

Construction of a Subtraction Scheme to All Orders

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1 Introduction

In these notes, we briefly summarize all necessary ingredients of a general all order subtraction scheme.

When calculating cross sections, we typically perform phase-space integrations over amplitudes. These phase space integrations are notoriously difficult to calculate, which is why one usually falls back to numerical methods. But because the phase space integrations contain poles, a direct numerical evaluation is not straight-forward. The idea behind subtraction schemes is to subtract the infrared divergences beforehand

$$\int d\Phi_{n+n_u} \langle \mathcal{M}_{n+n_u} | \mathcal{M}_{n+n_u} \rangle = \int d\Phi_{n+n_u} [\langle \mathcal{M}_{n+n_u} | \mathcal{M}_{n+n_u} \rangle - A_{n+n_u}] + \int d\Phi_{n+n_u} A_{n+n_u} \quad (1)$$

where $|\mathcal{M}_{n+n_u}\rangle$ is the matrix element of the considered process with n_u unresolved partons as a vector in color and spin space. A_{n+n_u} is an approximation that captures all infrared singularities—that is all singularities which lead to divergent integrals—of the integrand. Now the first integral on the right hand-side of Eq. (1) will be finite and we can compute it numerically, e.g. using *Monte-Carlo* (MC) methods. The second integral on the other hand will be divergent, but because the integrand is significantly simpler, its evaluation can be achieved using quasi analytical methods. It is a well known fact that all infrared divergences factorize [1]. For example the soft divergence of the radiation of a single gluon reads,

$$A_{n+1} = 4\pi\alpha_s \sum_{i,j=1}^n \frac{\varepsilon^*(p_{n+1}, \lambda_{n+1}) \cdot p_i}{p_{n+1} \cdot p_i} \frac{\varepsilon(p_{n+1}, \lambda_{n+1}) \cdot p_j}{p_{n+1} \cdot p_j} \langle \mathcal{M}_n | \mathbf{T}_j \cdot \mathbf{T}_i | \mathcal{M}_n \rangle. \quad (2)$$

That means the functional dependence of the unresolved momenta is independent of the hard scattering process. If the phase-space can be factorized as well, the problematic integrations over infrared sensitive variables can be performed using the distributional identity

$$z^{-1+\epsilon} = \frac{1}{\epsilon} \delta(z) + \sum_{k=0}^{\infty} \frac{\epsilon^k}{k!} \left[\frac{\ln^k z}{z} \right]_+, \quad (3)$$

while all other integrations can be carried out numerically.

From the above considerations the necessary ingredients are clear, we need:

1. Approximations of all infrared limits
2. A factorization of the phase space

The first point has been addressed up to N³LO for massless QCD [2, 3, 4, 5, 6, 7, 8]. The factorization of the phase space will be discussed in section 2.

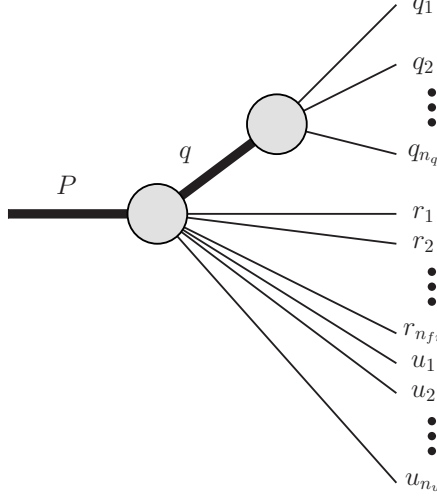


Figure 1: Pictorial representation of the phase-space factorization.

2 Phase-Space Parameterization

As discussed above, to perform the integration over the unresolved momenta, we need a factorization of the phase space. The phase-space parameterization we present here is based on Ref. [9] but generalizes the ideas to work at every order of α_s . Let us define

$$d\mu_m(k) \equiv \frac{d^d k}{(2\pi)^d} 2\pi \delta(k^2 - m^2) \theta(k^0) \equiv \frac{d^d k}{(2\pi)^d} 2\pi \delta_+(k^2 - m^2). \quad (4)$$

Then the complete phase space over $n = n_q + n_{fr} + n_u$ momenta, where n_u is the number of unresolved partons, n_{fr} the number of final state reference momenta and n_q the remaining momenta is

$$\begin{aligned} d\Phi_n &= \prod_{i=1}^{n_q} d\mu_{m_i}(q_i) \prod_{j=1}^{n_{fr}} d\mu_0(r_j) \prod_{k=1}^{n_u} d\mu_0(u_k) (2\pi)^d \delta^{(d)} \left(\sum_{i=1}^{n_q} q_i + \sum_{j=1}^{n_{fr}} r_j + \sum_{k=1}^{n_u} u_k - P \right) \\ &= \frac{dQ^2}{2\pi} d\mu_Q(q) \prod_{j=1}^{n_{fr}} d\mu_0(r_j) \prod_{k=1}^{n_u} d\mu_0(u_k) (2\pi)^d \delta^{(d)} \left(q + \sum_{j=1}^{n_{fr}} r_j + \sum_{k=1}^{n_u} u_k - P \right) \\ &\quad \times \prod_{i=1}^{n_q} d\mu_{m_i}(q_i) (2\pi)^d \delta^{(d)} \left(\sum_{i=1}^{n_q} q_i - q \right) \\ &= dQ^2 \left[\prod_{j=1}^{n_{fr}} d\mu_0(r_j) \prod_{k=1}^{n_u} d\mu_0(u_k) \delta_+ \left(\left(P - \sum_{j=1}^{n_{fr}} r_j - \sum_{k=1}^{n_u} u_k \right)^2 - Q^2 \right) \right] \\ &\quad \times \prod_{i=1}^{n_q} d\mu_{m_i}(q_i) (2\pi)^d \delta^{(d)} \left(\sum_{i=1}^{n_q} q_i - q \right). \end{aligned} \quad (5)$$

The factorization of the phase space in the resolved partons with momenta q_1, \dots, q_{n_q} and the reference + unresolved partons is pictorially depicted in Fig. 1. To truly factorize the phase-space integration of the unresolved partons, we perform a change of variables by rescaling the reference momenta

$$r_i = x_i \tilde{r}_i, \quad (6)$$

in a way to preserve the invariant mass of q

$$\begin{aligned} d\Phi_n &= dQ^2 \left[\prod_{j=1}^{n_{fr}} d\mu_0(\tilde{r}_j) \delta_+ \left(\left(P - \sum_{j=1}^{n_{fr}} \tilde{r}_j \right)^2 - Q^2 \right) \prod_{k=1}^{n_u} d\mu_0(u_k) \theta(\{u_l\} \in \mathcal{U}) \mathcal{J} \right] \\ &\quad \times \prod_{i=1}^{n_q} d\mu_{m_i}(q_i) (2\pi)^d \delta^{(d)} \left(\sum_{i=1}^{n_q} q_i - \tilde{q} \right) \end{aligned} \quad (7)$$

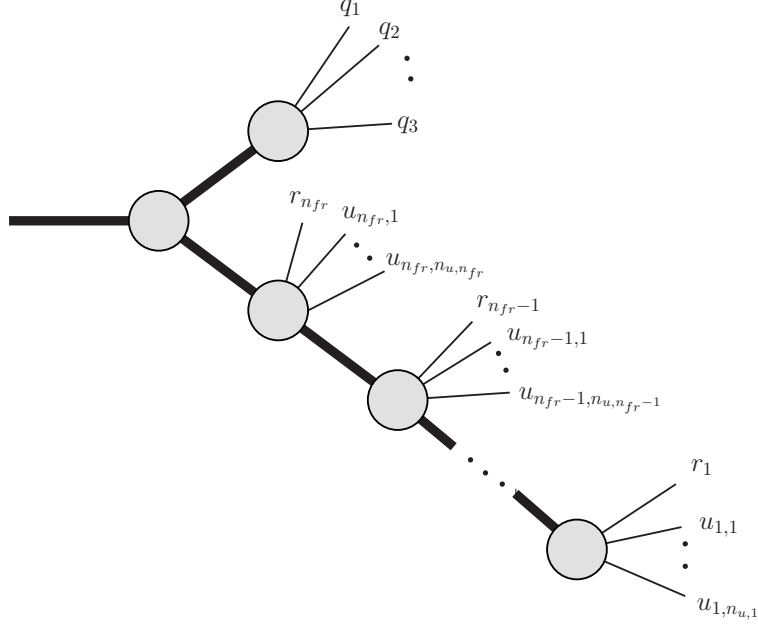


Figure 2: Pictorial representation of the rescaling procedure. Each thick line on the lower branch is rescaled in a way as to preserve the invariant mass of the line in the Born momentum configuration $\{P, \tilde{r}_j\}$ and the full momentum configuration $\{P, r_j, u_k\}$

The Heaviside-function $\theta(\{u_l\} \in \mathcal{U})$ ensures, that the boundaries of the phase-space integration of the unresolved momenta is correctly modified by the change of variables, and the Jacobian \mathcal{J} takes into account the effect on the integration measure. By changing from q to \tilde{q} without modifying the the phase-space integral over the resolved momenta q_i , we implied the existence of a Lorentz Λ , $q = \Lambda \tilde{q}$. Eq. (7) now completely decouples the integration over the unresolved momenta and the resolved momenta as we originally intended. The rescaling of the reference momenta is not unique. Ideally, we want a factorization that parameterizes the unresolved momenta with respect to one of the reference momenta. We can group the unresolved momenta according to the reference momenta it is parameterized against

$$\begin{aligned}
 r_1 &: \{u_{1,1}, \dots, u_{1,n_u,1}\} \\
 r_2 &: \{u_{2,1}, \dots, u_{2,n_u,2}\} \\
 &\vdots \\
 r_{n_{fr}} &: \{u_{n_{fr},1}, \dots, u_{n_{fr},n_u,n_{fr}}\}.
 \end{aligned} \tag{8}$$

Of course the total number of unresolved momenta remains unchanged

$$\sum_{j=1}^{n_{fr}} n_{u,j} = n_u. \tag{9}$$

Additionally, we require that in the infrared limits, either soft or colinear, the Born configuration is recovered from the full momentum configuration

$$\tilde{r}_j \longrightarrow r_j + \sum_{k=1}^{n_{u,j}} u_{j,k}. \tag{10}$$

The way to achieve this, is to rescale the momenta in a way to preserve the invariant mass square of every thick line in Fig. 2. We hence obtain a system of equations

$$\begin{aligned}
\left(P - x_1 \tilde{r}_1 - \sum_{i=1}^{n_{u,1}} u_{1,i}\right)^2 &= (P - \tilde{r}_1)^2 \\
\left(P - x_1 \tilde{r}_1 - \sum_{i=1}^{n_{u,1}} u_{1,i} - x_2 \tilde{r}_2 - \sum_{i=1}^{n_{u,2}} u_{2,i}\right)^2 &= (P - \tilde{r}_1 - \tilde{r}_2)^2 \\
&\vdots \\
\left(P - \sum_{i=1}^{n_{fr}} x_i \tilde{r}_i - \sum_{j=1}^{n_{fr}} \sum_{i=1}^{n_{u,j}} u_{j,i}\right)^2 &= \left(P - \sum_{i=1}^{n_{fr}} \tilde{r}_i\right)^2
\end{aligned} \tag{11}$$

Let us multiply out the j -th equation

$$\begin{aligned}
&-2P \cdot \sum_{i=1}^j x_i \tilde{r}_i + \sum_{i \neq k}^j x_i x_k \tilde{r}_i \cdot \tilde{r}_k - 2P \cdot \sum_{k=1}^j \sum_{i=1}^{n_{u,k}} u_{k,i} + \left(\sum_{k=1}^j \sum_{i=1}^{n_{u,k}} u_{k,i}\right)^2 + 2 \sum_{i=1}^j x_i \tilde{r}_i \cdot \sum_{k=1}^j \sum_{l=1}^{n_{u,k}} u_{k,l} \\
&= -2P \cdot \sum_{i=1}^j \tilde{r}_i + \sum_{i \neq k}^j \tilde{r}_i \cdot \tilde{r}_k
\end{aligned} \tag{12}$$

which we can then solve for x_j

$$x_j = \frac{2P \cdot (\tilde{r}_{\text{Weighted},j-1} - \tilde{r}_{\text{Tot},j} + u_{\text{Tot},j}) - (\tilde{r}_{\text{Weighted},j-1} + u_{\text{Tot},j})^2 + \tilde{r}_{\text{Tot},j}^2}{2\tilde{r}_j \cdot (\tilde{r}_{\text{Weighted},j-1} + u_{\text{Tot},j} - P)}. \tag{13}$$

Here we defined

$$u_{\text{Tot},j} = \sum_{k=1}^j \sum_{i=1}^{n_{u,k}} u_{k,i}, \quad \tilde{r}_{\text{Tot},j} = \sum_{i=1}^j \tilde{r}_i, \quad \tilde{r}_{\text{Weighted},j} = \sum_{i=1}^j x_i \tilde{r}_i. \tag{14}$$

We can therefore determine all rescaling factors recursively starting at $j = 1$. The maximum energy the a -th unresolved parton in cluster j can be reached if the reference parton in the cluster has zero energy, i.e. $x_j = 0$ and if all unresolved momenta that have not been fixed yet are zero as well $u_{j,k>a} = 0$. Let us define

$$u_{\text{Rest},j,a} \equiv u_{\text{Tot},j} - u_{j,a} \equiv \sum_{k=1}^{j-1} \sum_{l=1}^{n_{u,k}} u_{k,l} + \sum_{l=1}^{a-1} u_{j,l}. \tag{15}$$

Then the maximum energy can be determined from

$$0 = \frac{2P \cdot (\tilde{r}_{\text{Weighted},j-1} - \tilde{r}_{\text{Tot},j} + u_{\text{Rest},j,a} + u_{j,a}^{\text{Max}}) - (\tilde{r}_{\text{Weighted},j-1} + u_{\text{Rest},j,a} + u_{j,a}^{\text{Max}})^2 + \tilde{r}_{\text{Tot},j}^2}{2\tilde{r}_j \cdot (\tilde{r}_{\text{Weighted},j-1} + u_{\text{Rest},j,a} + u_{j,a}^{\text{Max}} - P)} \tag{16}$$

$$u_{j,a}^{\text{Max},0} = \frac{2P \cdot (\tilde{r}_{\text{Tot},j} - u_{\text{Rest},j,a} - \tilde{r}_{\text{Weighted},j-1}) + (u_{\text{Rest},j,a} + \tilde{r}_{\text{Weighted},j-1})^2 - \tilde{r}_{\text{Tot},j}^2}{2\tilde{u}_{j,a} \cdot (P - \tilde{r}_{\text{Weighted},j-1} - u_{\text{Rest},j,a})} \tag{17}$$

Lastly, we have to compute the Jacobian

$$\begin{aligned}
\prod_{i=1}^{n_{fr}} d\mu_0(r_i) &= \prod_{i=1}^{n_{fr}} [d\mu_0(r_i) dx_i \delta(x_i - f_{x_i}(r_i))] \\
&= \prod_{i=1}^{n_{fr}} [d\mu_0(\tilde{r}_i) dx_i x_i^{d-2} \delta(x_i - f_{x_i}(x_i \tilde{r}_i))] \\
&= \prod_{i=1}^{n_{fr}} \left[d\mu_0(\tilde{r}_i) dx_i x_i^{d-3} \left[-\frac{\partial}{\partial x_i} \frac{f_{x_i}(x_i \tilde{r}_i)}{x_i} \right]_{x_i=f_{x_i}(x_i \tilde{r}_i)}^{-1} \right].
\end{aligned} \tag{18}$$

$f_{x_i}(r_i)$ is the defining equation for x_i but expressed in terms of the full momentum configuration

$$f_{x_j}(r_j) = \frac{2r_j \cdot (r_{\text{Weighted},j-1} - P)}{2P \cdot (r_{\text{Weighted},j-1} - r_{\text{Tot},j} - u_{\text{Tot},j}) + (r_{\text{Tot},j} + u_{\text{Tot},j})^2 - r_{\text{Weighted},j-1}^2}, \tag{19}$$

where we defined

$$r_{\text{Tot},j} \equiv \sum_{i=1}^j r_i \equiv \tilde{r}_{\text{Weighted},j}, \quad r_{\text{Weighted},j} \equiv \sum_{i=1}^j \frac{1}{x_i} r_i \equiv \tilde{r}_{\text{Tot},j}. \quad (20)$$

For the Jacobian we need

$$\begin{aligned} \frac{f_{x_j}(x_j \tilde{r}_j)}{x_j} &= \frac{a}{bx_j + c} \Rightarrow \frac{\partial}{\partial x_j} \frac{f_{x_j}(x_j \tilde{r}_j)}{x_j} = -\frac{ab}{(bx_j + c)^2}, \quad \text{with} \\ a &= 2\tilde{r}_j \cdot (\tilde{r}_{\text{Tot},j} - P), \\ b &= 2\tilde{r}_j \cdot (\tilde{r}_{\text{Tot},j} - P + u_{\text{Tot},j}), \\ c &= 2P \cdot (\tilde{r}_{\text{Tot},j} - \tilde{r}_{\text{Weighted},j-1} - u_{\text{Tot},j}) + (\tilde{r}_{\text{Weighted},j-1} + u_{\text{Tot},j})^2 - \tilde{r}_{\text{Tot},j}^2. \end{aligned} \quad (21)$$

The algorithm for the generation of phase-space points is

1. generate a Born configuration;
2. generate unresolved momenta subject to constraints;
3. determine the rescaling parameters and, by the same, the full reference momenta;
4. determine the Lorentz transformation yielding q from \tilde{q} , and apply it to the final state momenta of the Born configuration;
5. multiply the weight by the Jacobian.

An important feature the phase-space parameterization needs to have is that every possible infrared limit needs to be easily expressible from the unresolved momenta, or else we can not apply Eq. (3). For example if we want to parameterize a triple-collinear limit, we can do this by generating the unresolved momenta with a small opening angle with respect to the reference momentum. Let us define the infrared sensitive variables

$$\xi = \frac{u}{u_{\text{Max},0}}, \quad \text{and} \quad \eta = \frac{u \cdot r}{2u^0 r^0}, \quad (22)$$

which parameterize the energy of the unresolved momentum and the angle with respect to the reference momentum. Both variables are in the interval $[0, 1]$ and the infrared pole is found at 0. Together with an angular variable $\phi \in [0, 1]$, we can parameterize the unresolved momenta very naturally and perform the MC integration in a simple hypercube of length 1.

Up to NLO every infrared limit can be parameterized in this manner, but starting at N³LO, we encounter divergences which can not be captured. Consider for example the triple-collinear limit: Let λ be the scale of the collinear limit. If

$$r \cdot u_1 \sim \lambda, \quad \text{and} \quad u_1 \cdot u_2 \sim \lambda^2 \quad \text{but} \quad r \cdot u_2 \sim \lambda, \quad (23)$$

then at this point we have no method of parameterizing this limit. We can fix this issue by applying our algorithm recursively. The idea is to generate momenta level by level with $1 \rightarrow 2$ splittings. Starting at the root, i.e. at some reference momentum, we generate a single unresolved momentum with our standard algorithm. Afterwards, we promote the unresolved momentum to a reference momentum. In the next step, we can allow for splittings of the original reference momentum and for a splitting of the original unresolved momentum, which is now also a reference momentum. If one of the momenta does not split anymore, then we simply treat it as a reference momenta without unresolved momenta. This procedure is repeated until we have generated all unresolved momenta. So to summarize: one simply has to generate all possible binary trees that correspond to a splitting of momenta and at each "level", we use our previous algorithm to compute the splittings of momenta, where each node corresponds to a reference momentum.

Let's consider an the example of the generation of two unresolved momenta. First we draw all possible binary trees. These can be seen in Figs. 3, 4, 5. Each tree now represents a different phase-space parameterization, and thus allows to describe a different infrared limit. In the first tree, both unresolved momenta are generated through a parameterization against a common reference momentum. We are thus able to generate soft unresolved momenta, as well as momenta collinear to the reference momentum, including any hierarchy of limits. We cannot, however, capture the hierarchy of Eq. (23). To describe this limit, we use the tree shown in Fig. 4. Here we first generate one of the unresolved momenta through a parameterization against the reference momentum, then we promote the generated unresolved momentum to a new reference momentum, and subsequently use it to parameterize the second unresolved momentum against. We note that the ordering can play a role. If for example the unresolved momenta also have a hierarchy of the energy scales, then the harder momentum must be generated first, as any unresolved momentum can only carry a fraction of the reference momentum it is generated against. Finally, if there is a double collinear limit with two reference momenta, we can use the tree displayed in Fig. 5.

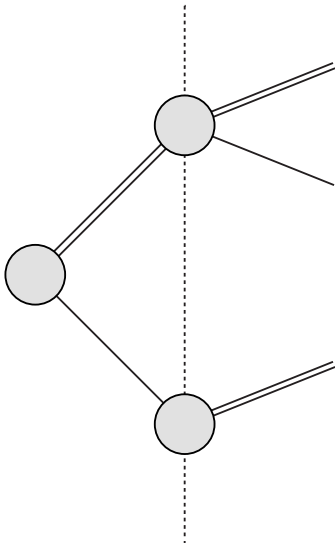


Figure 3: Example of a tree representing a certain phase-space parameterization. Double lines represent reference momenta, and single lines are unresolved momenta. Here both unresolved momenta are generated with respect to the same reference momentum.

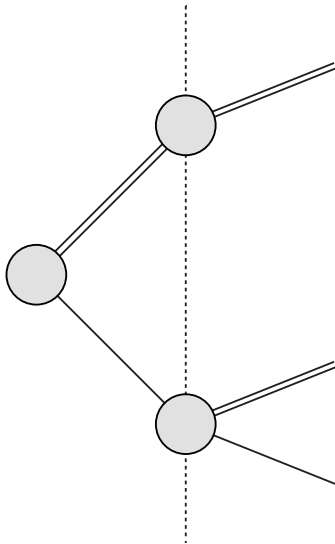


Figure 4: Example of a tree representing a certain phase-space parameterization. Double lines represent reference momenta, and single lines are unresolved momenta. Here the first unresolved momentum is parameterized against the a reference momentum, while the second unresolved momentum is parameterized against the previously generated unresolved momentum.

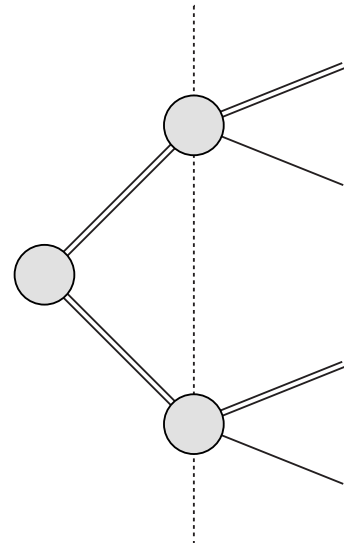


Figure 5: Example of a tree representing a certain phase-space parameterization. Double lines represent reference momenta, and single lines are unresolved momenta. Here both unresolved momenta are parameterized against two different reference momenta.

One last comment is in order: If all momenta in the final state of a process are reference momenta, i.e. if there are no spectator partons in the process $n_q = 0$, then the algorithm fails. In Ref. [9], they used the phase-space parameterization of Ref. [10] for this special case. Here we use the above described algorithm, but instead of considering all reference momenta at once, we single out one of the reference momenta and treat as as a spectator and then generate the unresolved momenta of that reference parton at a later step (See Fig. 6). In that last step we demote another parton to be the spectator. The downside is, that because the this momentum is now a spectator, it will be subject to Lorentz transformations. It is not yet clear if we can always find an ordering that will guarantee, that this Lorentz transformation will not spoil our parameterization of the IR poles.

Our algorithm is pretty much guaranteed to capture any possible infrared limit as it very much resembles the Feynman diagrams which generate these infrared singularities in the first place. It is, however, not always clear which tree is the right choice for a given limit. Furthermore, it is also clear that different trees can often parameterize the same limit. For example, if all a bunch of partons become simultaneously collinear with no special hierarchy, then any tree with just one reference momentum will be able to describe this limit.

3 Construction of Subtraction Terms

Now that we have a suitable phase-space parameterization we start constructing the subtraction terms. The main difficulty is that any sector might contain additional infrared singularities that are **not** parameterized by the construction of the phase space. We want to make sure that when we are in a certain sector, determined by some tree graph, than no other infrared singularities should appear in the phase-space. The way to achieve this is through so called *selector functions*. These functions are multiplied to the approximations in eq. (1), therefore they must approach unity close to the infrared singularity but can be something else anywhere else. In particular, we want to chose selector functions which are close to zero whenever we encounter infrared singularities which can not parameterized by in the given sector. Let us define an auxiliary function

$$d_{i,k} = \left(\frac{E_i}{\sqrt{s}} \right) (1 - \cos \theta_{ik}), \quad (24)$$

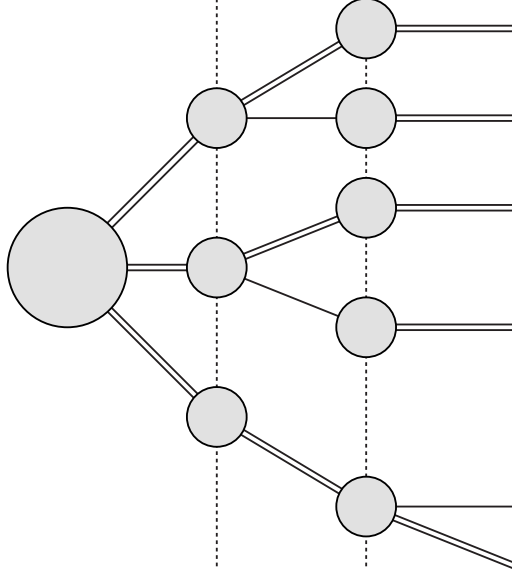


Figure 6: Example of how to generate unresolved momenta without the existence of spectator partons. The lowest branch is treated as a spectator momentum in the first recursion step. In the next step the other two branches become spectators and we generate the unresolved momenta of the lowest branch.

which we call the *IR-root function of a single splitting*, because it vanishes in the IR limit of a splitting of the reference parton k and the unresolved parton i . Notice, that the function is proportional to the propagator of the splitting amplitude. The IR-root function of an entire tree can then be build recursively by taking the product of all splitting nodes inside that tree

$$d_{i_1, \dots, i_{n_u}, k}^{\mathcal{T}} = \prod_{\text{Node } j \in \mathcal{T}} d_{j_1, j_2} \quad (25)$$

where j_1 and j_2 are the unresolved and reference momenta of the j th node, and \mathcal{T} is a tree representing a certain phase space parameterization. Again introducing multiple reference momenta is trivial and only amounts to multiplying the different IR-root functions. Finally, we can define our selector function as

$$\mathcal{S}_{i_1, \dots, i_{n_u}}^{\mathcal{T}} = \frac{1}{D_{n_u} d_{i_1, \dots, i_{n_u}}^{\mathcal{T}}}, \quad D_{n_u} = \sum_{\substack{\text{Trees } \mathcal{T}_i \\ \text{with } n_u \text{ unresolved}}} \frac{1}{d_{i_1, \dots, i_{n_u}}^{\mathcal{T}_i}} \quad (26)$$

Clearly, the selector functions are positive definite and form a decomposition of unity

$$\sum_{\substack{\text{Trees } \mathcal{T}_i \\ \text{with } n_u \text{ unresolved}}} \mathcal{S}_{i_1, \dots, i_{n_u}}^{\mathcal{T}_i} = 1. \quad (27)$$

These properties ensure, that if one of the selector functions goes to one, i.e. if we encounter an IR pole described by the selector function, than all the others must vanish. The situation is not quite so extreme, as we can have multiple trees describing the same infrared limit, in which case multiple IR-root functions approach zero. This is no problem however as long as all sectors which cannot describe the limit are suppressed.

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