### Soft parton-to-hadron FFs at NNLO\*+NNLL

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Abstract: The evolution of the parton-to-hadron fragmentation functions (FF) at low fractional hadron momenta z is theoretically studied in a framework combining next-to-next-to-leading-order (NNLO)  $\alpha_s$  corrections with next-to-modified-leading logarithmic resummations of soft and collinear parton radiation. The energy evolution of the moments of the low-z FFs are thereby computed, and compared to the existing experimental  $e^+e^-$  and DIS  $e^{\pm}p$  jet data. The impact of hadron-mass effects and higher-order corrections is presented. The data-theory comparison of the four FF moments (total hadron multiplicity, peak, width, and skewness) allow us to extract the QCD coupling  $\alpha_s$  at approximate NNLO accuracy,  $\alpha_s(m_z^2) = 0.1205\pm 0.0010^{+0.0022}_{-0.0000}$ , in excellent numerical agreement with the current world average.

#### Introduction

The distribution of hadrons in a jet is theoretically described by a fragmentation function (FF),  $D_{i\rightarrow h}(z, Q)$ , representing the probability that parton *i* fragments into hadron *h* carrying a fraction  $z = p_{hadron}/p_{parton}$  of the parent parton momentum. Starting with a parton at a given energy Q, its evolution to another energy scale Q' is driven by a branching process of parton radiation and splitting, resulting in a jet shower, which can be computed perturbatively using the DGLAP equations [1] at large  $z \gtrsim 0.1$ . The bulk of hadrons produced in the fragmentation of a jet come, however, from shower partons with low z < 0.1 values, a regime dominated by soft and collinear gluon bremsstrahlung that require proper resummation of their associated  $\log(1/x)$  and  $\ln \theta$ -singularities. Indeed, the emission of successive gluons inside a jet follows a parton cascade where the emission angles decrease as the jet evolves towards the hadronisation stage ("angular ordering"). Due to colour coherence and interference of gluon radiation, the energy spectrum of the majority of intrajet partons adopts a typical "hump-backed plateau" (HBP), or distorted Gaussian (DG), shape as a function of the log of the inverse of z,  $\xi = \ln(1/z)$ . This final distribution is infrared-safe in the sense that it is directly imprinted, without modifications, into the final charged particles spectrum after parton hadronization.

Various perturbative resummation schemes have been developed to treat the soft and collinear singularities present in the shower evolution of a jet: (i) the Leading Logarithmic Approximation (LLA) resums single logs of the type  $\left[\alpha_{\rm s} \ln \left(k_{\perp}^2/\mu^2\right)\right]^n$  where  $k_{\perp}$  is the transverse momentum of the emitted gluon with respect to the parent parton, (ii) the Double Logarithmic Approximation (DLA) resums soft-collinear and infrared gluons,  $g \to gg$  and  $q(\bar{q}) \to gq(\bar{q})$ , for small values of z and  $\theta \left[\alpha_{\rm s} \ln(1/z) \ln \theta\right]^n \sim \mathcal{O}(1)$  [2,3], (iii) Single Logarithms (SL) [4,5] take into account the emission of hard collinear gluons ( $\theta \to 0$ ),  $\left[\alpha_{\rm s} \ln \theta\right]^n \sim \mathcal{O}(\sqrt{\alpha_{\rm s}})$ , and (iv) the Modified Leading Logarithmic Approximation (MLLA), a SL correction to the DLA, resumming terms of order  $\left[\alpha_{\rm s} \ln(1/z) \ln \theta + \alpha_{\rm s} \ln \theta\right]^n \sim \left[\mathcal{O}(1) + \left(\mathcal{O}(\sqrt{\alpha_{\rm s}})\right)\right]$  [4]. We have developed a scheme to analytically compute the evolution of the HBP distribution of soft radiated partons in jets combining the next-to-MLLA approach [6] with fixed-order  $\alpha_{\rm s}$  corrections at an increasing level of accuracy: first at



Figure 1: Charged-hadron spectra in jets as a function of  $\xi = \ln(1/z)$  in  $e^+e^-$  at  $\sqrt{s} \approx 2-200$  GeV (left), and  $e^{\pm}$ ,  $\nu$ -p (Breit frame, scaled  $\times 2$  for the full hemisphere) at  $\sqrt{s} \approx 4-180$  GeV (right), individually fitted to Eq. (1) with the hadron mass corrections ( $m_{\text{eff}} = 130,110$  MeV) quoted.

approximate next-to-leading-order, NLO<sup>\*</sup> [7], followed by full-NLO [9], and then approximately next-to-NLO, NNLO<sup>\*</sup> [10].

We have used this framework to calculate the evolution of the jet FF, or rather its moments, as a function of the jet energy. The soft fragmentation function of a jet can be expressed, without any loss of generality, in terms of a distorted Gaussian (DG):

$$D(\xi, Y, \lambda) = \mathcal{N}/(\sigma\sqrt{2\pi}) \cdot e^{\left[\frac{1}{8}k - \frac{1}{2}s\delta - \frac{1}{4}(2+k)\delta^2 + \frac{1}{6}s\delta^3 + \frac{1}{24}k\delta^4\right]}, \text{ with } \delta = (\xi - \bar{\xi})/\sigma, \tag{1}$$

where  $\mathcal{N}$  is the average hadron multiplicity inside a jet, and  $\bar{\xi}$ ,  $\sigma$ , s, and k are respectively the mean peak position, dispersion, skewness, and kurtosis of the distribution. Within our DGLAP+NMLLA framework, the evolution of the moments of the FF as a function of initial jet energy and shower energy cutoff depend only on  $\Lambda_{\text{QCD}}$ . By comparing the theoretical energy dependence of the FF moments to jet fragmentation measurements in  $e^+e^-$  and deep-inelastic  $e^{\pm}p$  collisions, we are therefore able to extract a high-precision value of  $\alpha_s$  at NNLO<sup>\*</sup> accuracy.

### Energy evolution of the soft parton-to-hadron fragmentation functions

The system of equations for the FFs  $D_{i\to h}(z, Q)$  can be written as an evolution Hamiltonian which mixes gluon and (anti)quark states expressed in terms of DGLAP splitting functions for the branchings  $g \to gg$ ,  $q(\bar{q}) \to gq(\bar{q})$  and  $g \to q\bar{q}$ , where g, q and  $\bar{q}$  label a gluon, a quark, and an anti-quark respectively. The set of DGLAP+NMLLA integro-differential equations for the FF evolution can be solved analytically (iteratively) by expressing the Mellin-transformed hadron distribution in terms of the anomalous dimension  $\gamma$ :  $D \simeq C(\alpha_s(t)) \exp \left[\int^t \gamma(\alpha_s(t'))dt\right]$  for  $t = \ln Q$ , leading to a perturbative expansion in half powers of  $\alpha_s$ :  $\gamma \sim \mathcal{O}(\alpha_s^{1/2}) + \mathcal{O}(\alpha_s) + \mathcal{O}(\alpha_s^{3/2}) + \mathcal{O}(\alpha_s^{5/2}) + \cdots$ . The full expansion including up to the complete set of  $\mathcal{O}(\alpha_s^2) + \mathcal{O}(\alpha_s^{5/2})$  terms corresponds to theoretical results at NNLO+NNLL accuracy. The anomalous dimension  $\gamma$  allows one to calculate the moments of the DG through:

$$\mathcal{N} = K_0, \quad \bar{\xi} = K_1, \ \sigma = \sqrt{K_2}, \ s = \frac{K_3}{\sigma^3}, \ k = \frac{K_4}{\sigma^4}; \ K_{n \ge 0}(Y, \lambda) = \int_0^Y dy \left(-\frac{\partial}{\partial\omega}\right)^n \gamma_\omega \Big|_{\omega = 0}, \tag{2}$$

which are then inserted into Eq. (1). Corrections of  $\gamma$  up to order  $\alpha_s^{3/2}$  were computed in Refs. [7,8], followed by the full set of NLO  $\mathcal{O}(\alpha_s^2)$  terms, including the two-loop splitting functions, in Ref. [9]. At NLO, the diagonalisation of the evolution Hamiltonian results in two eigenvalues  $\gamma_{\pm\pm}$  in the  $\mathcal{D}^{\pm}$ basis, where the relevant one for the calculation of the FF moments  $\gamma_{++} \to \gamma_{\omega}^{\text{NLO+NNLL}}$ , reads:

$$\gamma_{\omega}^{\text{NLO+NNLL}} = \frac{1}{2}\omega(s-1) + \frac{\gamma_0^2}{4N_c} \left[ -\frac{1}{2}a_1(1+s^{-1}) + \frac{\beta_0}{4}(1-s^{-2}) \right] \\ + \frac{\gamma_0^4}{256N_c^2}(\omega s)^{-1} \left[ 4a_1^2(1-s^{-2}) + 8a_1\beta_0(1-s^{-3}) + \beta_0^2(1-s^{-2})(3+5s^{-2}) - 64N_c\frac{\beta_1}{\beta_0}\ln 2(Y+\lambda) \right] \\ + \frac{1}{4}\gamma_0^2\omega \left[ a_2(2+s^{-1}+s) + a_3(s-1) - a_4(1-s^{-1}) - a_5(1-s^{-3}) - a_6 \right], \quad (3)$$

where  $\gamma_0^2 = \frac{4N_c \alpha_s}{2\pi} = \frac{4N_c}{\beta_0(Y+\lambda)}$  is the LL anomalous dimension,  $s = \sqrt{1 + \frac{4\gamma_0^2}{\omega^2}}$ ,  $\beta_i$  the QCD  $\beta$ -function coefficients,  $a_{1,2}$  and hard constants obtained in [7], and  $a_{3,4,5,6}$  are new constants obtained from the full-resummed NNLL splitting functions [11]. In addition, terms from the NNLO  $\alpha_s$  running expression and the full systematic expansion of the anomalous dimension from the NNLL small-zresummed splitting functions have been added to the order  $\mathcal{O}(\alpha_s^{5/2})$  [12]. In particular, the account of NNLO  $\alpha_s$  provides corrections  $\propto \beta_2$  which were not considered before, and which are needed for the extraction of accurate values of  $\alpha_s$  from the data. Such terms should be added with those containing the small-z resummed N<sup>3</sup>LO splitting functions on equal footing and to the same order. (Since the splitting functions are only incorporated at NLO for the moment; our calculations can be considered of order NNLO<sup>\*</sup>+NNLL so far). Upon inverse-Mellin transformation, one obtains the energy evolution of the FF, and its associated moments, at NNLO\*+NNLL accuracy, as a function of  $Y = \ln(E/\Lambda_{OCD})$ , for an initial parton energy E, down to a shower cut-off scale  $\lambda = \ln(Q_0/\Lambda_{OCD})$  for  $N_f = 3, 4, 5$  quark flavors. The resulting formulae for the energy evolution of the moments depend on  $\Lambda_{\text{QCD}}$  as single free parameter. Relatively simpler expressions are obtained in the limitingspectrum case (for  $\lambda = 0$ , i.e. evolving the FF down to  $Q_0 = \Lambda_{\text{OCD}}$ ) motivated by the "local parton hadron duality" hypothesis for infrared-safe observables which states that the HBP distribution of partons in jets is simply renormalized in the hadronization process without changing its shape. Thus, by fitting the experimental hadron jet data at various energies to Eq. (1), one can determine  $\alpha_{\rm s}$  from the corresponding energy-dependence of its FF moments.

Figure 2 shows the energy evolution of the zeroth (multiplicity), first (peak position, closely connected to the mean of the distribution), second (width), and third (skewness) moments of the FF, at four levels of accuracy ( $\rm LO^*+LL$ ,  $\rm NLO^*+NLL$ ,  $\rm NLO+NNLL$ , and  $\rm NNLO^*+NNLL$ ). The hadron multiplicity increases exponentially with jet energy whereas the FF peak and width do it logarithmically, and the skewness features a slow power-law dropoff. The theoretical convergence of their evolutions are robust as proven by the small changes (10% max.) introduced by incorporating higher-order terms. On the other hand, the kurtosis (not shown), obtained from the fourth derivative of the anomalous dimension, features large non-convergent fluctuations in their jet-energy dependence from LO to NNLO<sup>\*</sup>.



Figure 2: Comparison of theoretical predictions at increasing level of accuracy (LO<sup>\*</sup> to NNLO<sup>\*</sup>) for the energy evolution of the jet charged-hadron multiplicity (top, left), FF peak position (top, right), FF width (bottom, left), and FF skewness (bottom, right).



Figure 3: Energy evolution of the jet charged-hadron multiplicity (left) and FF peak position (right) in  $e^+e^-$  and DIS jet data, fitted to the NNLO<sup>\*</sup>+NNLL predictions. The obtained  $\mathcal{K}_{ch}$  normalization constant, the individual NNLO<sup>\*</sup>  $\alpha_s(m_z^2)$  values, and  $\chi^2/ndf$  of the two fits, are quoted.

## Data-theory comparison and $\alpha_s$ extraction

We have first fitted to Eq. (1) the existing experimental jet FFs measured in 34 data sets from  $e^+e^-$  annihilation at  $\sqrt{s} = 2.2$ -206 GeV (amounting to 1200 HBP data points, Fig. 1 left) as well as from 15 DIS data-sets of the ZEUS collaboration over  $\sqrt{s} = 2.2$ -206 GeV, measured in the so call "brick-wall" Breit frame where the incoming quark scatters off the photon and returns along the same axis, (Fig. 1, right). Finite hadron-mass effects in the DG fit are accounted for through a rescaling of the theoretical (massless) parton momenta with an effective mass  $m_{\rm eff} \approx m_{\rm pion}$  as discussed in Refs. [7,8]. Also, the impact of particle decays on the extracted FF moments has been assessed comparing the BaBar data for prompt and inclusive hadrons [13], finding negligible effects for  $\xi < 5$ . To this first set of fitted FF moments, we have added the DG moments independently fitted by many other different  $e^+e^-$  and DIS measurements and published in the literature, finally collecting a total of about 340 experimental FF moments.

The individual fits for the first two FF moments are shown in Fig. 3 as a function of the original parton energy (i.e.  $\sqrt{s}/2$  in the case of  $e^+e^-$ , and invariant 4-momentum transfer  $Q_{\text{DIS}}$  for DIS). The overall normalization ( $\mathcal{K}_{ch}$ ) of the charged-hadron multiplicity of the jet, is an extra free parameter for this moment which, nonetheless, plays no role in the final  $\Lambda_{\text{QCD}}$  extracted given that its value just depends on the evolution of the multiplicity, and not on its absolute value at any given energy. The NNLO\*+NNLL limiting-spectrum ( $\lambda = 0$ ) predictions for  $N_f = 5$  active quark flavours<sup>\*</sup>, leaving  $\Lambda_{\text{QCD}}$  as a free parameter, reproduce very well the data. The most "robust" FF moment for the determination of  $\Lambda_{\text{QCD}}$  is the peak position  $\xi_{\text{max}}$  which proves quite insensitive to most of the uncertainties associated with the extraction method (DG and energy evolution fits, finitemass corrections) [8] as well as to higher-order corrections. The hadron multiplicities measured in DIS jets appear somewhat smaller (especially at high energy) than those measured in  $e^+e^-$ , due to limitations in the FF measurement only in half (current Breit)  $e^{\pm}$ p hemisphere and/or in the determination of the relevant Q scale [8].

The value of  $\alpha_s(m_z^2)$  obtained from the combined multiplicity+peak fit is  $\alpha_s(m_z^2) = 0.1205\pm0.0010$ , where the error includes all uncertainties as discussed in Ref. [8]. A conservative theoretical scale uncertainty of  $^{+0.0022}_{-0.0000}$  (obtained in [8] at NLO accuracy only) is added. This value is in perfect agreement with the current world-average,  $\alpha_s(m_z^2) = 0.1186\pm0.0012$ , obtained at NNLO accuracy from the combination of 6 different sets of observables [14,15]. The precision of our result  $\binom{+2\%}{-1\%}$  is clearly competitive with the other existing measurements, with a totally different set of experimental and theoretical uncertainties. Upcoming full-NNLO corrections of the energy evolution of the FF moments will entail a reduction of our final  $\alpha_s$  extraction and an eventual incorporation of the measurement into the world-average value. In the further future, the huge jet samples available at FCC-ee in the range of energies  $\sqrt{s} = 90-350$  GeV (combined with detectors with advanced charged particle reconstruction down to momenta  $p_T \approx 100$  MeV) will allow one to further reduce the experimental uncertainties, and extract  $\alpha_s$  with permille precision.

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<sup>\*</sup>Few-% corrections are applied to deal with slightly different  $N_f = 3.4$  evolutions below charm, bottom thresholds.

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