Global extraction of the parton-to-pion fragmentation functions at NLO accuracy in QCD

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Abstract.
In this review, we discuss the results on the parton-to-pion fragmentation functions obtained in a combined NLO fit to data of single-inclusive hadron production in electron-positron annihilation, proton-proton collisions, and lepton-nucleon deep-inelastic scattering. A more complete discussion can be found in Ref. [1].

1. Introduction
Fragmentation functions (FFs) are fundamental objects which describe the collinear transition of a quark $i$ into a hadron $H$ with a fraction $z$ of its momentum, and it is usually named as $D^H_i(z)$. These FFs can only be obtained by performing global fits. However, since the FFs are non perturbative objects, they cannot be computed from first principles and they need to be extracted by fitting the experimental data of different kind of processes. However, the scale dependence of the FFs can be obtained in perturbative QCD (pQCD) and can be determined by renormalization group equations, similar to those for parton densities (PDF).

In here we present the results of Ref. [1] where we obtained an updated set of parton-to-pion FFs with the determination of their uncertainties by applying the Iterative Hessian (IH) method in light of all the newly available, precise experimental results in single-inclusive pion production in electron-positron annihilation (SIA), semi-inclusive deep-inelastic lepton-nucleon scattering (SIDIS), and $pp$ collisions. This will allow us to scrutinize the consistency of the information on FFs extracted across the different hard scattering processes, i.e., to validate the fundamental notion of universality, which is at the heart of any pQCD calculation based on the factorization of short- and long-distance physics [2].

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2. Functional Form and Fit Parameters

We parametrize the hadronization of a parton of flavor $i$ into a positively charged pion at an initial scale of $Q_0 = 1$ GeV as

$$D_i^{\pi^+}(z, Q_0) = \frac{N_i z^{\alpha_i(1 - z)\beta_i[1 + \gamma_i(1 - z)\delta_i]} B[2 + \alpha_i, \beta_i + 1] + \gamma_i B[2 + \alpha_i, \beta_i + 1]}{B[2 + \alpha_i, \beta_i + 1]}.$$  \hspace{1cm} (1)

Here, $B[a, b]$ denotes the Euler Beta-function, and the $N_i$ in (1) are chosen in such a way that they represent the contribution of $zD_i^{\pi^+}$ to the momentum sum rule.

The improved experimental information now allows us to impose less constraints on the parameter space. More specifically, as before we still have to assume isospin symmetry, i.e.,

$$D_u^+ = D_d^+,$$  \hspace{1cm} (2)

and we need to relate the total $u$-quark and $d$-quark FFs by a global, $z$-independent factor $N_{d+d}$:

$$D_{d+d}^{\pi^+} = N_{d+d} D_{u+\bar{u}}^{\pi^+},$$  \hspace{1cm} (3)

which quantifies any charge symmetry violation found in the fit. The fragmentation of a strange quark into a pion is now related to the unfavored FFs in Eq. (2) by

$$D_s^{\pi^+} = D_\bar{s}^{\pi^+} = N_s z^{\alpha_s} D_{\bar{u}}^{\pi^+},$$  \hspace{1cm} (4)

rather than just using a constant as in the DSS analysis. Besides, the charm- and bottom-topion FFs no longer assume $\gamma_c = \gamma_b = 0$ in Eq. (1) but can now exploit the full flexibility of the ansatz. As in the DSS and all other analyses [3, 4, 5, 6, 7], we include heavy flavor FFs discontinuously as massless partons in the QCD scale evolution above their $\overline{\text{MS}}$ “thresholds”, $Q = m_c, m_b$, with $m_c$ and $m_b$ denoting the mass of the charm and bottom quark, respectively.

In total we now have 28 free fit parameters describing our updated FFs for quarks, antiquarks, and gluons into positively charged pions. The corresponding FFs for negatively charged pions are obtained by charge conjugation and those for neutral pions by assuming $D_i^{\pi^0} = [D_i^{\pi^+} + D_i^{\pi^-}]/2$.

3. Data Selection

For the global fit, we use all the available experimental information on single-inclusive charged and neutral pion production in SIA, SIDIS, and hadron-hadron collisions.

Compared to the data sets already used in the DSS global analysis [3], we include the new results from BABAR [8] and BELLE [9] in SIA at a c.m.s. energy of $\sqrt{S} \simeq 10.5$ GeV. Both sets are very precise, with relative uncertainties of about $2 - 3\%$, and reach all the way up to pion momentum fractions $z$ close to one, well beyond of what has been measured so far. As customary, we limit ourselves to data with $z \geq 0.1$ to avoid any potential impact from kinematical regions where finite, but neglected, hadron mass corrections, proportional to $M_\pi/(S^{1/2}z)$, might become of any importance [3, 6, 7].

In case of SIDIS, we replace the preliminary multiplicity data from HERMES [10] by their released final results [11]. More specifically, we use the data for charged pion multiplicities as a function of momentum transfer $Q^2$ in four bins of $z$ taken on both a proton and a deuteron target. In addition, we include the still preliminary multiplicity data for $\pi^\pm$ from the COMPASS Collaboration [12], which are given as a function of $z$ in bins of $Q^2$ and the initial-state momentum fraction $x$. In addition, for the SIDIS data sets we do not have to impose any cuts on both data sets to accommodate them in the global analysis.

Finally, we add a couple of new sets of data for inclusive high-$p_T$ pion production in $pp$ collisions to the results from the PHENIX experiment [13] already included in the DSS analysis.
Most noteworthy are the first results for neutral pions from the Alice Collaboration at CERN-LHC [14], covering unprecedented c.m.s. energies of up to 7 TeV. In addition, we add STAR data taken at $\sqrt{S} = 200$ GeV in various rapidity intervals for both neutral and charged pion production and for the $\pi^−/\pi^+$ ratio [15, 16, 17, 18]. It is worth mentioning that it turns out that a good global fit of RHIC and LHC $pp$ data, along with all the other world data, can only be achieved if one imposes a cut on the minimum $p_T$ of the produced pion of about 5 GeV.

4. Fit Procedure and Uncertainty Estimates

The 28 free parameters describing the updated parton-to-pion FFs in Eq. (1) at the chosen input scale of 1 GeV are again determined from a standard $\chi^2$ minimization where

$$\chi^2 = \sum_{i=1}^{N} \left[ \left( \frac{1 - N_i}{\delta N_i} \right)^2 + \sum_{j=1}^{N_i} \frac{(N_i T_j - E_j)^2}{\delta E_j^2} \right],$$

for $i = 1, \ldots, N$ data sets, each contributing with $N_i$ data points. $E_j$ is the measured value of a given observable, $\delta E_j$ the error associated with this measurement, and $T_j$ is the corresponding theoretical estimate for a given set of parameters in Eq. (1). In this new fit, we derive the optimum normalization shifts analytically from the condition $\partial \chi^2 / \partial N_i = 0$, which yields

$$N_i = \frac{\sum_{j=1}^{N_i} \frac{\delta N_i^2}{\delta E_j^2} T_j E_j + 1}{1 + \sum_{j=1}^{N_i} \frac{\delta N_i^2}{\delta E_j^2} T_j^2}.$$ (6)

Here, $\delta N_i$ denotes the quoted experimental normalization uncertainty for data set $i$.

Now, in order to estimate the uncertainties we use the IH method [19]. The main idea of the method is to assume a quadratic behavior of the $\chi^2$ hyper-surface of parameter displacements and to express the $\chi^2$ increment from its minimum value in terms of combinations of fit parameters that maximize the variation. These sets correspond to fixed displacements along the eigenvector directions of the Hessian matrix. To define the eigenvector sets one has to choose a tolerance parameter $\Delta \chi^2$ for the increment in $\chi^2$ which is still acceptable in the global fit. Here we proceed as follows: the tolerances for the eigenvector sets corresponding to 68% and 90% confidence level (C.L.) intervals are determined from the Gaussian probability density function for a $\chi^2$ distribution with $k$ degrees of freedom (d.o.f.):

$$P_k(x) = \frac{x^{k/2-1}e^{-x/2}}{\Gamma(k/2)2^{k/2}}.$$ (7)

The $\Delta \chi^2$ related to the 68$^{th}$ and 90$^{th}$ percentiles are then obtained by solving $\int_0^{\chi^2 + \Delta \chi^2} dx P_k(\chi^2) = 0.68$ and 0.90, respectively.

Finally, we choose the next-to-leading order (NLO) set of PDFs from the MSTW group [20] and the corresponding uncertainty estimates in computations of the SIDIS and $pp$ cross sections. For consistency, we also fix the strong coupling $\alpha_S$ to the values obtained in the MSTW fit.

5. Results

In this section we present and discuss the results of our global analysis of parton-to-pion fragmentation functions. First, we present the obtained fit parameters, normalization shifts, and individual $\chi^2$ values. Next, the obtained $D_i^{\pi^+}(z, Q^2)$ and their uncertainties are shown and compared to the results of the DSS fit.
5.1. Parton-To-Pion Fragmentation Functions

Table 1 reveals already a notable difference to one of the findings of the DSS analysis which preferred an unexpectedly sizable breaking of the charge symmetry between $u + \bar{u}$ and $d + \bar{d}$ FFs of about 10% [3], within large uncertainties though. Now, with much improved experimental information on charged pion multiplicities both from HERMES [11] and COMPASS [12] and new data on the ratio $\pi^-/\pi^+$ in $pp$ collisions from STAR [17], the parameter $N_{d+q}$ in Eq. (3) prefers to stay very close to unity, i.e., very little or no breaking.

Table 1. Parameters describing the NLO FFs for positively charged pions, $D_{i\pi^+}(z,Q_0)$, in Eq. (1) in the $\overline{\text{MS}}$ scheme at the input scale $Q_0 = 1$ GeV. Results for the charm and bottom FFs refer to $Q_0 = m_c = 1.43$ GeV and $Q_0 = m_b = 4.3$ GeV, respectively.

| flavor $i$ | $N_i$ | $\alpha_i$ | $\beta_i$ | $\gamma_i$ | $\delta_i$ |
|-----------|-------|------------|-----------|------------|------------|
| $u + \bar{u}$ | 0.387 | -0.388 | 0.910 | 7.15 | 3.96 |
| $d + \bar{d}$ | 0.388 | -0.388 | 0.910 | 7.15 | 3.96 |
| $\bar{u} + \bar{d}$ | 0.105 | 1.649 | 3.286 | 49.95 | 8.67 |
| $s + \bar{s}$ | 0.273 | 1.449 | 3.286 | 49.95 | 8.67 |
| $c + \bar{c}$ | 0.306 | 1.345 | 5.519 | 19.78 | 10.22 |
| $b + \bar{b}$ | 0.372 | -0.127 | 4.490 | 24.49 | 12.80 |
| $g$ | 0.260 | 2.552 | 6.194 | 87.06 | 20.36 |

Figure 1. The individual FFs for positively charged pions $zD_{i\pi^+}(z,Q^2)$ at $Q^2 = 10$ GeV$^2$ along with uncertainty estimates at 68% and 90% C.L. indicated by the inner and outer shaded bands, respectively. The panels on the right-hand-side show the corresponding relative uncertainties. Also shown is a comparison to the previous global analysis by DSS [3] (dashed lines).
In Fig. 1 we present the new parton-to-pion FFs at $Q^2 = 10$ GeV$^2$. As can be inferred, for the light quark flavors the old DSS results are either close to the updated fit or within its 90% C.L. uncertainty band. The best determined pion FFs is $D_{\pi^+u} + \bar{u}$, where the relative uncertainties are below 10% at 90% C.L. throughout most of the relevant $z$ range. Only for $z \gtrsim 0.8$ the errors rapidly increase because of the lack of experimental constraints in this region. The corresponding uncertainties for $D_{\pi^+d}$ turn out to be slightly larger as they also include possible violations of SU(2) charge symmetry through Eq. (3). Bigger deviations from the DSS analysis are found for both the gluon and the charm FFs. In the latter case, this is driven by the greater flexibility of the functional form, five fit parameters rather than three. The significantly reduced $D_{\pi^+g}$ as compared to the DSS fit is a result of the new ALICE $pp$ data [14], which have a strong preference for less pions from gluon fragmentation for basically all values of $z$. Similar conclusions are obtained for $Q^2 = M_Z^2$.

| experiment   | # data in fit | $\chi^2$ |
|--------------|--------------|----------|
| TPC [21]     | 44           | 37.1     |
| TASSO [22]   | 18           | 54.7     |
| SLD [23]     | 79           | 62.1     |
| ALEPH [24]   | 22           | 23.0     |
| DELPHI [25]  | 51           | 72.2     |
| OPAL [26, 27]| 46           | 192.3    |
| BABAR [8]    | 45           | 44.0     |
| BELLE [9]    | 78           | 46.8     |
| HERMES [11]  | 128          | 181.1    |
| COMPASS [12] prel. | 398     | 369.9    |
| PHENIX [13]  | 15           | 13.9     |
| STAR [16, 18, 15, 17]| 38     | 33.3     |
| ALICE [14]   | 7 TeV        | 11       |

**Table 2.** Data sets used in our NLO global analysis.

The overall quality of the fit is summarized in Tab. 2 where we list all data sets included in our global analysis, along with their individual $\chi^2$ values. Firstly, it is worth mentioning that there is a more than twofold increase in the number of available data points as compared to the original DSS analysis [3]. Secondly, the quality of the global fit has improved dramatically from $\chi^2$/d.o.f. $\simeq 2.2$ for DSS, see Tab. II in Ref. [3], to $\chi^2$/d.o.f. $\simeq 1.2$ for the current fit. A more detailed comparison reveals that the individual $\chi^2$ values for the SIA data [21, 22, 23, 24, 25, 26], which were already included in the DSS fit, have, by and large, not changed significantly. The biggest improvement concerns the SIDIS multiplicities from HERMES which, in their recently published version [11], are now described very well by the updated fit. Also, the preliminary charged pion multiplicities from COMPASS [12] and the new SIA data from BABAR [8] and BELLE [9] integrate nicely into the global analysis of parton-to-pion FFs. Finally, there is some tension among the $pp$ data sets from RHIC and the LHC, which forced us to introduce a cut $p_T > 5$ GeV on the pion’s transverse momentum in the current fit to accommodate both of them. The obtained individual $\chi^2$ values are all reasonable, as can be inferred from Tab. 2, with the new ALICE data [14] being on the high side, which largely stems from the penalty for the still sizable normalization shift. This large shift reflects the preference of the new ALICE data for a smaller gluon-to-pion FF than extracted by the original DSS fit based on RHIC PHENIX data [13] alone. As a result of the $p_T$
cut, the number of \( pp \) data in the fit for RHIC has decreased as compared to the DSS analysis. Both the BRAHMS [28] and STAR [29] results at forward pseudo-rapidities do not pass the \( p_T \) cut anymore, and, hence, are excluded from the updated fit.

6. Summary

We have presented a new, comprehensive global QCD analysis of parton-to-pion fragmentation functions at next-to-leading order accuracy including the latest experimental information. The analyzed data for inclusive pion production in semi-inclusive electron-positron annihilation, deep-inelastic scattering, and proton-proton collisions span energy scales ranging from about 1 GeV up to the mass of the Z boson. The achieved, very satisfactory and simultaneous description of all data sets strongly supports the validity of the underlying theoretical framework based on pQCD and, in particular, the notion of factorization and universality for parton-to-pion fragmentation functions.

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