Top-pair events with B-hadrons at the LHC

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Based on arXiv:2102.08267 and preliminary results

RWTH Aachen University

15th International Workshop on Top-Quark Physics (TOP2022)
Durham, UK, 5 September 2022

Institute for Theoretical Particle Physics and Cosmology | RWTH AACHEN UNIVERSITY

TRR 257 - Particle Physics Phenomenology after the Higgs Discovery

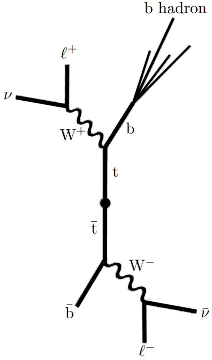
Top-pairs with B-hadrons

- Process considered:
  $p\, p \to t(\to B\ W^+ + X)\ \bar{t}(\to \bar{b}\ W^-)$
  $\quad\quad\quad\quad\quad\quad\quad \Lsh \ell^+\nu_\ell \quad\quad\quad\quad \Lsh \ell^-\bar{\nu}_\ell$

- 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

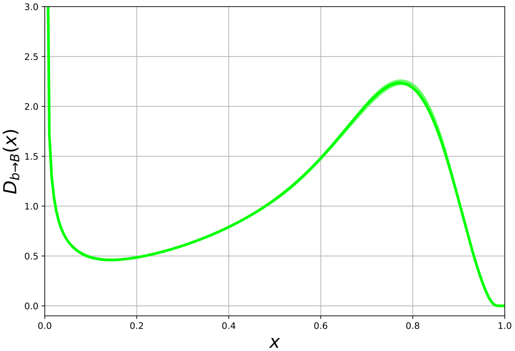


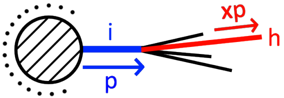
Introduction to fragmentation

- 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$\longrightarrow$hadron in the final state
- A hadron's momentum is measurable, but a parton's is not
- Mathematically similar to transition hadron$\longrightarrow$parton in the initial state

Fragmentation functions

- 'Probability distribution' to find a hadron h with a fraction x of the parton i's momentum: $D_{i \to h}(x)$
- 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:
  - 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)*
  - Top-pairs with B-hadrons at the LHC *Czakon, TG, Mitov, Poncelet (2021)*
  - W + c-jet at the LHC *Czakon, Mitov, Pellen, Poncelet (2020)*
  - ...
- First implementation of fragmentation in a general code for NNLO cross sections
- Fully general implementation; not limited to cases presented in this talk

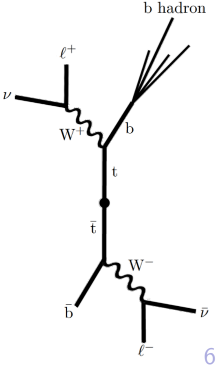
First application: LHC top-pair events with B-hadrons

- Previously studied at NLO

  A. Kharchilava (2000), S. Biswas, K. Melnikov and M. Schulze (2010)

  K. Agashe, R. Franceschini and D. Kim (2013), K. Agashe, R. Franceschini, D. Kim and M. Schulze (2016)

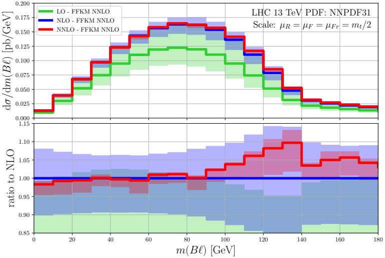
- On-shell W^+ (narrow width approximation)
- 15-point scale variation with central scales $\mu_R = \mu_F = \mu_{Fr} = m_t/2$ and $1/2 \leq \mu_i/\mu_j \leq 2$
- PDF set: NNPDF3.1
- $p_T(B) > 10$ GeV and $|\eta(B)| < 2.4$



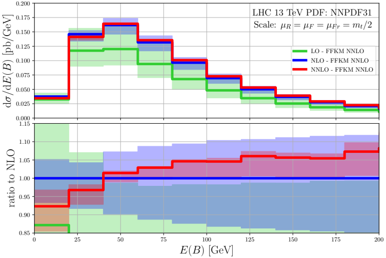
Top-pair events with B-hadrons at the LHC: plots

Observables:

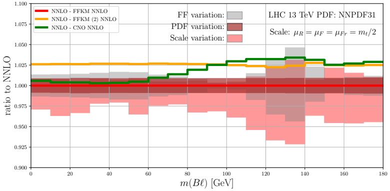
Invariant mass of B-ℓ system

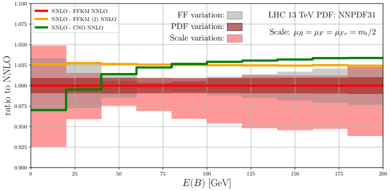


Energy of B-hadron



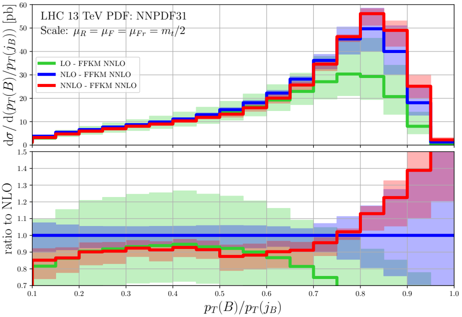
Breakdown of theory uncertainties:

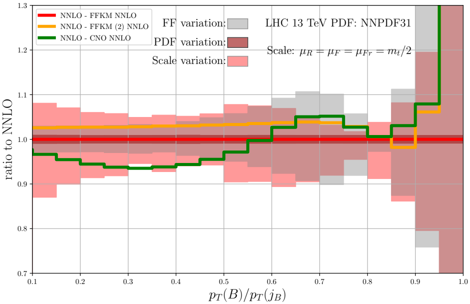




Top-pair events with B-hadrons at the LHC: jet ratio

- Jet algorithm: anti-k_T with $R = 0.8$



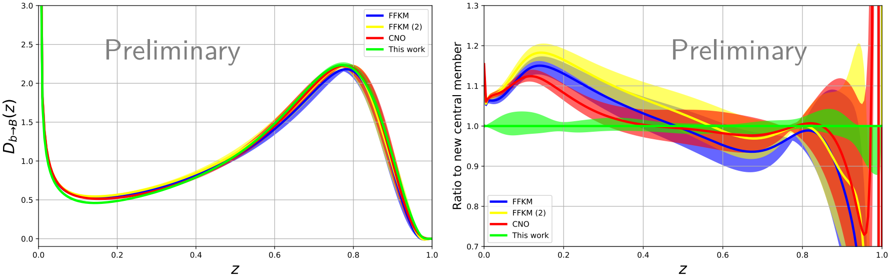


First improvement: fragmentation function fits

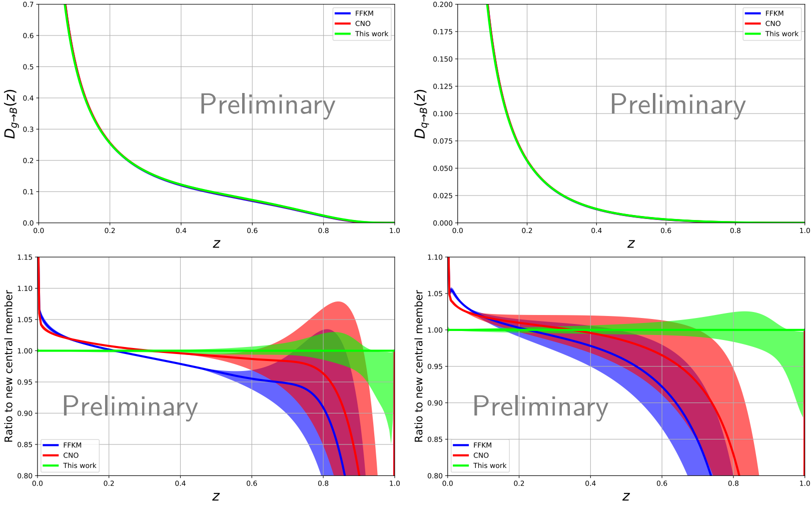
- At the time: no fits based on PFF approach available at NNLO
- Required for fully consistent results
- Three different FF sets based on three different compromises
- Two based on NNLO calculation within SCET/HQET
  M. Fickinger, S. Fleming, C. Kim and E. Mereghetti (2016)
- One based on NLO calculation 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: Corcella, Czakon, TG, Mitov, Poncelet (preliminary)

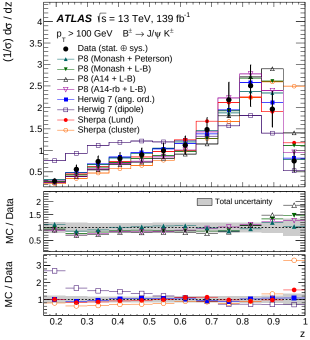


First NNLO fit within the PFF approach



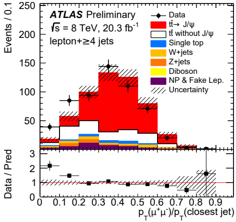
Second improvement: B-hadron decays

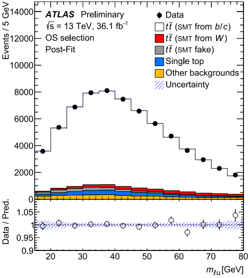
- Full reconstruction of B-hadrons difficult in practice
- Not enough $t\bar{t}$ events for distributions
  $\Rightarrow$ Cannot compare first results to experiment at present
- Could compare to data if process changed to $p\,p \longrightarrow B + X$
- Fully reconstructed B-hadrons in arXiv:2108.11650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



Second improvement: B-hadron decays

- Solution: incorporate B-hadron decays
- Only reconstruct some decay products
  $\Rightarrow$ Significantly boost statistics
- Examples:
  ATLAS-CONF-2015-040 ($B \to J/\psi + X$)
  ATLAS-CONF-2019-046 ($B \to \mu + X$)
- 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
- How can the decay be included in the fragmentation?

Including B-hadron decays in theory predictions

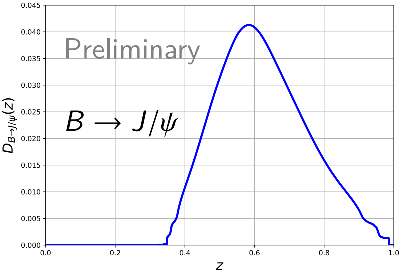
- Assume isotropic decay: $d\Gamma(B \to \mu + X) = f(E_\mu) dE_\mu d\cos\theta_\mu d\phi_\mu$
- Valid for spin-0 particles (e.g. weakly-decaying B-mesons)
- Normalize E_μ using $m_B \Rightarrow f(E_\mu) dE_\mu \to f(y) dy$
- Boost from B-hadron rest frame to $E_B \gg m_B$ and integrate over the angles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

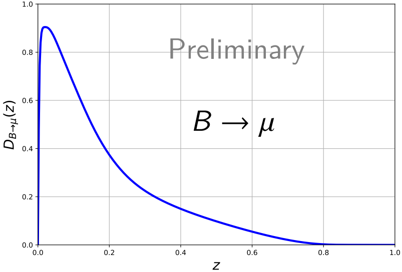
$$\Rightarrow \frac{d\Gamma(B \to \mu + X)}{dy} \to D_{B\to\mu}(z)$$

- $D_{B\to\mu}$ is the 'fragmentation function' for transition $B \to \mu$
- Can calculate $D_{B\to\mu}$ once and for all
- $D_{B\to\mu}$ combines with known $D_{i\to B}$ via convolution

Including B-hadron decays in theory predictions

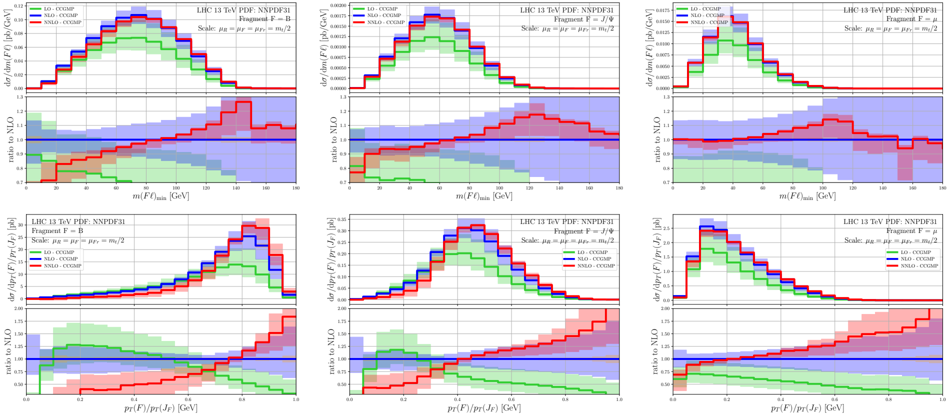
- Only requirement: must know $f(E_\mu)$
- Can be obtained using e.g. EvtGen
- Works for any descendant, not just muons
- Vast amount of data from B-factories
  $\Rightarrow f(E_\mu)$ expected to be more precise than $D_{i\to B}$





Preliminary results

B J/ψ μ



Conclusion

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

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

Decay fragmentation function derivation

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

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

$$\delta\left(z - \frac{E_d}{E_B}\right) = \delta\left(z - \gamma_B \frac{E_d^{\text{rest}} + \beta_B \cos(\theta) \sqrt{(E_d^{\text{rest}})^2 - m_d^2}}{E_B}\right)$$

$$\approx \delta\left(z - \frac{E_d^{\text{rest}} + \cos(\theta) \sqrt{(E_d^{\text{rest}})^2 - m_d^2}}{m_B}\right)$$

$$= \delta\left(z - y - \cos(\theta) \sqrt{y^2 - \frac{m_d^2}{m_B^2}}\right)$$

Decay fragmentation function derivation

Integrating over the angles and y yields

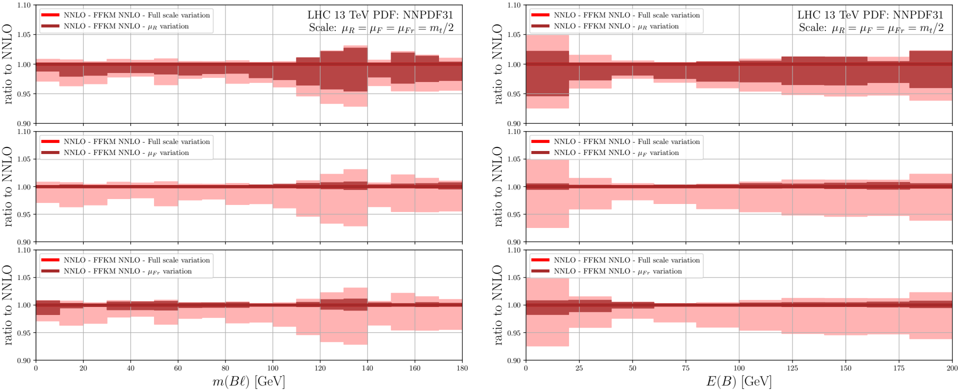
$$\frac{d\Gamma(B \to d + X)}{dz}$$

$$= \int_0^{2\pi}\int_{-1}^{1}\int_0^{1} \frac{m_B}{4\pi} f(y\, m_B)\delta\left(z - y - \cos(\theta)\sqrt{y^2 - \frac{m_d^2}{m_B^2}}\right) dy\, d\cos(\theta) d\phi$$

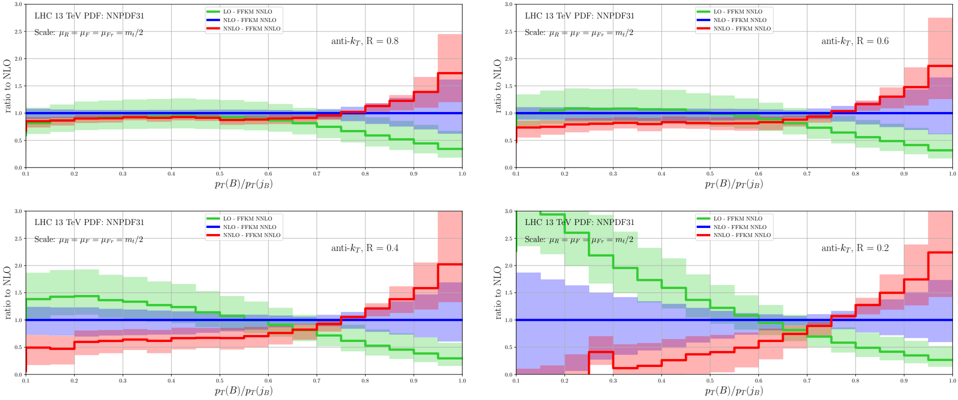
$$= \int_0^1 \frac{m_B}{2\sqrt{y^2 - \frac{m_d^2}{m_B^2}}} f(y\, m_B)\theta\left(1 - \frac{(z-y)^2}{y^2 - \frac{m_d^2}{m_B^2}}\right) dy$$

$$= \int_{\frac{z}{2}+\frac{m_d^2}{2z\, m_B^2}}^{1} \frac{m_B}{2\sqrt{y^2 - \frac{m_d^2}{m_B^2}}} f(y\, m_B) dy \equiv \Gamma_B\, D_{B\to d}(z)$$

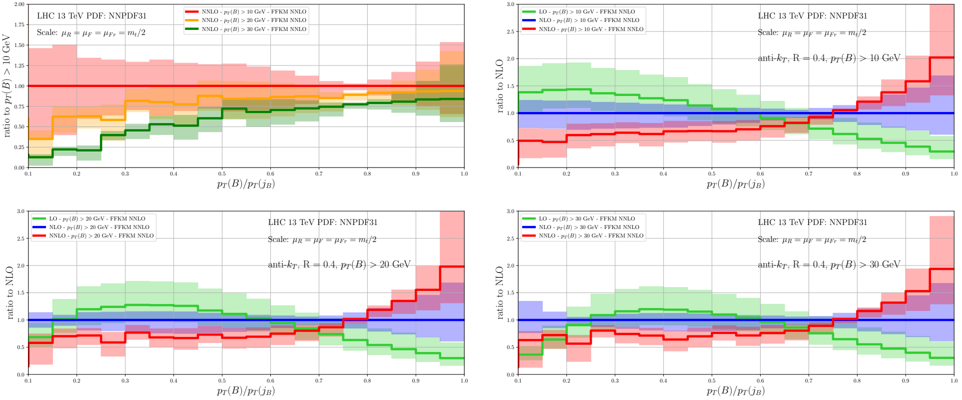
Top-pair events with B-hadrons at the LHC: separated scale dependence



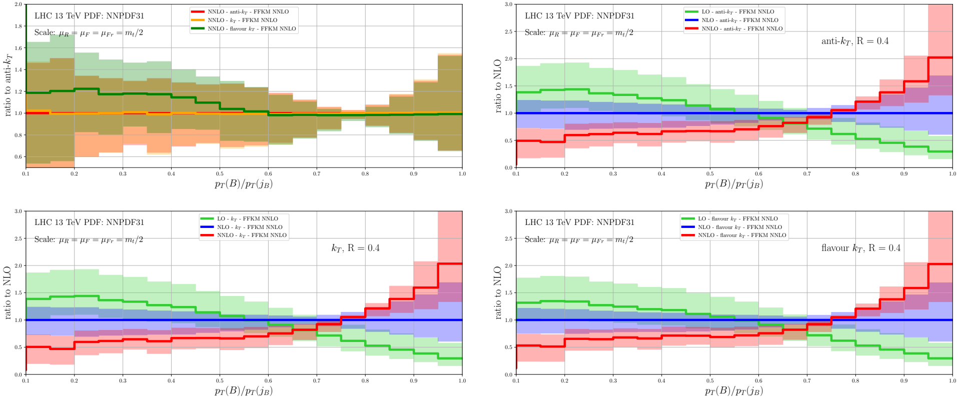
Jet ratio: R-dependence



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:

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

- $D_{i\to Q}$ calculable $\Rightarrow$ only need to fit $D_{Q\to h}$ (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:

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

- 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

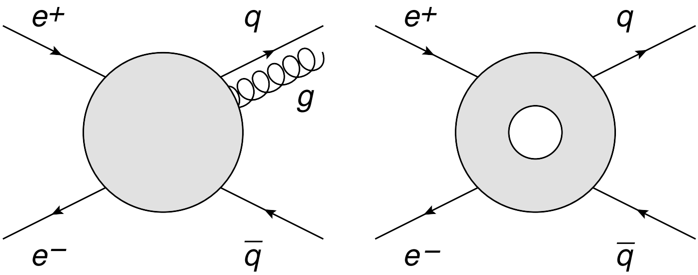
$$D_{Q\to Q}(x,\mu_{Fr},m_Q) = \delta(1-x) + \frac{\alpha_s C_F}{2\pi}\left[\frac{1+x^2}{1-x}\left(\ln\frac{\mu_{Fr}^2}{m_Q^2} - 2\ln(1-x) - 1\right)\right]_+$$

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

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

Fragmentation and collinear divergences

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



Collinear renormalisation

- Solved by collinear renormalisation:

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

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

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

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

Collinear renormalisation

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

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

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

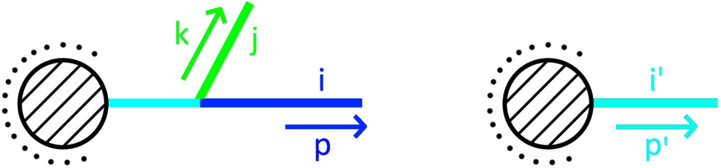
$$\sigma = \int_0^1 \frac{f_\epsilon(x)}{x^{1-a\epsilon}} dx$$

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

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

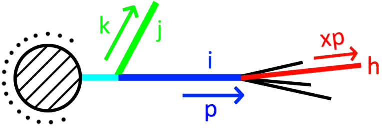
Introduction to subtraction schemes

- $$\sigma = \underbrace{\int_0^1 \left(\frac{f_\epsilon(x)}{x^{1-a\epsilon}} - \frac{f_\epsilon(0)}{x^{1-a\epsilon}} \right) dx}_{\text{expand in } \epsilon \text{ around } d=4} + \frac{f_\epsilon(0)}{a\epsilon}$$
- 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 $q(p_1) + \overline{q}(p_2)$ 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

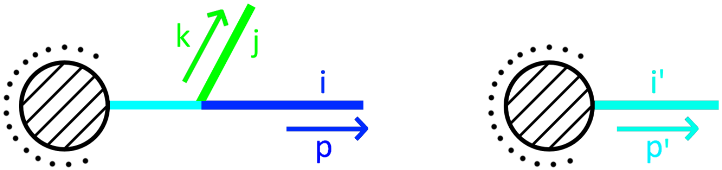
$$\mathcal{V}_{ij}(\epsilon) = \int_0^1 d\tilde{z}_i \; (\tilde{z}_i(1-\tilde{z}_i))^{-\epsilon} \int_0^1 \frac{dy}{y} \; (1-y)^{1-2\epsilon} \, y^{-\epsilon} \; \frac{< \boldsymbol{V}_{ij,k}(\tilde{z}_i; y) >}{8\pi\alpha_S\mu^{2\epsilon}}$$

with $\Big\downarrow$ fragmentation

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

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"