Top quark spin and QCD corrections in event generation
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Chapter 6

One-Loop Matching for $Z \rightarrow 3$ Partons

In the previous chapter the VINCIA antenna-shower algorithm was presented followed by a first description for NLO matching for $Z \rightarrow 2$ partons. The two parton case is special for two reasons. Firstly because of the absence of renormalization terms and secondly, since the lack of additional radiation required a special treatment to match the event to NLO accuracy, by adapting the weight. Consecutive NLO matching will employ a rescaling of the accept probability to incorporate knowledge of the NLO calculation in a unitary approach. This chapter will focus on generalizing the approach for an additional parton in the final state and is therefore the key step to a fully general framework that allows for an arbitrary number of partons.

6.1 Constructing a Matching Term

The approximation to the 3-parton exclusive rate produced by a shower matched to (at least) NLO for the 2-parton inclusive rate and to LO for the 3-parton one, is

$$\text{Approximate} \rightarrow (1 + V_2) |M^0_3|^2 \Delta_2(m^2_Z, Q_3^2) \Delta_3(Q^2_{R3}, Q^2_{\text{had}}),$$

where $M^0_3$ is the tree-level $Z \rightarrow qg\bar{q}$ matrix element and $Q_{R3}$ denotes the “restart scale”. For strong ordering, $Q_{R3}$ is equal to $Q_3$, while, for smooth ordering, it is given by the nested antenna phase spaces, i.e., by the successive antenna invariant masses. The subscripts on the two Sudakov factors $\Delta_2$ and $\Delta_3$ make it explicit that they refer to the event as a whole, see the illustration in fig. 6.1. Again, we have the choice whether we wish to work in 4 dimensions, with a non-zero hadronization scale, $Q_{\text{had}}$, or in $d$ dimensions with the hadronization scale taken to zero. We have maintained the hadronization scale in eq. (6.1), though we shall see below that the dependence on it does indeed cancel in the final result.
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The 2-parton Sudakov factor, $\Delta_2$, is generated by the (matched) evolution from 2 to 3 partons,

$$\Delta_2(m_Z^2, Q_R^2) = 1 - \int_{Q_R^2}^{m_Z^2} d\Phi \, g_s^2 \, 2C_F \, A_{g/q\bar{q}} + \mathcal{O}(\alpha_s^2), \quad (6.2)$$

with $A_{g/q\bar{q}}$ again defined by eq. (5.52). Notice that the integral only runs from the starting scale, $m_Z^2$, to the 3-parton resolution scale, $Q_R^2$, hence this integral is IR finite, though it does contain logarithms. In the remainder of this chapter, we shall work only with the leading-colour part of the Sudakov and matrix-element expressions, hence from now on we replace $2C_F$ in the above expression by $C_A$,

$$\Delta_{2LC}(m_Z^2, Q_R^2) = 1 - \int_{Q_R^2}^{m_Z^2} d\Phi \, g_s^2 \, C_A \, A_{g/q\bar{q}} + \mathcal{O}(\alpha_s^2). \quad (6.3)$$

The 3-parton Sudakov factor, $\Delta_3$, imposes exclusivity and is given by

$$\Delta_3(Q_{R3}^2, Q_{had}^2) = 1 - \sum_{j=1}^{2} \int_{Q_{had}^2}^{Q_{R3}^2} d\Phi \, g_s^2 \, (C_A \, A_{Ej} + 2T_R \, A_{SJ}) + \mathcal{O}(\alpha_s^2), \quad (6.4)$$

where the index $j$ runs over the $qq$ and $g\bar{q}$ antennae, and we use subscripts $E$ and $S$ for gluon emission and gluon splitting, respectively. We have implicitly assumed smooth ordering here, which implies that the upper boundaries on the integrals are given by the respective dipole invariant masses (squared), $s_j$. Note also that we must take into account all modifications that are applied to the LL antenna functions, including $P_{\text{imp}}$, $P_{\text{Ari}}$, and LO matrix-element matching factors. (We do not write out these factors here, to avoid clutter.) I.e., the antenna functions in the above expression must be the ones actually generated by the shower algorithm, including the effect of any modifications imposed by vetos.
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For strong ordering, there are no $P_{\text{imp}}$ factors, and the upper integral boundary is instead $\min(Q_3^2, s_j)$,

$$\Delta_3(Q_3^2, Q_{\text{had}}^2) = 1 - \sum_{j=1}^{2} \int_{Q_{\text{had}}^2}^{\min(Q_3^2, s_j)} \text{d}\Phi \text{ant}_j g_s^2 (C_A A_{Ej} + 2T_R A_{Sj}) + \mathcal{O}(\alpha_s^2).$$

(6.5)

However, since strong ordering is not able to fill the entire 4-parton phase space [110, 141], full NLO matching can only be obtained for the smoothly ordered variant. It is nonetheless interesting to examine both types of shower algorithms, since even in the strongly ordered case, we may compare the Sudakov logarithms arising at $\mathcal{O}(\alpha_s^2)$ to those present in the fixed-order calculation.

On the fixed-order side, the expression for the 3-parton exclusive rate is simply

$$\text{Exact} \rightarrow |M_3^0|^2 + 2 \text{Re}[M_3^0 M_3^{1*}] + \int_0^{Q_{\text{had}}^2} \frac{\text{d}\Phi_3}{\text{d}\Phi_3} |M_3^0|^2,$$

where the last term represents 4-parton configurations in which a single parton is unresolved with respect to the hadronization scale. For $Z$ decay, $d$-dimensional expressions for the virtual matrix element have been available since long [125, 139, 142, 143]. Details on the calculation and in particular its renormalization, are given in appendix B, in a notation convenient for our purposes.

We now seek a fully differential matching factor, $K_3 = 1 + V_3$, such that the expansion

$$\text{Matched} = (1 + V_3) \text{Approximate},$$

(6.7)

reproduces the exact expression, eq. (6.6), to one-loop order. (“Approximate” here stands for the tree-level matched shower approximation, eq. (6.1).) Trivial algebra yields

$$V_3^{\text{LC}} = \left[ \frac{2 \text{Re}[M_3^0 M_3^{1*}]}{|M_3^0|^2} \right]^{\text{LC}} - V_2$$

(6.8)

$$+ \int_{Q_3^2}^{m_Z^2} \text{d}\Phi \text{ant}_s g_s^2 2C_A A_{g/q\bar{q}} + \sum_{j=1}^{2} \int_0^{s_j} \text{d}\Phi \text{ant}_j g_s^2 (C_A A_{Ej} + 2T_R A_{Sj})$$

$$+ \int_0^{Q_{\text{had}}^2} \frac{\text{d}\Phi_4}{\text{d}\Phi_3} \frac{|M_4^0|^2}{|M_3^0|^2} - \sum_{j=1}^{2} \int_0^{Q_{\text{had}}^2} \frac{\text{d}\Phi_4}{\text{d}\Phi_3} \frac{|M_4^0|^2}{|M_3^0|^2} \frac{g_s^2}{2} (C_A A_{Ej} + 2T_R A_{Sj})$$

where we have reinstated $d$-dimensional forms of the one-loop matrix element and of the divergent $3 \to 4$ terms. For a shower matched to $|M_4^0|^2$ at leading order, the last two terms will cancel, by definition of the matched antenna functions (even for an unmatched shower, the difference could at most be a finite power correction in the hadronization scale, since the matrix element and the shower antenna functions have the same singular-
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\[ V_{3Z}^{LC} = \left[ \frac{2 \text{Re}[M^0_M^0 M^1_3^*]}{|M^0_3|^2} \right]^{LC} - V_{2Z} \]

\[ + \int_{Q_3^2}^{m_3^2} d\Phi_\text{ant} \ g_s^2 2C_A \ A_{g/qq} + \sum_{j=1}^{2} \int_{0}^{s_j} d\Phi_\text{ant} \ g_s^2 \ (C_A \ A_{E_j} + 2T_R \ A_{S_j}). \]

(6.9)

Rewriting the remaining integrals in terms of a set of standardized antenna subtraction terms, writing out the ordering functions for gluon emission and gluon splitting, \( O_E \) and \( O_S \), explicitly, and denoting the ARIADNE factor for gluon splitting by \( P_A \), we arrive at the following master equation for the second-order correction to the 3-jet rate:

\[ V_{3Z}^{LC} = \left[ \frac{2 \text{Re}[M^0_M^0 M^1_3^*]}{|M^0_3|^2} \right]^{LC} - V_{2Z} + \sum_{j=1}^{2} \int_{0}^{s_j} d\Phi_\text{ant} \ g_s^2 \ (C_A \ A_{E_j}^{\text{std}} + n_F A_{S_j}^{\text{std}}) \]

\[ + \int_{Q_3^2}^{m_3^2} d\Phi_\text{ant} \ g_s^2 C_A A_{g/qq}^{\text{std}} + \int_{Q_3^2}^{m_3^2} d\Phi_\text{ant} \ g_s^2 C_A \ \delta A_{g/qq} \]

\[ - \sum_{j=1}^{2} \int_{0}^{s_j} d\Phi_\text{ant} \ g_s^2 \ (C_A \ (1 - O_{E_j}) \ A_{E_j}^{\text{std}} + n_F \ (1 - O_{S_j}) \ P_A \ A_{S_j}^{\text{std}}) \]

\[ + \sum_{j=1}^{2} \int_{0}^{s_j} d\Phi_\text{ant} \ g_s^2 \ (C_A \ \delta A_{E_j} + n_F \ \delta A_{S_j}) - \sum_{j=1}^{2} \int_{0}^{s_j} d\Phi_\text{ant} \ g_s^2 n_F \ (1 - P_A) \ A_{S_j}^{\text{std}}, \]

(6.10)

with the standardized Gehrmann-Gehrmann-de Ridder-Glover (GGG) subtraction terms defined by \[125\]:

\[ A_{g/qq}^{\text{std}} = a_3^0 \ ( = a_3^0 ), \quad \int_{0}^{s} d\Phi_\text{ant} \ g_s^2 A_{g/qq}^{\text{std}} = \frac{\alpha_s}{2\pi} \left( -2I_{qq}^{(1)}(\epsilon, \mu^2/s) + \frac{19}{4} \right) \]

\[ A_{g/gg}^{\text{std}} = d_3^0, \quad \int_{0}^{s} d\Phi_\text{ant} \ g_s^2 A_{g/gg}^{\text{std}} = \frac{\alpha_s}{2\pi} \left( -2I_{qg}^{(1)}(\epsilon, \mu^2/s) + \frac{17}{3} \right) \]

\[ A_{q/qq}^{\text{std}} = e_3^0 \ ( = \frac{1}{2} E_3^0 ), \quad \int_{0}^{s} d\Phi_\text{ant} \ g_s^2 A_{q/qq}^{\text{std}} = \frac{\alpha_s}{2\pi} \left( -2I_{qg,F}^{(1)}(\epsilon, \mu^2/s) - \frac{1}{2} \right) \]

(6.11)

whose IR limits and integrated pole structures were examined thoroughly in \[125, 139, 140\], though we have here rewritten the IR singularity operators \( I^{(1)} \) in explicitly dimensionless forms, see appendix \[\text{A}\] (The alphabetical labeling in eqs. \(6.11\) corresponds to the notation used in \[125\].)

The first line and first term on the second line in eq. \(6.10\) represent a standard antenna-subtracted one-loop matrix element, normalized to the Born level, with the standardized subtraction terms tabulated in eq. \(6.11\), and the additional finite term \(V_{2Z}\) originating from the NLO matching at the preceding order; see section \[5.2.2\] eq. \(5.49\).
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The subsequent terms express the difference between the simple fixed-order subtraction carried out in the first line and the actual terms that are generated by a matched Markovian antenna shower. Physically, these terms represent the difference between the evolution of a single dipole (the original \( q \bar{q} \) system) and evolution of two dipoles (the post-branching \( qg \bar{q} \) system), with a transition occurring at the branching scale \( Q_3 \). As mentioned above, the \( O_{E_j} \) and \( O_{S_j} \) factors in the third line represent the ordering criterion imposed in the evolution, either strong or smooth. For smooth ordering, they are

\[
1 - O_{E_j} = 1 - \frac{Q_3^2}{Q_{E_j}^2 + Q_3^2}, \tag{6.12}
\]

\[
1 - O_{S_j} = 1 - \frac{Q_3^2}{m_{qg}^2 + Q_3^2}, \tag{6.13}
\]

with \( Q_{E_j} \) the evolution variable used for gluon emissions, while for strong ordering, the factor \( 1 - O_j \) can be removed if the integral boundaries are replaced by \( [Q_3^2, s_j] \) (note: this replacement should only be done in the third line).

The last term in eq. (6.10) is an artifact of the ARIADNE factor, \( P_{Ari} \), which was introduced in section 5.1.2 and is applied to gluon-splitting antennae in VINCIA. Summed over the two “sides” of the splitting gluon, this produces the same collinear singularities as the standard gluon-splitting antenna, but in highly asymmetric configurations in which the splitting gluon is near-collinear to a neighbouring colour line, the ARIADNE factor produces a strong suppression, which improves the agreement with the tree-level 4-parton matrix element [133], and which then generates an additional logarithm.

Notice that all but the \( \delta A \) terms are defined in terms of standarized antenna functions, and the corresponding integrals can be carried out analytically, once and for all. We give explicit forms for each of these terms, for each choice of evolution variable, in the following section.

The only terms of eq. (6.10) that need to be integrated numerically are thus the \( \delta A \) terms, which express the difference between the standarized antenna functions and those generated by the actual (matched) shower evolution, which may have different finite terms and/or be matched to the LO 4-parton matrix element. Nonetheless, since the previous lines already contain most of the structure, we expect these functions to be relatively well-behaved and numerically sub-leading. Specifically, the \( \delta A \) terms for gluon emission and gluon splitting, respectively, are defined by

\[
\delta A_{E_j}^{LC} = O_{E_j} \left( R_{4E}^{LC} A_{E_j}^{LL} - A_{E_j}^{std} \right), \tag{6.14}
\]

\[
\delta A_{S_j}^{LC} = O_{S_j} P_{A_j} \left( R_{4S}^{LC} A_{S_j}^{LL} - A_{S_j}^{std} \right), \tag{6.15}
\]

with \( A_{LL} \) the unmatched shower antenna function (as defined in [113, 133]) and the second-order LO matching factors, \( R_{4E} \) and \( R_{4S} \) (for \( Z \rightarrow qgg \bar{q} \) and \( Z \rightarrow q'q' \bar{q} \), respectively), defined as in eq. (5.40), but including only the leading-colour terms in \( P_{4E}^{LC} \). For strong ordering, similarly to above, the \( O_j \) factors can be removed by changing the integration boundaries of the \( \delta A \) terms to \([0, Q_3^2]\).
6.1. Constructing a Matching Term

Finally, we note that one could in principle equally well have defined eq. (6.10) without the terms on the third line. The $\delta A$ terms in eqs. (6.14) and (6.15) would then likewise have to be defined without $P_{imp}$ and $P_{Ari}$ factors. However, while this would give a seemingly cleaner relation with standard fixed-order subtraction, the behaviour of the (numerical) integrals over the $\delta A$ terms would be more difficult, due to over-subtraction in the unordered regions. (Showers without either a strong-ordering condition or a smooth-ordering suppression greatly overestimate the real-radiation matrix elements in the unordered region [110, 133, 144].) Numerically, it is therefore more convenient to integrate the contributions represented by the third line in eq. (6.10) analytically, leaving only the suppressed terms in eq. (6.15) to be integrated over numerically.

To be specific, the numerical integration over the $\delta A$ terms is performed by rewriting the $\delta A$ integrals in dimensionless MC form, as:

$$\frac{\alpha_s}{2\pi} C_A \sum_{j=1}^{2} \frac{1}{4N} \sum_{i=1}^{N} \left( s_j \delta A_j(\Phi_i) \right),$$

and similarly for the gluon-splitting terms, with $\Phi_i$ a number of random (uniformly distributed) antenna phase-space points. The common factor $1/4$ arises from combining the prefactor $8\pi^2$ above with the area of the phase-space triangle, $1/2$, and the factor $1/(16\pi^2)$ from the phase-space factorization, $d\Phi_{ant}$. For smooth $p_{\perp}$-ordering with an arbitrary normalization factor $N_\perp$ (so $Q_E^2 = N_\perp p_\perp^2$), the ordering factors, $O_j$, reduce to:

$$O_E(q_i g_j, \bar{q}_k \to q_a g_b g_c, \bar{q}_k) = \frac{y_{jk}}{y_{jk} + x_{ab} x_{bc}}, \quad (6.17)$$

$$O_E(q_i g_j, \bar{q}_k \to q_i, g_a g_b \bar{q}_c) = \text{same with } i \leftrightarrow k, \quad (6.18)$$

$$O_S(q_i g_j, \bar{q}_k \to q_a \bar{q}_b g_c, \bar{q}) = \frac{N_\perp y_{jk}}{N_\perp y_{jk} + x_{bc}}, \quad (6.19)$$

$$O_S(q_i g_j, \bar{q}_k \to q_i, \bar{q}_b \bar{q}_c \bar{q}_a) = \text{same with } i \leftrightarrow k, \quad (6.20)$$

where we have used $y$ with $ijk$ indices for the scaled invariants in the original $qg\bar{q}$ topology and $x$ with $abc$ indices for the integration variables in the antenna phase space. Note also that the $y$ values are normalized to the full 3-parton CM energy (squared), while the $x$ values are normalized to their respective dipole CM energies (squared).

6.1.1 The Renormalization Term

A further ingredient to be discussed is the choice of renormalization scale on both the fixed order and parton shower sides of the calculation, as these scales are in general chosen differently in both sides. Hence a translation term arises at second order, which must account for this difference, keeping in mind that, as the scale evolves from one to the other, flavour thresholds are passed. Our aim is to have the flexibility to use fixed order matrix elements renormalized according to their usual scheme, while maintaining the freedom to make a different choice on the shower side.
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The fixed order calculations for $Z$-decay to jets to which we match are customarily renormalized in a version of the MS scheme called the Zero-Mass Variable Flavour Number Scheme (ZM-VFNS). In this scheme the bare QCD coupling is renormalized as

$$g_b = \mu^\epsilon g(\mu^2_R) \left[1 + \frac{\alpha_s(\mu^2_R)}{8\pi} \left\{ -\frac{1}{\epsilon} + \gamma_E - \ln 4\pi + \ln \frac{\mu^2}{\mu^2_R} \right\} \right]$$

(6.21)

with $\beta_0 = (11C_A - 2n_F)/3 \equiv \beta_0^F$ and $n_F$ is the number of light flavours. One thus ignores flavours that are heavier than the scale of the calculation, both in the virtual and in the real calculations. Once all the UV poles are cancelled, one has a running coupling that depends on the number of light flavours for the scale $\mu_R$ at hand. One then changes the flavour number when a threshold is crossed. For our present case of $Z$ boson decay to jets we take $n_F = 5$ for $\mu_R$ not too different from the $Z$-boson mass.

Let us be more specific about the matching of $\alpha_s$ across flavour thresholds. At one loop,

$$\alpha_s^{(n_F)}(\mu_R) = \frac{4\pi/\beta_0^F}{\ln(\mu^2_R/\Lambda^2_F)}.$$  (6.22)

The value of $\Lambda_F$ depends on the number of active flavours, as follows. When passing flavour thresholds the following one-loop matching conditions are imposed

$$\alpha_s^{(5)}(m_b) = \alpha_s^{(4)}(m_b), \quad \alpha_s^{(4)}(m_c) = \alpha_s^{(3)}(m_c).$$  (6.23)

These conditions can be satisfied if $\Lambda_F$ obeys the matching conditions

$$\ln \frac{\Lambda^2_F}{\Lambda^2_{F+1}} = \frac{2}{3\beta_0^F} \ln \frac{m^2_{F+1}}{\Lambda^2_{F+1}}.$$  (6.24)

With these conditions one can also express $\alpha_s$ values for different flavour numbers into eachother. E.g. if $m_c < \mu_R < m_b$, one can express $\alpha_s^{(4)}(\mu_R)$ in terms of $\alpha_s^{(5)}(\mu_R)$ by the relation

$$\alpha_s^{(4)}(\mu_R) = \alpha_s^{(5)}(\mu_R) \frac{1}{\frac{\beta_0^4}{\beta_0^5} + \left(1 - \frac{\beta_0^4}{\beta_0^5}\right) \frac{\alpha_s^{(5)}(\mu_R)}{\alpha_s^{(5)}(m_b)}}.$$  (6.25)

For completeness we briefly review how this $n_F$-dependent UV singularity occurs in the context of the (inclusive) 3-jet rate, in the case where we only consider massless quarks [142,143]. In the virtual contribution, the only one-loop diagram for $Z \rightarrow q\bar{q}g$ that is sensitive to the number of flavours is the quark self-energy correction on the external gluon. The self-energy diagram itself, being scaleless, is zero in dimensional regularization. However, renormalization of the coupling amounts to adding a $n_F$ counterterm on the external gluon line proportional to

$$n_F \frac{2}{3\epsilon} \left(\frac{\mu^2}{\mu^2_R}\right)^\epsilon.$$  (6.26)
The real contribution contributes a \( n_F \) dependent (collinear) \( 1/\epsilon \) pole as well, from gluon-splitting

\[
- n_F \frac{2}{3\epsilon} \left( \frac{\mu^2}{s} \right)^\epsilon .
\]

(6.27)

In the sum over real and virtual contributions the poles cancel, as guaranteed by the KLN theorem, leaving a logarithm of the form

\[
n_F \frac{2}{3} \ln \left( \frac{s}{\mu^2_R} \right) .
\]

(6.28)

On the shower side a related prescription is used, in which the running coupling is evaluated at a shower scale \( \mu_{PS} \), such that the scale again depends on the number of flavours. Depending on the value of \( \mu_{PS} \), a corresponding value of \( n_F \) is chosen, as well as of the QCD scale \( \Lambda_F \). This is often different from that for a fixed order calculation.

Shifting to a different scale for \( \alpha_s \) of a given flavour number is quite straightforward. Translating from a shower scale \( \mu_{PS} \) to a matrix-element scale \( \mu_{ME} \) amounts to replacing,

\[
a_{g/\bar{q}q} \bigg|_{\mu_R=\mu_{PS}} \rightarrow \left( 1 + \alpha_s \frac{11N_C - 2n_F}{12\pi} \ln \left( \frac{\mu_{ME}^2}{\mu_{PS}^2} \right) + \mathcal{O}(\alpha_s^2) \right) a_{g/\bar{q}q} \bigg|_{\mu_R=\mu_{ME}} .
\]

(6.29)

For coherent parton-shower models, the arguments presented in [145] also motivate a change to a “Monte Carlo” scheme for \( \alpha_s \), in which \( \Lambda_{QCD} \) is rescaled, for each \( n_F \), by the so-called CMW factor \( \sim 1.5 \) (with some mild flavour dependence), relative to its \( \overline{\text{MS}} \) value. If the shower model being matched employs this scheme, then a further rescaling of the renormalization-scale argument, \( \mu_{PS} \rightarrow \mu_{PS}/k_{CMW} \), should be used in eq. (6.29), with

\[
k_{CMW} = \exp \left( \frac{67 - 3\pi^2 - 10n_F/3}{2(33 - 2n_F)} \right) = \begin{cases} 1.513 & n_F = 6 \\ 1.569 & n_F = 5 \\ 1.618 & n_F = 4 \\ 1.661 & n_F = 3 \end{cases}
\]

(6.30)

for \( N_c = 3 \). The translation of renormalization scale (and scheme) yields then an additional term to be added to the definition of \( V_3 \) in eq. (6.10),

\[
V_{3\mu} = - \frac{\alpha_s}{2\pi} \frac{11N_C - 2n_F}{6} \ln \left( \frac{\mu_{ME}^2}{\mu_{PS}^2} \right) = - \frac{\alpha_s}{2\pi} \frac{\beta_0}{2} \ln \left( \frac{\mu_{ME}^2}{\mu_{PS}^2} \right) .
\]

(6.31)

By inserting the above term, which enters at overall order \( \alpha_s^2 \ln(\mu_{ME}^2/\mu_{PS}^2) \), the two calculations can be compared consistently at one-loop accuracy.
Note that if several different shower paths populate the same fixed-order phase-space point, then each path will in general be associated with a distinct $\mu_{\text{PS}}$ value. Thus, one $V_{3\mu}$ term arises for each shower path, weighted by the relative contribution of each path to the total. Since for our case there is only one antenna contributing to $Z \rightarrow qg\bar{q}$, this particular complication does not arise here.

We finally alert the reader regarding the use of different flavour number $\alpha_s$’s in the master equation (6.10). In that equation cancellation of $1/\epsilon$ divergences take place, already in the first line of the right hand side. For this cancellation it is important that the subtraction terms, originating from the shower expansion and listed in eq. (6.11), use $\alpha_s^{(5)}$ renormalized as in the fixed order calculation. All subsequent terms in the master equation are finite, and constitute differences of unordered and strongly ordered shower based terms, which are also finite, and beyond NLO.

### 6.1.2 Leading-Colour One-Loop Correction for $Z \rightarrow 3$ Jets

Combining the results above, in particular eqs. (6.10), (6.11), and (6.31), we obtain the complete expression for the leading-colour one-loop correction for $Z \rightarrow 3$ Jets,

\[
V_{3Z}(q, g, \bar{q}) = \left[ \frac{2 \text{Re}[M_3^0 M_3^{1*}]}{|M_3^0|^2} \right]^\text{LC} - \frac{\alpha_s}{\pi} - \frac{\alpha_s}{2\pi} \left( \frac{11N_{\text{C}} - 2n_F}{6} \right) \ln \left( \frac{\mu_{\text{ME}}^2}{\mu_{\text{PS}}^2} \right) + \frac{\alpha_s C_A}{2\pi} \left[ -2I_{qg}^{(1)}(\epsilon, \mu^2/s_{qg}) - 2I_{gq}^{(1)}(\epsilon, \mu^2/s_{gq}) + \frac{34}{3} \right] + \frac{\alpha_s n_F}{2\pi} \left[ -2I_{qg,F}^{(1)}(\epsilon, \mu^2/s_{qg}) - 2I_{gq,F}^{(1)}(\epsilon, \mu^2/s_{gq}) - 1 \right] + \frac{\alpha_s C_A}{2\pi} \left[ 8\pi^2 \int_{Q_3^2}^{m_Z^2} d\Phi_{\text{ant}} A_{\text{g/qq}}^{\text{std}} + 8\pi^2 \int_{Q_3^2}^{m_Z^2} d\Phi_{\text{ant}} \delta A_{g/qg} \right] - \sum_{j=1}^{2} 8\pi^2 \int_{s_j^0}^{s_j} d\Phi_{\text{ant}} (1 - O_{E_j}) A_{g/qg}^{\text{std}} + \sum_{j=1}^{2} 8\pi^2 \int_{s_j^0}^{s_j} d\Phi_{\text{ant}} \delta A_{g/qg} \right] + \frac{\alpha_s n_F}{2\pi} \left[ -\sum_{j=1}^{2} 8\pi^2 P_{A_j} \int_{s_j^0}^{s_j} d\Phi_{\text{ant}} (1 - O_{S_j}) A_{q/gq}^{\text{std}} \right] + \sum_{j=1}^{2} 8\pi^2 \int_{s_j^0}^{s_j} d\Phi_{\text{ant}} \delta A_{q/qg} - \frac{1}{6} \frac{s_{qg} - s_{gq}}{s_{qg} + s_{gq}} \ln \left( \frac{s_{qg}}{s_{gq}} \right) \right],
\]

(6.32)

where:

\begin{itemize}
  \item We use the usual MC definition of leading colour and include terms $\propto C_A$ and $\propto n_F$ but neglect ones $\propto 1/C_A$.
\end{itemize}
6.1. Constructing a Matching Term

- the first line contains the full (leading-colour) one-loop matrix element, the $V_{2Z}$ correction from one-loop matching at the preceding order, and the $V_{3\mu}$ term from the choice of shower renormalization scale;

- the second line contains the standardized subtraction term arising from the $qg \rightarrow qgg$ and $g \bar{q} \rightarrow gg \bar{q}$ antennae;

- the third line contains the standardized subtraction term arising from the $qg \rightarrow q\bar{q}'q'$ and $g \bar{q} \rightarrow \bar{q}'q\bar{q}$ antennae;

- the fourth to last lines contain the terms arising from the difference between the (matched) shower evolution and the standardized subtraction terms, including the consequences of ordering choices and modification factors such as those arising from the Ariadne factor and from matching to the LO matrix elements.

We denote the singular subtracted 1-loop matrix element by $S_{Virtual}$

\[
S_{Virtual} = \left[ 2 \Re \left[ \frac{M_0^0 M_3^{1*}}{|M_3^0|^2} \right] \right]^{LC} + \frac{\alpha_s C_A}{2\pi} \left[ -2 I_{qg}^{(1)}(\epsilon, \mu^2/s_{qq}) - 2 I_{qg}^{(1)}(\epsilon, \mu^2/s_{qg}) + \frac{34}{3} \right] \\
+ \frac{\alpha_s n_F}{2\pi} \left[ -2 I_{qg,F}^{(1)}(\epsilon, \mu^2/s_{qq}) - 2 I_{gq,F}^{(1)}(\epsilon, \mu^2/s_{qg}) - 1 \right] \tag{6.33}
\]

In section 6.2, we compute the analytical integrals corresponding to each of the shower-generated terms, for different choices of evolution variable, ordering criterion, and antenna functions.

With the one-loop matrix element expressed as in appendix B.2, it is easy to see that the infrared singularity operators in eq. (6.33) cancel, leaving only explicitly finite remainders (which may still contain logarithms of resolved scales). This then constitutes the description of the one-loop matching for $Z \rightarrow 3$ jets, having already discussed the case for two jets. In the context of eq. (5.46) we have now corrected the first two terms on the rhs to NLO accuracy.

6.1.3 One-Loop Correction for Born + 2 Partons

To illustrate how the formalism presented here generalizes to higher multiplicities, we take the case of the NLO correction to $Z \rightarrow 4$ partons. For simplicity, however, we continue to restrict our analysis of the correction factor to the leading-colour level. At NLO, the exclusive $Z \rightarrow 4$ partons rate at “infinite” perturbative resolution (similarly to above) is

\[
\text{Exact} \rightarrow |M_4^0|^2 + 2\Re \left[ M_4^0 M_4^{1*} \right]. \tag{6.34}
\]

Labeling the 4 partons by $Z \rightarrow i, j, k, \ell$, there are two possible antenna-shower histories leading to each 4-parton configuration, with $j$ and $k$ the last emitted parton, respectively. Those two contributions both enter in the definition of the tree-level 4-parton
matching factor,
\[ R_4 = \frac{|M^0_3(i, j, k, \ell)|^2}{A_{j/IK}^0 |M_3^0(I, K, \ell)|^2 + A_{k/JL}^0 |M_3^0(i, J, L)|^2}, \tag{6.35} \]
such that their sum reproduces the full 4-parton matrix element. Note that a separate such factor is applied to \( Z \to qgq\bar{q} \) and \( Z \to q'q'\bar{q} \), and that we have suppressed colour and coupling factors here, for compactness (we ignore the small, non-singular extra interference terms for the special case where all four quarks have the same flavour).

The antenna functions, \( A \), are understood to include all such factors, as well as any \( P_{\text{imp}} \) and \( P_{\text{ari}} \) factors appropriate to the branchings at hand. For a general \( n \)-parton matrix element, the denominator contains one term for each possible clustering.

Labeling the \( IK \to ijk \) history by \( A \) and the \( JL \to jk\ell \) one by \( B \), the sum over the two histories yields
\[ R_4 \Delta_4(Q_4, 0) \sum_{\alpha \in A, B} A_{3 \to 4}^\alpha |M_3^\alpha|^2 \Delta_2(m_Z^2, Q_3^\alpha) \Delta_3(Q_3^\alpha, Q_4^\alpha) \prod_{m=2}^3 (1 + V_m^\alpha), \tag{6.36} \]
where it is understood that \( \alpha \) is an index, not a power, and the last product factor takes into account the NLO matching at the preceding multiplicities. Expanding the Sudakov factors to first order and using the definition of the NLO correction factor at the preceding multiplicity, eq. (6.9), this becomes
\[ R_4 \left( 1 - \sum_k \int_0^{s_k} d\Phi_{\text{ant}} R_5 A_{4 \to 5} \right) \sum_{\alpha \in A, B} A_{3 \to 4}^\alpha |M_3^\alpha|^2 \times \left[ 1 + \frac{2 \text{Re}[M_3^0 M_3^1]^\alpha}{|M_3^\alpha|^2} + \sum_j \int_0^{Q_4^\alpha} d\Phi_{\text{ant}} A_{3 \to 4}^\alpha \right], \tag{6.37} \]
which we can rewrite as
\[ |M_4|^2 \left( 1 - \sum_k \int_0^{s_k} d\Phi_{\text{ant}} R_5 A_{4 \to 5} \right) + R_4 \sum_{\alpha \in A, B} A_{3 \to 4}^\alpha |M_3^\alpha|^2 \left( \frac{2 \text{Re}[M_3^0 M_3^1]^\alpha}{|M_3^\alpha|^2} + \sum_j \int_0^{Q_4^\alpha} d\Phi_{\text{ant}} A_{3 \to 4}^\alpha \right), \tag{6.38} \]
where we again emphasize that the antenna functions are understood to include all relevant coupling, \( P_{\text{imp}} \), and \( P_{\text{ari}} \) factors. The first term represents the new subtraction that the shower generates at 4 partons, while the second represents part of the NLO correction to the preceding multiplicity. For one of the histories (the one followed by the “current” event), this correction has already been evaluated and can be reused. The contribution from the other history will have to be recomputed, however. In general, there will be one subtraction to perform at the \( n \)-parton level, and there will be \( m \sim n - n_{\text{Born}} - 1 \) new
subtractions that have to be done at the \((n - 1)\)-parton level, in addition to the one that was already done during the evolution of the current event.

Clearly, there is an undesirable scaling behavior built into this, which will make NLO matching at many partons quite computing intensive. An alternative, which eliminates the sum over histories, is that of sector showers, see e.g., [133, 146].

### 6.2 Sudakov Integrals

In this section, we work out the standardized Sudakov integrals appearing in the second and third line of eq. (6.10), for each choice of evolution variable. We also study the soft and collinear limits of the Sudakov integrals and compare them to those of the one-loop matrix element. This provides an explicit check of whether the first-order expansion of the Sudakov factors generates the correct logarithms present in the fixed-order calculation.

Given our choice of the GGG antenna functions as our standard ones, the relevant terms are

$$g_s^2 \left[ C_A \int_{Q^2_3}^s d\Phi_{\text{ant}} - \sum_{j=1}^2 C_A \int_{0}^{s_j} (1 - O_{E_j}) a^0_3 d\Phi_{\text{ant}} - \sum_{j=1}^2 2 T R n_{E j P A_j} \int_{0}^{s_j} (1 - O_{S_j}) e^0_3 d\Phi_{\text{ant}} \right]$$

(6.39)

The general form of the first term, which originates from the \(2 \rightarrow 3\) branching step, is

$$g_s^2 C_A \int_{Q^2_3}^s d\Phi_{\text{ant}} = \frac{\alpha_s C_A}{2\pi} \left( \sum_{i=1}^5 K_i I_i(s, Q^2_3) \right)$$

(6.40)

where the definitions for the \(K_i\) and the \(I_i\) functions are given in appendix C for each type of antenna function and ordering variable. Their derivation and soft/collinear structure will be discussed more closely below, for each choice of ordering and evolution variable.

The form of the \(3 \rightarrow 4\) integrals depends on whether we work in the context of strong or smooth ordering. We shall now consider each of those cases in turn, beginning with strong ordering.

### 6.2.1 Strong Ordering

For strong ordering, the inverted ordering conditions in eq. (6.10), \((1 - O_{E_j/\text{S}_j})\), reduce to step functions expressing integration over the unordered region. The integration surface is thus limited from below by the phase-space contour defined by the evolution scale of the first branching, \(Q^2\), and from above by the edge defined by the invariant mass of the antenna.
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The expression generated by the $3 \rightarrow 4$ splitting case for gluon emission is

$$- g_s^2 \sum_{j=1}^{2} C_A \int_0^{s_j} (1 - O_{E_j}) \, d^3 \Phi_{\text{ant}}$$

$$= - \frac{\alpha_s C_A}{2\pi} \left( \sum_{i=1}^{5} K_i I_i(s_{qg}, Q_s^2) \right) - \frac{\alpha_s C_A}{2\pi} \left( \sum_{i=1}^{5} K_i I_i(s_{gq}, Q_s^2) \right).$$

(6.41)

where $K_i$ and $I_i$ are the same as those for the $2 \rightarrow 3$ term above, though they here appear with different arguments. The remaining case is the $3 \rightarrow 4$ gluon splitting defined by

$$- g_s^2 \sum_{j=1}^{2} n_F P_{A_j} \int_0^{s_j} (1 - O_{S_j}) \, e_3^0 \, d\Phi_{\text{ant}}$$

$$= - \frac{\alpha_s n_F}{2\pi} P_{A_{qq}} H(s_{qq}, Q_s^2) - \frac{\alpha_s n_F}{2\pi} P_{A_{qg}} H(s_{qg}, Q_s^2).$$

(6.42)

with $H$ defined in appendix C and $P_{A_i}$ as defined in eq. (5.20). We will discuss the derivation of these terms in more detail in the following three sections, for strong $m_D$-, $p_\perp$, and energy-ordering, respectively.

Dipole Virtuality

We begin with dipole virtuality as evolution variable, which is perhaps the simplest case. We start by repeating the integrals of eq. (6.10) with the one-particle phase space defined as in eq. (5.8). In the case of dipole virtuality the contours are triangular (fig. 5.2a). We recall that, for the $g \rightarrow q\bar{q}$ terms, it is the $q\bar{q}$ invariant mass that is used as evolution variable, regardless of what choice is made for gluon emissions. The $m_D$ scale of the previous emission still enters, however, since that defines the ordering scale applied to both emissions and splittings. The explicit forms of the terms in eq. (6.39) are:

$$= \frac{\alpha_s}{4\pi} \left\{ \begin{array}{c}
\frac{C_A}{s} \int_{s_{\text{min}}(s_{gq}, s_{qg})}^{s_{\text{min}}(s_{qg}, s_{gq})} \int_{s_{gq}}^{s_{gq}} ds_1 \int_{s_{qg}}^{s_{qg}} ds_2 \, d_3^0(s_1, s_2) \\
- \frac{C_A}{s_{gq}} \Theta(s_{gq} - 2s_{qg}) \int_{s_{gq}}^{s_{gq}} ds_1 \int_{s_{qg}}^{s_{qg}} ds_2 + \frac{C_A}{s_{qg}} \Theta(s_{qg} - 2s_{gq}) \int_{s_{gq}}^{s_{gq}} ds_1 \int_{s_{qg}}^{s_{qg}} ds_2 \\
x \int_{s_{gq}}^{s_{gq}} ds_1 \int_{s_{qg}}^{s_{qg}} ds_2 \\
- \frac{n_F}{s_{qg}} \Theta(s_{qg} - s_{gq}) P_{A_1} \int_{s_{qg}}^{s_{qg}} ds_1 \int_{s_{gq}}^{s_{gq}} ds_2 + \frac{n_F}{s_{gq}} \Theta(s_{gq} - s_{qg}) P_{A_2} \int_{s_{gq}}^{s_{gq}} ds_1 \int_{s_{qg}}^{s_{qg}} ds_2 \\
x \int_{s_{gq}}^{s_{gq}} ds_1 \int_{s_{qg}}^{s_{qg}} ds_2
\end{array} \right\}$$

(6.43)
with \( P_{A_1} = \frac{2s_{qq}}{s_{qq} + s_{gq}} \) and \( P_{A_2} = \frac{2s_{gq}}{s_{qq} + s_{gq}} \) as defined in eq. (5.20) and the gluon-splitting antenna \( a_0^3 \) has its singularities in \( s_1 \).

For compactness, we only show the integration for the double-pole (soft-collinear eikonal) terms present in both \( a_0^3 \) and \( d_0^3 \) here, which are the only sources of transcendentality-2 terms. The full antenna integrals, including also the lower-transcendentality terms originating from single poles and finite terms, are given in appendix C. The \( T = 2 \) part of the \( a_0^3 \) integral is

\[
\frac{\alpha_s C_A}{4\pi} \left[ \int_{\min(s_{qq}, s_{gq})}^{s - \min(s_{qq}, s_{gq})} ds_1 \int_{\min(s_{qq}, s_{gq})}^{s - s_1} ds_2 \frac{2}{s_1 s_2} \right].
\]

(6.44)

To evaluate this expression, we first rewrite it in a dimensionless form in terms of the rescaled integration variables \( y_i = s_i / (s - \frac{1}{2} Q_3^2) \), with upper boundary 1 and lower boundary

\[
\xi_{\text{min}} = \frac{\min(s_{qq}, s_{gq})}{s - \min(s_{qq}, s_{gq})}.
\]

(6.45)

The integration is over a triangular surface. The lower integration boundary cuts off the evolution variable at the value of the 3-parton evolution scale. The other boundary is determined by the total energy of the dipole before branching which here is \( \sqrt{s} \). We use the integral

\[
\int_{x}^{1} \frac{dy}{y} \ln \left( \frac{1 - y + x}{x} \right) = \ln^2(x) - \ln(x) \ln(1 + x) - \text{Li}_2 \left( \frac{1}{1 + x} \right) + \text{Li}_2 \left( \frac{x}{1 + x} \right).
\]

(6.46)

to obtain

\[
\frac{\alpha_s C_A}{2\pi} \left[ \ln \left( \frac{s}{\min(s_{qq}, s_{gq})} \right) \ln \left( \frac{s - \min(s_{qq}, s_{gq})}{\min(s_{qq}, s_{gq})} \right) \right. \\
- \text{Li}_2 \left( \frac{s - \min(s_{qq}, s_{gq})}{s} \right) + \text{Li}_2 \left( \frac{\min(s_{qq}, s_{gq})}{s} \right) \right].
\]

(6.47)

To discuss the \( 3 \to 4 \) Sudakov terms, let us for definiteness assume that we are in a 3-parton phase-space point with \( s_{qq} > s_{gq} \). The opposite case is symmetric. Again we only include the \( T = 2 \) terms explicitly here, with the details of the full antenna integrals relegated to appendix C.

\[
\frac{\alpha_s C_A}{4\pi} \left[ \int_{s_{gq}}^{s_{qq} - s_{gq}} ds_1 \int_{s_{gq}}^{s_{qq} - s_1} ds_2 \frac{2}{s_1 s_2} \right].
\]

(6.48)

The integration is again over a triangular surface. The total energy of the dipole before branching is now \( \sqrt{s_{qq}} \). The integral in eq. (6.48) corresponding to the sum over antenna integrals only contains one \( d_0^3 \) integral because the other has equal upper and lower integration boundaries. Note that this integral actually vanishes for \( s_{qq} \leq Q_3^2 \), which amounts to the dipole-virtuality ordering allowing the \( 3 \to 4 \) branchings to populate their full respective phase spaces (i.e. no correction term is necessary).
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Focusing on the case $s_{qg} > 2s_{g\bar{q}}$ for which the second integral is nonvanishing (which now amounts to the ordering condition imposing a nontrivial restriction on the $3 \to 4$ phase space, see fig. 5.3a), we obtain, including the $2 \to 3$ term

$$\frac{\alpha_s C_A}{4\pi} \left[ \int_{\xi_{\min}}^{1} dy_1 \int_{\xi_{\min}}^{1-y_1+\xi_{\min}} dy_2 \frac{2}{y_1 y_2} - \int_{\xi'_{\min}}^{1} dy'_1 \int_{\xi'_{\min}}^{1-y'_1+\xi'_{\min}} dy'_2 \frac{2}{y'_1 y'_2} \right] (6.49)$$

with lower-transcendality terms again available in appendix C. For the mirror case $s_{g\bar{q}} > 2s_{qg}$ essentially symmetric expressions are obtained, while for the intermediate cases in which the two invariants are within a factor 2 of each other, the second integral in eq. (6.49) simply vanishes.

The full double-logarithmic term from the expanded Sudakov terms in eq. (6.43), for strong ordering in dipole virtuality, is then

$$\frac{\alpha_s C_A}{2\pi} \left[ \ln \left( \frac{s}{s_{qg}/2 Q_3^2} \right) \ln \left( \frac{s - \frac{1}{2} Q_3^2}{s} \right) - \ln \left( \frac{s_{max} - \frac{1}{2} Q_3^2}{s} \right) \right]$$

$$+ \Theta \left( s_{max} - Q_3^2 \right) \left( - \ln \left( \frac{s_{max}}{s_{max}} \right) \ln \left( \frac{s_{max} - \frac{1}{2} Q_3^2}{s_{max}} \right) \right)$$

$$+ \ln \left( \frac{s_{max}}{s_{max}} \right) - \ln \left( \frac{s_{max} + \frac{1}{2} Q_3^2}{s_{max}} \right) \right] , (6.51)$$

where the $\Theta$ function ensures that the second term is only active if

$$s_{max} = \max(s_{qg}, s_{g\bar{q}}) > 2 \min(s_{qg}, s_{g\bar{q}}) = Q_3^2 , (6.52)$$

so that the expression applies over all of phase space.

We shall now consider the infrared limits of this result, and compare them to those of the one-loop matrix element. For this comparison we keep only terms that involve logarithms of the invariants. The soft limit corresponds to vanishing $Q_3^2 (\xi_{\min} \to 0)$. The first line of eq. (6.51) represents the contribution of the $2 \to 3$ expanded Sudakov. To find the contribution in the soft limit, we choose to approach the limit along the diagonal of the phase space triangle. Parametrizing this by $s_{qg}/s = s_{g\bar{q}}/s \to y$ we find for this term

$$\ln^2(y) - \frac{\pi^2}{6} .$$

The contributions of the $3 \to 4$ Sudakovs in the soft limit are examined in two separate cases corresponding to the two regions in fig. 5.3a. In the first case given by $s_{max} < 2s_{min}$, corresponding to the light grey area in the figure, the step function in eq. (6.51)
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yields zero. In the second case given by $s_{\text{max}} > 2s_{\text{min}}$, corresponding to the dark grey area in the figure, the step function is equal to one. The double logs and dilogarithms now yield a finite contribution that does not diverge in the soft limit. We can understand this by parametrizing the soft limit by $\lambda$

\[ s_{qg} = \lambda s \quad s_{gq} = p\lambda s \quad s'_1 = \lambda\kappa s \quad s'_2 = \lambda\mu s \quad p > 2 \, , \quad (6.53) \]

so that the integral becomes

\[ \int_{s_{\text{min}}}^{s_{\text{max}}-s_{\text{min}}} ds_1 \int_{s_{\text{min}}}^{s_{\text{max}}-s_1} ds_2 \frac{1}{s_1 s_2} \to \int_1^{p-1} d\kappa \int_1^{p-\kappa} d\mu \frac{1}{\kappa \mu} . \quad (6.54) \]

This implies that the integration variable scales with the integration limits and is independent of the soft limit. We can also expect this behaviour from examining fig. 5.2a. The shape of the different regions does not change for different values of $Q_3^2$, in contrast with the case of transverse momentum, as we will see below.

After the poles cancel in eq. (6.32), the pole-subtracted version of the one-loop matrix element, SVirtual, defined in eq. (6.33), contains all the relevant terms on the matrix-element side. The transcendentality-2 terms of SVirtual are given by

\[ -R(y_1, y_2) = \text{Li}_2(y_1) + \text{Li}_2(y_2) - \frac{\pi^2}{6} - \ln y_1 \ln y_2 + \ln y_1 \ln(1-y_1) + \ln y_2 \ln(1-y_2) . \quad (6.55) \]

Including the transcendentality-1 terms (see appendix [B]), taking the soft limit by sending $s_{qg}/s = s_{gq}/s = y \to 0$, and keeping only logarithmic terms, the pole-subtracted matrix element (ME) reduces to

\[ \text{ME:} \quad s_{qg}/s = s_{gq}/s = y \to 0 \quad \frac{\alpha_s C_A}{2\pi} \left[ -\ln^2(y) - \frac{10}{3} \ln(y) \right] + \frac{\alpha_s n_F}{6\pi} \ln(y) , \quad (6.56) \]

The single log proportional to $C_A$ originates from the renormalization term and the single log of the closed quark loops (proportional to $n_F$) arises due to the definition of the infrared singularity operator, defined in the appendix in eq. (A.3).

Taking the same limit of the Sudakov integrals for dipole virtuality eq. (6.43), but omitting for the time being the renormalization term, $V_{3\mu}$, we find for the parton shower (PS),

\[ -\text{PS:} \quad s_{qg}/s = s_{gq}/s = y \to 0 \quad \frac{\alpha_s C_A}{2\pi} \left[ \ln^2 y + \frac{3}{2} \ln(y) \right] . \quad (6.57) \]

We see that the soft limit almost cancels against eq. (6.56). For an NLL-accurate shower, however, all divergent terms should match precisely, leaving at most a finite remainder in the final matching correction, eq. (6.32). In the expressions above, this holds for the $\ln^2(y)$ term but not for the single logarithms (different coefficient). Interestingly, the remainder is proportional to the QCD $\beta$ function, specifically

\[ \text{ME} - \text{PS} \to -\frac{\alpha_s}{2\pi} \frac{1}{2} \beta_0 \ln(y) . \quad (6.58) \]
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It can therefore be absorbed in the choice of renormalization scale by solving for $\mu_{PS}$ in $V_{3\mu}$, which yields:

$$\mu_{PS}^2 \propto y s .$$

(6.59)

This tells us that, in the soft limit, the specific choice of a renormalization scale that is linear in the branching invariants will absorb all logarithms up to and including $\alpha_s^2 \ln(y)$. Interestingly, this reasoning would rule out $\mu_R^2 \propto p_\perp^2$, since our $p_\perp$-definition is quadratic in the invariants, $p_\perp^2 = s_{ij}s_{jk}/s$. A better choice of renormalization scale would appear to be $\mu_R \propto m_D$, specifically

$$\mu_{PS}^2 = \min(s_{ij}, s_{jk}) = \frac{1}{2}m_D^2 .$$

(6.60)

Taken at face value, this seems to contradict the standard literature [128] on $p_\perp$ as the optimal universal renormalization-scale choice. However, as we shall see below in fig. 6.2 there is in fact no choice of renormalization scale that absorbs all logarithms for this particular evolution variable; the choice $\mu_R \propto m_D$ merely manages to reabsorb the additional logarithms that are generated by the ordering condition as $y \rightarrow 0$, but leftover logs in other parts of phase space will remain uncanceled, ruining the NLL precision. In that sense, choosing $\mu_R \propto p_\perp$ would simply leave a different set of uncanceled logs, nonvanishing as $y \rightarrow 0$.

Before we show the results over all of phase space however, we first investigate a complementary interesting limit, the hard-collinear one, which is characterized by one of the invariants becoming maximal while the other vanishes. In this limit, the pole-subtracted one-loop matrix element, $S_{Virtual}$, becomes

$$\text{ME: } s_{qg}/s \rightarrow 1, s_{gq}/s = y \rightarrow 0 \quad \frac{\alpha_s}{2\pi} \left[ -\frac{5}{3}C_A + \frac{1}{6}n_F \right] \ln(y)$$

(6.61)

There are no log-squared terms in this limit, and both of the single-log terms are half as large here as they were in the soft limit.

The Sudakov integrals for $m_D$-ordering yield one divergent term, $-\frac{1}{6}C_A \ln(y)$, in the hard-collinear region, modulo a factor $\alpha_s/(2\pi)$. The Sudakov integral for gluon splitting in the neighbouring antenna, represented by the first term on the second-to-last line of eq. (6.32) is specified in the last line of eq. (6.43). The step function is only non-zero for the first term in the hard-collinear limit $s_{qg} \rightarrow s, s_{gq} \rightarrow 0$ and produces a term $\frac{1}{6}P_{A_j}n_F \ln(y)$. The numerator of the corresponding Ariadne factor contains the invariant of the neighboring dipole $s_{gq}$ which vanishes in this limit and causes the dipole splitting contribution to reduce to zero. The $n_F$-dependent contribution is instead shifted to the last term of eq. (6.32), which has the same limit but without the Ariadne pre-factor. The hard-collinear limit of the shower terms, including only terms involving logarithms of the invariants and not including the $V_{3\mu}$ term, is therefore

$$\text{PS: } s_{qg}/s \rightarrow 1, s_{gq}/s = y \rightarrow 0 \quad \frac{\alpha_s}{2\pi} \left[ -\frac{1}{6}C_A + \frac{1}{6}n_F \right] \ln(y) .$$

(6.62)
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Again, the combination (ME – PS) relevant for computing the correction factor is proportional to the QCD $\beta$ function, and in fact has exactly the same form as eq. (6.58). The conclusion is therefore that, also in this limit, all logarithms through $\alpha_s^2 \ln(y)$ can be absorbed by choosing a renormalization scale which is linear in the vanishing invariant. The particular choice which is linear in both the soft and collinear limits is $\mu_{PS} \propto m_D$. To illustrate this, we show the full NLO $Z \rightarrow 3$ jets correction factors, $(1 + V_{3Z})$, for $m_D$-ordering with a few different choices of renormalization scale and scheme, in fig. 6.2. Note that the axes are logarithmic, in $\ln(y_{ij}) = \ln(s_{ij}/s)$, to make the infrared limits clearly visible.

Without the $V_{3\mu}$ term, the correction factor looks as depicted in the top left-hand plot in fig. 6.2. The increasing contours towards the axes indicate uncanceled logarithms in the correction factor. The middle pane shows the correction factor derived for $\mu_{PS} = p_\perp$. As discussed above, there is an uncanceled logarithm in the soft limit (lower left-hand corner of the plot), since $p_\perp$ is quadratic in the vanishing invariants there. However, in
the hard-collinear limits (upper left-hand and lower right-hand corners), $p_\perp$ is linear in the vanishing invariant, and hence the contours remain bounded there. In the right-hand pane, we show the choice $\mu_{PS} = m_D$, which can be seen to lead to bounded correction factors (below $\sim 1.3$) in all three phase-space corners. Nonetheless, there is still an uncanceled divergence between the soft and hard collinear limits. We shall see in the section on $p_\perp$-ordering below that the cure for this is basically to choose a better evolution variable.

In the bottom row of fig. 6.2 we show a few variations on $\mu_{PS} = m_D$, specifically we include the CMW rescaling of $\Lambda_{QCD}$, as defined by eq. (6.30), and show how a variation of the renormalization scale by a factor of 2 affects the correction factor. In the left-hand pane, we show $\mu_{PS} = \frac{1}{2}m_D$ and in the right-hand one $\mu_{PS} = m_D$. Of these, the choice $\mu_{PS} = \frac{1}{2}m_D$, with CMW rescaling, leads to the smallest correction factors (best LO behaviour), and this could therefore be taken as a useful default for $m_D$-ordering, e.g. for uncertainty estimates.

Transverse Momentum

For a shower ordered in $p_\perp$, the antenna phase-space integrals in eq. (6.10) are performed over contours such as those depicted in fig. 5.2e. The curved contours motivate a coordinate transformation from $(s_1, s_2)$ to a basis defined as the dimensionless evolution variable $y = \frac{Q^2}{s} = \frac{4s_1s_2}{s_1s_2}$, complemented by an energy-sharing variable, which we define as $z = \frac{s_1}{s}$. Note that the coordinate transformation depends explicitly on the total invariant mass $s$ of the $2 \rightarrow 3$ dipole. For the $3 \rightarrow 4$ integrations, the invariant mass $s$ is replaced by the invariant mass of the appropriate dipole (either $s_{qg}$ or $s_{gq}$). The integration boundaries in $z$ are determined by the intersection of the invariant mass of the dipole with the evolution parameter $Q^2$. The choice of $y$ and its integration boundaries make the effect of strong ordering especially clear since we see integration from $Q^2$ to the total invariant mass of the dipole (the unordered region). As before, the integration over the gluon-splitting antenna ($e_3^0$) makes use of a different phase space integration, in $m_{qg}$, and only uses the evolution parameter as a cut-off in the singularity of the corresponding dipole.
6.2. Sudakov Integrals

The contributing terms are:

\[
g_2^2 \left[ C_A \int_{Q_3^2}^s d^3 \Phi_{\text{ant}} - \sum_{j=1}^2 C_A \int_0^{s_j} \left(1 - O_{E_j}\right) d^3 \Phi_{\text{ant}} \right. \\
\left. - \sum_{j=1}^2 2 T_R n_F P_{A_j} \int_0^{s_j} \left(1 - O_{S_j}\right) e_3^0 d^3 \Phi_{\text{ant}} \right] \\
= \frac{\alpha_s}{4\pi} C_A s A_1 \left[ \frac{Q_3^2}{s}, 1 \right] - C_A s q g A_2 \left[ \frac{4 s q g}{s}, \max \left( \frac{4 s q g}{s}, 1 \right) \right] \\
- s q g C_A A_3 \left[ \frac{4 s q g}{s}, \max \left( \frac{4 s q g}{s}, 1 \right) \right] \\
- n_F \left( \frac{P_{A_1}}{s q g} \int_{Q_3^2}^{\max(Q_3^2, s_g q)} d s_1 \int_0^{s_g q - s_1} d s_2 e_3^0(s_1, s_2) \right. \\
\left. + \frac{P_{A_2}}{s q g} \int_{Q_3^2}^{\max(Q_3^2, s_g q)} d s_1 \int_0^{s_g q - s_1} d s_2 e_3^0(s_1, s_2) \right) \] (6.63)

with

\[
A_n[a,b] = \int_a^b d y_n \int_{z_n^{\min}}^{z_n^{\max}} d z_n |J_n| A_n(y_n, z_n) \quad \text{for } n = 1, 2, 3, \quad (6.64)
\]

and

\[
y_n = 4 \frac{s_1 s_2}{m_{1K}^4}, \quad z_n = \frac{s_1}{m_{1K}^4}, \quad |J_1| = \frac{m_{1K}^4}{4 z_n^2}, \quad z_n^{\max} = \frac{1}{2} \left(1 \pm \sqrt{1 - y_n}\right). \quad (6.65)
\]

For \(n = 1\) we set \(m_{1K}^2 = s\), for \(n = 2\) \(m_{1K}^2 = s q g\) and for \(n = 3\) \(m_{1K}^2 = s q g\). The Ariadne factor \(P_{A_j}\) is defined in eq. (5.20). The max condition on the outer integration boundary of \(A_2\) and \(A_3\) reflect that the correction term disappears if the generated \(Q_3^2\) is larger than the invariant mass of the dipole. As for \(m_D\)-ordering, we here work out the most divergent behavior explicitly, by focussing on the double log terms arising from the eikonal term in the antenna, and relegate the full form of the antenna integrals to appendix C. The double poles give rise to terms

\[
\frac{\alpha_s C_A}{2\pi} \int_{\frac{Q_3^2}{x}}^1 d y_1 \int_{\frac{z_n^{\min}}{y_1}}^{\frac{z_n^{\max}}{y_1}} d z_1 \frac{1}{y_1 z_1},
\]

which lead to the following generic transcendentality-2 integrals,

\[
\int_x^1 d y_1 \ln \left( \frac{1 + \sqrt{1 - y_1}}{1 - \sqrt{1 - y_1}} \right) = \text{Li}_2 \left( \frac{1}{2} \left(1 - \sqrt{1 - x}\right) \right) - \text{Li}_2 \left( \frac{1}{2} \left(1 + \sqrt{1 - x}\right) \right) + \frac{1}{2} \ln \left( \frac{x}{4} \right) \ln \left[ - \left( \frac{-2 + 2\sqrt{1-x} + x}{x} \right) \right]. \quad (6.66)
\]
The double logarithm in the shower expansion is generated by a combination of the $2 \to 3$ and $3 \to 4$ Sudakov integrals, with the respective pieces adding up to

$$
\frac{\alpha_s C_A}{2\pi} \left[ -\frac{\pi^2}{6} + \frac{1}{2} \ln \left( \frac{s_{gg}s_{gq}}{s^2} \right)^2 + \frac{\pi^2}{3} - \frac{1}{2} \ln \left( \frac{s_{gg}}{s} \right)^2 - \frac{1}{2} \ln \left( \frac{s_{gq}}{s} \right)^2 \right].
$$

(6.67)

We see that a partial cancellation arises between the first two terms (which come from the $2 \to 3$ Sudakov expansion) and the last three (which come from the $3 \to 4$ expansion). What remains is a log squared in both invariants

$$
\ln \left( \frac{s_{qg}}{s} \right) \ln \left( \frac{s_{gq}}{s} \right).
$$

At the single-log level, the $3 \to 4$ terms give a numerically larger coefficient than the $2 \to 3$ ones, leading to a single log remainder. The gluon-splitting term also reduces to a single log. The overall result in the soft limit is then

$$
-\text{PS: } s_{gg} = s_{gq} = y \to 0 \quad \frac{\alpha_s C_A}{2\pi} \left[ \ln^2(y) - \frac{1}{3} \ln(y) \right] + \frac{\alpha_s n_F}{6\pi} \ln(y).
$$

(6.68)

Comparing with the result of the virtual correction in the soft limit, eq. (6.56), we see that the shower generates the double log terms correctly, and, similarly to the case of $m_D$-ordering, there is a single-log remainder which is proportional to the QCD $\beta$ function. However, for $p_\perp$-ordering the constant of proportionality is 1, rather than $\frac{1}{2}$, a difference which translates to the optimal renormalization-scale choice being quadratic in the invariants in this case, rather than linear. Before commenting further on this difference, let us first consider the complementary, hard-collinear, limit.

In the hard-collinear limit, we find the same as for $m_D$-ordering,

$$
-\text{PS: } s_{gg} = y \to 0, s_{gq} \to s \quad \frac{\alpha_s}{2\pi} \left[ -\frac{1}{6} C_A + \frac{1}{6} n_F \right] \ln(y).
$$

(6.69)

Double logs (eikonal parts of the antenna) also appear at both the $2 \to 3$ and $3 \to 4$ levels, but cancel among each other as almost all other antenna terms do; what remains at the single-log level is the integrated difference between a quark-antiquark antenna and a quark-gluon antenna, plus the $n_F$-dependent ‘Ariadne Log’. The only contributing Sudakov gluon splitting contribution is the second term in the last line of eq. (6.63). Integration over the $s_{gq}$ dipole, however, is associated with an Ariadne factor carrying $s_{qg}$ in the numerator and therefore reduces to zero. As before, we can write the remainder as half the QCD $\beta$ function, which implies that a renormalization scale linear in the vanishing invariants can absorb the logarithm.

To summarize, for $p_\perp$-ordering we find that the optimal renormalization-scale choice must be quadratic in the vanishing invariants in the soft limit and linear in the hard-collinear limit. Those conditions are fulfilled by $p_\perp$ itself, thus

$$
\mu_{PS}^2 \propto p_\perp^2 = \frac{s_{ij}s_{jk}}{s_{ijk}}
$$

(6.70)

absorbs all logarithmic terms up to and including $\alpha_s^2 \ln(y)$ in the LO couplings.

Illustrations of the full NLO correction factors, $(1 + V_{3Z})$, are given in fig. 6.3. The
ordering of the plots in the top row are the same as in fig. 6.3 showing, from left to right, $\mu_{PS} = \sqrt{s}$, $\mu_{PS} = p_\perp$, $\mu_{PS} = m_D$. Similarly to the case of strong $m_D$-ordering, both of the latter two choices exhibit no logarithmic divergences in the hard-collinear regions (top left and bottom right corners of the plots), but in the soft region (bottom left corner) it is here $\mu_{PS} = p_\perp$ which leaves the correction factor free of logarithms. Indeed, we see that the combination of evolution and renormalization in $p_\perp$ leads to a rather flat correction factor over all of phase space, showing that this combination is indeed “better” than $m_D$-ordering.

In the bottom row of plots in fig. 6.3, we include the CMW factor and show the correction factors for $\mu_{PS} = p_\perp$ (left) and $\mu_{PS} = 2p_\perp$ (right). In particular on the left-hand pane, the NLO correction factor is essentially unity in the soft limit, while the corrections in the hard-collinear regions remain less than $\sim 20\%$. This gives some additional weight to the arguments for $p_\perp$-ordered showers with $p_\perp$ as renormalization scale being the best default choice for strongly ordered dipole-antenna showers. It also provides some ratio-

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Figure 6.3: NLO correction factor for strong $p_\perp$-ordering, with GGG antennae. Top row: $\mu_{PS} = \sqrt{s}$ (left), $\mu_{PS} = p_\perp$ (middle), and $\mu_{PS} = m_D$ (right). Bottom row: using the CMW $\Lambda_{MC}$, with $\mu_{PS} = p_\perp$ (left) and $\mu_{PS} = 2p_\perp$ (right). For all plots, $\alpha_s = 0.12$, $n_F = 5$, and gluon splittings were evolved in $m_{qq}$. 
nale why one typically finds a rather large value of $\alpha_s(m_Z) \sim 0.13$ (with CMW rescaling, or $\alpha_s(m_Z) \sim 0.14$ without it) when tuning such models to LEP event shapes; there is still a genuine order 20% NLO correction in the hard resolved region (upper right-hand corner). We return to this in more detail in the context of full LO + NLO matching in section 6.3.

Energy

To put the differences between $m_D$ and $p_\perp$ in context, we now briefly examine the case of energy ordering, which is known to produce the wrong DGLAP evolution in the collinear limit [144, 147, 148], and hence we should find larger (possibly divergent) NLO corrections.

Slicing phase space with the energy variable $Q_3^2 = s_{ijk}(y_{ij} + y_{jk})^2$, see fig. 5.2f, requires the use of an explicit infrared cut-off because the contours otherwise allow for the invariants to hit singular regions for every value of the contour. We will here use a cut-off in transverse momentum (a cut-off in dipole virtuality is also possible). The cutoff motivates us to switch to a different choice of integration variables. Therefore integration is transformed from $(s_1, s_2)$ to the dimensionless evolution parameters $y_E^2 = \frac{Q_3^2}{s} = \frac{(s_1 + s_2)^2}{m_{IK}^2}$ and completed with the energy sharing variable $\zeta = \frac{s_2}{m_{IK}^2}$. The interesting integrals arising from expanding the Sudakov form factor then are

$$g_s^2 \left[ C_A \int_{Q_3^2}^{\infty} a_3 d\Phi_{\text{ant}} - 2 \sum_{j=1}^{2} C_A \int_{0}^{s_j} (1 - O_{E_j}) d_{3j}^0 d\Phi_{\text{ant}} \right]$$

$$- \sum_{j=1}^{2} 2 T_R n_F P_{A_j} \int_{0}^{s_j} (1 - O_{S_j}) e_{3j}^0 d\Phi_{\text{ant}}$$

$$= \frac{\alpha_s}{4\pi} \left[ C_A \{ A\mathcal{E}_1(s, 1) - A\mathcal{E}_2(\min[s_{qg}, 1], 1) - A\mathcal{E}_3(\min[s_{g\bar{q}}, 1], 1) \} \right.$$

$$\left. - n_F \left( \frac{P_{A_{qg}}}{s_{qg}} \int_{Q_3^2}^{\max(Q_3^2, s_{qg})} ds_1 \int_{0}^{s_{qg} - s_1} ds_2 e_{3}^0(s_1, s_2) \right) + \frac{P_{A_{g\bar{q}}}}{s_{g\bar{q}}} \int_{Q_3^2}^{\max(Q_3^2, s_{g\bar{q}})} ds_1 \int_{0}^{s_{g\bar{q}} - s_1} ds_2 e_{3}^0(s_1, s_2) \right]$$

(6.71)

with

$$A\mathcal{E}_n(m_{IK}^2, 1) = \int_{Q_3^2}^{m_{IK}^2} dy_E^2 \int_{0}^{1} d\zeta' \frac{1}{2} A\mathcal{E}_n^0(y_E^2, \zeta').$$

With $A\mathcal{E}_1^0 = a_3^0$, $A\mathcal{E}_2^0 = d_3^0$ and $A\mathcal{E}_3^0 = e_3^0$. The inner integral has been rescaled to make it independent of the outer integral with $\zeta = y_E\zeta'$. To establish the cut-off, we use the relation $4 \frac{s_1 + s_2}{s} = 4p_\perp^2/s$, which we demand to be larger than the cut-off $\Delta$. In terms of
6.2. Sudakov Integrals

our variables we then have the condition

\[ 4\zeta'(1 - \zeta') > \frac{\Delta}{y_E^2}. \] (6.72)

The upper and lower limits on \( \zeta' \) are then

\[ \zeta'_- < \zeta' < \zeta'_+, \quad \zeta'_\pm = \frac{1}{2} \left( 1 \pm \sqrt{1 - \frac{\Delta}{y_E^2}} \right). \] (6.73)

Focussing on the eikonal integral

\[ \frac{\alpha_s C_A}{4\pi} \int_{y_E^2 = \frac{\alpha_s^2}{y_E^2}}^1 d\zeta'_- + d\zeta'_+ \int_{\zeta'_-}^{\zeta'_+} \frac{d\zeta'}{\zeta'} . \] (6.74)

the result for this integral is

\[ \frac{\alpha_s}{2\pi} \left[ \text{Li}_2 \left( \frac{1}{2} \left( 1 - \sqrt{1-\Delta} \right) \right) - \text{Li}_2 \left( \frac{1}{2} \left( 1 + \sqrt{1-\Delta} \right) \right) + \frac{1}{2} \left[ -2 \tanh \left( \sqrt{1 - \frac{\Delta}{y_E^2}} \right) \times \ln(4) + \tanh \left( \sqrt{1 - \Delta} \ln(16) + \ln^2 \left( 1 - \sqrt{1-\Delta} \right) - \ln^2 \left( 1 + \sqrt{1-\Delta} \right) 
\right. 
\right. 
\left. 
\left. - \ln^2 \left( 1 - \sqrt{1 - \frac{\Delta}{y_E^2}} \right) + \ln^2 \left( 1 + \sqrt{1 - \frac{\Delta}{y_E^2}} \right) \right] - 2\text{Li}_2 \left( \frac{1}{2} \left( 1 - \sqrt{1 - \frac{\Delta}{y_E^2}} \right) \right) 
\right. 
\right. 
\left. + \text{Li}_2 \left( \frac{1}{2} \left( 1 + \sqrt{1 - \frac{\Delta}{y_E^2}} \right) \right) \right]. \] (6.75)

In the soft limit \( y_E^2 = 4y^2 \to 0 \) this reduces to

\[ -\frac{1}{2} \ln^2(\Delta) - \ln^2 \left( \frac{\Delta}{4y^2} \right) - 2 \ln(4y^4) \ln(2) - \text{Li}_2 \left( \frac{\Delta}{64y^2} \right) \] (6.76)

Thus we see that there are explicit non-cancelling double-logarithmic terms that involve the hadronization cutoff, \( \Delta \). Depending on the ratio between the dipole mass and the cutoff, these would lead to asymptotically divergent correction factors.

One might wonder whether using a linearized form of energy ordering would make a difference, see fig. 5.2d. Rather than go through the derivations again, we merely show the full NLO corrections in fig. 6.4 for both linear (top row) and squared (bottom row) energy ordering, for an (arbitrary) dimensionless cutoff value of \( \Delta = 10^{-7} \).

From left to right in both rows, we show the three renormalization-scale choices, \( \mu_{PS} = p_\perp \) (left), \( \mu_{PS} = m_D \) (middle), and \( \mu_{PS} = Q_E \) (right), with the latter equal to linear energy in the top row and squared energy in the bottom one. Interestingly, the contours in the linear case are increasing towards the soft region, while they ultimately decrease in the squared case. It is clear, however, that no intelligent choice of renormalization scale
can absorb the infrared divergences. Moreover, any other choice of $\Delta$ would have led to different contours, due to the explicit $\ln(\Delta)$ terms, hence even if a “least bad” choice was found, it would not be universal.

As mentioned above, the main point of showing these comparisons is to place the comparison between $m_D$ and $p_\perp$ in the previous subsections in perspective. Thus, while we saw that $p_\perp$ was generating a better-behaved correction factor than $m_D$, the one for $m_D$ is still far better behaved than is the case for energy ordering. From this perspective, we still believe it could make sense, e.g., to use $m_D$-ordering, with the NLO correction factor included, as a conservative uncertainty variation for a central prediction based on $p_\perp$-ordering.

Figure 6.4: NLO correction factor for strong energy-ordering, with GGG antennae, for various renormalization-scale choices and linear (top row) and squared (bottom row) scaling of the evolution variable with gluon energy.
6.2. Sudakov Integrals

6.2.2 Smooth Ordering

We will now discuss the same Sudakov integrals as in the previous subsections but for the case of smooth ordering (section 5.1.4). This is especially interesting given that smooth ordering is the way VINCIA is able to fill all of phase space without significant under- or overcounting at the LO level [110]. As discussed in section 5.1.4 however, this does involve some ambiguity in what Sudakov factors are associated with the unordered points, and the NLO 3-jet correction factors should tell us explicitly whether this ambiguity generates problems at this level.

The Sudakov integrations are actually more straightforward for smooth ordering than was the case for strong ordering, since the $P_{\text{imp}}$ factor regulates the integrands on the boundaries. Therefore the integrations always run over the full phase space of the system. The $2 \to 3$ splitting generates the same terms as in the strong-ordering case, eq. (6.40). Including also the $3 \to 4$ terms, the expanded Sudakov generates the following antenna integrals,

$$g_s^2 \left[ C_A \int_0^s a_0^j d\Phi_{\text{ant}} - \sum_{j=1}^2 C_A \int_0^{s_j} \frac{Q_{E_j}^2}{Q_{E_j}^2 + Q_3^2} d_3^0 d\Phi_{\text{ant}} \right]$$

$$- \sum_{j=1}^2 2 T_R n_F P_{A_j} \int_0^{s_j} \frac{m^2_{q\bar{q}}}{m^2_{q\bar{q}} + Q_3^2} e_0^j d\Phi_{\text{ant}} \right] , \quad (6.77)$$

where $Q_3$ is the evolution scale evaluated on the 3-parton configuration and $Q_{E_j}(m_{q\bar{q}})$ is the scale of the $3 \to 4$ emissions (splittings) being integrated over. The full answer for the $3 \to 4$ case for gluon emission is

$$- g_s^2 \sum_{j=1}^2 C_A \int_0^{s_j} \frac{Q_{E_j}^2}{Q_{E_j}^2 + Q_3^2} d_3^0 d\Phi_{\text{ant}}$$

$$= - \frac{\alpha_s C_A}{4\pi} \left( \sum_{i=1}^5 K_i L_i(s_{qg}, Q_3^2) \right) - \frac{\alpha_s C_A}{4\pi} \left( \sum_{i=1}^5 K_i L_i(s_{gq}, Q_3^2) \right) . \quad (6.78)$$

where $K_i$ and $L_i$ can be found in appendix C. The full answer for the $3 \to 4$ case for gluon splitting is

$$- g_s^2 \sum_{j=1}^2 n_F P_{A_j} \int_0^{s_j} \frac{m^2_{q\bar{q}}}{m^2_{q\bar{q}} + Q_3^2} e_0^j d\Phi_{\text{ant}}$$

$$= - \frac{\alpha_s n_F}{4\pi} G(s_{qg}, Q_3^2) - \frac{\alpha_s n_F}{4\pi} G(s_{gq}, Q_3^2) . \quad (6.79)$$

where $G$ can be found in the appendix. We will discuss the derivation of these terms in more detail in the following two subsections, for smooth $m_D$- and $p_\perp$-ordering, respectively.
Chapter 6. One-Loop Matching for $Z \to 3$ Partons

Dipole Virtuality

Since the $2 \to 3$ emission terms remain the same as in the case of strong $m_D$-ordering, we only need to rederive the $3 \to 4$ contributions to $V_{32}$, which are

$$-g_s^2 \sum_{j=1}^2 C_A \int_0^{s_j} (1 - O_{Ej}) \frac{d^0}{d\Phi_{ant}} + \sum_{j=1}^2 2 T_R n_F P_{A_j} \int_0^{s_j} (1 - O_{Sj}) \epsilon_3^0 \frac{d^0}{d\Phi_{ant}}$$

$$= -\frac{\alpha_s}{4\pi} \left[ \frac{C_A}{s_{qq}} \left( \int_0^{s_{qq}} ds_2 \int_{s_1}^{s_{qq}-s_2} ds_1 O_{E1} + \int_0^{s_{qq}} ds_1 \int_{s_1}^{s_{qq}-s_1} ds_2 O_{E2} \right) d^0_{s_2} \right. $$

$$+ \frac{C_A}{s_{gq}} \left( \int_0^{s_{gq}} ds_2 \int_{s_1}^{s_{gq}-s_2} ds_1 O_{E1} + \int_0^{s_{gq}} ds_1 \int_{s_1}^{s_{gq}-s_1} ds_2 O_{E2} \right) d^0_{s_2}$$

$$+ 2n_F \left( \frac{P_{A_1}}{s_{qq}} \int_0^{s_{qq}} ds_2 \int_{s_1}^{s_{qq}-s_2} ds_1 + \frac{P_{A_2}}{s_{gq}} \int_0^{s_{gq}} ds_2 \int_{s_1}^{s_{gq}-s_2} ds_1 \right) O_S \epsilon_3^0 \left. \right]$$

(6.80)

with $O_{Ej} = \frac{Q_j^2}{Q_{Ej}^2 + Q_3^2}$, $O_{Sj} = \frac{Q_j^2}{m_{Sj}^2 + Q_3^2}$ as defined in eq. (6.12). $O_{E1} = \frac{2s_2}{Q_3^2 + 2s_2}$, $O_{E2} = \frac{2s_1}{Q_3^2 + 2s_1}$, $O_S = \frac{s_1}{s_1 + Q_3^2}$ and eq. (6.13). $Q_3^2 = 2 \min(s_{qq}, s_{gq})$, and $\epsilon_3^0$ carrying the singularity in $s_1$. We will focus again on deriving the transcendality-2 terms explicitly, with the full expressions given in the appendix. We start by recalling the expression for the strongly-ordered $2 \to 3$ branching,

$$\frac{\alpha_s C_A}{2\pi} \left[ \ln \left( \frac{s}{\frac{1}{2}Q_3^2} \right) \ln \left( \frac{s - \frac{1}{2}Q_3^2}{\frac{1}{2}Q_3^2} \right) - \text{Li}_2 \left( \frac{s - \frac{1}{2}Q_3^2}{s} \right) + \text{Li}_2 \left( \frac{\frac{1}{2}Q_3^2}{s} \right) \right].$$

To this we add the results from the eikonal term $\frac{2s_{qq}}{s_1 s_2}$ of one $3 \to 4$ gluon emission, the first line in eq. (6.80),

$$-\frac{2\alpha_s C_A}{\pi} \int_0^2 dy_2 \int_y y_2 \frac{1}{y_1 (y_3^2 + 2y_2)} \left[ -\ln(4) \ln \left( 1 - \frac{1}{1 + y_3^2} \right) + \ln(4) \ln \left( 1 + \frac{1}{1 + y_3^2} \right) - 2 \text{Li}_2 \left( -\frac{1}{y_3^2} \right) \right. $$

$$+ 2 \text{Li}_2 \left( \frac{1}{2 + y_3^2} \right) - 2 \text{Li}_2 \left( \frac{2}{2 + y_3^2} \right) \right]$$

(6.81)

where we have transformed $y_i = \frac{y}{s_{qq}^2}$ for $i = 1, 2$ and $y_3^2 = \frac{Q_j^2}{s_{qq}} = 2 \min(1, \frac{y_1}{y_3^2})$. Taking the limit for the soft region $y_3^2 \to 2$ (since we take the invariants as vanishing simultaneously), we see that the remainder is just a finite term that contains no logarithms of the vanishing invariants,

$$\frac{\alpha_s C_A}{8\pi} \left[ 2 \ln^2(2) + \text{Li}_2 \left( \frac{1}{4} \right) \right].$$

(6.82)
6.2. Sudakov Integrals

We will receive this contribution twice. Including all divergent logarithmic contributions and disregarding constant terms such as in eq. (6.82), we find the same as in the strongly-ordered case,

\[ - \text{PS: } s_{qq} = s_{gq} = y \to 0 \quad \frac{\alpha_s C_A}{2\pi} \left[ \ln^2(y) + \frac{3}{2} \ln(y) \right], \quad (6.83) \]

and hence the preferred choice of scale in the soft limit remains one which is linear in the vanishing invariants, such as \( \mu_{PS} \propto m_D \).

In the hard collinear limit the Sudakov integrals plus the ‘Ariadne Log’ reduce to

\[ - \text{PS: } s_{qq} = y \to 0, s_{gq} \to s \quad \frac{\alpha_s C_A}{2\pi} \left[ -\frac{1}{6} C_A + \frac{1}{6} n_F \right] \ln(y), \quad (6.84) \]

again the same as in the strongly ordered case, cf. eq. (6.62).

To summarize, we do not expect any qualitatively different limiting behaviour in the smoothly ordered case with respect to the strongly ordered one, though details may of course still vary. To illustrate this, we include the plots in fig. 6.5. In all cases, we use a renormalization scale \( \propto m_D \), but with different prefactors, from left to right: \( \mu_{PS} = m_D, \mu_{PS} = m_D/2 \), and finally \( \mu_{PS} = m_D/2 \) with CMW rescaling. In particular the latter generates correction factors very close to unity in both the soft and hard collinear limits, while we still see the leftover divergence inbetween those limits that was also present in the case of strong \( m_D \)-ordering, cf. fig. 6.2. Nonetheless, it is worth noting that for a large region of phase space, say with \( m_{ij} > 0.1 \) \( m \) (corresponding to \( \ln(y_{ij}) > -4.6 \)), the corrections are still quite well behaved and relatively small, less than \( \sim 20\% \).
Transverse Momentum

Again we only need to recompute the contributions from the $3 \to 4$ Sudakov terms, as the $2 \to 3$ ones are the same as in the strongly ordered case. The $3 \to 4$ Sudakov integrals are

$$
- g_s^2 \left[ \sum_{j=1}^{2} C_A \int_0^{s_j} \frac{1}{2} (1 - O_{E_j}) \, d\Phi_{ant} + \sum_{j=1}^{2} 2 T_R n_F P_{A_j} \int_0^{s_j} (1 - O_{S_j}) \, C_3^0 \, d\Phi_{ant} \right]
+ \frac{\alpha_s}{4\pi} \left[ \left( \frac{C_A}{s_{qg}} \int_0^{s_{qg}} ds_2 \int_0^{s_{qg} - s_2} ds_1 O_E + C_A \int_0^{s_{qg}} ds_2 \int_0^{s_{qg} - s_2} ds_1 O_E \right) d_3^0 \right. \\
\left. + 2n_F \left( \frac{P_{A_1}}{s_{qg}} \int_0^{s_{qg}} ds_2 \int_0^{s_{qg} - s_2} ds_1 + \frac{P_{A_2}}{s_{gq}} \int_0^{s_{qg}} ds_2 \int_0^{s_{qg} - s_2} ds_1 \right) O_S \right] \right]
$$

(6.85)

with $O_{E_j}$, $O_{S_j}$ as defined eq. (6.12) en eq. (6.13), specified by $O_E = \frac{4s_1 s_2}{s_1 + Q_3^2}$, $O_S = \frac{s_1}{s_1 + Q_3^2}$. As before we focus on explicitly calculating the transcendentality-2 contribution arising from the eikonal part of the antenna in the first term in the first line of eq. (6.85),

$$
- \frac{\alpha_s C_A}{2\pi} \int_0^1 dy_2 \int_0^{1-y_2} dy_1 \frac{4y_1 y_2}{y_3^2 + 4y_1 y_2} - \frac{1}{1 + \sqrt{1 + y_3^2}} \\
= - \frac{\alpha_s C_A}{2\pi} \left[ - \text{Li}_2 \left( - \frac{2}{1 + \sqrt{1 + y_3^2}} \right) - \text{Li}_2 \left( \frac{2}{1 + \sqrt{1 + y_3^2}} \right) \right]
$$

(6.86)

where we have transformed $y_i = \frac{s_i}{s_{qg}}$ and $y_3^2 = \frac{Q_3^2}{s_{qg}}$. In the limit $s_{\text{min}} / s, s_{\text{max}} / s = y \to 0$ so that $y_3^2 \to 0$, this yields

$$
\frac{\alpha_s C_A}{2\pi} \left[ - \frac{1}{2} \ln^2(y) \right].
$$

(6.87)

Adding the contributions from the $2 \to 3$ splitting and transcendentality-1 terms, we find the following result for the soft limit

$$
- \text{PS:} \quad s_{qg} = s_{gq} = y \to 0 \quad \frac{\alpha_s C_A}{2\pi} \left[ \ln^2(y) - \frac{1}{3} \ln(y) \right] + \frac{\alpha_s}{6\pi} n_F \ln(y),
$$

(6.88)

as in the strongly ordered case. The double logarithm matches with SVirtual and the single logarithm can be absorbed by choosing a renormalization scale that is quadratic in the vanishing invariants, such as $\mu_{PS} \propto p_\perp$.

In the hard collinear limit, the shower integrals behave as

$$
- \text{PS:} \quad s_{qg} = y \to 0, s_{gq} \to s \quad \frac{\alpha_s}{2\pi} \left[ - \frac{1}{6} C_A + \frac{1}{6} n_F \right] \ln(y),
$$

(6.89)
6.2. Sudakov Integrals

Figure 6.6: NLO correction factor for smooth $p_{\bot}$-ordering, with GGG antennae, without (top row) and with (bottom row) the CMW rescaling of $\Lambda_{QCD}$. The left-hand panes use $\mu_{PS} = p_{\bot}$ and the right-hand ones $\mu_{PS} = 2p_{\bot}$. For all plots, $\alpha_s = 0.12$, $n_F = 5$, and the evolution scale for gluon splittings was $m_{qq}$. 
the same as in all the other cases. This completes the argument that indeed $\mu_{PS} \propto p_\perp$ is the appropriate choice also for smooth $p_\perp$-ordering.

In fig. 6.6 we show the NLO correction factors, $(1 + V_{3Z})$, for smooth $p_\perp$-ordering. The top row shows the correction factors without using the CMW rescaling of $\Lambda_{QCD}$, and the plots in the bottom row include it. For the left-hand panes, we used a shower renormalization scale of $\mu_{PS} = p_\perp$, and for the right-hand ones we used $\mu_{PS} = 2p_\perp$.

We see that all correction factors are essentially well-behaved, with no runaway logs, similarly to the case of strong $p_\perp$-ordering. However, for the case of smooth $p_\perp$-ordering, it looks as if the CMW rescaling (bottom row) is almost doing “too much” in the soft region. Given that the CMW arguments [145] were derived explicitly by considering the subleading behaviour of strongly ordered (coherent) parton showers, we do not perceive of this as any major drawback. Instead, one should merely be aware of the slight shifts in the NLO corrections that result from applying it or not, recalling that a rescaling of $\Lambda$ by the CMW factor $\sim 1.5$ is within the ordinary factor 2 variation of the renormalization scale that is often taken as a standard for uncertainty estimates.

The shifts caused by CMW rescaling and/or by renormalization-scale prefactors are of course fully taken into account in our implementation in the VINCIA code, and are thus reabsorbed into the one-loop matching coefficient at the matched order, stabilizing the prediction. Differences at higher orders will result from the fact that the CMW rescaling, if applied, is used for all shower branchings, while the NLO correction derived here is only applied at the $Z \rightarrow 3$ stage of the calculation.

Because smooth $p_\perp$-ordering is the default in VINCIA we wish to understand this case as best as we can, and therefore we include some further comparisons with non-default settings in fig. 6.7.

In fig. 6.7a we modify the normalization of the evolution variable from the VINCIA default $Q_E^2 = 4p_\perp^2$ to the ARIADNE choice $Q_E^2 = p_\perp^2$. Though the normalization

Figure 6.7: NLO correction factor for smooth $p_\perp$-ordering, with GGG antennae: variations of how gluon splittings are interleaved with gluon emissions, see text. We used $\alpha_s = 0.12$, $n_F = 5$, and $\mu_{PS} = p_\perp$. 

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factor cancels in the $P_{imp}$ factor for sequential gluon emissions, it is relevant for deciding the relative ordering between gluon emissions and gluon splittings. As this plot shows, however, the modification only produces quite small differences in the NLO correction factor, and with the “wrong” sign. Thus, we retain $N_\perp = 4$ as the default in VINCIA. In fig. 6.7b we change the evolution variable for gluon splittings to be the same as that for gluon emissions, i.e., $p_\perp$, with similar conclusions as for the previous variation. In fig. 6.7c we switch off the Ariadne factor for gluon splittings. We notice that the NLO corrections get slightly larger. There is no change along the diagonal $y_{ij} = y_{jk}$ since the Ariadne factor is unity there, but along the edges of the plots, the NLO corrections become larger, which further motivates the choice of keeping the Ariadne factor switched on by default in VINCIA.

The overall result is that the infrared limits are generally well-behaved for $p_\perp$ evolution with $\mu_{PS} \propto p_\perp$. Remaining differences amount to small finite shifts of order 10%-20% away from unity. At that level, the effective finite terms of the antenna functions also play a role, hence it is too early to draw definite conclusions just based on the plots presented here. The impact of finite terms will be studied in section 6.3 in the context of matching to the LO matrix elements for $Z \rightarrow 4$ partons, which effectively fixes the finite terms with respect to the pure-shower answers studied here.

### 6.2.3 Tables of Infrared Limits

The results of the preceding subsections on the infrared limits of the pole-subtracted matrix elements and of the Sudakov integrals generated by the various evolution-scale choices are collected here, in parametric form, for easy reference. The renormalization terms, $V_{3\mu}$, are not included. Tab. 6.1 expresses the limits of SVirtual, while tab. 6.2 contains the Sudakov-integral limits.

<table>
<thead>
<tr>
<th>SVirtual</th>
<th>soft</th>
<th>hard collinear</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>$\left(-L^2 - \frac{10}{3}L - \frac{\pi^2}{6}\right)C_A + \frac{1}{3}n_FL$</td>
<td>$-\frac{2}{3}LC_A + \frac{1}{6}n_FL$</td>
</tr>
</tbody>
</table>

Table 6.1: Limits of SVirtual, with $L$ denoting $\ln(y)$, and $s_{qq}/s = s_{gq}/s = y \rightarrow 0$, omitting an overall factor of $\alpha_s/2\pi$. 

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<table>
<thead>
<tr>
<th>$p_\perp$</th>
<th>strong</th>
<th>smooth</th>
</tr>
</thead>
<tbody>
<tr>
<td>soft</td>
<td>$(L^2 - \frac{1}{3}L + \frac{\pi^2}{6}) C_A + \frac{1}{3} n_F L$</td>
<td>$(L^2 - \frac{1}{3}L - \frac{\pi^2}{6}) C_A + \frac{1}{3} n_F L$</td>
</tr>
<tr>
<td>hard col.</td>
<td>$-\frac{1}{6} L C_A + \frac{1}{6} n_F L$</td>
<td>$(-\frac{1}{6} L - \frac{\pi^2}{6}) C_A + \frac{1}{6} n_F L$</td>
</tr>
<tr>
<td>$m_D$</td>
<td>soft</td>
<td>smooth</td>
</tr>
<tr>
<td></td>
<td>$(L^2 + \frac{3}{2}L - \frac{\pi^2}{6}) C_A$</td>
<td>$(L^2 + \frac{3}{2}L - \frac{\pi^2}{6}) C_A$</td>
</tr>
<tr>
<td></td>
<td>hard col.</td>
<td></td>
</tr>
<tr>
<td></td>
<td>$-\frac{1}{6} L C_A + \frac{1}{6} n_F L$</td>
<td>$(-\frac{1}{6} L - \frac{\pi^2}{6}) C_A + \frac{1}{6} n_F L$</td>
</tr>
</tbody>
</table>

Table 6.2: Limits of strong and smooth $p_\perp$ and $m_D$ ordering, with $L$ denoting $\ln(y)$, with $s_{qg} = s_{gq} = y \to 0$. Non divergent terms, such as $\pi^2$ have been omitted in the calculation of $V_{3Z}$, and the renormalization term in $V_{3Z}$ is set to zero. An overall factor of $\alpha_s/2\pi$ is suppressed. Therefore $p_T$ in the soft limit will yield a correction of $V_{3z} = -\beta_0$ while the hard collinear region of $p_T$ and both the soft and hard collinear region of $m_D$ add a correction of $V_{3z} = -\frac{1}{2}\beta_0$.

6.3 Results Including both LO and NLO Corrections

In the preceding section, we focussed on deriving the analytic forms of the shower integrals and comparing their infrared limits to the matrix-element expressions. It is now time to include also the finite terms arising from matching to the 4-parton tree-level matrix element, expressed by the $\delta A$ terms in eq. (6.32). Our ultimate aim in this section is to include the full leading-colour one-loop corrections through second order in $\alpha_s$ (i.e., up to and including $Z \to 3$ partons) and combine these with the full-colour tree-level corrections through third order in $\alpha_s$ (i.e., up to and including $Z \to 5$ partons, the default in VINCIA). However, since we shall perform the $\delta A$ integrals numerically, adding those terms to the analytic ones derived in the previous section, we first wish to examine the numerical size and precision required on the $\delta A$ terms themselves.

6.3.1 Finite Antenna Terms and LO Matching Corrections

Finite-term variations of the antenna functions (and in particular fixing the finite terms via unitary LO matching corrections, such as is done in VINCIA [110]) will affect the terms generated by the $3 \to 4$ Sudakov expansions in the following way. Larger finite terms will cause an increased amount of $3 \to 4$ branchings, which in turn will decrease the associated Sudakov factor (in the sense of driving it closer to zero). This will feed into the NLO correction factor, which compensates and drives the final answer back towards its NLO-correct value. (Note that similar variations will not occur for the $2 \to 3$ branching step, since we treat that as fixed to the LO 3-parton matrix element throughout.) This feedback mechanism is encoded in the $\delta A$ terms in eq. (6.32).

Following the reasoning above, we should expect larger antenna finite terms to increase the NLO correction factor (since, to stabilize the 3-parton exclusive rate, it must compensate for losing more 3-parton phase-space points to 4-parton ones), and vice versa:

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6.3. Results Including both LO and NLO Corrections

Figure 6.8: NLO correction factor for strong (top row) and smooth (bottom row) $p_{\perp}$-ordering, for MIN (left), VINCIA default (middle), and MAX (right) antenna functions. We use $\mu_R = p_{\perp}$ combined with CMW rescaling, $\alpha_s = 0.12$, and gluon splitting in $m_{qq}$.

smaller finite terms should result in a decrease of the NLO correction. At the pure-shower level (i.e., without LO matrix-element corrections to fix the finite terms), this is illustrated by fig. 6.8.

For ease of comparison, all plots use the CMW rescaling of $A_{QCD}, \mu_{PS} = p_{\perp}, n_F = 5$, and $\alpha_s(m_Z) = 0.12$. The default antenna functions in VINCIA\footnote{Note that VINCIA was recently updated with a set of helicity-dependent antenna functions [149], so the defaults shown here are not identical to the GGG ones, but are instead helicity sums/averages over the functions defined in [149].} are shown in the middle panes, for strong (top row) and smooth (bottom row) ordering, respectively. A variation with smaller finite terms for the $3 \rightarrow 4$ antenna functions is shown to the left, and one with larger finite terms on the right. As expected, the NLO correction factors react by becoming lower for smaller finite terms and higher for larger finite terms, for both strong and smooth ordering.

We emphasise that the plots in fig. 6.8 are shown purely for illustration, to give a feeling for the changes produced by finite-term variations. In the actual matched shower
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Figure 6.9: Size of $\delta A$ terms differences between GGG and VINCIA default antennae.

evolution, the constraint imposed by matching to the LO 4-parton matrix elements fixes the finite terms, via the unitary procedure derived in [110], which was briefly recapped in section 5.2.1. The effective finite terms then depend on the full LO 4-parton matrix elements, and have a more complicated structure than the simple antenna functions we have so far been playing with. We shall therefore not attempt to integrate them analytically, but prefer instead to let VINCIA compute a numerical MC estimate for us.

Each point in that MC integration will involve computing at least one LO 4-parton matrix element, hence it is crucial to know how many points will be needed to obtain sufficient accuracy. Since everything else is handled analytically, this will be the deciding factor in determining the speed of the NLO-corrected algorithm. We shall perform a speed test below in section 6.3.4, but first we need to determine the accuracy we need on the $\delta A$ integral.

A first analytic estimate of the size of the $\delta A$ terms can be obtained by simply computing the ones produced by switching from GGG to the VINCIA default antennae (summed and averaged over helicities [149]), with the following $O(1)$ finite-term differences:

$$qg \to qgg : \quad F_{\text{Emit}}^{\text{VINCIA}} - F_{\text{Emit}}^{\text{GGG}} = 1.5 - (2.5 - y_{ij} - 0.5y_{jk}) = -1 + y_{gij} + 0.5y_{jk}, \quad (6.90)$$

$$qg \to q\bar{q}'q' : \quad F_{\text{Split}}^{\text{VINCIA}} - F_{\text{Split}}^{\text{GGG}} = 0.0 - (0.5 + y_{ij}) = 0.5 - y_{ij}, \quad (6.91)$$

with $F_{\text{Emit}}$ and $F_{\text{Split}}$ defined in eqs. (5.4) and (5.5). The $\delta A$ terms produced by these differences are plotted in fig. 6.9 for strong ordering in $m_D$ (left) and $p_\perp$ (centre), and for smooth ordering in $p_\perp$ (right), respectively. As expected, they do come out to be numerically subleading, roughly of order $\alpha_s/(2\pi)$, relative to LO (unity), yielding corrections ranging from a few permille to about a percent of the LO result.

Finally, in fig. 6.10 we include the full LO 4-parton matrix elements and plot the distribution of numerically computed $\delta A$ terms during actual VINCIA runs, for 100,000 events. The result is now represented by a one-dimensional histogram, with $\delta A$ on the x-axis and relative rate on the y-axis. On the left-hand pane, the $\delta A$ distribution with default settings is shown on a linear scale, while the right-hand pane shows the same result on a logarithmic scale, including variations with higher numerical accuracy.
6.3. Results Including both LO and NLO Corrections

As mentioned above, the integration is done by a uniform Monte Carlo sampling of the $\delta A$ integrands. We require a numerical precision better than 1\% on the estimated size of the term (relative to LO) and, by default, always sample at least 100 MC points for each antenna integral. In the left-hand pane of fig. 6.10 we see that, even with the full 4-parton LO matrix-element corrections included, the size of the $\delta A$ terms remains below one percent for the vast majority of 3-parton phase-space points.

On the logarithmic scale in the right-hand pane of fig. 6.10, however, it is evident that there is also a tail of quite rare phase-space points which are associated with larger $\delta A$ corrections. Numerical investigations reveal that this tail is mainly generated by the integrals over the $g \rightarrow q\bar{q}$ terms, in particular in phase-space points in which the gluon is collinear to one of the original quarks. This agrees with our expectation that these terms are the ones to which the pure shower gives the “worst” approximation, and hence they are the ones that receive the largest matrix-element corrections. As a test of the numerical stability of the NLO corrections for these points, we increased the minimum number of MC points used for the $\delta A$ integration from the default 100 (shown with “+” symbols) to 400 (“×” symbols) and 1600 (“∗” symbols), cutting the expected statistical MC error in half with each step, at the cost of increased event-generation time. Though we do observe a slight broadening of the distribution between the default and the higher-precision settings, the shifts should be interpreted horizontally and remain well under the required percent-level precision with respect to LO. The default settings are therefore kept at a minimum of 100 MC points, though we note that future investigations, in particular of more complicated partonic topologies, may require developing a better understanding of, and perhaps a better shower approximation to, these integrals, especially the $g \rightarrow q\bar{q}$ contribution.

For completeness, we note that the runs used to obtain these distributions were performed using the new default “Nikhef” tune of VINCI A’s NLO-corrected shower, which
will be described in more detail in the following subsection. Parameters for the tune are given in appendix D.

6.3.2 LEP Results

Since we have restricted our attention to massless partons in this work, we shall mainly consider the light-flavour-tagged event-shape and fragmentation distributions produced by the L3 experiment at LEP for our validations and tuning, see [150]. We consider three possible VINCIA settings:

- New default (NLO): uses two-loop running for $\alpha_s$, with CMW rescaling of $\Lambda_{QCD}$. From the comparisons to event-shape variables presented in this section, we settled on a value of $\alpha_s(M_Z) = 0.122$. A few modifications to the string-fragmentation parameters were made, relative to the old default, to compensate for differences in the region close to the hadronization scale. The revised parameters are listed in appendix D under the “Nikhef” tune.

- New default (NLO off). Identical to the previous bullet point, but with the NLO correction factor switched off.

- Old default (LO tune): uses one-loop running for $\alpha_s$, without CMW rescaling of $\Lambda_{QCD}$, and $\alpha_s(M_Z) = 0.139$. The string-fragmentation parameters are those of the “Jeppsson 5” tune, see appendix D.

The three main event-shape variables that were used to determine the value of $\alpha_s(M_Z)$ are shown in fig. 6.11 with upper panes showing the distributions themselves (data and MC) and lower panes showing the ratios of MC/data, with one- and two-sigma uncertainties on the data shown by darker (green) and lighter (yellow) shaded bands, respectively. The Thrust (left) and $C$-parameter (middle) distributions both have perturbative expansions that start at $O(\alpha_s)$ and hence they are both explicitly sensitive to the corrections considered in this chapter. The expansion of the $D$ parameter (right) begins at $O(\alpha_s^2)$. It is sensitive to the NLO 3-jet corrections mainly via unitarity, since all 4-jet events begin their lives as 3-jet events in our framework. It also represents an important cross-check on the value extracted from the other two variables.

For a pedagogical description of the variables, see [150]. Pencil-like 2-jet configurations are to the left (near zero) for all three observables. This region is particularly sensitive to non-perturbative hadronization corrections. More spherical events, with several hard perturbative emissions, are towards the right (near 0.5 for Thrust and 1.0 for $C$ and $D$). The maximal $\tau = 1 - T$ for a 3-particle configuration is $\tau = 1/3$ (corresponding to the Mercedes configuration), beyond which only 4-particle (and higher) states can contribute. This causes a noticeable change in slope in the distribution at that point, see fig. 6.11a. The same thing happens for the $C$ parameter at $C = 3/4$, in fig. 6.11b. The $D$ parameter is sensitive to the smallest of the eigenvalues of the sphericity tensor, and is therefore zero for any purely planar event, causing it to be sensitive only to 4- and higher-particle configurations over its entire range.
6.3. Results Including both LO and NLO Corrections

Figure 6.11: L3 light-flavour event shapes: Thrust, $C$, and $D$. 
Both the new NLO tune (solid blue line with filled-dot symbols) and the old LO one (dashed magenta line with open-triangle symbols) reproduce all three event shapes very well. With the NLO corrections switched off (solid red line with open-circle symbols), the new tune produces a somewhat too soft spectrum, consistent with its low value of \( \alpha_s(M_Z) \) not being able to describe the data without the benefit of the NLO 3-jet corrections.

As a further cross check, we show two further event-shape variables that were included in the L3 study in fig. 6.12: the Wide and Total Jet Broadening parameters, \( B_W \) and \( B_T \), respectively. These have a somewhat different and complementary sensitivity to the perturbative corrections, compared to the variables above, picking out mainly the transverse component of jet structure. They are equal at \( \mathcal{O}(\alpha_s) \), but \( B_T \) receives somewhat larger \( \mathcal{O}(\alpha_s^2) \) corrections than \( B_W \). Again, we see that both the old (LO) and new (NLO) defaults are able to describe the data, and that the spectrum with the new default value for \( \alpha_s(M_Z) \) is too soft if the NLO corrections are switched off.

Finally, as an aid to constraining the Lund fragmentation-function parameters, the L3 study also included two infrared-sensitive observables: the charged-particle multiplicity and momentum distributions, to which we compare in fig. 6.13, with the momentum fraction defined as

\[
x = \frac{2|p|}{\sqrt{s}}.
\]

(6.92)

There is again no noteworthy differences between the old and new default tunes.

Having determined the value of \( \alpha_s(M_Z) \) and the parameters of the non-perturbative fragmentation function, we extended the validations to include a set of jet-rate and jet-resolution measurements by the ALEPH experiment [151] (now without the benefit of light-flavour tagging), using the standard Durham \( k_T \) algorithm for \( e^+e^- \) collisions [152], as implemented in the FASTJET code [153]. We also compared to default PYTHIA 8 and, for completeness, checked that the relative production fractions of various meson and baryon species were indeed unchanged relative to the old VINCIA default.

Rather than presenting all of this information in the form of many additional plots, tab. 6.3 instead provides a condensed summary of all the validations we have carried out, via \( \langle \chi^2 \rangle \) values for each of the models with respect to each of the LEP distributions, including a flat 5% “theory uncertainty” on the MC numbers. Already from this simple set of \( \chi^2 \) values, it is clear that the LO models/tunes are already doing very well\(^3\). This agreement, however, comes at the price of using a very large (“LO”) value for \( \alpha_s \), which is not guaranteed to be universally applicable.

The main point of the overview in tab. 6.3 is that an equally good agreement can be obtained with an \( \alpha_s(m_Z) \) value that is consistent with other NLO determinations [158], specifically

\[
\alpha_s(m_Z) = 0.122,
\]

(6.93)

once the NLO 3-jet corrections are included. This should carry over to other NLO-corrected processes, and hence the fragmentation parameters we have settled on should be

\(^3\)Both VINCIA and PYTHIA are known to give quite good fits to LEP data [110, 149, 154, 155]. For comparisons including other generators and tunes, see [mcplots.cern.ch](http://mcplots.cern.ch).
6.3. Results Including both LO and NLO Corrections

Figure 6.12: L3 light-flavour event shapes: jet broadening

Figure 6.13: L3 light-flavour fragmentation observables: charged-track multiplicity and momentum distribution.

applicable to future NLO-corrected studies with VINCIA, and can also serve as a starting point for NLO-level matching studies with PYTHIA 8. In the latter context, the 2-loop
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<th>$\langle \chi^2 \rangle$ Shapes</th>
<th>$T$</th>
<th>$C$</th>
<th>$D$</th>
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<th>$B_T$</th>
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</thead>
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<tr>
<td>PYTHIA 8</td>
<td>0.8</td>
<td>0.4</td>
<td>0.9</td>
<td>1.2</td>
</tr>
<tr>
<td>VINCIA (LO)</td>
<td>0.0</td>
<td>0.5</td>
<td>0.3</td>
<td>0.6</td>
</tr>
<tr>
<td>VINCIA (NLO)</td>
<td>0.1</td>
<td>0.7</td>
<td>0.2</td>
<td>0.6</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>$\langle \chi^2 \rangle$ Jets</th>
<th>$r_{4j}^{\text{exc}}$</th>
<th>$\ln(y_{12})$</th>
<th>$r_{2j}^{\text{exc}}$</th>
<th>$\ln(y_{23})$</th>
<th>$r_{3j}^{\text{exc}}$</th>
<th>$\ln(y_{34})$</th>
</tr>
</thead>
<tbody>
<tr>
<td>PYTHIA 8</td>
<td>0.1</td>
<td>0.2</td>
<td>0.1</td>
<td>0.2</td>
<td>0.1</td>
<td>0.3</td>
</tr>
<tr>
<td>VINCIA (LO)</td>
<td>0.1</td>
<td>0.2</td>
<td>0.1</td>
<td>0.2</td>
<td>0.0</td>
<td>0.2</td>
</tr>
<tr>
<td>VINCIA (NLO)</td>
<td>0.2</td>
<td>0.4</td>
<td>0.1</td>
<td>0.3</td>
<td>0.1</td>
<td>0.3</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>$\langle \chi^2 \rangle$ Jets</th>
<th>$r_{4j}^{\text{exc}}$</th>
<th>$\ln(y_{45})$</th>
<th>$r_{5j}^{\text{exc}}$</th>
<th>$\ln(y_{56})$</th>
<th>$r_{6j}^{\text{inc}}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>PYTHIA 8</td>
<td>0.2</td>
<td>0.3</td>
<td>0.2</td>
<td>0.4</td>
<td>0.3</td>
</tr>
<tr>
<td>VINCIA (LO)</td>
<td>0.3</td>
<td>0.1</td>
<td>0.1</td>
<td>0.0</td>
<td>0.0</td>
</tr>
<tr>
<td>VINCIA (NLO)</td>
<td>0.2</td>
<td>0.2</td>
<td>0.1</td>
<td>0.2</td>
<td>0.1</td>
</tr>
</tbody>
</table>

Table 6.3: $\langle \chi^2 \rangle$ values for: Top: L3 light-flavour event shapes and fragmentation variables [150], and LEP average meson and baryon fractions [156, 157]. Bottom: Durham $k_T n$-jet rates, $r_{nj}$, and jet resolutions, $y_{ij}$, measured by the ALEPH experiment [151]. For the latter, the $\langle \chi^2 \rangle$ calculation was restricted to the perturbative region, $\ln(y) > -8$. A flat 5% theory uncertainty was included on the MC numbers. Both default PYTHIA and the VINCIA (LO) tune use $\alpha_s(m_Z) = 0.139$ while the VINCIA (NLO) tune uses $\alpha_s(m_Z) = 0.122$.

running in particular could be retained, while the soft fragmentation parameters would presumably have to be somewhat readjusted to absorb differences between VINCIA and PYTHIA 8 near the hadronization scale.

### 6.3.3 Uncertainties

As in previous versions of VINCIA, we use the method proposed in [110] to compute a comprehensive set of uncertainty bands, which are provided in the form of a vector of alternative weights for each event. Each set is separately unitary, with average weight one. The difference with respect to previous versions is that each variation now benefits

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4The differences in soft fragmentation parameters between existing LO VINCIA and PYTHIA-8 tunes could be used as an initial guideline for such an effort, see, e.g., appendix D.

5VINCIA currently does not attempt to give a separate estimate of the uncertainty on the total inclusive cross section. The uncertainties it computes only pertain to shapes of distributions and the effects of cuts on the

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6.3. Results Including both LO and NLO Corrections

fully from the inclusion of NLO corrections.

When setting the parameter \texttt{Vincia:uncertaintyBands = on}, the uncertainty weights are accessible through the method

\begin{verbatim}
    double vincia.weight(int i=0);
\end{verbatim}

with \( i = 0 \) corresponding to the ordinary event sample, normally with all weights equal to unity, and the following variations, for \( i = \):

1. Default: since the user may have chosen other settings than the default, the default is included as the first variation.

2. \texttt{alphaS-Hi}: all renormalization scales are decreased to \( \mu = \mu_{\text{def}}/k_{\mu} \), where \( \mu_{\text{def}} = \mu_{\perp} \) for gluon emission and \( \mu_{\text{def}} = m_{qq} \) for gluon splitting. The default value of \( k_{\mu} = 2 \) can be changed by the user. A second-order compensation for this variation is provided by the renormalization-scale sensitive term \( V_{3\mu} \).

3. \texttt{alphaS-Lo}: \( \mu = \mu_{\text{def}} \cdot k_{\mu} \), with similar comments as above.

4. \texttt{ant-Hi}: antenna functions with large finite terms (MAX [149]). This variation is already compensated for by LO matching and is not explicitly affected by the NLO corrections.

5. \texttt{ant-Lo}: antenna functions with small finite terms (MIN [149]), with similar comments as above.

6. \texttt{NLO-Hi}: branching probabilities are multiplied by a factor \( (1 + \alpha_s) \) to represent unknown (but finite) NLO corrections. Is canceled by NLO matching.

7. \texttt{NLO-Lo}: branching probabilities are divided by a factor \( (1 + \alpha_s) \). Is canceled by NLO matching.

8. \texttt{Ord-pT1}: \( p_{\perp} \) ordering with alternative (user-definable) \( N_{\perp} \) normalization factor in \( Q_{E}^2 = N_{\perp} p_{\perp}^2 \). Compensated at first order by LO matching, and at second order (Sudakov corrections) by NLO matching via ordering-sensitive terms in \( V_{3Z} \).

9. \texttt{Ord-mD}: smooth \( m_D \) ordering, with similar comments as above.

10. \texttt{NLC-Hi}: \( qg \) emission antennae use \( C_A \) as colour factor. Compensated at first order by LO matching. Not affected by NLO matching since we only operate at leading colour.

11. \texttt{NLC-Lo}: \( qg \) emission antennae use \( 2C_F \) as colour factor, with similar comments as above.

---

total inclusive rate.
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We emphasize that these variations are not all independent (for instance the $\alpha_s$ and NLO variations are highly correlated) and hence the corresponding uncertainties should not be summed in quadrature. In the VINCIARoot plotting tool included with VINCIAM, the uncertainty band is constructed by taking the max and min of the variations. See the VINCIAM HTML manual for more information about the uncertainty bands and [110] for details on their algorithmic construction.

### 6.3.4 Speed

Although the CPU time required by matrix-element and shower/hadronization generators is still typically small in comparison to that of, say, full detector simulations, their speed and efficiency are still decisive for all generator-level studies, including tuning and validation, parameter scans, development work, phenomenology studies, comparisons to measurements corrected to the hadron level, and even studies interfaced to fast detector simulations. For this wide range of applications, the high-energy simulation itself constitutes the main part of the calculation. An important benchmark relevant to practical work is for instance whether the calculation can be performed easily on a single machine or not.

Higher matched orders are characterized by increasing complexity and decreasing unweighting efficiencies, resulting in an extremely rapid growth in CPU requirements (see e.g. [149]). At NLO, the additional issues of negative weights and/or so-called counter-events can contribute further to the demands on computing power. With this in mind, high efficiencies and fast algorithmic structures were a primary concern in the development of the formalism for leading-order matrix-element corrections in VINCIAM [110, 133, 149], and this emphasis carries through to the present work. We can make the following remarks.

- The only fixed-order phase-space generator is the Born-level one. All higher-multiplicity phase-space points are generated by (trial) showers off the lower-multiplicity ones. This essentially produces a very fast importance-sampling of phase-space that automatically reproduces the dominant QCD structures.

- Likewise, the only cross-section estimate that needs to be precomputed at initialization is the total inclusive one. Thus, initialization times remain at fractions of a second regardless of the matching order.

- The matrix-element corrected algorithm works just like an ordinary parton shower, with modified (corrected) splitting kernels. In particular, all produced events have the same weights, and no additional unweighting step is required.

- Since the corrections are performed multiplicatively, in the form of $(1+\text{correction})$, with 1 being the LO answer, there are no negative-weight events and no counter-events. The only exception would be if the correction becomes larger than the LO answer, and negative. This would correspond to a point with a divergent fixed-order expansion, in which case the use of NLO corrections would be pointless anyway. Moreover, as demonstrated by the plots in the previous sections, our definitions of
6.4. Outlook and Conclusions

<table>
<thead>
<tr>
<th>LO level</th>
<th>NLO level</th>
<th>Time / Event [milliseconds]</th>
<th>Speed w.r.t. PYTHIA</th>
</tr>
</thead>
<tbody>
<tr>
<td>$Z \rightarrow Z$</td>
<td>2</td>
<td>0.4</td>
<td>1</td>
</tr>
<tr>
<td>VINCIA (NLO)</td>
<td>2, 3, 4, 5</td>
<td>2, 3.0</td>
<td>$\sim 1/5$</td>
</tr>
<tr>
<td>VINCIA (NLO)</td>
<td>2, 3, 4, 5</td>
<td>2, 3.0</td>
<td>$\sim 1/7$</td>
</tr>
</tbody>
</table>

Table 6.4: Event-generation time in VINCIA 1.0.30 compared to PYTHIA 8.176.

the corrections are analytically stable (and numerically subleading with respect to LO) over all of phase space, including the soft and collinear regions, for reasonable renormalization- and evolution-variable choices.

- The parameter variations described in section 6.3.3 can be performed together with the matching corrections to provide a set of uncertainty bands in which each variation benefits from the full corrections up to the matched orders. These are provided in the form of a vector of alternative weights for each event [110], at a cost in CPU time which is only a fraction of that of a comparable number of independent runs.

These attributes, in combination with helicity dependence in the case of the leading-order formalism [149], allow VINCIA to run comfortably on a single machine even with full-fledged matching and uncertainty variations switched on.

The inclusion of NLO corrections will necessarily slow down the calculation. The relative increase in running time relative to PYTHIA 8, is given in tab. 6.4, including the default level of tree-level matching, with and without the NLO 3-jet correction. Without it (but still including the default tree-level corrections which go up to $Z \rightarrow 5$ partons), VINCIA is 5 times slower than PYTHIA. With the NLO 3-jet correction switched on, this increases only slightly, to a factor 7. For a fully showered and hadronized calculation which includes second-order virtual and third-order tree-level corrections, we consider that to still be acceptably fast. Importantly, an event-generation time of a few milliseconds per event implies that serious studies can still be performed on an ordinary laptop computer.

6.4 Outlook and Conclusions

In this work, we have investigated the expansion of a Markov-chain QCD shower algorithm to second order in the strong coupling, for $e^+ e^- \rightarrow 3$ partons, and made systematic comparisons to matrix-element results obtained at the same order. Using these results, we have subjected the subleading properties of shower algorithms with different evolution/ordering variables and different renormalization-scale choices to a rigorous examination. At the analytical level, we have compared the logarithmic structures at the edge...
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of phase space, and at the numerical level we have illustrated the difference between the expanded shower algorithm and the one-loop matrix element.

We find that the choice of $p_\perp$-ordering, with a renormalization scale proportional to $p_\perp$ yields the best agreement with the one-loop matrix element, over all of phase space. This elaborates on, and is consistent with, earlier findings [128, 145]. Using the antenna invariant mass, $m_D$, for the evolution variable still gives reasonable results in the hard regions of phase space, but leads to logarithmically divergent corrections for soft emissions, the exact form of which depends on the choice of renormalization variable. In the VIN-CIA code, we retain the option of using $m_D$ mainly as a way of providing a conservative uncertainty estimate.

With the NLO 3-jet corrections included as multiplicative corrections to the shower branching probabilities, we find that we can obtain good agreement with a large set of LEP event-shape, fragmentation, and jet-rate observables with a value of the strong coupling constant of $\alpha_s(M_Z) = 0.122$. This is in strong contrast with earlier (LO) tunes of both PYTHIA and VINCIA which employed much larger values $\sim 0.14$ to obtain agreement with the LEP measurements.

This chapter is intended as a first step towards a systematic embedding of one-loop amplitudes within the VINCIA shower and matching formalism. To arrive at a full-fledged prescription, this will need to be extended to hadron collisions, ideally in a way that allows for convenient automation. A first step towards developing the underlying shower formalism for $pp$ collisions was recently taken [159], and more work is in progress.

In addition, further studies should be undertaken of the impact of unordered sequences of radiation that can occur for the smooth-ordering case (it may be necessary to adopt a strategy similar to the truncated showers of the MC@NLO approach), and the mutually related issues of total normalization and how much of the (hard) corrections are exponentiated (similar to the differences between the POWHEG and MC@NLO formalisms, but here occurring at one additional order, where the relevant total normalization is the NNLO one). Finally, it would be interesting to develop an extension of this formalism that would allow second-order-corrected antenna functions to be used at every stage in the shower, thereby upgrading the precision of the all-orders resummation, a project that would involve examining the second-order corrections to branchings of $qg$ and $gg$ mother antennae as well.