

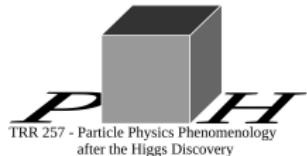
# Bottom-quark fragmentation and top-pair production at the LHC

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Alexander Mitov, René Poncelet

Based on arXiv:2102.08267 and arXiv:2210.06078

30th International Workshop on Deep-Inelastic Scattering  
and Related Subjects (DIS2023)  
East Lansing, Michigan, USA, 30 March 2023



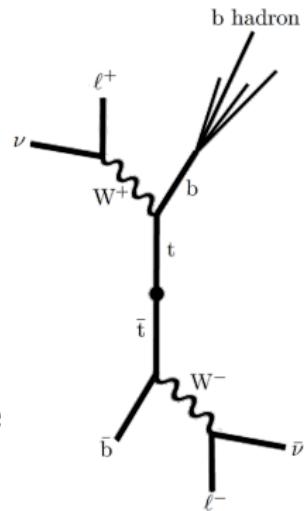
# Top-pairs with $B$ -hadrons

- Process considered:

$$p p \rightarrow t(\rightarrow B W^+ + X) \bar{t}(\rightarrow \bar{b} W^-)$$

$$\downarrow \ell^+ \nu_\ell \qquad \qquad \downarrow \ell^- \bar{\nu}_\ell$$

- Measurements involving  $b$ -jets suffer from large jet energy scale uncertainties
- Measurements of  $B$ -hadron momenta very precise  
 $\Rightarrow$  high-precision top-mass determination
- Production of hadrons is a non-perturbative effect

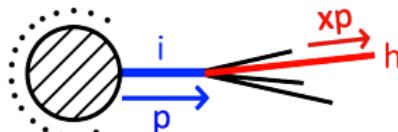
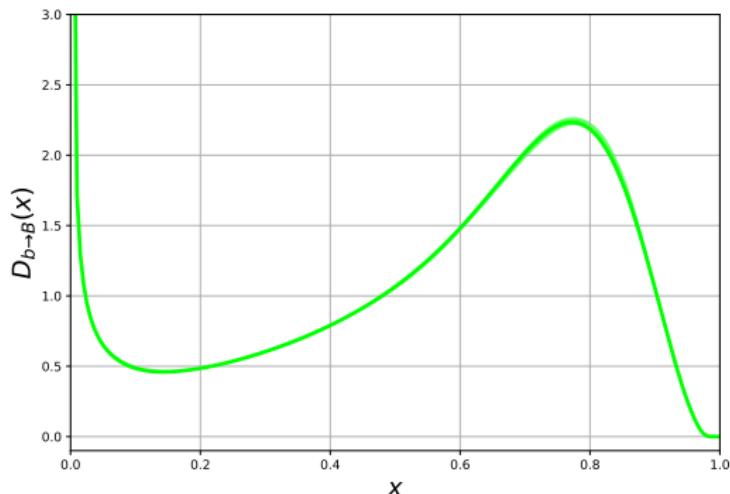


# Introduction to fragmentation

- Idea: describe production of hadrons using two steps
  - ① The production of partons using perturbation theory
  - ② The (non-perturbative) fragmentation of these partons into the observed hadrons
- Transition parton→hadron in the final state
- Mathematically similar to transition hadron→parton in the initial state
- Factorisation accurate up to  $\mathcal{O}\left(\frac{m_h}{Q}\right)$

# Fragmentation functions

- ‘Probability distribution’ to find a hadron  $h$  with a fraction  $x$  of the parton  $i$ ’s momentum:  $D_{i \rightarrow h}(x)$
- Only considers longitudinal kinematics;  $i, h$  massless
- Non-perturbative: fitted to data
- Scale dependent
- Analogous to PDFs
- No parton showers used



# The software

- Calculations were performed using C++ library STRIPPER
- Many NNLO firsts over the years. Recently:
  - Event shapes at the LHC  
*Alvarez, Cantero, Czakon, Llorente, Mitov, Poncelet (2023)*
  - $W\bar{b}$  production at the LHC *Hartanto, Poncelet, Popescu, Zoi (2022)*
  - Three-jet production at the LHC *Czakon, Mitov, Poncelet (2021)*
  - Diphoton + jet at the LHC *Chawdhry, Czakon, Mitov, Poncelet (2021)*
  - Exact top-mass effects in Higgs production at the LHC  
*Czakon, Harlander, Klappert, Niggetiedt (2021)*
  - ...
- First implementation of fragmentation in a general code for NNLO cross sections
- Fully general implementation; not limited to cases presented in this talk

# New fragmentation function fits

- No fits based on PFF approach available at NNLO
- Required for fully consistent results
- First paper: FF sets based on three different compromises
- Two based on NNLO calculation within SCET/HQET

*M. Fickinger, S. Fleming, C. Kim and E. Mereghetti (2016)*

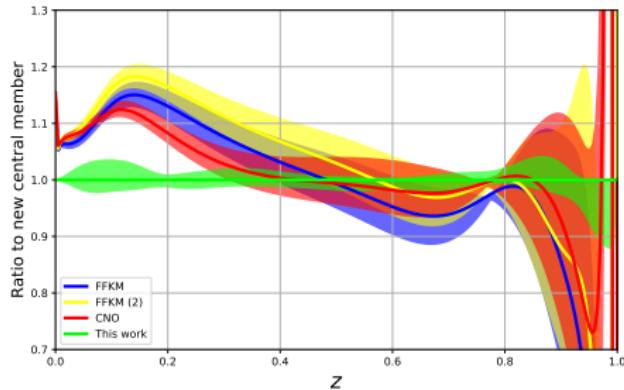
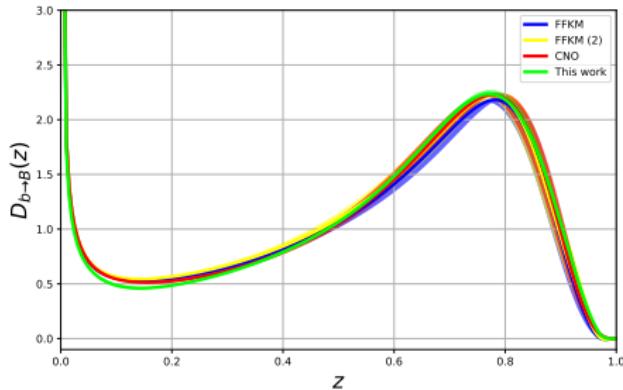
- One based on NLO calculation within PFF approach

*M. Cacciari, P. Nason and C. Oleari (2006)*

- Different compromises consistent within uncertainties
- Nonetheless better to use a consistent fit

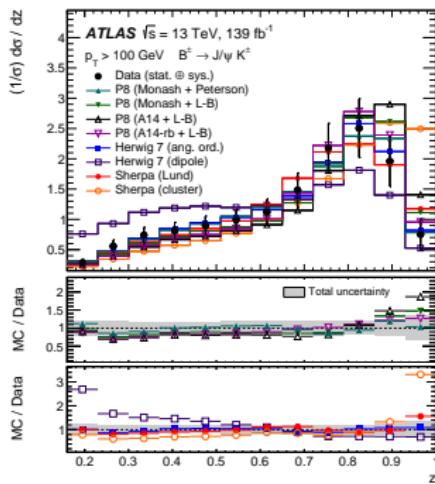
# First NNLO fit within the PFF approach

- Based on data from ALEPH, DELPHI, OPAL and SLD.
- Blue/Yellow: based on Fickinger, Fleming, Kim, Mereghetti (2016)
- Red: based on Cacciari, Nason, Oleari (2006)
- Green: Czakon, TG, Mitov, Poncelet (2022)



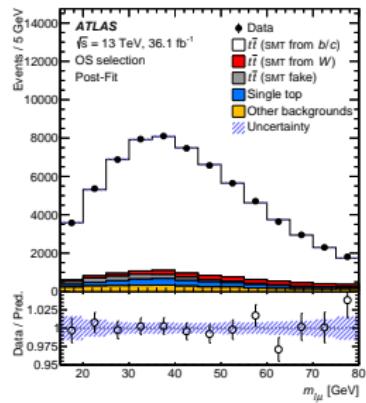
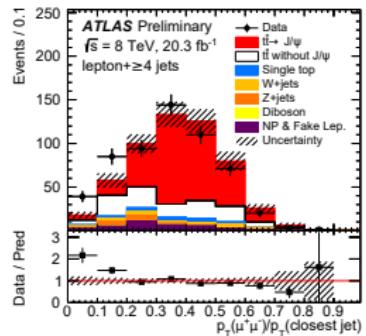
# Incorporating $B$ -hadron decays

- First paper: predictions for fully reconstructed  $B$ -hadrons only
- Full reconstruction of  $B$ -hadrons difficult in practice
- Not enough  $t\bar{t}$  events for distributions  
⇒ Cannot compare first results to experiment at present
- Could compare to data if process changed to  $p p \rightarrow B + X$
- Fully reconstructed  $B$ -hadrons in arXiv:2108.11650 (ATLAS)
- Not a problem for the software, but process lacks information on  $m_t$



# Incorporating $B$ -hadron decays

- Solution: incorporate  $B$ -hadron decays
- Only reconstruct some decay products  
⇒ Significantly boost statistics
- Examples by ATLAS:  
 ATLAS-CONF-2015-040 ( $B \rightarrow J/\psi + X$ )  
 arXiv:2209.00583 ( $B \rightarrow \mu + X$ )
- Still considering top-pair production,  
but comparison with experiment now possible

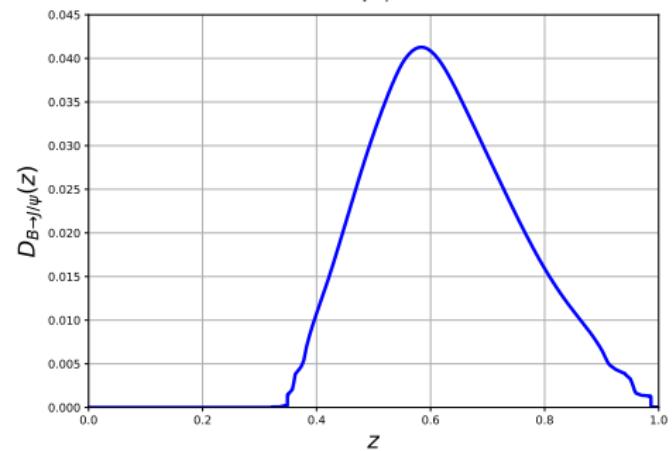


# Including $B$ -hadron decays in theory predictions

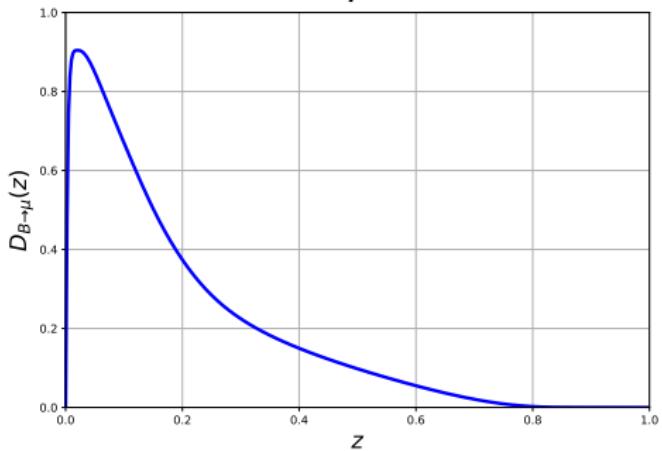
- $B$ -hadron treated as massless  $\Rightarrow$  cannot decay
- Most obvious solution:
  - ① Map massless  $B$ -hadron momentum to massive one
  - ② Decay massive  $B$ -hadron using external package
- Not ideal:
  - Momentum remapping ambiguous
  - Need to interface to external package (e.g. EvtGen)
- Easier and more consistent solution:
  - ① Modify fragmentation function to incorporate the decay
  - ② Run the program as usual, no modifications required
- Need the ‘fragmentation function’  $D_{B \rightarrow d}$  for the decay  $B \rightarrow d$
- Can be obtained from the differential decay rate using EvtGen

# $B$ -hadron decay fragmentation functions

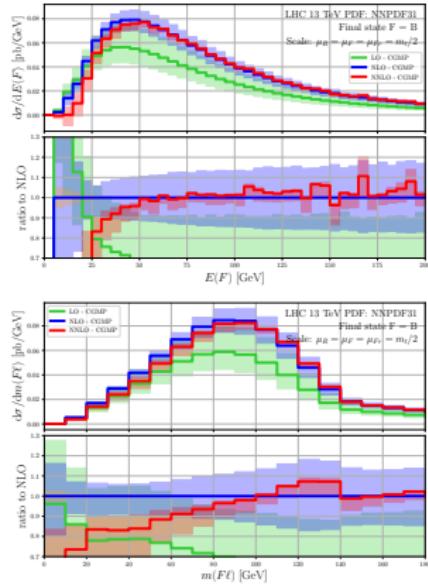
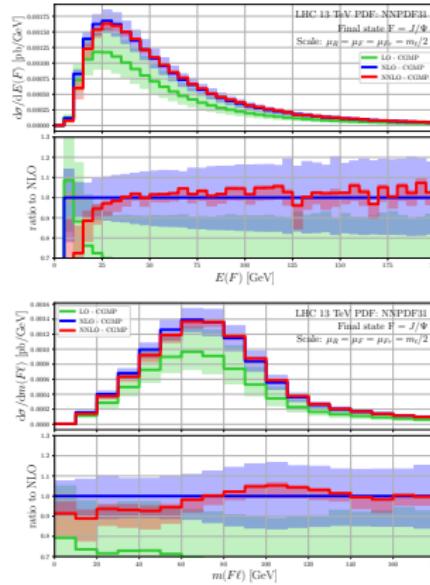
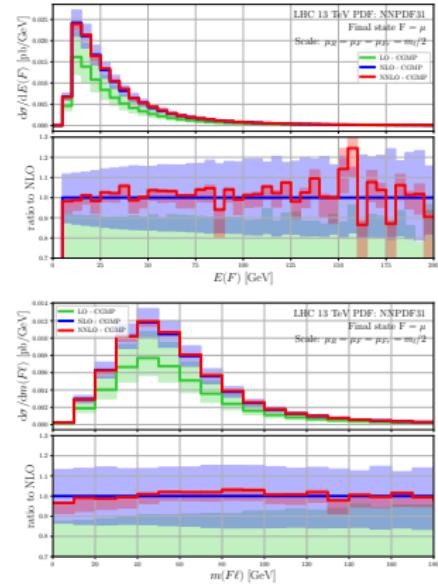
$J/\psi$



$\mu$

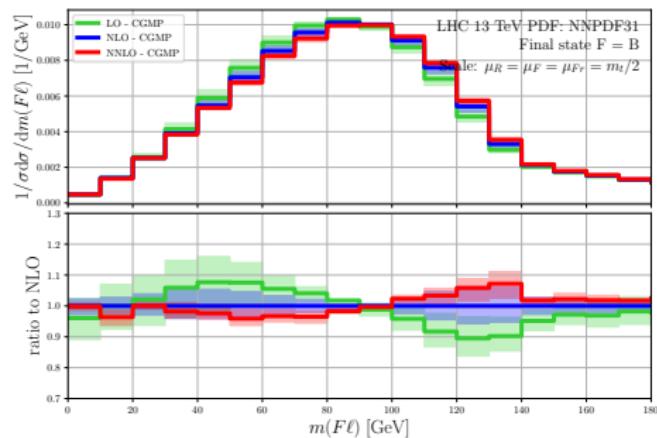


# Results: energy and invariant mass spectra

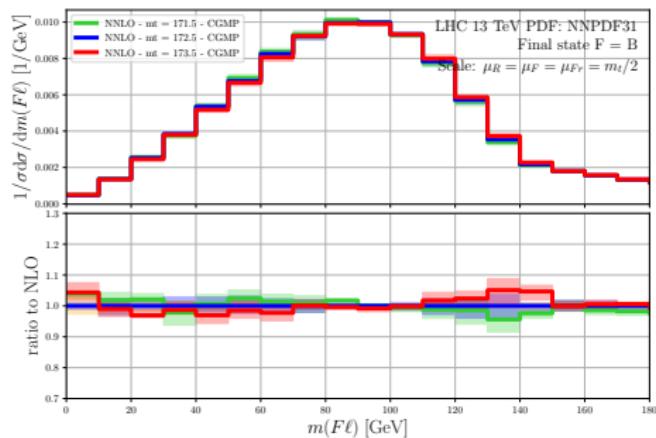
*B**J/ψ* $\mu$ 

# Measuring $m_t$ using the $m(B\ell)$ spectrum

LO, NLO, NNLO for fixed  $m_t$



NNLO, varying  $m_t$  by 1 GeV



- Note: NNLO effects almost identical to a  $\sim 1$  GeV shift in  $m_t$

# Conclusion

- Can describe the production of any hadron in any process at NNLO
- Fitted a new NNLO  $B$ -hadron FF consistent with our approach
- Calculation can now include  $B$ -hadron decays
- First application: top-quark pairs at the LHC
- Much smaller uncertainties at NNLO than at NLO
- NNLO effects very important for accurate  $m_t$  measurements

We are very interested in comparing to data in dedicated studies!

# Phase-space cuts

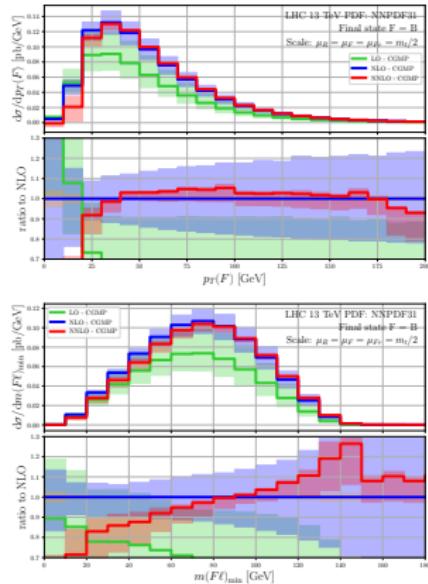
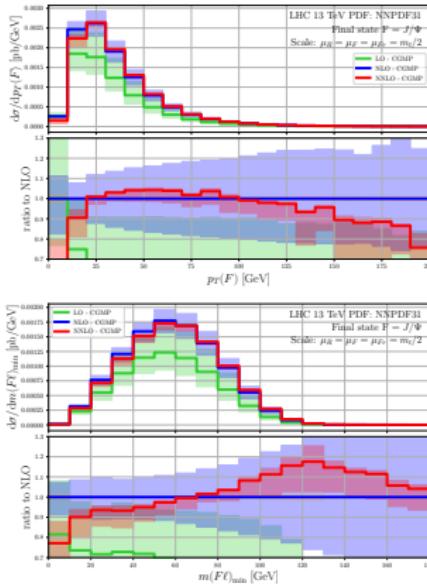
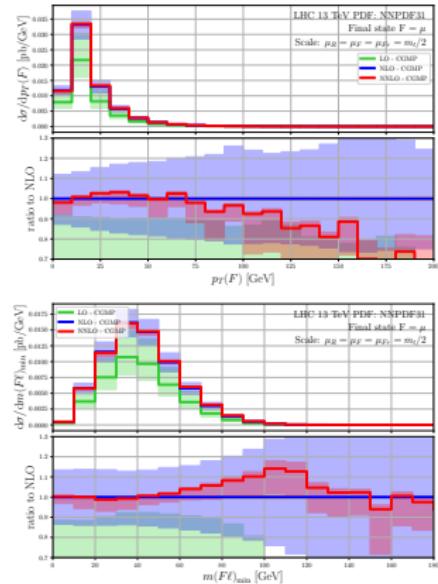
Differential distributions:

- $p_T(\ell) > 25 \text{ GeV}, |\eta(\ell)| < 2.5$
- at least 2 anti- $k_T$  jets ( $R = 0.4$ ) with  $p_T(j) > 25 \text{ GeV}$  and  $|\eta(j)| < 2.5$
- $\Delta R(\ell, j) > 0.4$
- $p_T(F) > 8 \text{ GeV}$  and  $|\eta(F)| < 2.5$ ,  $F$  must be part of one jet

Top-quark-mass extraction:

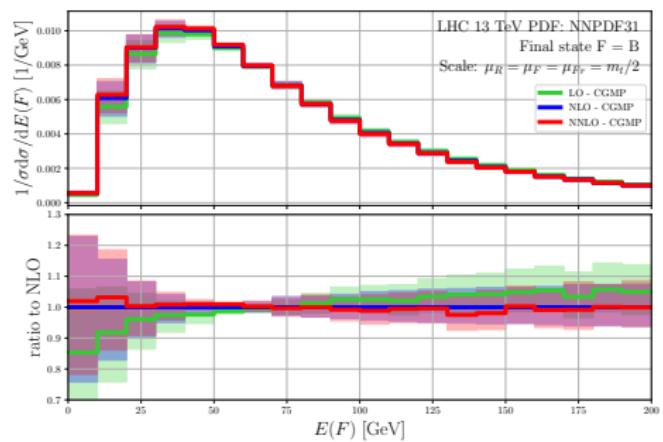
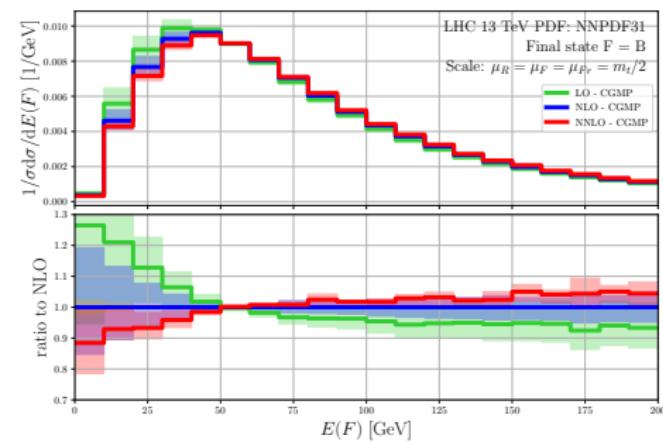
- $p_T(\ell) > 25 \text{ GeV}, |\eta(\ell)| < 2.5$
- $p_T(F) > 8 \text{ GeV}$  and  $|\eta(F)| < 2.5$

# Results: $p_T$ and $m(F\ell)_{\min}$ spectra

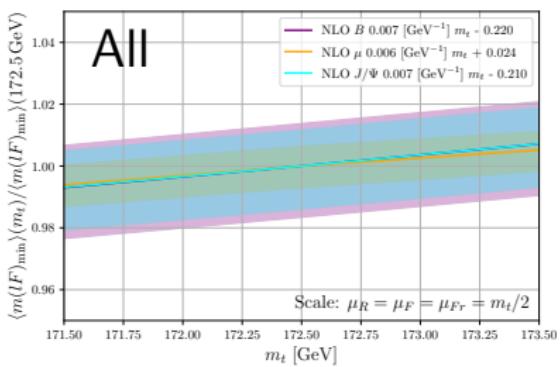
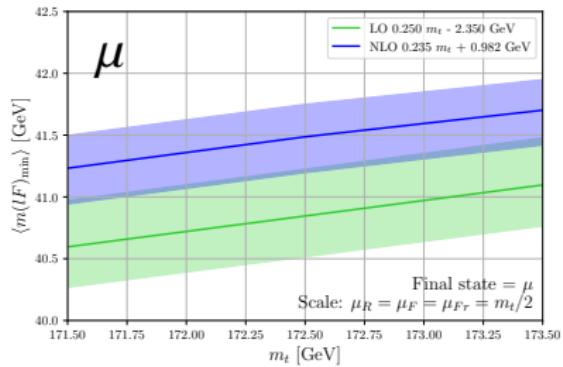
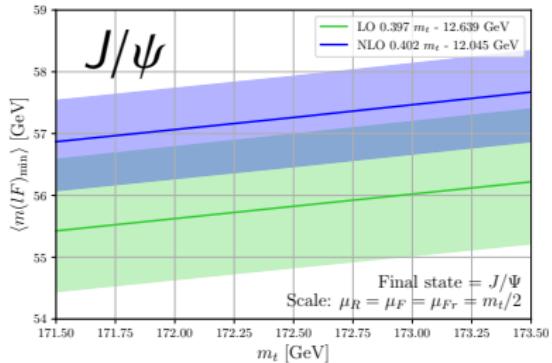
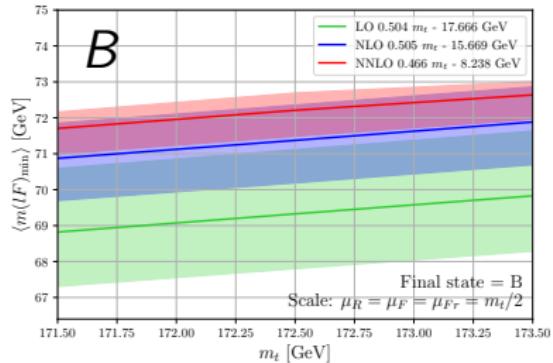
*B**J/ψ* $\mu$ 

# Measuring $m_t$ using the $E(B)$ peak

- Idea: position of the  $E(B)$  peak independent of production process  
*K. Agashe, R. Franceschini and D. Kim (2012)*
- Can be used for model-independent measurement of  $m_t$
- Caveat: only works for LO decays (right plot)

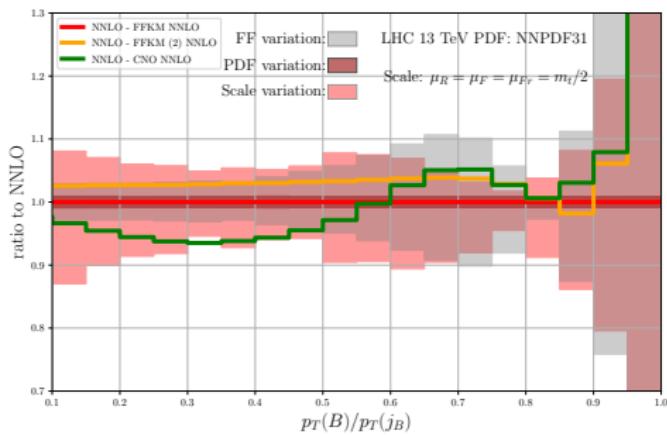
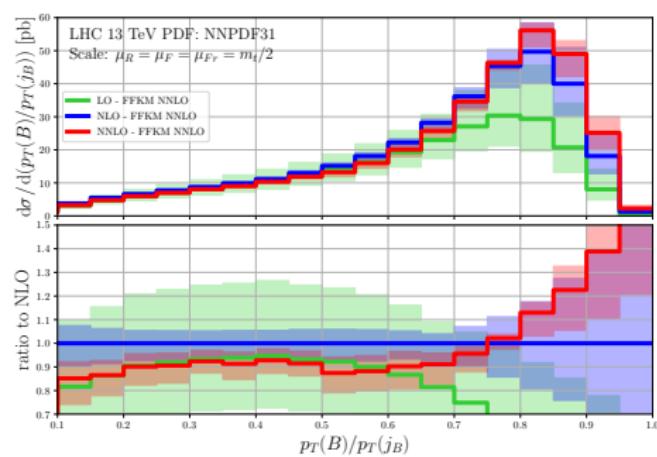


# Measuring $m_t$ using $\langle m(F\ell)_{\min} \rangle$

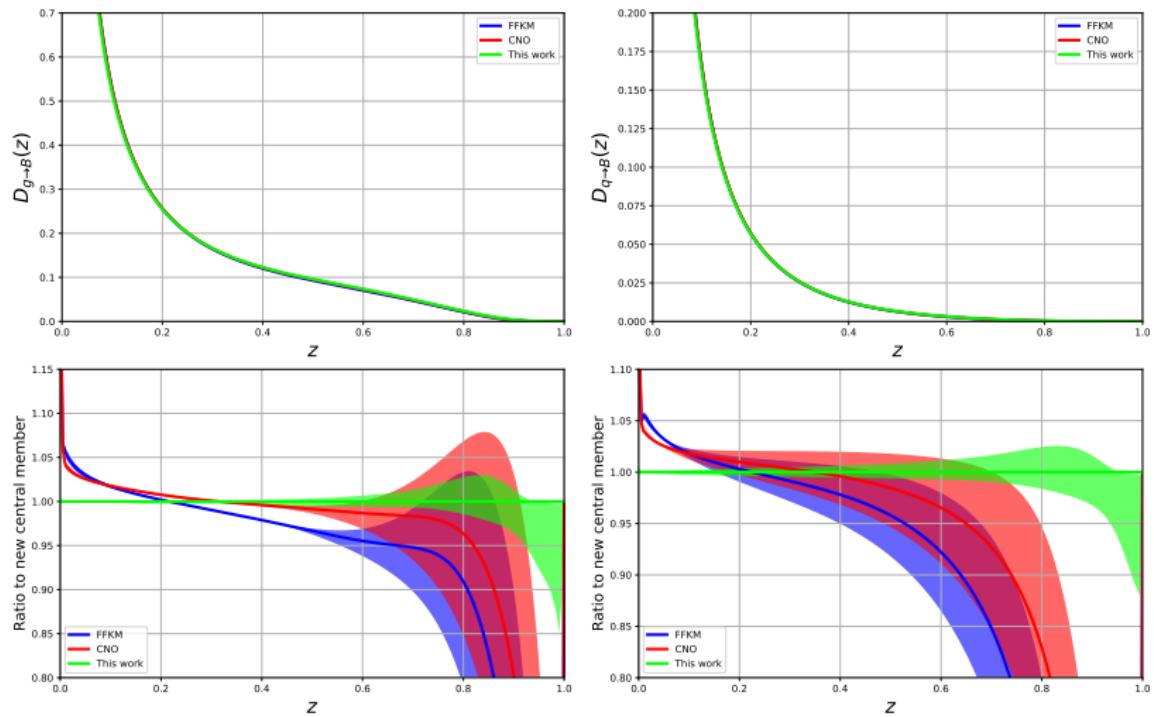


# Measuring fragmentation functions at the LHC: jet ratio

- $p_T(B) > 10 \text{ GeV}$  and  $|\eta(B)| < 2.4$
- Jet algorithm: anti- $k_T$  with  $R = 0.8$



# First NNLO fit within the PFF approach



# Including B-hadron decays in theory predictions

- Assume isotropic decay:  $d\Gamma(B \rightarrow \mu + X) = f(E_\mu) dE_\mu d\cos\theta_\mu d\phi_\mu$
- Valid for spin-0 particles (e.g. weakly-decaying B-mesons)
- Normalize  $E_\mu$  using  $m_B \Rightarrow f(E_\mu) dE_\mu \rightarrow f(y) dy$
- Boost from B-hadron rest frame to  $E_B \gg m_B$  and integrate over the angles and  $y$ , fixing  $z = E_\mu/E_B$

$$\Rightarrow \frac{d\Gamma(B \rightarrow \mu + X)}{dy} \rightarrow D_{B \rightarrow \mu}(z)$$

- $D_{B \rightarrow \mu}$  is the 'fragmentation function' for transition  $B \rightarrow \mu$

# Including B-hadron decays in theory predictions

- Can calculate  $D_{B \rightarrow \mu}$  once and for all
- $D_{B \rightarrow \mu}$  combines with known  $D_{i \rightarrow B}$  via convolution
- Only requirement: must know  $f(E_\mu)$
- Can be obtained using e.g. EvtGen
- Works for any descendant, not just muons
- Vast amount of data from B-factories  
 $\Rightarrow f(E_\mu)$  expected to be more precise than  $D_{i \rightarrow B}$

# Decay fragmentation function derivation

$$d\Gamma(B \rightarrow d + X) = \frac{1}{4\pi} f(E_d^{\text{rest}}) dE_d^{\text{rest}} d\cos(\theta) d\phi \stackrel{y = \frac{E_d^{\text{rest}}}{m_B}}{=} \frac{m_B}{4\pi} f(y m_B) dy d\cos(\theta) d\phi$$

Boost to  $E_B \gg m_B$  along the z-axis and fix  $z = \frac{E_d}{E_B}$  using

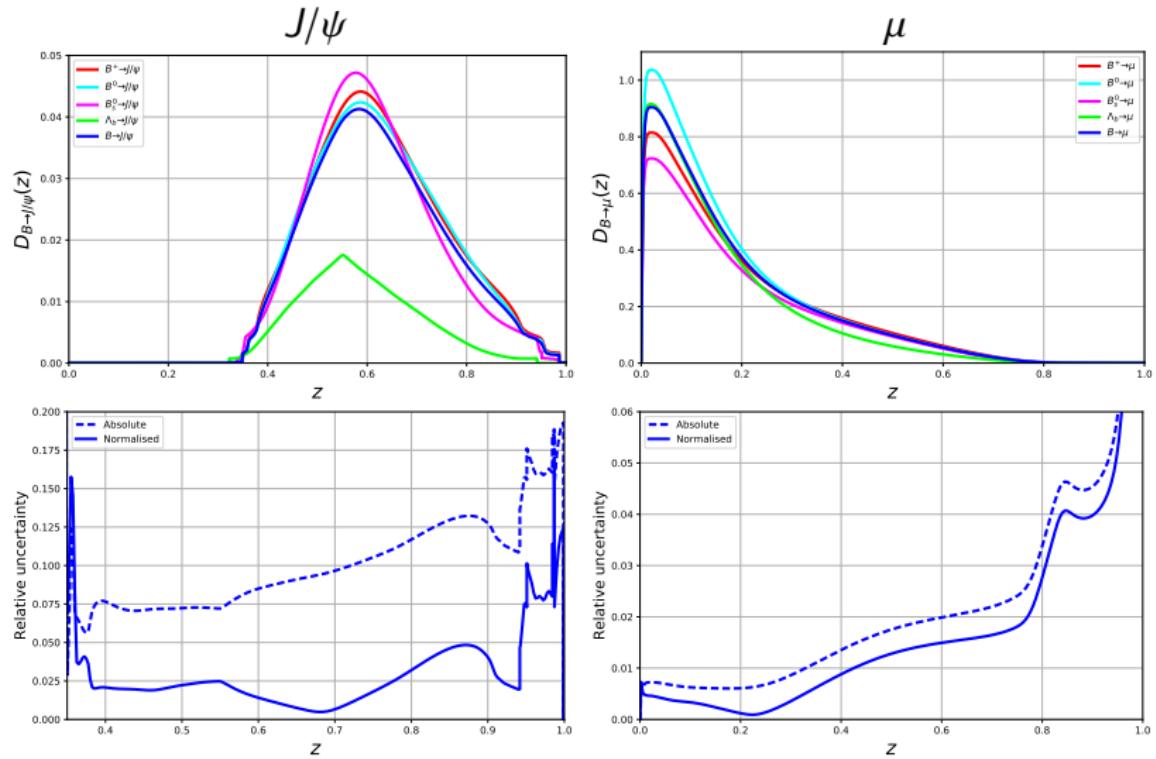
$$\begin{aligned} \delta\left(z - \frac{E_d}{E_B}\right) &= \delta\left(z - \gamma_B \frac{E_d^{\text{rest}} + \beta_B \cos(\theta) \sqrt{(E_d^{\text{rest}})^2 - m_d^2}}{E_B}\right) \\ &\approx \delta\left(z - \frac{E_d^{\text{rest}} + \cos(\theta) \sqrt{(E_d^{\text{rest}})^2 - m_d^2}}{m_B}\right) \\ &= \delta\left(z - y - \cos(\theta) \sqrt{y^2 - \frac{m_d^2}{m_B^2}}\right) \end{aligned}$$

# Decay fragmentation function derivation

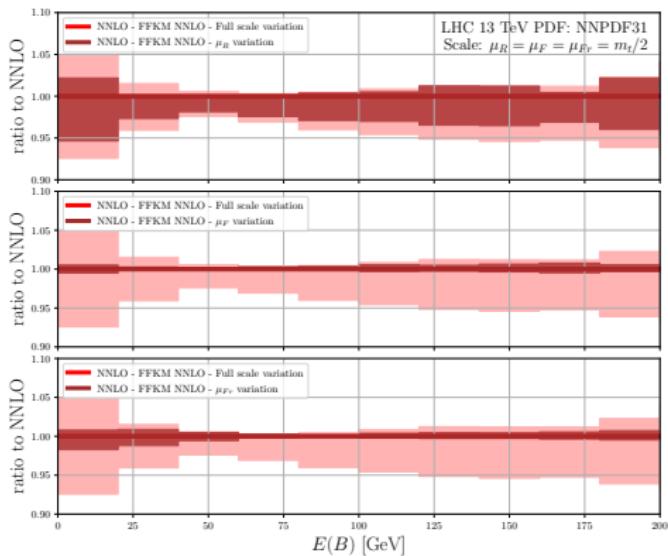
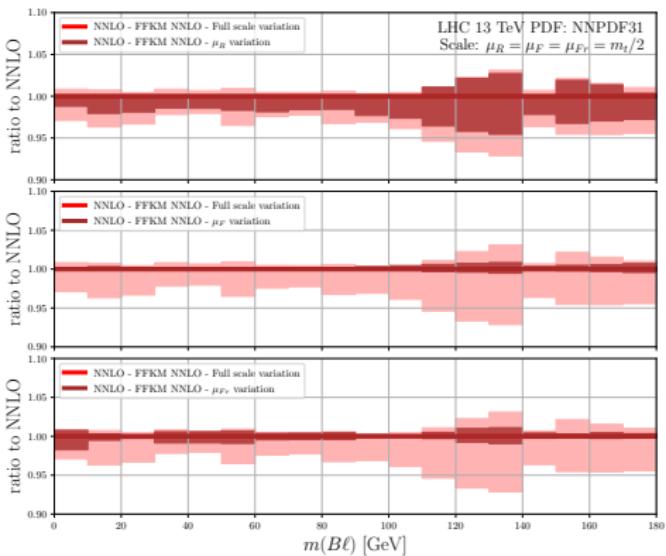
Integrating over the angles and  $y$  yields

$$\begin{aligned}
 & \frac{d\Gamma(B \rightarrow d + X)}{dz} \\
 &= \int_0^{2\pi} \int_{-1}^1 \int_0^1 \frac{m_B}{4\pi} f(y m_B) \delta\left(z - y - \cos(\theta)\sqrt{y^2 - \frac{m_d^2}{m_B^2}}\right) dy d\cos(\theta) d\phi \\
 &= \int_0^1 \frac{m_B}{2\sqrt{y^2 - \frac{m_d^2}{m_B^2}}} f(y m_B) \theta\left(1 - \frac{(z-y)^2}{y^2 - \frac{m_d^2}{m_B^2}}\right) dy \\
 &= \int_{\frac{z}{2} + \frac{m_d^2}{2zm_B^2}}^1 \frac{m_B}{2\sqrt{y^2 - \frac{m_d^2}{m_B^2}}} f(y m_B) dy \equiv \Gamma_B D_{B \rightarrow d}(z)
 \end{aligned}$$

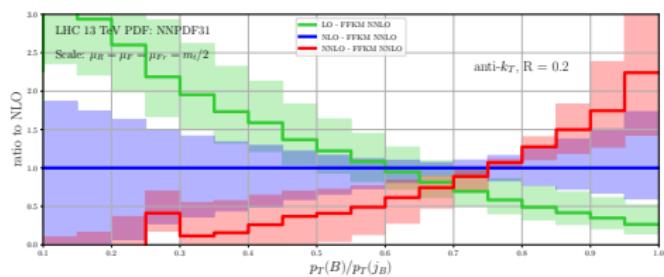
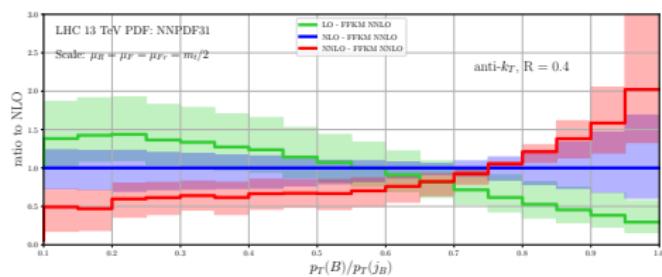
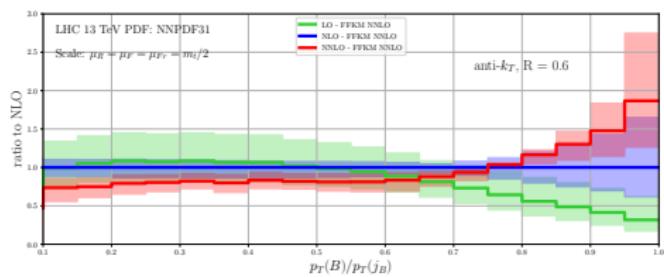
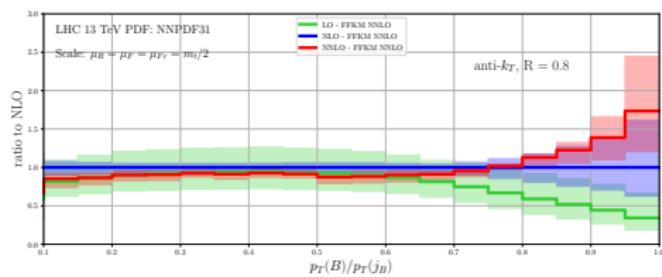
# $B$ -hadron decay fragmentation functions



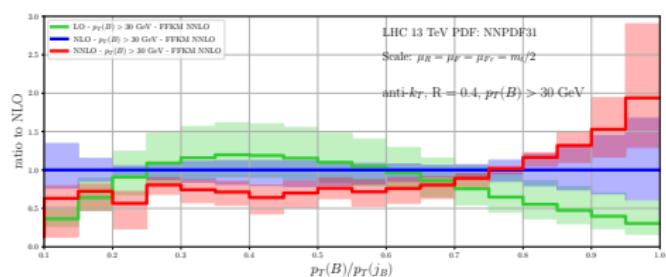
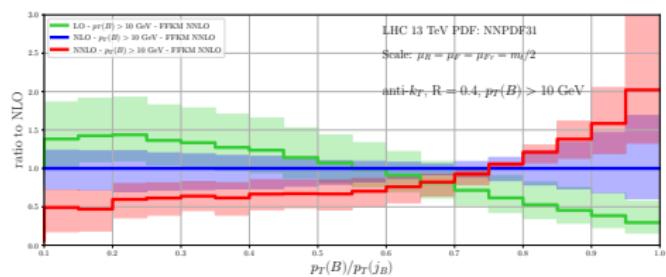
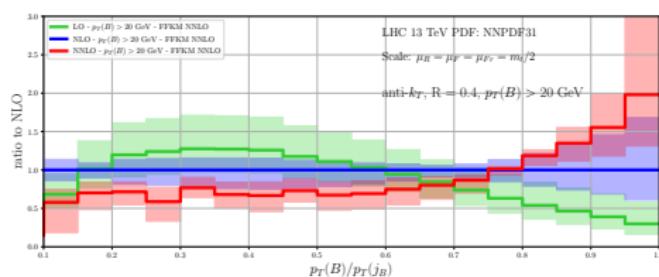
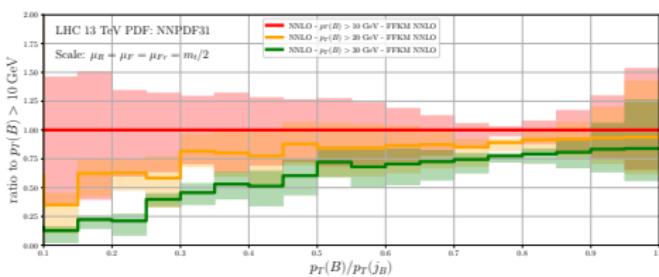
# Top-pair events with $B$ -hadrons at the LHC: separated scale dependence



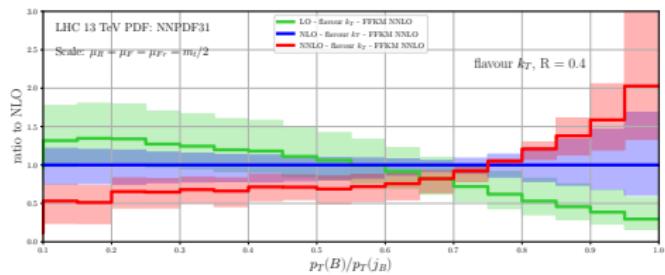
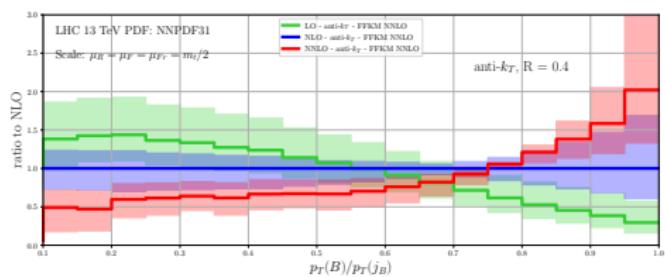
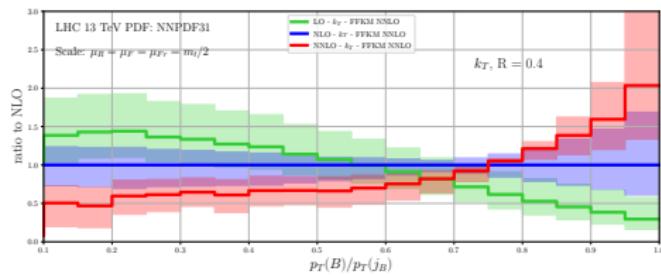
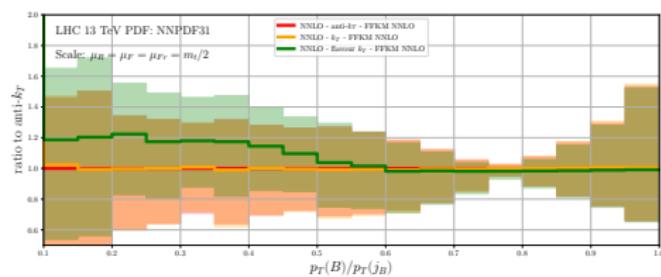
# Jet ratio: $R$ -dependence



# Jet ratio: $p_T$ -cut-dependence



# Jet ratio: jet-algorithm-dependence



# Perturbative fragmentation functions: introduction

- Need to fit many parameters (one function per parton)
- Reduction possible for heavy flavours using perturbative fragmentation functions (PFFs) *Mele and Nason (1991)*
- Heavy-flavoured hadrons contain heavy quarks
- The heavy-quark mass satisfies  $m_Q \gg \Lambda_{\text{QCD}}$
- $\Rightarrow$  Production of heavy quarks can be described perturbatively
- $\Rightarrow$  Split fragmentation into production of heavy quark and fragmentation of heavy quark into hadron

# Reduction of non-perturbative parameters

- Split fragmentation function into a non-perturbative FF (NPFF) and PFFs:

$$D_{i \rightarrow h} = D_{i \rightarrow Q} \otimes D_{Q \rightarrow h}$$

- $D_{i \rightarrow Q}$  calculable  $\Rightarrow$  only need to fit  $D_{Q \rightarrow h}$  (single function)
- Without PFFs: gluon FF poorly constrained by  $e^+e^-$ -colliders
- $\Rightarrow$  Large uncertainties at the LHC

# Perturbative fragmentation function formalism

- Factorise production of massive quarks into production of massless partons and fragmentation:

$$\frac{d\sigma_Q}{dE_Q} = \sum_i \left( \frac{d\sigma_i}{dE_i}(m_Q = 0) \otimes D_{i \rightarrow Q} \right)$$

- Initially used to resum mass logarithms ( $\ln(p_T/m_Q)$ )
- Added benefit: massive cross section from massless ones
- PFFs already known through NNLO

NLO: Mele and Nason (1991)

NNLO: Melnikov and Mitov (2004, 2005)

# The NLO perturbative fragmentation functions

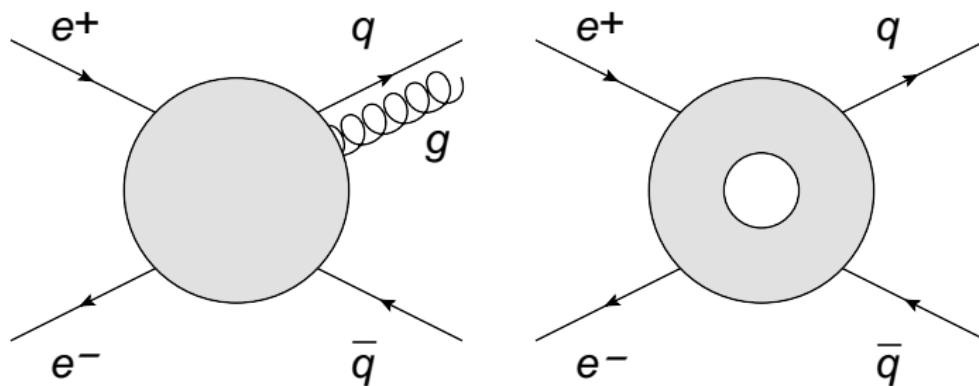
$$D_{Q \rightarrow Q}(x, \mu_{Fr}, m_Q) = \delta(1-x) + \frac{\alpha_s C_F}{2\pi} \left[ \frac{1+x^2}{1-x} \left( \ln \frac{\mu_{Fr}^2}{m_Q^2} - 2 \ln(1-x) - 1 \right) \right]_+$$

$$\int_0^1 f(x) g_+(x) dx = \int_0^1 (f(x) - f(1)) g(x) dx$$

- New and arbitrary ‘renormalisation’ scale  $\mu_{Fr}$
- Two kinds of logarithm could spoil perturbative convergence  
⇒ Resummation

# Fragmentation and collinear divergences

- Reminder:  $\frac{d\sigma_h}{dE_h} = \sum_i \frac{d\sigma_i}{dE_i} \otimes D_{i \rightarrow h}$
- $d\sigma_i$  is infrared-unsafe
- No cancellation of divergences by KLN theorem



# Collinear renormalisation

- Solved by collinear renormalisation:

$$D_i^B(x) = \sum_j (Z_{ij} \otimes D_j)(x)$$

- Analogous to coupling renormalisation
- Yields RGEs for FFs (DGLAP equations):

$$\mu_{Fr}^2 \frac{dD_{i \rightarrow h}}{d\mu_{Fr}^2}(x, \mu_{Fr}) = \sum_j (P_{ij}^T \otimes D_{j \rightarrow h})(x, \mu_{Fr})$$

- $\Rightarrow$  Only need to fit NPFFs at a single scale
- $\mu_{Fr}$ -dependence known  $\Rightarrow$  can resum  $\ln \frac{\mu_{Fr}^2}{m_Q^2}$  in PFFs

# Collinear renormalisation

$$D_i^B(x) = \sum_j (Z_{ij} \otimes D_j)(x), \quad (f \otimes g)(x) = \int_x^1 \frac{dz}{z} f\left(\frac{x}{z}\right) g(z)$$

$$\begin{aligned} Z_{ij}(x) = & \delta_{ij} \delta(1-x) + \frac{1}{\epsilon} \left( \frac{\mu_R^2}{\mu_{Fr}^2} \right)^\epsilon \frac{\alpha_s}{2\pi} P_{ij}^{(0)\text{T}}(x) \\ & + \left( \frac{\alpha_s}{2\pi} \right)^2 \left[ \frac{1}{2\epsilon} \left( \frac{\mu_R^2}{\mu_{Fr}^2} \right)^{2\epsilon} P_{ij}^{(1)\text{T}}(x) \right. \\ & + \frac{1}{2\epsilon^2} \left( \frac{\mu_R^2}{\mu_{Fr}^2} \right)^{2\epsilon} \sum_k (P_{ik}^{(0)\text{T}} \otimes P_{kj}^{(0)\text{T}})(x) \\ & \left. + \frac{\beta_0}{4\epsilon^2} \left\{ \left( \frac{\mu_R^2}{\mu_{Fr}^2} \right)^{2\epsilon} - 2 \left( \frac{\mu_R^2}{\mu_{Fr}^2} \right)^\epsilon \right\} P_{ij}^{(0)\text{T}}(x) \right] \end{aligned}$$

# Introduction to subtraction schemes

- Strategy for numerical integration of cross sections
- Cross sections contain singularities in  $d = 4$  (soft, collinear)
- In  $d = 4 - 2\epsilon$ , cross sections behave like

$$\sigma = \int_0^1 \frac{f_\epsilon(x)}{x^{1-a\epsilon}} dx$$

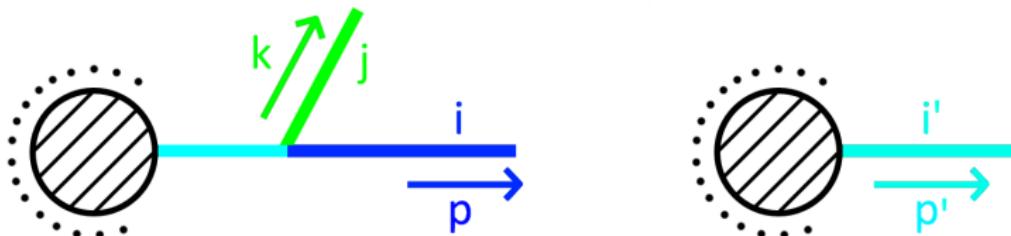
- Idea: subtract divergences differentially (subtraction terms), add them in integrated form (integrated subtraction terms):

$$\sigma = \int_0^1 \underbrace{\left( \frac{f_\epsilon(x)}{x^{1-a\epsilon}} - \frac{f_\epsilon(0)}{x^{1-a\epsilon}} \right) dx}_{\text{regular at } x=0} + f_\epsilon(0) \underbrace{\int_0^1 \frac{1}{x^{1-a\epsilon}} dx}_{1/(a\epsilon)}$$

# Introduction to subtraction schemes

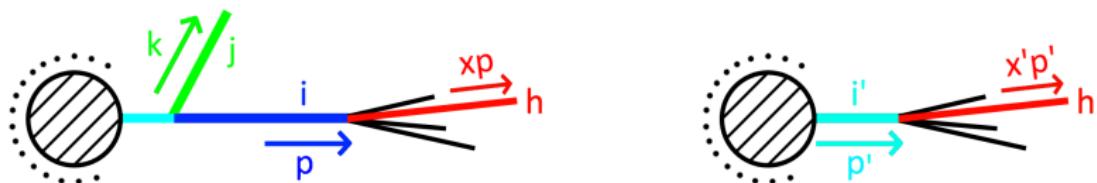
- $$\sigma = \int_0^1 \underbrace{\left( \frac{f_\epsilon(x)}{x^{1-a\epsilon}} - \frac{f_\epsilon(0)}{x^{1-a\epsilon}} \right) dx}_{\text{expand in } \epsilon \text{ around } d=4} + \frac{f_\epsilon(0)}{a\epsilon}$$

- Can perform numerical integration in  $d = 4$
- Subtraction term can in principle be any function, but:
- Both value and kinematics of subtraction term must match cross section in singular limit



# Subtraction schemes and fragmentation

- Without fragmentation: cannot distinguish collinear quark-pair  $q(p_1) + \bar{q}(p_2)$  from  $g(p_1 + p_2)$
- With fragmentation: both momentum of fragmenting particle and flavour matter  
 $\Rightarrow$  must store flavour and e.g.  $p_1^0/(p_1^0 + p_2^0)$
- Introduce concept of reference observables: match reference observable for cross section and subtraction term by rescaling the momentum fraction



# Subtraction schemes and fragmentation

- Without fragmentation: cannot distinguish  $q(p) + g(0)$  from  $q(p)$
- With fragmentation: cannot remove gluon if it is the fragmenting particle
- Usually: have to recalculate integrated subtraction terms

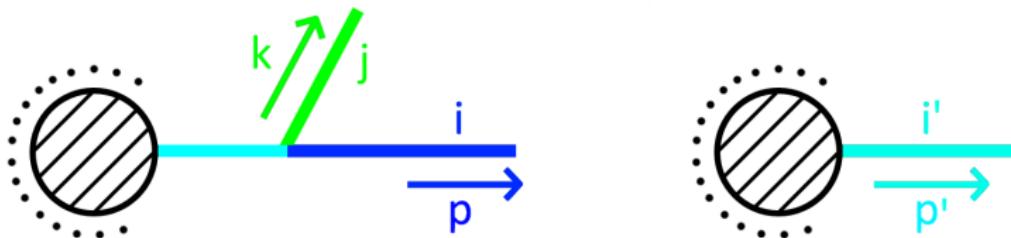
$$\mathcal{V}_{ij}(\epsilon) = \int_0^1 d\tilde{z}_i (\tilde{z}_i(1-\tilde{z}_i))^{-\epsilon} \int_0^1 \frac{dy}{y} (1-y)^{1-2\epsilon} y^{-\epsilon} \frac{\langle V_{ij,k}(\tilde{z}_i; y) \rangle}{8\pi\alpha_S\mu^{2\epsilon}}$$

with  fragmentation

$$\overline{\mathcal{V}}_{ij}(z; \epsilon) = \Theta(z)\Theta(1-z) \frac{z^{1-\epsilon}}{(1-z)^{1+\epsilon}} \int_0^1 d\tilde{z}_i (\tilde{z}_i(1-\tilde{z}_i))^{-\epsilon} \frac{\langle V_{ij,a}(\tilde{z}_i; 1-z) \rangle}{8\pi\alpha_S\mu^{2\epsilon}}$$

# Subtraction schemes and fragmentation

- Calculation of integrated subtraction terms laborious
- Important observation: not necessary if each subtraction term cancels only one singularity
- Exceptionally the case for the **sector-improved residue subtraction scheme**
- $\Rightarrow$  Major simplification of fragmentation implementation



# Reference observables

- Momentum fraction of subtraction terms not fully constrained
- Must be the same distribution for full/integrated subtraction terms
- Must match fraction of real contribution in relevant singular limit
- $\Rightarrow$  Can use freedom to improve numerical convergence
- Idea: rescale fractions per event to make all terms land in the same histogram bin
- Significantly reduce poor convergence due to “missed binning”
- Process requires “reference observable”