8}$$

The integration over z can be done analytically:

$$\begin{aligned}
&\int dz(1-y)\left[\frac{2}{1-z(1-y)} - (1+z)\right]\\
&= -\frac{1}{2}z^2 - z + \frac{\kappa}{4}[\ln z - 2\ln(1-z)] - \frac{4}{4+\kappa}\left[\frac{1}{2}\kappa\ln z \right.\\
&\quad \left. + \ln(\kappa + 4(1-z)^2) + \sqrt{\kappa}\arctan\left(\frac{2}{\sqrt{\kappa}}(1-z)\right)\right].
\end{aligned} \tag{A9}$$

The same holds for the other splittings. Therefore we obtain for the Sudakov factors

$$\Delta_{ij,k}(t_1, t_2) = \exp\left\{-\mathcal{C}_{\tilde{i},\tilde{k}} C \int_{\kappa_-}^{\kappa_+}\frac{d\kappa}{\kappa}\frac{\alpha_s(\frac{1}{4}\kappa s_{ijk})}{2\pi} \times (\mathcal{V}_{ij,k}(\kappa, z_+) - \mathcal{V}_{ij,k}(\kappa, z_-))\right\}, \tag{A10}$$

where C is a color factor and equal to

$$C = \begin{cases} C_F & \text{for } q \to qg,\\ C_A & \text{for } g \to gg,\\ T_R & \text{for } g \to q\bar{q}. \end{cases} \tag{A11}$$

The functions $\mathcal{V}_{ij,k}(\kappa, z)$ are given by

$$\mathcal{V}_{qg,k}(\kappa, z) = -\frac{1}{2}z^2 - z + \frac{\kappa}{4}[\ln z - 2\ln(1-z)] - \frac{4}{4+\kappa}\left[\frac{1}{2}\kappa \ln z + \ln(\kappa + 4(1-z)^2) - \sqrt{\kappa}\arctan\left(\frac{2}{\sqrt{\kappa}}(1-z)\right)\right],$$

$$\mathcal{V}_{gg,k}(\kappa, z) = -\frac{2}{3}z^3 + z^2 - 4z - \frac{1}{2}\kappa z + \kappa \ln\frac{z}{1-z} + \frac{4}{4+\kappa}\left[\frac{1}{2}\kappa \ln\frac{1-z}{z} + \ln\frac{\kappa + 4z^2}{\kappa + 4(1-z)^2} - \sqrt{\kappa}\arctan\left(\frac{2z}{\sqrt{\kappa}}\right) + \sqrt{\kappa}\arctan\left(\frac{2(1-z)}{\sqrt{\kappa}}\right)\right],$$

$$\mathcal{V}_{gq,k}(\kappa, z) = \frac{2}{3}z^3 - z^2 + z + \frac{\kappa}{2}z - \frac{\kappa}{4}\ln\frac{z}{1-z}. \tag{A12}$$

APPENDIX B: INSERTION OF EMITTED PARTICLES

In this appendix we list the relevant formulas for the insertion of one additional four-vector into a set of n four-vectors. This insertion satisfies momentum conservation and can be considered as the inverse of the $(n+1) \to n$ phase space mapping of Catani and Seymour. These insertion mappings are also useful for an efficient phase space integration of the real emission contribution in NLO calculations. Therefore we quote in addition the relevant phase space weights. For the shower algorithm, these weights are not needed, as they are taken into account through the generation of the shower.

1. Insertion for final-state particles

a. The massless case

We start with the simplest case, where both the emitter and the spectator are in the final state and all particles involved in the dipole splitting are massless. The insertion procedure is identical to the one used in [82]. Given the four-vectors $\tilde{p}_{ij}$ and $\tilde{p}_k$ together with the three variables y, z, and ϕ_s we would like to construct p_i, p_j, and p_k, such that

$$p_i + p_j + p_k = \tilde{p}_{ij} + \tilde{p}_k, \qquad p_i^2 = p_j^2 = p_k^2 = 0. \tag{B1}$$

In four dimensions we have for the phase space measure

$$d\phi_{\text{unres}} = \frac{s_{ijk}}{32\pi^3}\int_0^1 dy(1-y)\int_0^1 dz \int_0^{2\pi} d\phi_s, \tag{B2}$$

where $s_{ijk} = (\tilde{p}_{ij} + \tilde{p}_k)^2 = (p_i + p_j + p_k)^2$. It is convenient to work in the rest frame of $P = \tilde{p}_{ij} + \tilde{p}_k = p_i + p_j + p_k$. We shall orient the frame in such a way, that the spatial components of $\tilde{p}_k$ are along the z direction. When used as a phase space generator we set

$$y = u_1, \qquad z = u_2 \qquad \phi_s = 2\pi u_3, \tag{B3}$$

where u_1, u_2, and u_3 are three uniformly distributed random numbers in [0, 1]. From

$$y = \frac{s_{ij}}{s_{ij} + s_{ik} + s_{jk}}, \qquad z = \frac{s_{ik}}{s_{ik} + s_{jk}} \tag{B4}$$

we obtain

$$s_{ij} = yP^2, \qquad s_{ik} = z(1-y)P^2, \qquad s_{jk} = (1-z)(1-y)P^2. \tag{B5}$$

If $s_{ij} < s_{jk}$ we want to have $p_k' \to p_k$ as $s_{ij} \to 0$. Define

$$E_i = \frac{s_{ij} + s_{ik}}{2\sqrt{s_{ijk}}}, \qquad E_j = \frac{s_{ij} + s_{jk}}{2\sqrt{s_{ijk}}}, \qquad E_k = \frac{s_{ik} + s_{jk}}{2\sqrt{s_{ijk}}}, \tag{B6}$$

$$\theta_{ik} = \arccos\left(1 - \frac{s_{ik}}{2E_iE_k}\right), \qquad \theta_{jk} = \arccos\left(1 - \frac{s_{jk}}{2E_jE_k}\right). \tag{B7}$$

In our coordinate system we have

$$p_i' = E_i(1, \sin\theta_{ik}\cos(\phi_s + \pi), \sin\theta_{ik}\sin(\phi_s + \pi), \cos\theta_{ik}),$$
$$p_j' = E_j(1, \sin\theta_{jk}\cos\phi_s, \sin\theta_{jk}\sin\phi_s, \cos\theta_{jk}),$$
$$p_k' = E_k(1, 0, 0, 1). \tag{B8}$$

The momenta p_i', p_j', and p_k' are related to the momenta p_i, p_j, and p_k by a sequence of Lorentz transformations back to the original frame

$$p_i = \Lambda_{\text{boost}}\Lambda_{xy}(\phi)\Lambda_{xz}(\theta)p_i' \tag{B9}$$

and analogously for the other two momenta. The explicit formulas for the Lorentz transformations are obtained as follows: Let $|P| = \sqrt{(\tilde{p}_{ij} + \tilde{p}_k)^2}$ and denote by $\hat{p}_k$ the coordinates of the hard momentum $\tilde{p}_k$ in the center of mass system of $\tilde{p}_{ij} + \tilde{p}_k$. $\hat{p}_k$ is given by

$$\hat{p}_k = \left(\frac{E_P}{|P|}\tilde{E}_k - \frac{\vec{\tilde{p}}_k \cdot \vec{P}}{|P|}, \vec{\tilde{p}}_k + \left(\frac{\vec{\tilde{p}}_k \cdot \vec{P}}{|P|(E_P + |P|)} - \frac{\tilde{E}_k}{|P|}\right)\vec{P}\right). \tag{B10}$$

The angles are then given by

$$\theta = \arccos\left(\frac{2\hat{E}_kE_k' - 2\hat{p}_k \cdot p_k'}{2|\vec{\hat{p}}_k||\vec{p}_k'|}\right), \qquad \phi = \arctan\left(\frac{\hat{p}_k^y}{\hat{p}_k^x}\right). \tag{B11}$$

For the case considered here particle k is massless and the formula for θ reduces to

$$\theta = \arccos\left(1 - \frac{2\hat{p}_k \cdot p'_k}{2\hat{p}^t_k p^{t'}_k}\right). \tag{B12}$$

The explicit form of the rotations is

$$\Lambda_{xz}(\theta) = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & \cos\theta & 0 & \sin\theta \\ 0 & 0 & 1 & 0 \\ 0 & -\sin\theta & 0 & \cos\theta \end{pmatrix}, \quad \Lambda_{xy}(\phi) = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & \cos\phi & -\sin\phi & 0 \\ 0 & \sin\phi & \cos\phi & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}. \tag{B13}$$

The boost $p = \Lambda_{\mathrm{boost}} q$ is given by

$$p = \left(\frac{E_P}{|P|}E_q + \frac{\vec{q}\cdot\vec{P}}{|P|}, \vec{q} + \left(\frac{\vec{q}\cdot\vec{P}}{|P|(E_P + |P|)} + \frac{E_q}{|P|}\right)\vec{P}\right). \tag{B14}$$

The weight is given by

$$w = \frac{s_{ijk}}{16\pi^2}(1-y). \tag{B15}$$

b. The massive case

We now consider the case of final-state particles with arbitrary masses:

$$\tilde{p}^2_{ij} = m^2_{ij}, \quad p^2_i = m^2_i, \quad p^2_j = m^2_j, \quad \tilde{p}^2_k = p^2_k = m^2_k. \tag{B16}$$

The dipole phase space reads [63]

$$d\phi_{\mathrm{unres}} = \frac{s_{ijk}}{32\pi^3}(1 - \mu_i^2 - \mu_j^2 - \mu_k^2)^2[\lambda(1, \mu_{ij}^2, \mu_k^2)]^{-(1/2)} \times \int_{y_-}^{y_+} dy(1-y)\int_{z_-}^{z_+} dz \int_0^{2\pi} d\phi_s, \tag{B17}$$

where

$$s_{ijk} = (\tilde{p}_{ij} + \tilde{p}_k)^2, \quad \mu_l = \frac{m_l}{\sqrt{s_{ijk}}}, \quad \lambda(x,y,z) = x^2 + y^2 + z^2 - 2xy - 2yz - 2zy. \tag{B18}$$

The integration boundaries are given by

$$y_+ = 1 - \frac{2\mu_k(1-\mu_k)}{1 - \mu_i^2 - \mu_j^2 - \mu_k^2}, \quad y_- = \frac{2\mu_i\mu_j}{1 - \mu_i^2 - \mu_j^2 - \mu_k^2}, \tag{B19}$$

$$z_\pm = \frac{2\mu_i^2 + (1 - \mu_i^2 - \mu_j^2 - \mu_k^2)y}{2[\mu_i^2 + \mu_j^2 + (1 - \mu_i^2 - \mu_j^2 - \mu_k^2)y]} \times (1 \pm v_{ij,i} v_{ij,k}). \tag{B20}$$

The general formula for the relative velocities is $v_{p,q} = \sqrt{1 - p^2q^2/(pq)}$. In our case the relative velocities are given by

$$v_{ij,k} = \frac{\sqrt{[2\mu_k^2 + (1 - \mu_i^2 - \mu_j^2 - \mu_k^2)(1-y)]^2 - 4\mu_k^2}}{(1 - \mu_i^2 - \mu_j^2 - \mu_k^2)(1-y)}, \quad v_{ij,i} = \frac{\sqrt{(1 - \mu_i^2 - \mu_j^2 - \mu_k^2)^2 y^2 - 4\mu_i^2\mu_j^2}}{(1 - \mu_i^2 - \mu_j^2 - \mu_k^2)y + 2\mu_i^2}. \tag{B21}$$

For the phase space generation we set

$$y = (y_+ - y_-)u_1 + y_-, \quad z = (z_+ - z_-)u_2 + z_-, \quad \phi_s = 2\pi u_3. \tag{B22}$$

We again work in the rest frame of $P = \tilde{p}_{ij} + \tilde{p}_k = p_i + p_j + p_k$, such that the spatial components of $\tilde{p}_k$ are along the z direction:

$$\tilde{p}_{ij} = (\tilde{E}_{ij}, 0, 0, -|\vec{\tilde{p}}_k|), \quad \tilde{p}_k = (\tilde{E}_k, 0, 0, |\vec{\tilde{p}}_k|). \tag{B23}$$

For the invariants we have

$$2p_ip_j = y(P^2 - m_i^2 - m_j^2 - m_k^2), \quad 2p_ip_k = z(1-y)(P^2 - m_i^2 - m_j^2 - m_k^2), \quad 2p_jp_k = (1-z)(1-y)(P^2 - m_i^2 - m_j^2 - m_k^2). \tag{B24}$$

The invariants are related to y and z as follows:

$$y = \frac{2p_ip_j}{2p_ip_j + 2p_ip_k + 2p_jp_k}, \quad z = \frac{2p_ip_k}{2p_ip_k + 2p_jp_k}. \tag{B25}$$

In our chosen frame

$$p'_i = |\vec{p}_i|\left(\frac{E_i}{|\vec{p}_i|}, \sin\theta_{ik}\cos(\phi_s + \pi), \sin\theta_{ik}\sin(\phi_s + \pi), \cos\theta_{ik}\right), \quad p'_j = |\vec{p}_j|\left(\frac{E_j}{|\vec{p}_j|}, \sin\theta_{jk}\cos\phi_s, \sin\theta_{jk}\sin\phi_s, \cos\theta_{jk}\right), \quad p'_k = |\vec{p}_k|\left(\frac{E_k}{|\vec{p}_k|}, 0, 0, 1\right). \tag{B26}$$

The energies are obtained from the invariants as follows:

$$E_i = \frac{s_{ijk} - 2p_jp_k + m_i^2 - m_j^2 - m_k^2}{2\sqrt{s_{ijk}}}, \quad E_j = \frac{s_{ijk} - 2p_ip_k - m_i^2 + m_j^2 - m_k^2}{2\sqrt{s_{ijk}}}, \quad E_k = \frac{s_{ijk} - 2p_ip_j - m_i^2 - m_j^2 + m_k^2}{2\sqrt{s_{ijk}}}. \tag{B27}$$

For the angles we have

$$\theta_{ik} = \arccos\left(\frac{2E_iE_k - 2p_ip_k}{2|\vec{p}_i||\vec{p}_k|}\right),$$
$$\theta_{jk} = \arccos\left(\frac{2E_jE_k - 2p_jp_k}{2|\vec{p}_j||\vec{p}_k|}\right). \quad \text{(B28)}$$

The momenta p'_i, p'_j, and p'_k are related to the momenta p_i, p_j, and p_k by the same sequence of Lorentz transformations as in Eq. (B9). The weight is

$$w = \frac{s_{ijk}}{16\pi^2}(1 - \mu_i^2 - \mu_j^2 - \mu_k^2)^2[\lambda(1, \mu_{ij}^2, \mu_k^2)]^{-(1/2)} \times (1-y)(y_+ - y_-)(z_+ - z_-). \quad \text{(B29)}$$

2. Insertion for an antenna between an initial state and a final state

a. The massless case

Here the $(n+1)$-particle phase space is given by a convolution:

$$d\phi_{n+1} = \int_0^1 dx\, d\phi_n(xp_a)\, d\phi_{\text{dipole}}. \quad \text{(B30)}$$

The dipole phase space reads:

$$d\phi_{\text{dipole}} = \frac{|2\tilde{p}_{ij}p_a|}{32\pi^3}\int_0^1 dz \int_0^{2\pi} d\phi_s. \quad \text{(B31)}$$

The angle ϕ_s parametrizes the solid angle perpendicular to $\tilde{p}_{ij}$ and xp_a. Therefore we can treat the case of a final-state emitter with an initial-state spectator as well as the case of an initial-state emitter with a final-state spectator at the same time. x and z are related to the invariants as follows:

$$x = \frac{-2p_ip_a - 2p_jp_a - 2p_ip_j}{-2p_ip_a - 2p_jp_a},$$
$$z = \frac{-2p_ip_a}{-2p_ip_a - 2p_jp_a}. \quad \text{(B32)}$$

For the phase space generation we set

$$x = 1 - u_1, \qquad z = u_2, \qquad \phi_s = 2\pi u_3. \quad \text{(B33)}$$

We denote $Q = \tilde{p}_{ij} + xp_a = p_i + p_j + p_a$. It is convenient to work in the rest frame of $P = p_i + p_j = Q - p_a$ and to orient the frame such that p_a is along the z axis. For the invariants we have

$$2p_ip_j = (-Q^2)\frac{1-x}{x}, \qquad 2p_ip_a = \frac{z}{x}Q^2,$$
$$2p_jp_a = \frac{1-z}{x}Q^2. \quad \text{(B34)}$$

In this frame

$$p'_i = E_i(1, \sin\theta_{ia}\cos\phi_s, \sin\theta_{ia}\sin\phi_s, \cos\theta_{ia}),$$
$$p'_j = E_i(1, -\sin\theta_{ia}\cos\phi_s, -\sin\theta_{ia}\sin\phi_s, -\cos\theta_{ia}),$$
$$p'_a = (-|E_a|, 0, 0, |E_a|\text{sign}(p_a^{z\prime})). \quad \text{(B35)}$$

We have

$$E_i = \frac{1}{2}|P|, \qquad E_a = \frac{1}{|P|}(P\cdot p_a),$$
$$\theta_{ia} = \arccos\left[\text{sign}(p_a^{z\prime})\left(-1 + \frac{2p_ip_a}{2E_iE_a}\right)\right]. \quad \text{(B36)}$$

The momenta p'_i, p'_j are again related to the momenta p_i, p_j by a sequence of Lorentz transformations as in Eq. (B9). The weight is given by

$$w = \frac{|Q^2|}{16\pi^2 x}. \quad \text{(B37)}$$

b. The massive case

The dipole phase space now reads

$$d\phi_{\text{dipole}} = \frac{|2\tilde{p}_{ij}p_a|}{32\pi^3}\int_{z_-}^{z_+} dz \int_0^{2\pi} d\phi_s. \quad \text{(B38)}$$

The integration boundaries are given by

$$z_+ = 1, \qquad z_- = \frac{\mu^2}{1 - x + \mu^2}, \quad \text{(B39)}$$

where

$$\mu^2 = \frac{m_i^2}{|2\tilde{p}_{ij}p_a|} = \frac{xm_i^2}{|Q^2 - m_i^2|}. \quad \text{(B40)}$$

We consider only the case where $m_{\tilde{ij}} = m_i = m$ and all other masses are zero. For the phase space generation we set

$$x = 1 - u_1, \qquad z = (z_+ - z_-)u_2 + z_-, \qquad \phi_s = 2\pi u_3. \quad \text{(B41)}$$

For the invariants we have now

$$2p_ip_j = (-Q^2 + m_i^2)\frac{1-x}{x}, \qquad 2p_ip_a = \frac{z}{x}(Q^2 - m_i^2),$$
$$2p_jp_a = \frac{1-z}{x}(Q^2 - m_i^2). \quad \text{(B42)}$$

We parametrize the momenta as

$$p'_i = |\vec{p}_i|\left(\frac{E_i}{|\vec{p}_i|}, \sin\theta_{ia}\cos\phi_s, \sin\theta_{ia}\sin\phi_s, \cos\theta_{ia}\right),$$
$$p'_j = |\vec{p}_i|(1, -\sin\theta_{ia}\cos\phi_s, -\sin\theta_{ia}\sin\phi_s, -\cos\theta_{ia}),$$
$$p'_a = (-|E_a|, 0, 0, |E_a|\text{sign}(p_a^{z\prime})). \quad \text{(B43)}$$

Then

$$E_i = \frac{P^2 + m_i^2}{2|P|}, \qquad E_a = \frac{1}{|P|}(P \cdot p_a),$$
$$\theta_{ia} = \arccos\left[\mathrm{sign}(p_a^{z\prime}) \frac{(2E_iE_a - 2p_ip_a)}{2|\vec{p}_i|(-E_a)} \right]. \tag{B44}$$

The momenta p_i', p_j' are again related to the momenta p_i, p_j by a sequence of Lorentz transformations as in Eq. (B9). The weight is given by

$$w = \frac{|Q^2 - m_i^2|}{16\pi^2 x}(z_+ - z_-). \tag{B45}$$

3. Insertion for an initial-state antenna

Here we only have to consider the case where all particles are massless. In this case we transform all the final-state momenta. The $(n+1)$-particle phase space is given by a convolution:

$$d\phi_{n+1} = \int_0^1 dx\, d\phi_n(xp_a)\, d\phi_{\text{dipole}}. \tag{B46}$$

The dipole phase space reads:

$$d\phi_{\text{dipole}} = \frac{|2p_ap_b|}{32\pi^3} \int_0^{1-x} dv \int_0^{2\pi} d\phi_s. \tag{B47}$$

The variable v is given by

$$v = \frac{-2p_ap_i}{2p_ap_b}. \tag{B48}$$

For the phase space generation we set

$$x = 1 - u_1, \qquad v = (1-x)(1-u_2), \qquad \phi_s = 2\pi u_3. \tag{B49}$$

We denote

$$K = -p_a - p_b - p_i, \qquad \tilde{K} = -\tilde{p}_{ai} - p_b. \tag{B50}$$

We have

$$p_a = \frac{1}{x}\tilde{p}_{ai},$$
$$p_i = \Lambda_{\text{boost}} E_i(1, \sin\theta_{ia}\cos\phi_s, \sin\theta_{ia}\sin\phi_s, \cos\theta_{ia})$$
$$p_b = p_b, \tag{B51}$$

with E_i and θ_{ia} given in the rest frame of $p_a + p_b$ by

$$E_a = -\frac{1}{2}\sqrt{2p_ap_b}, \qquad E_i = \frac{\tilde{K}^2 - 2p_ap_b}{4E_a},$$
$$\theta_{ia} = \arccos\left[\mathrm{sign}(\hat{p}_a^z)\left(-1 + \frac{2p_ip_a}{2E_iE_a}\right)\right]. \tag{B52}$$

$\hat{p}_a$ denotes p_a in the rest frame of $p_a + p_b$. Λ_{boost} transforms from the rest frame of $p_a + p_b$ to the lab frame. All other final-state momenta are transformed with

$$\Lambda^{-1} = g^{\mu\nu} - 2\frac{(K+\tilde{K})^\mu (K+\tilde{K})^\nu}{(K+\tilde{K})^2} + 2\frac{K^\mu \tilde{K}^\nu}{K^2}. \tag{B53}$$

The weight is given by

$$w = \frac{|\tilde{K}^2|}{16\pi^2 x}(1-x). \tag{B54}$$

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