Zero-Jettiness Soft Function to Third Order in Perturbative QCD

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We present the high-precision result for the zero-jettiness soft function at next-to-next-to-next-to-leading order (N3LO) in perturbative QCD. At this perturbative order, the soft function is the last missing ingredient required for the computation of a hadronic color singlet production or a color singlet decay into two jets using the zero-jettiness variable as the slicing parameter. Furthermore, the knowledge of the N3LO soft function enables the resummed description of the thrust distribution in the process $e^+e^- \to$ hadrons through next-to-next-to-next-to-leading logarithmic order, which is important for the extraction of the strong coupling constant using this shape variable. On the methodological side, the complexity of the zero-jettiness variable forced us to develop a new semi-analytic method for phase-space integration in the presence of constraints parameterized through Heaviside functions which, hopefully, will be useful for further development of the N-jettiness slicing scheme.

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Introduction—During the next decade, experiments at the Large Hadron Collider (LHC) will test the standard model (SM) of particle physics at an unprecedented level of precision provided that uncertainties of the theoretical predictions can be controlled. This opportunity motivated an enormous effort in theoretical collider physics, see Ref. [1] for a recent overview. Among other things, these advances enabled fully differential description of the Higgs boson and the vector boson production processes at next-to-next-to-next-to-leading order (N3LO) in perturbative QCD [2–7].

Perturbative computations in QCD have to go beyond pure virtual amplitudes because the latter are infrared divergent. For infrared safe observables, these divergences are known to cancel with the real-emission contributions and, in case of hadron collisions, with additional contributions that originate from the collinear renormalization of parton distribution functions [8–10]. Organizing such a cancellation in an observable- and process-independent way is nontrivial. A popular approach that allows one to do this is the so-called slicing method where an observable δ is introduced to distinguish subprocesses with Born kinematics ($\delta = 0$) from subprocesses with higher final-state multiplicity ($\delta \neq 0$). The $\delta = 0$ case includes virtual corrections, as well as unresolved soft and/or collinear real-emission contributions. The universal factorization of the real-emission matrix elements in the soft and collinear limits and the infrared safety of the slicing variable δ allow a simplified calculation of the $\delta = 0$ contributions.

In practice, one introduces a cut-off parameter $\delta_c \ll 1$ and treats all contributions with $\delta < \delta_c$ as unresolved, i.e., corresponding to the $\delta = 0$ case discussed above. Contributions from the phase-space regions with $\delta > \delta_c$ require at least one formally resolved emission, so that the perturbative order of the required computation drops by one unit compared to the target precision of the inclusive cross section (i.e., N3LO becomes NNLO, etc.) [11].

Among several slicing variables that have been discussed in recent years, there is just one that can be used to describe processes with an arbitrary number of jets beyond NLO. Dubbed N jettiness in the original papers [14,15], it was used as a slicing variable in Refs. [5,16–20] to compute NNLO QCD corrections to several processes with either zero or one jet. For the N-jettiness variables, the unresolved contribution can be expressed in terms of the beam, soft and jet functions [14,15,21] which can be computed in perturbative QCD independently of each other. The NNLO beam and jet functions were computed in Refs. [22–24]. The NNLO soft functions for zero and one jettiness were calculated in Refs. [25–31], and for two jettiness in Ref. [32]. Extension of this approach to higher-multiplicity

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processes requires computation of NNLO N-jettiness soft function for an arbitrary number of hard final-state particles. This was accomplished recently in Ref. [33], making the N-jettiness slicing scheme the very first perturbative framework for which, through NNLO, all divergencies of unresolved real-emission ingredients are known analytically for arbitrary collider processes (see also Ref. [34] where a fully numerical calculation of the N-jettiness soft function at NNLO was reported).

To extend the N-jettiness slicing scheme to N3LO in QCD we need to compute beam, jet and soft functions through this perturbative order. While beam and jet functions do not depend on the multiplicity N and were calculated a few years ago [35–39], the N3LO QCD soft functions remain unknown.

In fact, the computation of the N3LO N-jettiness soft function for an arbitrary number of hard final-state partons is a problem of outstanding technical complexity. Hence, as the first step it is reasonable to focus on the simplest possible soft function, namely the one where the number of hard emitters is exactly two. In this case, the N-jettiness variable reduces to the zero-jettiness one, defined as follows:

$$\mathcal{T}_0(n) = \sum_{i=1}^{n} \min\left[\frac{2p_a \cdot k_i}{P}, \frac{2p_b \cdot k_i}{P}\right]. \quad (1)$$

In Eq. (1), the summation index runs over all soft partons in a particular process, $p_{a,b}$ are four-momenta of two hard emitters and P is an arbitrary variable with the mass dimension one.

The soft function is then computed with the help of the following formula:

$$S_\tau = \sum_{n=0}^{\infty} S_\tau^{(n)}, \quad (2)$$

where

$$S_\tau^{(n)} = \frac{1}{\mathcal{N}} \int \prod_{i=1}^{n} [\mathrm{d}k_i] \delta[\tau - \mathcal{T}_0(n)] \mathrm{Eik}(p_a, p_b, \{k\}_n). \quad (3)$$

In Eq. (3), $[\mathrm{d}k] = \mathrm{d}^d k/(2\pi)^{d-1} \delta(k^2)\theta(k^0)$ with $d = 4 - 2\epsilon$, the eikonal function is defined as follows:

$$\mathrm{Eik}(p_a, p_b, \{k\}) = \lim_{\{k\}\to 0} \frac{|\mathcal{M}(p_a, p_b, \{k\})|^2}{|\mathcal{M}(p_a, p_b)|^2}, \quad (4)$$

and $\mathcal{N}$ is the symmetry factor that is required to properly account for the contribution of identical particles to $S_\tau^{(n)}$.

Each function $S_\tau^{(n)}$ describes a partonic process with n final-state soft partons computed to an arbitrary loop order, where also all loop amplitudes have to be calculated in the leading soft approximation. Thus $S_\tau^{(n)} \sim \alpha_s^n$ at the leading order and, thanks to the virtual corrections, it also contains arbitrary powers of α_s in higher orders. A simple way to visualize what needs to be computed is to recognize that S_τ is a (normalized) cross section computed in the soft approximation for both real and virtual partons, where the standard energy-momentum conservation condition is replaced with the requirement that the zero jettiness has a particular value τ.

Hence, similar to the contributions to perturbative cross sections at high orders of perturbation theory, the computation of the zero-jettiness soft function at N3LO requires the triple-real contribution, the one-loop correction to the double-real contribution and the two-loop correction to the single-real contribution, displayed in Fig. 1. We note that the triple-real contribution is known partially [40,41], whereas full results are available for the other two [42,43]. While the calculation of the one-loop correction to the double-real emission treats phase-space and loop integration on the same footing, the simple form of the integrated two-loop correction to the single-emission soft current [44] allows one to integrate over the soft-gluon phase space after the loop integration has been performed. Furthermore, the three-loop correction to the Born amplitude vanishes in the soft approximation since the appearing loop integrals are scaleless.

In this Letter, we report on the completion of the calculation of the triple-real contribution and present a high-precision result for the zero-jettiness soft function to third order in perturbative QCD. In what follows, we briefly describe the calculation summarizing technical challenges and tests of the calculation that have been performed; a more detailed discussion will be given elsewhere [45]. We present the result for the N3LO contribution to the zero-jettiness soft function, which can also be found in digital form alongside this submission, and conclude after that.

Overview of the calculation—The challenge with computing the soft function arises from the very definition of the zero-jettiness variable, which, for each soft parton, requires selecting the minimal value among scalar products of parton's and hard emitters' momenta. Thus, this function can change abruptly in the middle of the phase space making

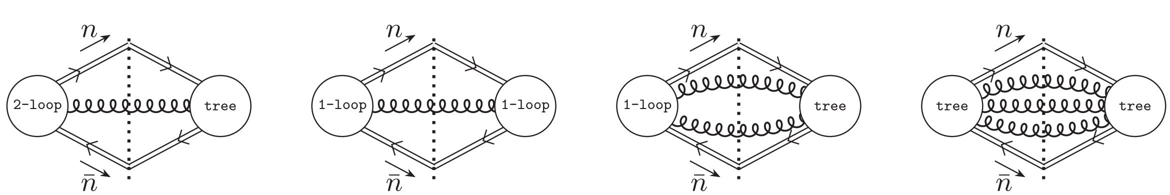

FIG. 1. Different contributions to the zero-jettiness soft function at N3LO, see text for details. Only contributions with final-state gluons are shown. Diagrams to the right of the cut are complex conjugated.

analytic integration of the soft function rather difficult. If, instead, one attempts a numerical integration, one has to face a plethora of poorly understood soft and collinear singularities, typical to a generic N3LO computation, and ultraviolet divergencies that arise because the energy-momentum conservation requirement has been dropped. These problems make the numerical calculation of the soft function highly nontrivial, especially in such a high order as N3LO.

To enable the computation of the zero-jettiness soft function, we make use of the fact that it is Lorentz invariant and its dependence on P, $s_{ab} = 2p_a \cdot p_b$ and τ can be easily reconstructed. Thus, we can set $\tau = 1$ and choose a reference frame and a factor P without loss of generality. We take $P = \sqrt{s_{ab}}$, and consider a center-of-mass frame where

$$p_a = \frac{\sqrt{s_{ab}}}{2} n, \qquad p_b = \frac{\sqrt{s_{ab}}}{2} \bar{n}, \tag{5}$$

with $n^2 = \bar{n}^2 = 0$ and $n \cdot \bar{n} = 2$. We then write

$$k_i = \frac{\alpha_i}{2} n + \frac{\beta_i}{2} \bar{n} + k_{\perp,i}. \tag{6}$$

We use this decomposition and rewrite Eq. (1) as

$$\mathcal{T}_0(n) = \sum_{i=1}^{n} \min\,[\alpha_i, \beta_i], \tag{7}$$

which allows us to project the phase-space integrations on the unique value of $\mathcal{T}_0$ by inserting partitions of unity

$$1 = \theta(\alpha_i - \beta_i) + \theta(\beta_i - \alpha_i), \tag{8}$$

to the integrand in Eq. (3) for each of the soft partons.

Thus, to compute the triple-real contribution, we should integrate the eikonal function in Eq. (4) over the phase space of three real gluons with a δ function $\delta(\tau - x_1 - x_2 - x_3)$ where $x_i = \min[\alpha_i, \beta_i]$, and a product of three θ functions whose arguments are $\pm(\alpha_i - \beta_i)$.

We note that the required eikonal function for three soft gluons was computed and simplified in Ref. [46]. For the $q\bar{q}g$ soft final-state partons the required eikonal function can be extracted from Ref. [47]. We have recomputed these eikonal functions for the case of two hard partons, that we require for the analysis in this Letter, and found agreement with the results reported in these references.

Using these results for the eikonal functions, we can construct all required real-emission integrals with constraints provided by the definition of the zero-jettiness variable. These integrals are complicated, and we make use of the various internal symmetries to simplify them. For example, we note that upon relabeling $n \leftrightarrow \bar{n}$, integrals do not change. This implies that we have only two classes of integrals to consider. The first class involves integrals where the phase-space constraint is

$$\delta\left(1 - \sum_{i=1}^{3} \beta_i\right) \prod_{i=1}^{3} \theta(\alpha_i - \beta_i). \tag{9}$$

We will refer to such integrals as nnn integrals. The second class of integrals are integrals where the constraint reads

$$\delta\left(1 - \sum_{i=1}^{2} \beta_i - \alpha_3\right) \prod_{i=1}^{2} \theta(\alpha_i - \beta_i)\theta(\beta_3 - \alpha_3). \tag{10}$$

We will refer to these integrals as $nn\bar{n}$ integrals. All integrals that are needed for the calculation of $S_\tau^{(3)}$ can be written as a linear combination of nnn and $nn\bar{n}$ integrals using the freedom to rename $n \leftrightarrow \bar{n}$ and $k_i \leftrightarrow k_j$, $i, j \in \{1, 2, 3\}$.

To further reduce the number of triple-real integrals that have to be calculated, we employ integration-by-parts (IBP) identities [48,49]. To make this technology applicable to phase-space integrals which contain θ functions as constraints, we use its extensions discussed in Refs. [40,50]. Following Ref. [50] and rewriting phase space integrals as cuts of loop integrals, we derive the integration-by-parts identities where we encounter additional terms associated with derivatives of (some) θ functions. Since $\mathrm{d}\theta(x)/\mathrm{d}x = \delta(x)$, we can apply reverse unitarity [50] one more time, obtaining a system of equations for integrals with θ functions and integrals where one of the θ functions is replaced by a δ function. Selecting the latter, and writing the integration-by-parts equations for them, we obtain integrals that contain two δ functions and one θ function, in addition to the original ones. Applying this procedure iteratively, we obtain a list of integrals that close the system of integration-by-parts equations. These integrals contain a various number of θ and δ functions; the original integrals possess three θ functions and the "simplest" ones—three δ functions.

Upon generating sufficiently many IBP equations, we obtain a system of linear equations that contains all integrals that are required to compute the triple-real emission contribution to the soft function. We then solve this system and express the required integrals through a set of basis (or master) integrals. Once master integrals are calculated, the result for the triple-real emission contribution to the soft function is obtained.

Although the setup that we describe above is standard, realizing it in practice turned out to be quite challenging. We list below some of the issues that we encountered and briefly comment on how we solved them.

(i) The (usually straightforward) step of constructing linear algebraic equations for the required triple-real integrals with the help of the integration-by-parts method turns out to be nontrivial in this case because none of the public computer codes dedicated to processing loop integrals and deriving and solving IBP equations for them, can work with θ-function constraints.

(ii) A replacement of θ functions with δ functions in integrands creates difficulties with defining unique integral families since, upon such replacements, propagators that define classes of integrals become linear dependent. A multivariate partial fractioning has to be applied to map integrals on the unique set of families. This has to be done on the fly when the integration-by-parts identities are constructed.

(iii) Once a large-enough system of linear equations is obtained, we solve it using the program KIRA [51–53]. To obtain the solution, we need to choose preferred master integrals, and we do so by using criteria such as the minimal number of θ functions, the simplest structure of propagators, etc.

(iv) As explained in Ref. [41], not all integrals with θ-function constraints are regularized dimensionally. To ameliorate this problem, we need to introduce an analytic regulator which provides an additional challenge for various steps discussed in the previous items. Although the dependence on the analytic regulator cancels in the final expression for the soft function, it significantly complicates the reduction to master integrals and their calculation.

(v) We have attempted to compute the required master integrals analytically. In many cases this can be done in a relatively straightforward way provided that singular limits of integrands can be identified, subtracted, and evaluated separately. To calculate finite remainders of divergent master integrals whose integrands can be expanded in series in ϵ, we relied very heavily on the program HYPERINT [54]. It is not an exaggeration to say that without it, obtaining analytic results for the majority of integrals would not have been possible.

(vi) Diagrams that describe processes where an off-shell gluon splits into three soft gluons lead to integrals that contain the following propagator:

$$\frac{1}{k_{123}^2} = \frac{1}{2k_1k_2 + 2k_1k_3 + 2k_2k_3}. \tag{11}$$

We were unable to compute integrals with such a propagator analytically by direct integration. Instead, we modified this propagator by introducing a "mass" term

$$\frac{1}{k_{123}^2} \to \frac{1}{k_{123}^2 + m^2}, \tag{12}$$

making master integrals functions of m^2. It is then straightforward to derive the differential equations for m-dependent master integrals [55]. Once the differential equations become available, we solve them numerically, starting from the $m^2 \to \infty$ limit, where boundary constants can be computed, and propagate these solutions to $m^2 = 0$, where a particular limit of mass-dependent integrals, that corresponds to Taylor series in m^2, is needed.

(vii) Calculation of boundary conditions at $m^2 = \infty$ is a highly nontrivial problem. Indeed, these real-emission integrals possess ultraviolet divergencies since the δ function $\delta(\tau - \mathcal{T}_0)$ does not constrain energies of all the partons. This fact results in the appearance of $\mathcal{O}(m^{-4\epsilon})$ and $\mathcal{O}(m^{-2\epsilon})$ "branches" in $m^2 \to \infty$ integrals, in addition to regular Taylor branches which correspond to a "naive" expansion of integrands in powers of $1/m^2$.

We have computed all the required boundary constants analytically. To reduce the number of independent boundary integrals that have to be calculated, we simplified the master integrals at $m^2 \to \infty$ along the lines described in Ref. [39], and used integration-by-parts identities to derive relations amongst expanded integrals of a specific branch.

(viii) We have tested the computed master integrals in several ways. First, we have constructed a Mellin-Barnes representation for all $m^2 = 0$ integrals, required for the calculation of the soft function, and computed them numerically. We were able to verify the analytic results, as well as the results of $m^2 \to 0$ extrapolation of the solution of the differential equations for a large number of highly nontrivial integrals.

We have also checked solutions of the differential equations for master integrals at finite m^2 by using them to predict results for other integrals that can be evaluated by a direct numerical integration. The numerical integration is performed using the sector decomposition [56,57] and, by choosing the integrals carefully, it is possible to keep the size of the resulting expressions under control. By computing many such integrals, we were able to check all the master integrals at finite m^2.

(ix) As part of the effort to compute the missing $nn\bar{n}$ real-emission integrals, we have recalculated the nnn contribution to the soft function at N3LO, reported earlier in Ref. [39] and found complete agreement.

Renormalization—We are now in a position to assemble the final result for the soft function. To write it in the simplest way possible, we note that S_τ is a distribution in the variable τ. The leading order term is normalized to be a δ function, $\delta(\tau)$, and terms of the type $\tau^{-1-2n\epsilon}$ with $n = 1$, 2, 3, etc. appear in higher perturbative orders. In fact, for a generic s_{ab} and P in the definition of the jettiness variable, Eq. (1), the nth order contribution to the soft function will have a prefactor

$$X_\tau^n = \frac{1}{\tau}\left(\frac{\tau P}{\mu\sqrt{s_{ab}}}\right)^{-2n\epsilon}, \tag{13}$$

where the renormalization scale μ appears when the bare QCD coupling constant is rewritten through the renormalized one. We note that the $\overline{\mathrm{MS}}$ renormalization scheme is used throughout this Letter. To avoid the need to deal with the distributions, it is convenient to work with the Laplace transform of the soft function defined as follows:

$$S = \int_0^\infty \mathrm{d}\tau S_\tau e^{-\tau u}, \tag{14}$$

where u is the parameter of the Laplace transform. Integrating the quantity in Eq. (13), we find

$$\int_0^\infty \mathrm{d}\tau X_\tau e^{-\tau u} = -\frac{e^{-2\epsilon n\gamma_E}\Gamma(1-2n)}{2n\epsilon} e^{2n\epsilon L_S}, \tag{15}$$

where $L_S = \log(\bar{u}\mu\sqrt{s_{ab}}/P)$, $\bar{u} = ue^{\gamma_E}$, and γ_E is the Euler-Mascheroni constant. Hence, we conclude that the Laplace transform of the soft function depends on the parameter L_S.

The bare soft function S is a divergent quantity; it requires a dedicated renormalization. In the Laplace space, this renormalization is multiplicative,

$$\tilde{S} = Z_s S, \tag{16}$$

where $\tilde{S}$ is the renormalized soft function that contains no $1/\epsilon$ poles, and Z_s is a function of the strong coupling constant $\alpha_s(\mu)$ and L_s.

The renormalization constant Z_s can be determined from the renormalization group equation [58,59]

$$\mu \frac{\mathrm{d}}{\mathrm{d}\mu} \log Z_s(\mu) = -4\Gamma_{\mathrm{cusp}} L_S - 2\gamma^s. \tag{17}$$

The cusp anomalous dimension Γ_{cusp} and the soft anomalous dimension γ^s in Eq. (17) can be found in Ref. [60], as extracted from Refs [61–70]. We provide them in digital form in Supplemental Material [71].

The renormalization group equation (17) can be solved order by order in the expansion in the strong coupling constant α_s. Once Z_S is obtained, it is straightforward to use it to predict $1/\epsilon$ poles of the bare soft function. The leading pole of the nth order contribution is $1/\epsilon^{2n-1}$, which means that for the N3LO soft function, there are five $1/\epsilon$ poles that the reported calculation should reproduce. It goes without saying that this should occur independently for different color and n_f factors, so in practice the number of checks that our calculation has to pass is quite significant. Indeed, we find that our result for the bare soft function does reproduce all the $1/\epsilon$ poles that are predicted by the renormalization group equation.

Results and discussion—To present the result for the renormalized soft function, we write an expansion of its logarithm in powers of $a_s = \alpha_s(\mu)/(4\pi)$

$$\log[\tilde{S}(L_S)] = \sum_{i=1}^{3} a_s^i \sum_{j=0}^{2i} C_{i,j} L_S^j. \tag{18}$$

At each order in the perturbative expansion, the coefficients of the logarithms L_S are predicted in terms of cusp and soft anomalous dimensions, and the soft function at lower perturbative orders. Thus, the soft function can be fully reconstructed from the expression where the logarithm L_S is set to zero, $L_S \to 0$. Writing

$$\log[\tilde{S}(0)] = C_R \mathcal{C}, \tag{19}$$

where C_R is the Casimir operator of the hard emitters [$C_R = C_F(C_A)$ for quarks (gluons)], we obtain

$$\mathcal{C} = -a_s\pi^2 + a_s^2\left[n_f T_F\left(\frac{80}{81} + \frac{154\pi^2}{27} - \frac{104\zeta_3}{9}\right) - C_A\left(\frac{2140}{80} + \frac{871\pi^2}{54} - \frac{286\zeta_3}{9} - \frac{14\pi^4}{15}\right)\right]$$
$$+ a_s^3\left[n_f^2 T_F^2\left(\frac{265408}{6561} - \frac{400\pi^2}{243} - \frac{51904\zeta_3}{243} + \frac{328\pi^4}{1215}\right) + n_f T_F(C_F X_{FF} + C_A X_{FA}) + C_A^2 X_{AA}\right], \tag{20}$$

where the three quantities X_{FF}, X_{FA}, and X_{AA}, truncated to 16 significant digits, read

$$X_{FF} = 68.9425849800376,$$
$$X_{FA} = 839.7238523813981,$$
$$X_{AA} = -753.7757872704537. \tag{21}$$

Equations (20) and (21) are the main result of the Letter. We note that it should be possible to obtain even more precise numerical results within our setup, and eventually reconstruct a fully analytic result using standard methods as was done in Ref. [41]. We also note that the computer-readable result for the renormalized soft function $\tilde{S}(L_S)$ through N3LO can be found in Supplemental Material [71].

The results reported in Eq. (21) can be compared with earlier attempts to deduce the nonlogarithmic contribution to the soft function using existing NNLO QCD prediction for thrust in $e^+e^- \to 3$ jets [72], the result for the N3LO hard function for $e^+e^- \to 2$ jets [73], and the result for the N3LO jet function [35]. Using the value of the N3LO nonlogarithmic contribution to the cumulative cross section for thrust in the singular limit extracted in Ref. [26] from a fit to a fixed order prediction obtained with the EERAD3 Monte Carlo program [72], the $\mathcal{O}(a_s^3)$ contribution to the soft function was obtained in Ref. [35]. In our notation, this result corresponds to the coefficient of the a_s^3 term in the expansion of $\tilde{S}(0)$ with $C_R = C_F$ and $n_f = 5$. Denoting this coefficient as $c_{3,qq}$, and using numerical results shown in Eq. (21), we find that our calculation yields

$$c_{3,qq} = -1369.575849. \tag{22}$$

The constant $c_{3,qq}$ in Eq. (22) should be contrasted with the value of $c_{3,qq}$ obtained in Ref. [35] using the result of the numerical fit reported in Ref. [26],

$$c_{3,qq}^{\mathrm{fitted}} = -19988 \pm 1440(\mathrm{stat}) \pm 4000(\mathrm{syst}). \tag{23}$$

Since the difference between the two results is substantial, we note that possible issues with the validity of the fit result obtained with the EERAD3 program were recently pointed out in Ref. [74]. Interestingly, a significantly smaller value of $c_{3,qq}$ may have important implications for the determination of the strong coupling constant from the thrust distribution, pushing it to slightly larger values, see Ref. [74].

Conclusion—In this Letter, we reported the result of the calculation of the N3LO QCD contribution to the soft function defined using the zero-jettiness variable. This soft function is the last ingredient that is needed to enable the use of the zero-jettiness slicing scheme for N3LO computations for color-singlet production at the LHC or for N3LO description of the two-jet production in e^+e^- annihilation. This soft function can also be used to resum zero-jettiness logarithms with N3LL′ accuracy for the thrust distribution in the vicinity of the two-jet limit, as was recently discussed in Ref. [74] using a fitted value for $c_{3,qq}$. As pointed out in that reference, the extraction of α_s from the thrust distribution will certainly benefit from the exact value of $c_{3,qq}$ obtained in this Letter.

Our calculation is the first ever computation of the N3LO soft function for the N-jettiness variable, albeit for $N = 0$. The next logical step is to attempt to extend it to the $N = 1$ case where, ideally, one would use the result for the $N = 0$ soft function as a boundary condition that contains the most demanding singular limits. This idea was the gist of the approach employed in Ref. [33] for computing the NNLO soft function for arbitrary N, and it would be very interesting to attempt to generalize it to the N3LO case.

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[11] We note in passing that slicing methods may suffer from so-called power corrections which, at this point, are poorly understood, but are expected to be significant for zero-jettiness slicing [12,13]. To ameliorate this problem in a numerical calculation, one needs to choose δ_c to be very small reducing the efficiency of a calculation.

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