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Automated Calculation of Jet Fragmentation at NLO in QCD

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目 录

01

Introduction

Categories of FF (arxiv: 1607.02521)

Integrated FF

- $$D_1^{h/q}(z) = \frac{z}{4}\sum_X \int \frac{d^3\vec{P}_X}{(2\pi)^3 2P_X^0}\frac{d\xi^+}{2\pi} e^{ik^-\xi^+}\mathrm{Tr}\Big[\langle 0\big|\mathcal{W}(\infty^+,\xi^+)\psi_q\big(\xi^+,0^-,\vec{0}_T\big)\big|P_h,S_h;X\rangle \times \langle P_h,S_h;X\big|\bar{\psi}_q\big(0^+,0^-,\vec{0}_T\big)\mathcal{W}(0^+,\infty^+)\big|0\rangle\gamma^-\Big].$$
- The number density of unpolarized hadrons in an unpolarized quark

Transverse Momentum Dependent(TMD) FF

- $G_1^{h/q}$ The density of longitudinally polarized hadrons in a longitudinally polarized quark
- $H_1^{h/q}$ The density of transversely polarized hadrons in a transversely polarized quark

Categories of FF

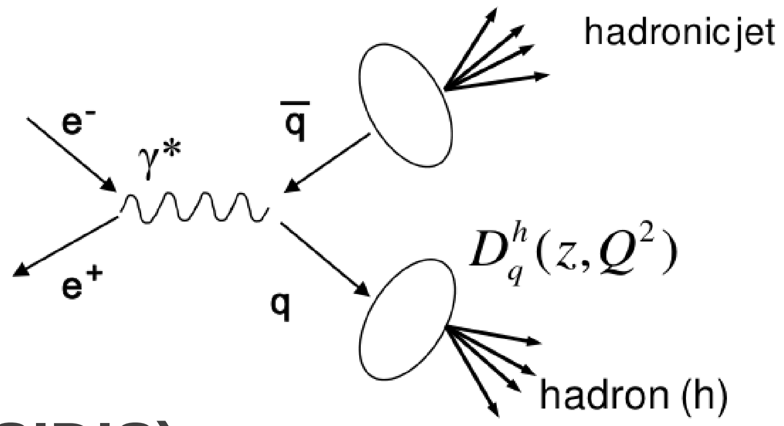
Higher Twist FF

- Twist 3 is defined by two-parton correlators, no density interpretation
- Another class is defined by quark-gluon-quark correlation functions, it can be considered as quantum interference effects

Di-hadron FF (DiFF)

- It describes fragmentation of a parton to two hadrons

Experiments



Single Inclusive Annihilation (SIA)

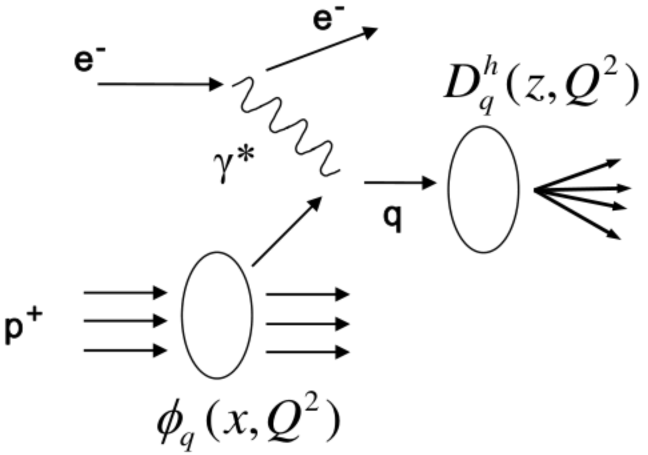
- $e^+e^- \rightarrow h + X$

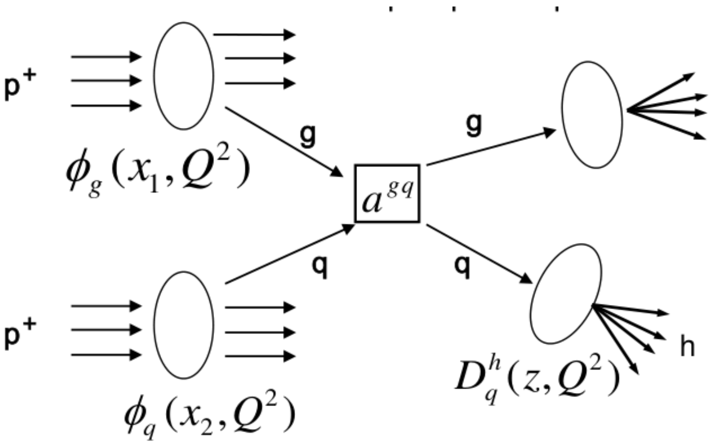
Semi-Inclusive Deep-Inelastic Scattering(SIDIS)

- $e^- + p \rightarrow h + X$

Hadron Production

- $p + p \rightarrow h(j) + X$





QCD Factorization

Factorization Theorem

- $\sigma(e^+e^- \to hX) = \hat{\sigma} \otimes FF$
- $\sigma(e^-p \to hX) = \hat{\sigma} \otimes PDF \otimes FF$
- $\sigma(pp \to hX) = \hat{\sigma} \otimes PDF \otimes PDF \otimes FF$

$$\frac{d\sigma(e^+e^- \to hX)}{dz} = \sum_i \int_x^1 \frac{dz}{z} C_i\left(z, \alpha_s(\mu), \frac{q^2}{\mu^2}\right) D_i^h\left(\frac{x}{z}, \mu^2\right)$$

Sum rule

$$\sum_h \int_0^1 z D_{q(g)}^h(z, Q^2) = 1$$

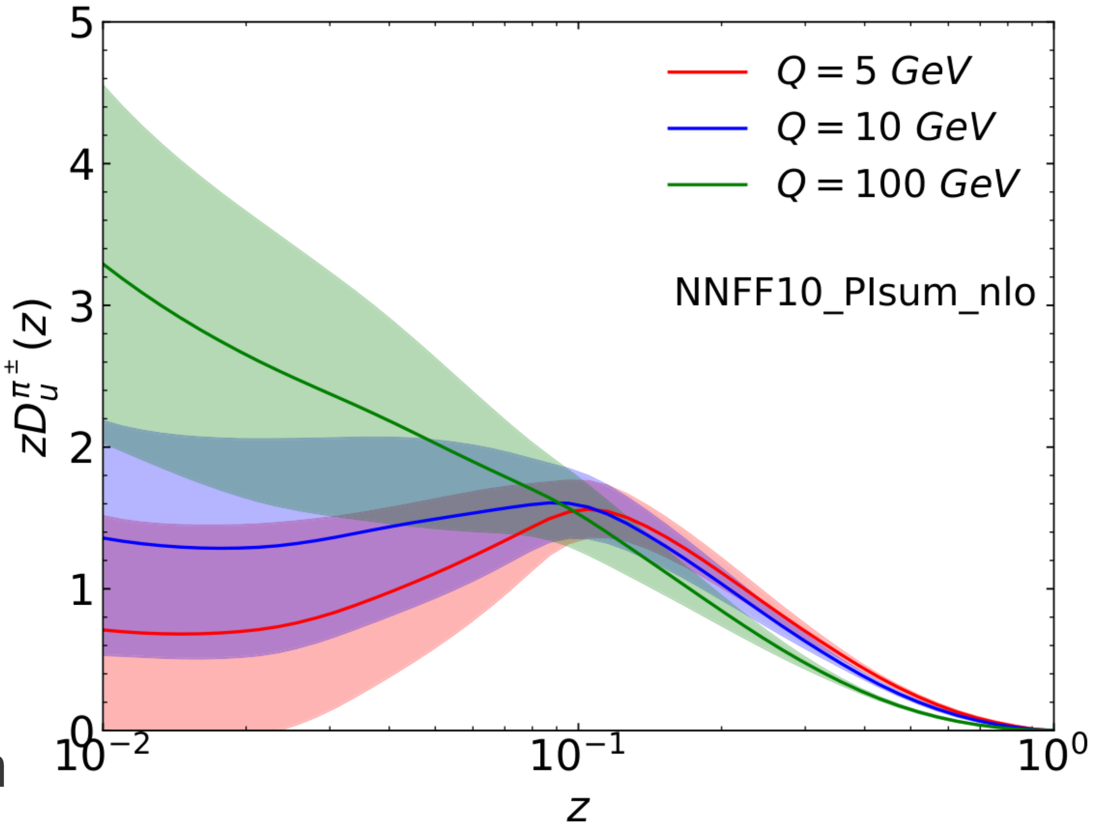
QCD Factorization

DGLAP Evolution

$$\frac{d}{d\ln Q^2}\vec{D}^h(z,Q^2)=\hat{P}\otimes\vec{D}^h(Q^2)$$

$$\vec{D}^h=\begin{pmatrix}D_s^h\\ D_g^h\end{pmatrix},D_s^h=\sum_q(D_q^h+D_{\bar{q}}^h)$$

$$\hat{P}=\begin{pmatrix}P_{q\to qg} & 2n_f P_{q\to gq}\\ P_{g\to q\bar{q}} & P_{g\to gg}\end{pmatrix}$$



The evolution kernels at three loop have been calculated
(arxiv: 0604053,0709.3899,1107.2263, 2006.10534,2012.03256,2012.07853)

Existing Global Analysis of FFs

- BKK, J . Binnewies, B. A. Kniehl and G. Kramer, 1995
- DSS, D. de Florian, R. Sassot and M. Stratmann, 2007
- KKP, B. A. Kniehl, G. Kramer and B. Pötter, 2000
- NNFF, V. Bertone, S. Carrazza, N.P. Hartland, E.R. Nocera, J. Rojo, 2017
- MAPFF, R. Abdul Khalek, V. Bertone, A. Khoudli, E. R. Nocera, 2022
- JAM, JAM Collaboration. N. Sato, C. Andres, J.J. Ethier, W. Melnitchouk, 2019

02

FMNLO Framework

Motivation For New Computational Framework

- The available processes of hard scattering are limited and are usually implemented case-by-case
- Interactions in the hard processes are usually constrained to be SM interaction
- Direct calculations at NLO are costly in computation time

FMNLO

- https://fmnlo.sjtu.edu.cn/~fmnlo
- **Based on hybrid scheme of NLO calculations**
  - phase-space slicing of collinear regions
  - local subtraction methods
- **Integrated with MG5_aMC@NLO, any processes could be calculated. (SM and BSM)**
  - $e^+e^- \to \gamma^* \to q\bar{q} \to hX$
  - $\mu^+\mu^- \to H \to gg \to hX$
  - $pp \to jj/Zj/\gamma j$

FMNLO

- Once the grid is generated by MG5_aMC@NLO, it can be convoluted with FF to obtain observables within seconds
- With built-in BKK,KKP,DSS FF sets, more could be added.
- Linked to LHAPDF library, data sets on LHAPDF could be accessed easily.
- We have provided some examples of modules used in our paper

Theory Ingredients

$$\frac{d\sigma}{dp_{T,h}} = \int dx \int dPS_m [|M|^2_{B,m} + |M|^2_{V,m} + |\tilde{\mathcal{I}}|^2_m] \sum_{i=1}^{m} \delta(p_{T,h} - xp_{T,i}) D^0_{h/i}(x)$$
$$+ \int dx \int dPS_{m+1} [|M|^2_{R,m+1} \sum_{i=1}^{m+1} \delta(p_{T,h} - xp_{T,i}) D^0_{h/i}(x) \%$$
$$- |\mathcal{I}|^2_{m+1} \sum_{\tilde{i}=1}^{m} \delta(p_{T,h} - x\tilde{p}_{T,\tilde{i}}) D^0_{h/\tilde{i}}(x)].$$

- $|M|^2_B$, $|M|^2_V$ and $|M|^2_R$ represent square of matrix elements at leading order (LO), one-loop level and in real corrections, respectively
- $|\mathcal{I}|^2_{m+1}$ denotes the local subtraction terms, and

$$|\tilde{\mathcal{I}}|^2_m = \int PS_1 |\mathcal{I}|^2_{m+1}$$

Theory Ingredients

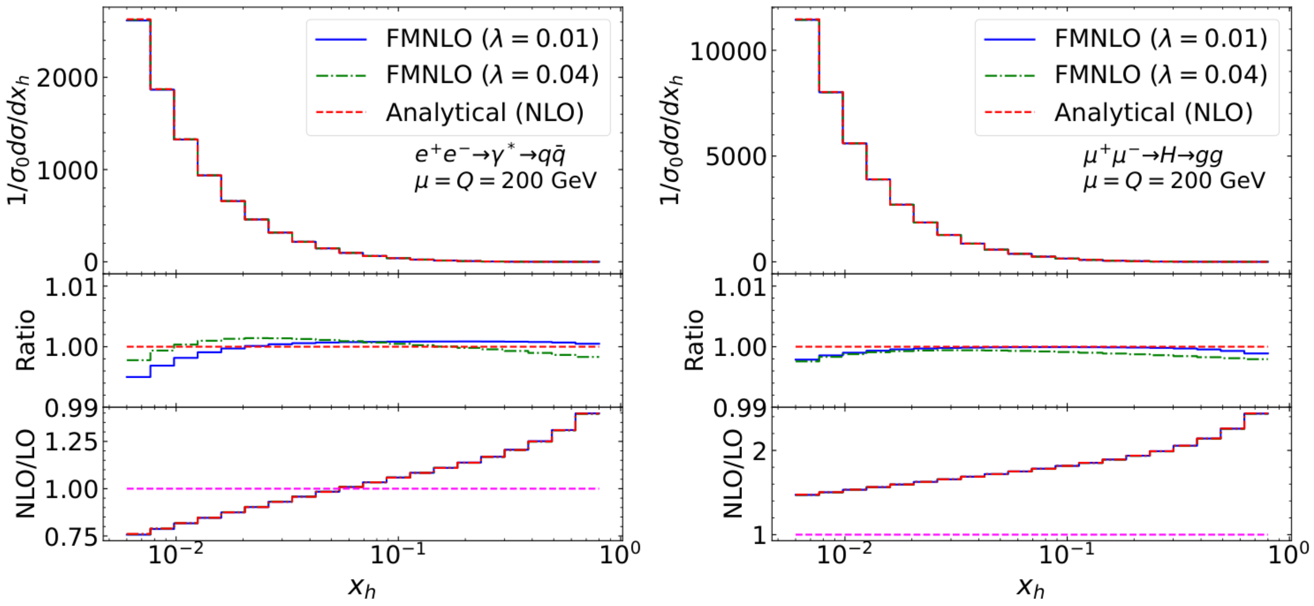
$$\int dx \int dPS_{m+1}(\Theta(\lambda - C) + \Theta(C-\lambda))[|M|^2_{R,m+1}\sum_{i=1}^{m+1}\delta(p_{T,h} - xp_{T,i})D^0_{h/i}(x) - |\mathcal{I}|^2_{m+1}\sum_{\tilde{i}=1}^{m}\delta(p_{T,h} - x\tilde{p}_{T,\tilde{i}})D^0_{h/\tilde{i}}(x)]$$

$$= \int dx \int dPS_{m+1}\Theta(C-\lambda)[|M|^2_{R,m+1}\sum_{i=1}^{m+1}\delta(p_{T,h} - xp_{T,i})D^0_{h/i}(x) - |\mathcal{I}|^2_{m+1}\sum_{\tilde{i}=1}^{m}\delta(p_{T,h} - x\tilde{p}_{T,\tilde{i}})D^0_{h/\tilde{i}}(x)] + |\tilde{\mathcal{J}}|^2_m$$

- **Two Θ functions are inserted to partition into the unresolved and resolved collinear regions with a cutoff λ.**
- **The phase space integral of $m+1$-body above the cutoff is free of infrared and collinear singularities and can be calculated numerically in four dimensions.**
- **The integral below the cutoff which contains collinear singularities can be factorized using the collinear approximations.**

Lepton Collisions

- **Consider two processes**
  - $e^+e^- \to \gamma^* \to q\bar{q} \to hX$
  - $\mu^+\mu^- \to H \to gg \to hX$
- **Toy model**
  - $xD_{h/i}(x,\mu) = N_i x^{-1/2}(1-x)^5$
  - $N_i = 1$ for q and $\bar{q}$, $N_i = 9/4$ for g

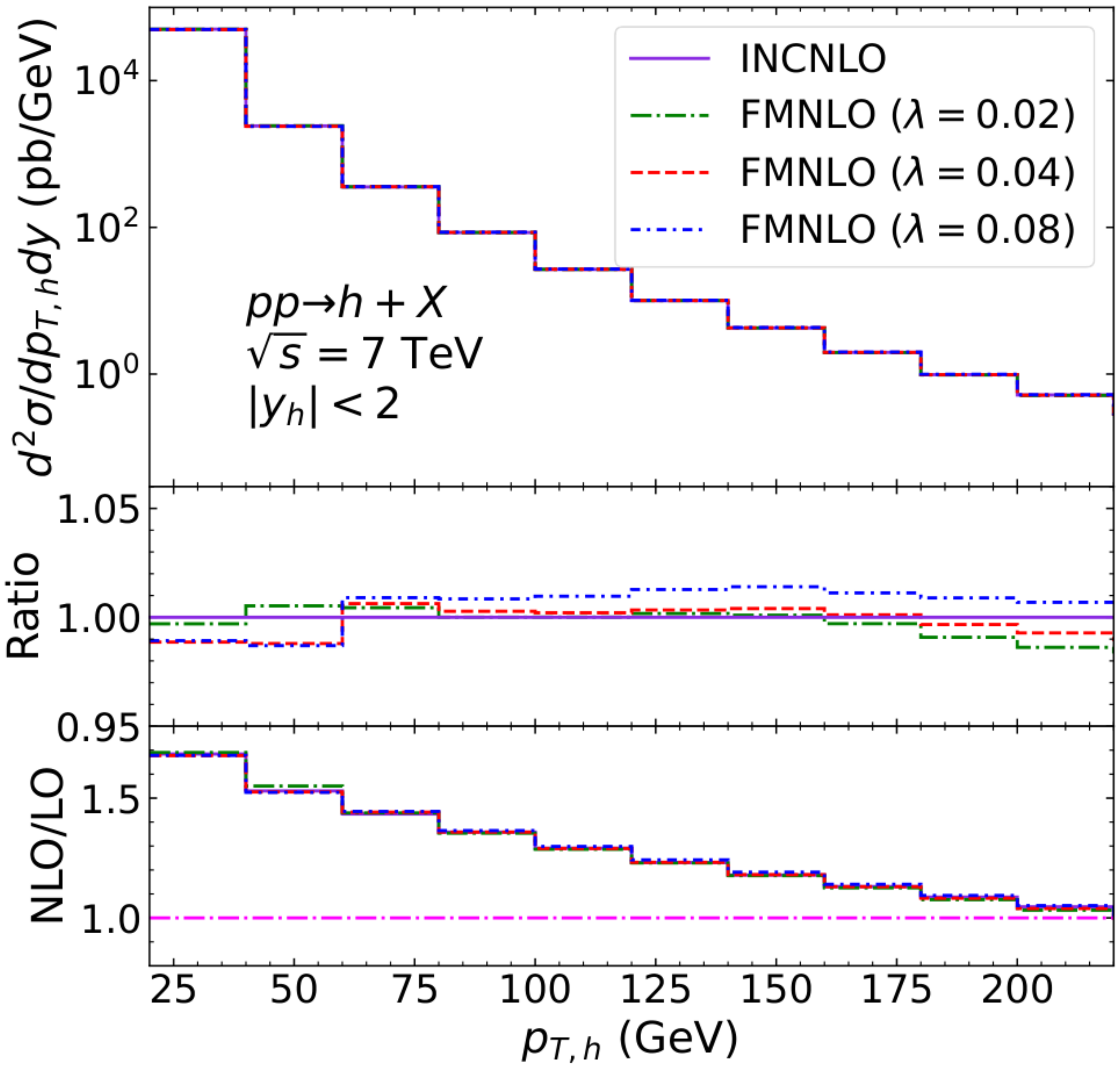


(a) $e^+e^- \to \gamma^* \to q\bar{q}$ (b) $\mu^+\mu^- \to H \to gg$

- **The deviation from analytical results are only a few per mille**

Hadron Collisions

- $p+p \to h+X$
- **Comparison with INCNLO (Hadro-production program by PHOX)**
- **PDF: CTEQ6M NLO, FF: BKK**
- **Agreement with numerical values**

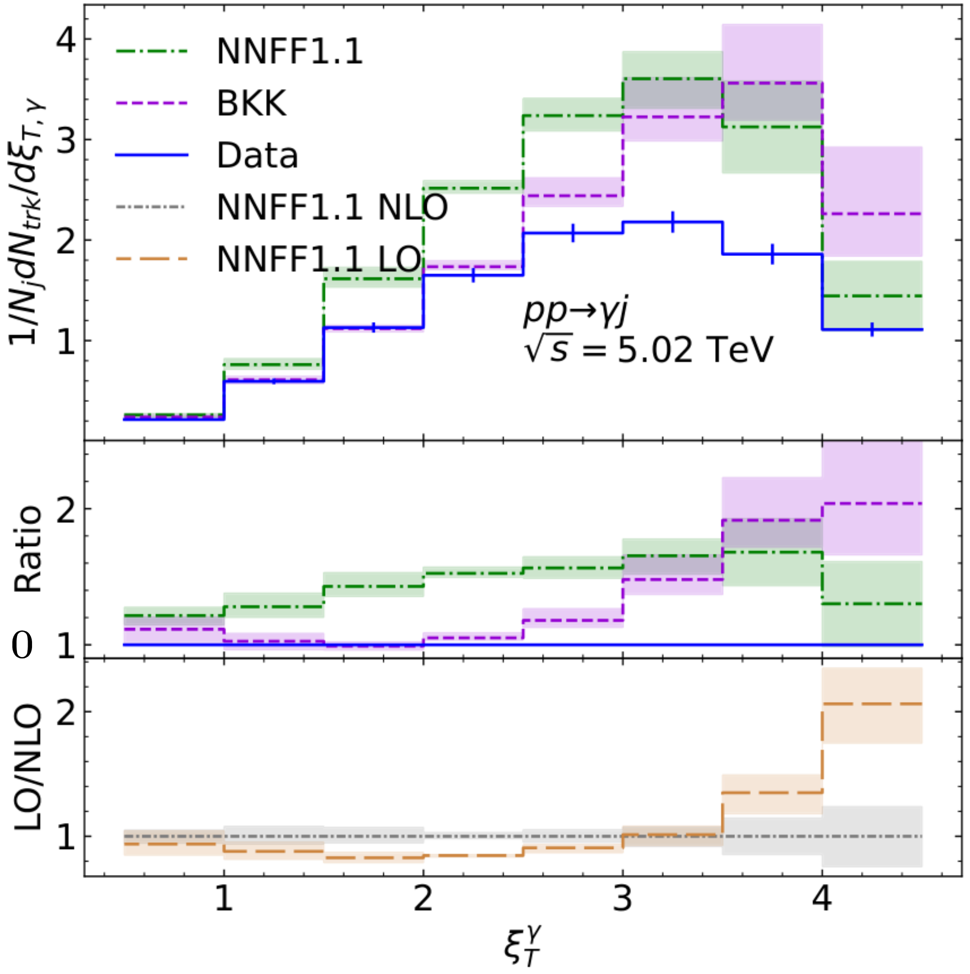


03

Applications at LHC

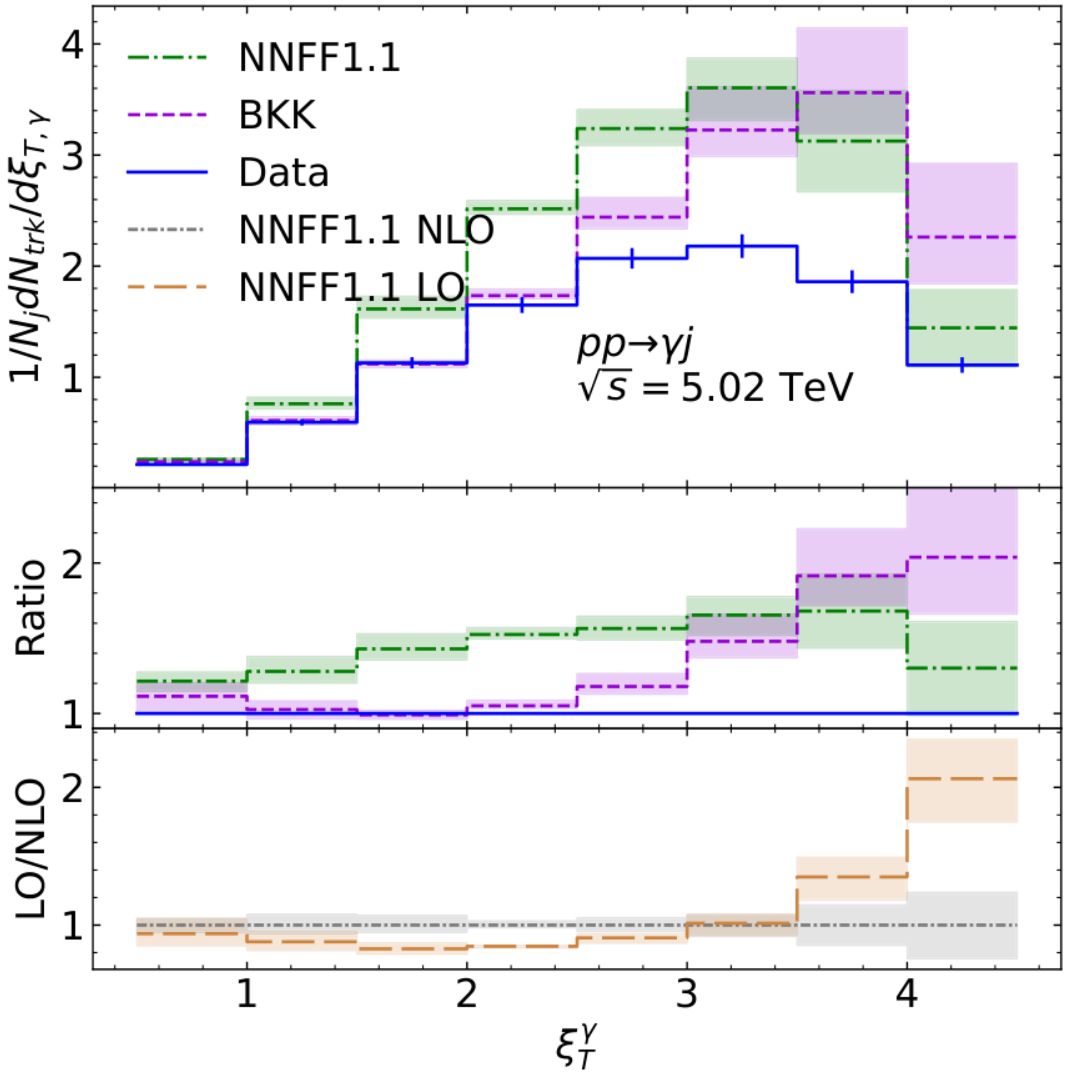
Isolated Photon Tagged Jets

- arxiv: 1801.04895
- $pp \to \gamma j$
- $\xi_T^\gamma \equiv \ln[-p_{T,\gamma}^2/(\vec{p}_{T,\gamma} \cdot \vec{p}_{T,h})]$
- Error bands indicate scale variations, which are obtained by taking the envelope of theory predictions of the 9 scale combinations of $\mu_F/\mu_{F,0} = \mu_R/\mu_{R,0} = \{1/2, 1, 2\}$ and $\mu_D/\mu_{D,0} = \{1/2, 1, 2\}$
- Experimental errors are represented by error bars



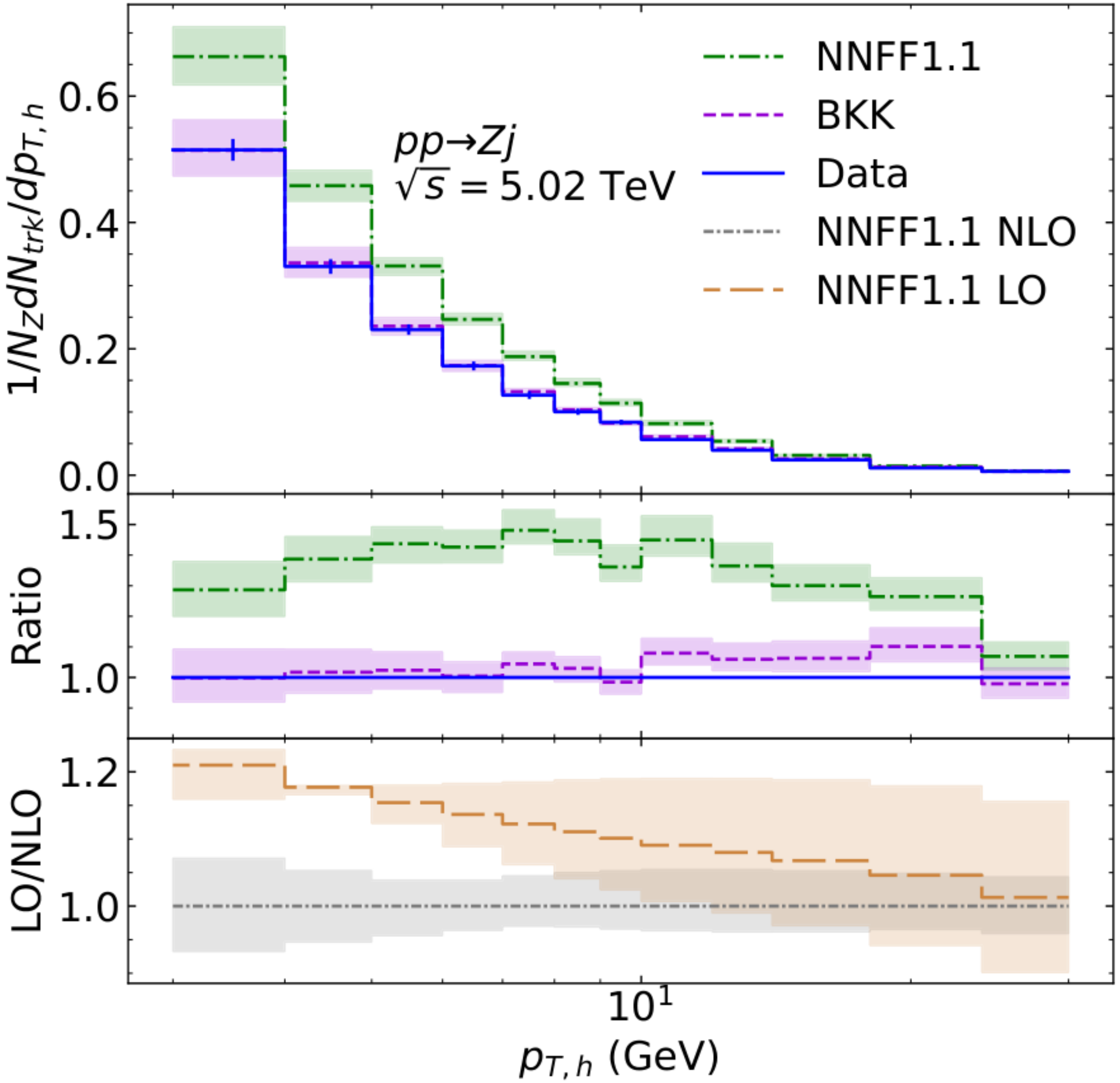
Isolated Photon Tagged Jets

- BKK results closely resemble the experimental data and exhibit a good agreement in the lower ξ_T^γ region $[0.5, 2.5]$, the discrepancy is large as ξ_T^γ increases
- The NNFF1.1 results match the experimental data in the lower and higher regions, deviations are large in the middle



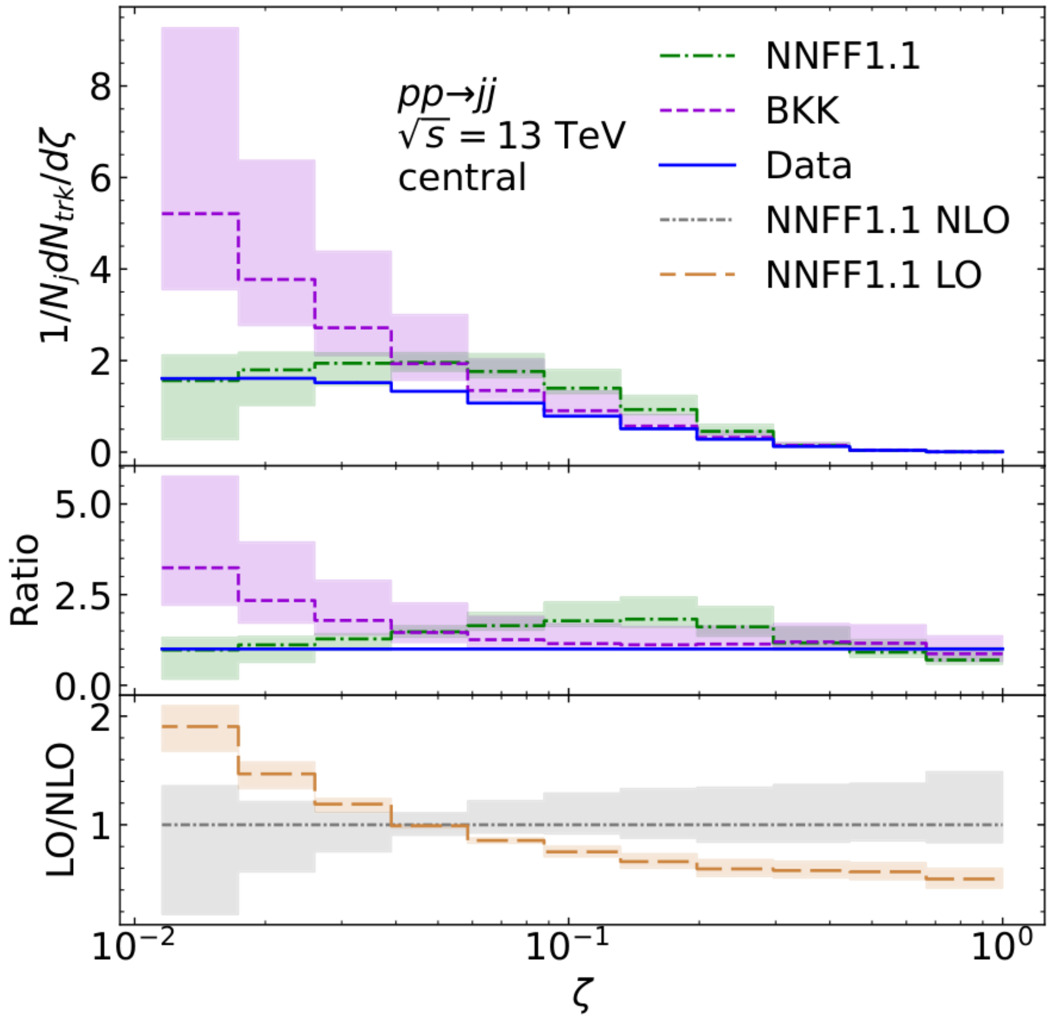
Z Tagged Jets

- arxiv:2103.04377
- $pp \to Zj$
- In most regions, the experimental data lies within the error band of the BKK results
- NNFF1.1 results show a greater discrepancy, particularly in the middle region



QCD Inclusive Dijets

- arxiv: 1906.09254
- $pp \to jj$
- $\zeta = p_{T,h}/p_{T,j}$
- Both the NNFF1.1 and BKK results fit well in the high ζ region, but BKK lies more closely with experimental data
- In lower ζ region (first three bins), NNFF1.1 predictions exhibit a closer resemblance



04

Analysis of Fragmentation Function

Data Selection

Selected Data Sets

- Publications within 5 years
- Focused on pp collisions
- Exclude momentum fraction $x < 0.01$ as it requires higher order corrections

Experiments	lum.	observables	N$_{pt}$	Range
CMS 5.02 TeV	27.4 pb^{-1}	$1/N_j dN_{trk}/d\xi_T^\gamma$	8(5)	$\xi_T^\gamma \in [0.5, 4.5]$
ATLAS 5.02 TeV	25 pb^{-1}	$1/N_j dN_{trk}/dp_{T,h}$	10(7)	$p_{T,h} \in [1, 100]$ GeV
CMS 5.02 TeV	320 pb^{-1}	$1/N_Z dN_{trk}/dp_{T,h}$	14(11)	$p_{T,h} \in [1, 30]$ GeV
ATLAS 5.02 TeV	160 pb^{-1}	$1/N_Z d^2N_{trk}/dp_{T,h}d\Delta\phi$	15(9)	$p_{T,h} \in [1, 60]$ GeV
ATLAS 13 TeV	33 fb^{-1}	$1/N_j dN_{trk}/d\zeta$ (central)	261(143)	$\zeta \in [0.002, 0.67]$
ATLAS 13 TeV	33 fb^{-1}	$1/N_j dN_{trk}/d\zeta$ (forward)	261(143)	$\zeta \in [0.002, 0.67]$

Framework of Fitting

- **Parameterization**

$$xD_{h/i}(x,Q_0)=a_{i,0}x^{\alpha_i}(1-x)^{\beta_i}\left(1+\sum_{n=1}^{p}a_{i,n}x^n\right)$$

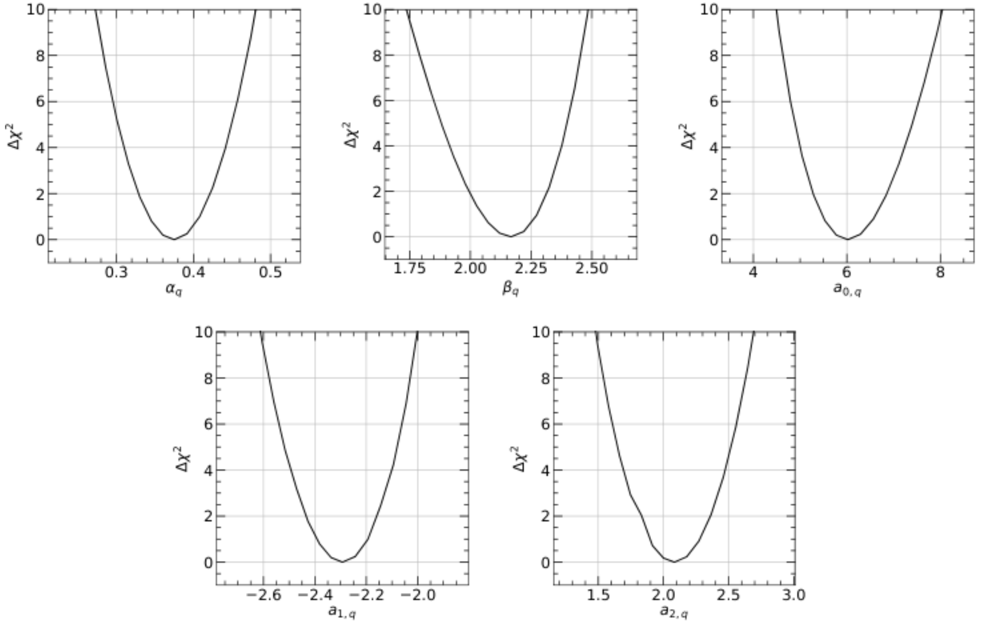
- **No flavor separation**
  - $Q_0=5\ \mathrm{GeV}$
  - $p=2,n_f=5$

- **Fitting quality: Log-likelihood Function**

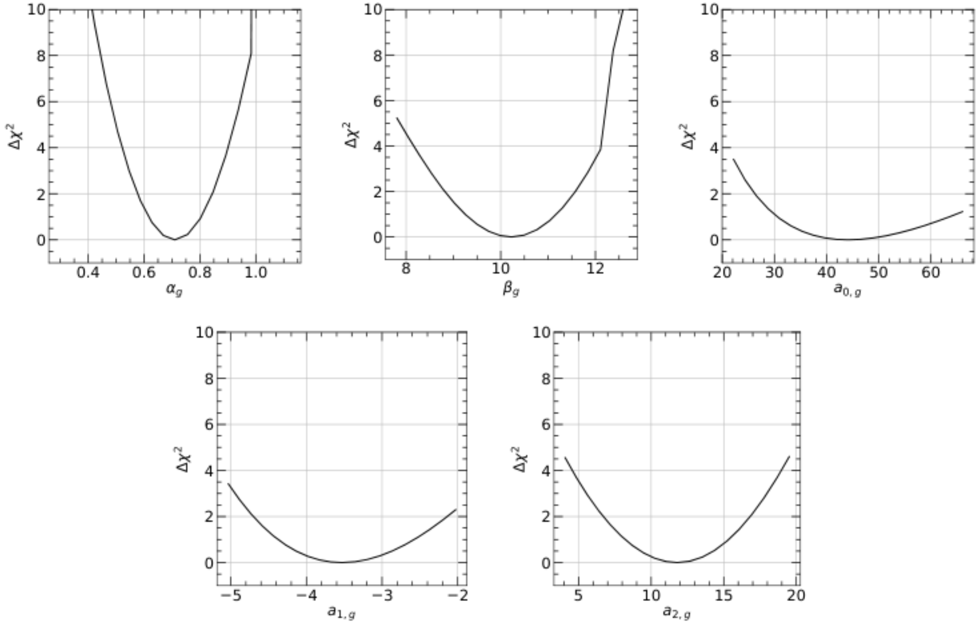
$$\chi^2(\{\alpha,\beta,a_n\},\{\lambda\})=\sum_{k=1}^{N_{\mathrm{pt}}}\frac{1}{s_k^2}\left(D_k-T_k-\sum_{\mu=1}^{N_\lambda}\sigma_{k,\mu}\lambda_\mu\right)^2+\sum_{\mu=1}^{N_\lambda}\lambda_\mu^2$$

LM Scan

Profile of total χ^2 change from scans on individual parameters with other parameters freely varying



(a) LM scan of quarks



(b) LM scan of gluon

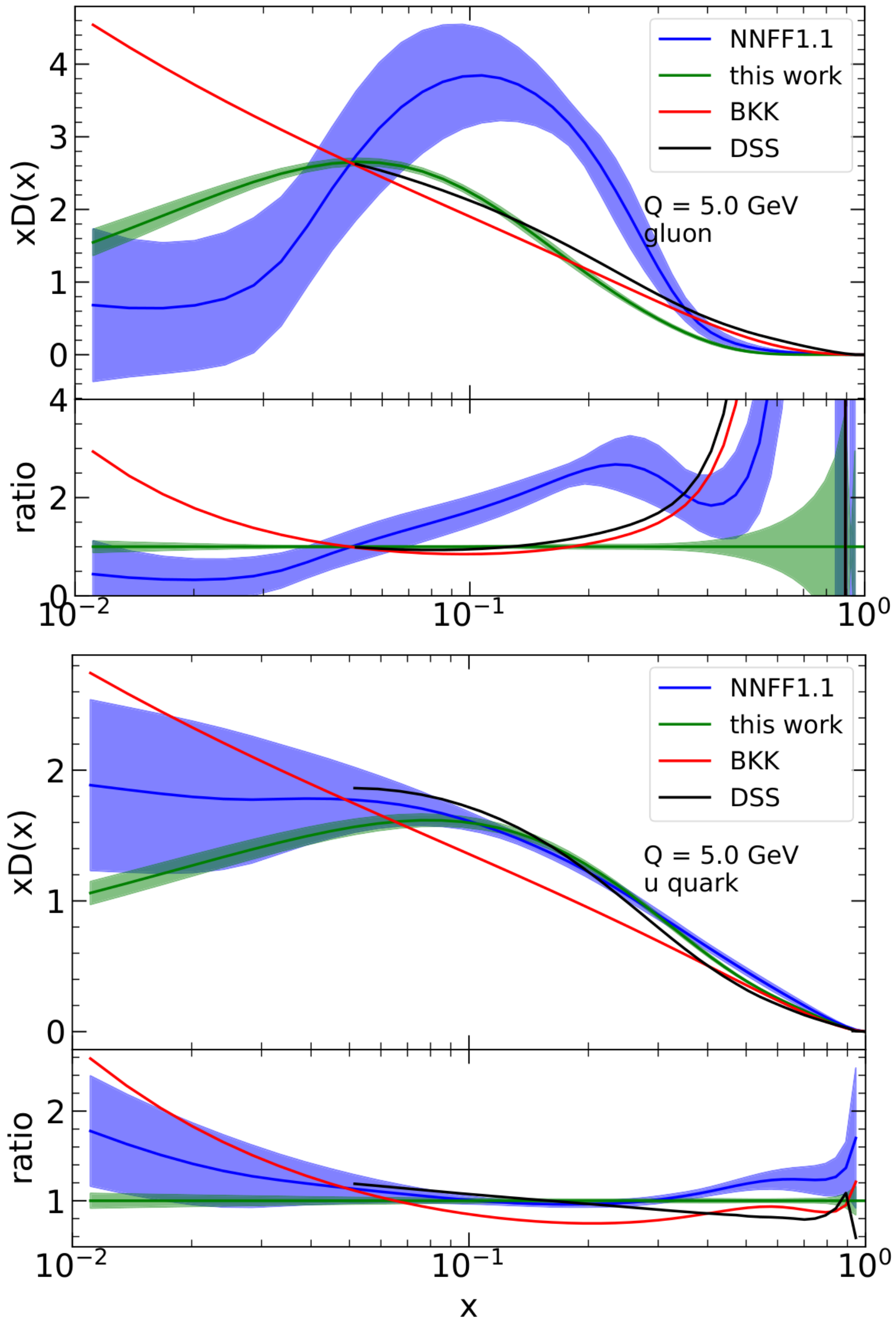
Results

Best fit results and LM scan on individual parameters (68% Confidence Level)

quark	α	β	a_0	a_1	a_2	$\langle x \rangle$
best-fit	0.375	2.166	6.016	-2.292	2.083	0.586
unc.(scan)	$^{+0.03}_{-0.03}$	$^{+0.11}_{-0.12}$	$^{+0.55}_{-0.56}$	$^{+0.10}_{-0.10}$	$^{+0.18}_{-0.20}$	--
unc.(Hessian)	$^{+0.03}_{-0.03}$	$^{+0.09}_{-0.10}$	$^{+0.45}_{-0.44}$	$^{+0.08}_{-0.08}$	$^{+0.16}_{-0.16}$	$^{+0.007}_{-0.008}$
gluon	α	β	a_0	a_1	a_2	$\langle x \rangle$
best-fit	0.710	10.224	44.080	-3.527	11.786	0.510
unc.(scan)	$^{+0.09}_{-0.16}$	$^{+1.09}_{-0.91}$	$^{+19.54}_{-13.54}$	$^{+0.95}_{-0.85}$	$^{+3.54}_{-3.60}$	--
unc.(Hessian)	$^{+0.09}_{-0.10}$	$^{+0.91}_{-0.93}$	$^{+18.9}_{-14.1}$	$^{+0.92}_{-0.83}$	$^{+3.32}_{-3.52}$	$^{+0.011}_{-0.012}$

Comparison of FF

- Uncertainties and deviations of different FF sets at small x region are large
- FF sets of quarks exhibit good agreements in x>0.1 except BKK
- Deviation of D_g^h from different FF sets are large, more constraints are required
- The error band in our nominal fit is tight. On the one hand, LHC data restricts gluon FF well. On the other hand, it's due to our chosen form of parameterization and error estimation method



05

Summary and Prospects

Summary and Prospects

Summary

- In this presentation, we propose a new framework for the calculation of differential cross section combining general-purpose Monte-Carlo generators with fragmentation functions (FFs) at NLO in QCD
- Its numerical stability is validated in cases of lepton collisions and hadron collisions
- It is further applied on the predictions of hadron cross section on LHC and the results are compared with experimental data
- With the framework and data on LHC, Fragmentation Function fit is obtained and compared with existing FF sets

Summary and Prospects

Prospects

- Include more experimental data points
- Detailed analysis with respect to Fragmentation Function fit, including different forms of parametrization, range of kinematic cuts and scale choices
- Include identified charged hadron
- Extend precision of calculation to NNLO

Thanks for Listening

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