

# Top-Pair Events with B-hadrons at the LHC

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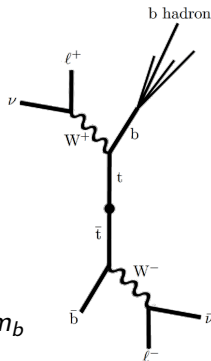
# Top-pairs with B-Hadrons

- Process considered:

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

$$\quad \hookrightarrow \ell^+ \nu_\ell \quad \quad \quad \hookrightarrow \ell^- \bar{\nu}_\ell$$

- Measurements of B-hadrons very precise  
 $\Rightarrow$  high-precision top-mass determination
- High top mass  $\Rightarrow$  small power corrections in  $m_b$
- Production of hadrons is a non-perturbative effect

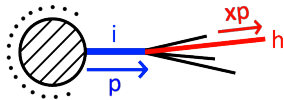
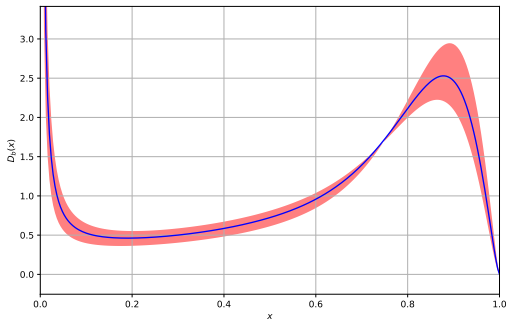


# Introduction to Fragmentation

- Idea: describe production of hadrons using two steps
  - ① The production of partons (gluon and quarks) using perturbation theory
  - ② The (non-perturbative) fragmentation of these partons into the observed hadrons
- Transition parton  $\rightarrow$  hadron in the final state
- Hadron's momentum is measurable (parton's is not)
- Mathematically similar to transition hadron  $\rightarrow$  parton in the initial state

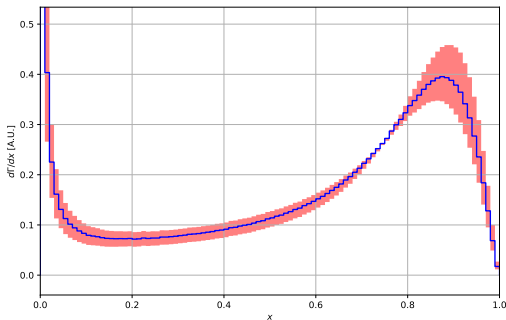
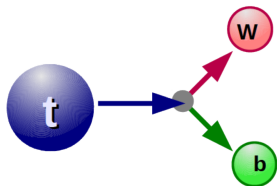
# Fragmentation Functions

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



## Example: Top-decay to a B-hadron at LO

- $t \rightarrow B W^+ + X$
- Partonically at LO:  
 $t \rightarrow b W^+$



# 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:

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

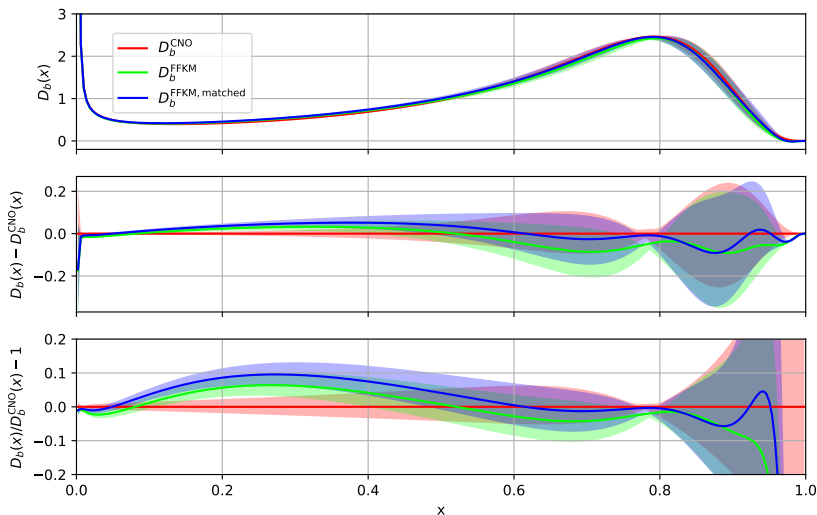
- $D_{i \rightarrow Q}$  calculable  $\Rightarrow$  only need to fit  $D_{Q \rightarrow h}$  (single function)
- Without PFFs: gluon FF poorly constrained by  $e^+e^-$ -colliders
- $\Rightarrow$  Large uncertainties at the LHC



# Fragmentation Functions Used in the Paper

- At present: no fits based on PFF approach available at NNLO
- 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)*
- $\ln \frac{\mu_{Fr}^2}{m_Q^2}$  is resummed at NNLL,  $\ln(1-x)$  at (NN)NLL.

## Fragmentation Functions Used in the Paper



# 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, T.G., Mitov, Poncelet (2021)*
  - W + c-jet at the LHC *Czakon, Mitov, Pellen, Poncelet (2020)*
  - ...
- This work: first implementation of fragmentation in a general code for NNLO cross sections
- Fully general implementation; not limited to cases presented in this talk

# Isolated Top Decay: Setup

- Previously considered through NLO

*S. Biswas, K. Melnikov and M. Schulze (2010)*

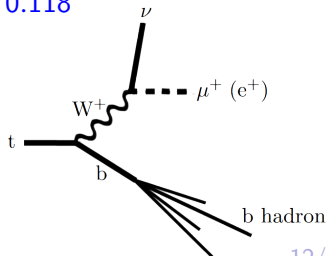
- On-shell  $W^+$  (narrow width approximation)

- Parameters:

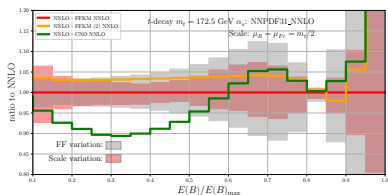
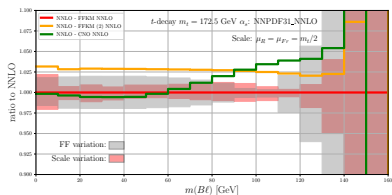
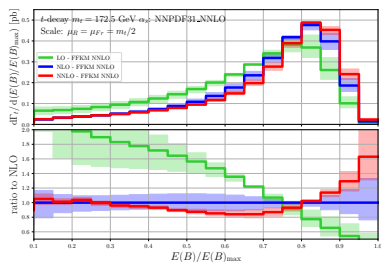
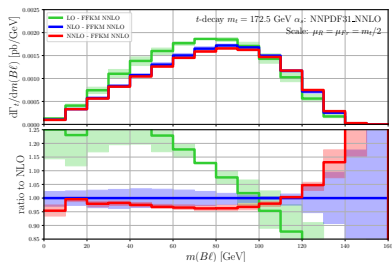
$m_t = 172.5$  GeV,  $m_W = 80.385$  GeV,  $\Gamma_W = 2.0928$  GeV,  
 $m_b = (4.66$  GeV,  $4.75$  GeV),  $\alpha_s(M_Z) = 0.118$

- 7-point scale variation with  
central scales  $\mu_R = \mu_{Fr} = m_t/2$

- Single cut:  $E(B) > 5$  GeV



# Isolated Top Decay: Plots



# Top-Pair Events with B-hadrons at the LHC: Setup

- 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)*

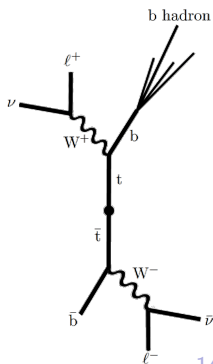
- On-shell  $W^+$  (narrow width approximation)

- Parameters as before

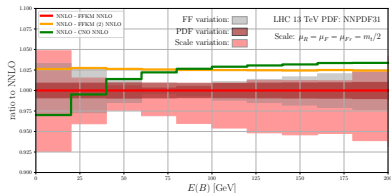
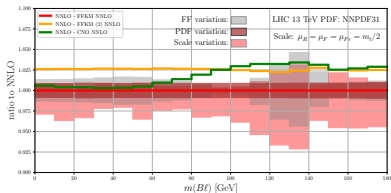
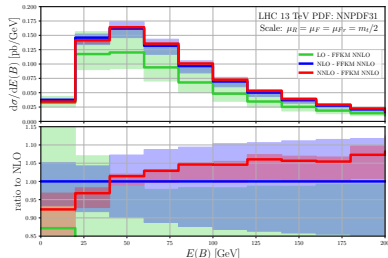
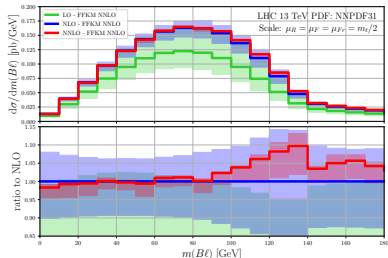
- 15-point scale variation with  
central scales  $\mu_R = \mu_F = \mu_{Fr} = m_t/2$   
and  $1/2 \leq \mu_i/\mu_j \leq 2$

- PDF set: NNPDF3.1

- $p_T(B) > 10 \text{ GeV}$  and  $|\eta(B)| < 2.4$

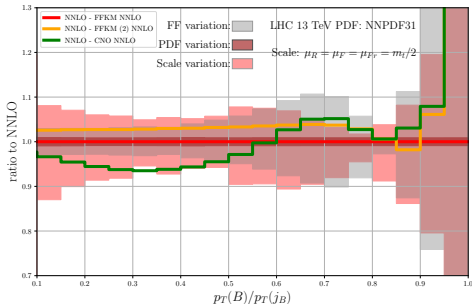
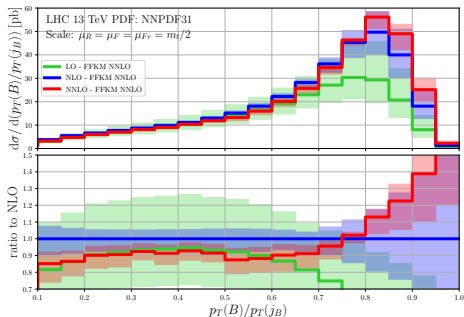


# Top-Pair Events with B-hadrons at the LHC: Plots



## Top-Pair Events with B-hadrons at the LHC: Jet Ratio

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

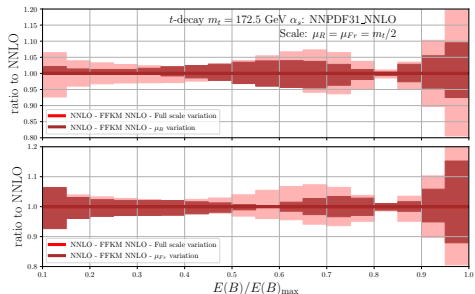
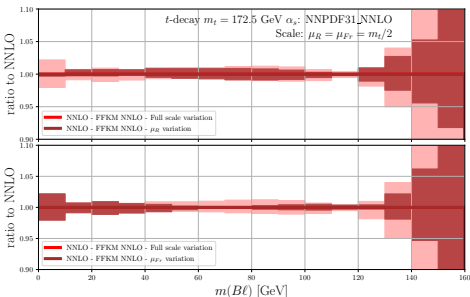




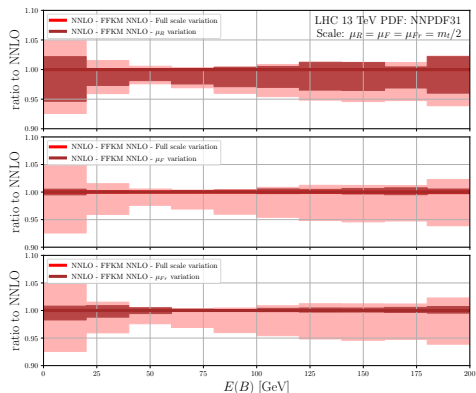
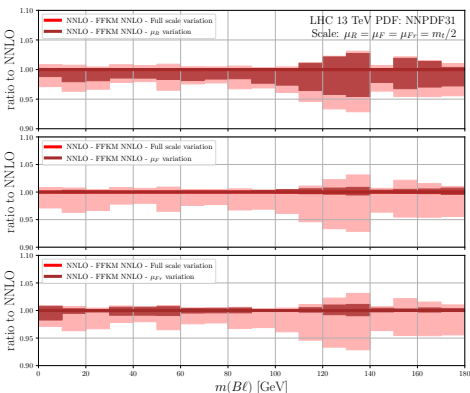
## Conclusion and Outlook

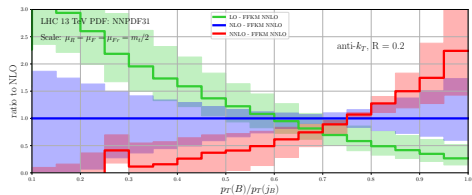
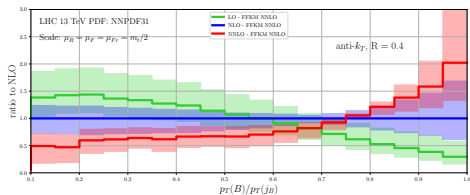
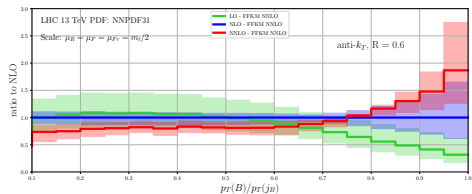
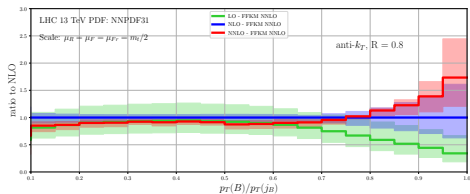
- Fragmentation has been implemented in STRIPPER
- First application: top-quark pairs at the LHC
- Big reduction in scale uncertainties from NLO to NNLO
- $\Rightarrow$  potential for more accurate top-mass determination
- PDF-insensitive extraction of FFs at LHC plausible
- Framework completely general: can describe the production of any hadron in any process at NNLO

# Isolated Top Decay: Separated Scale Dependence

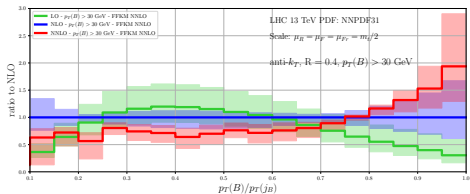
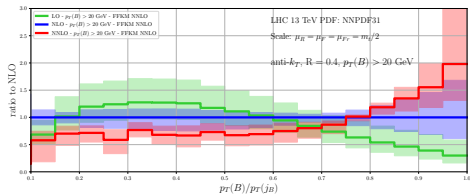
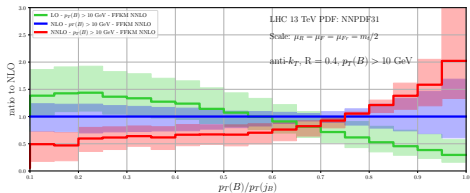
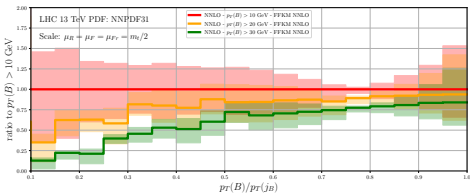


# Top-Pair Events with B-hadrons at the LHC: Separated Scale Dependence

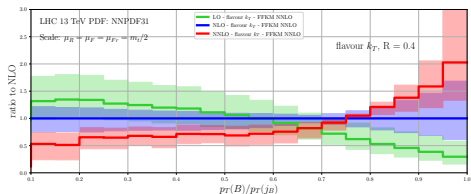
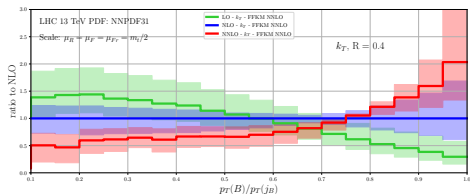
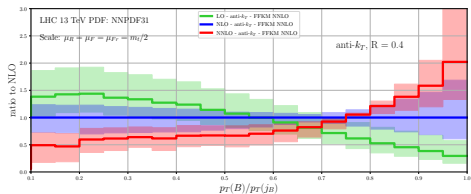
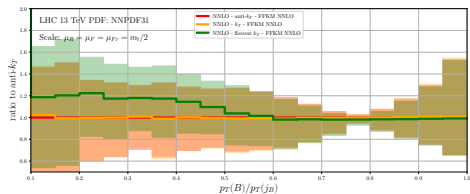


Jet Ratio:  $R$ -Dependence

# Jet Ratio: $p_T$ -Cut-Dependence



# Jet Ratio: Jet-Algorithm-Dependence



# Perturbative Fragmentation 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

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

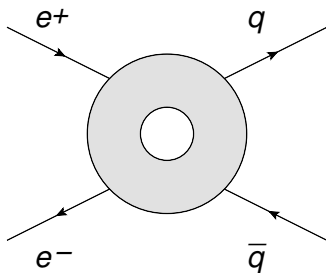
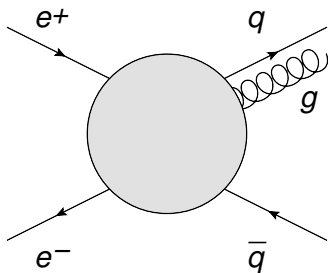
$$\int_0^1 f(x) g_+(x) dx = \int_0^1 (f(x) - f(1)) g(x) dx$$

- 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

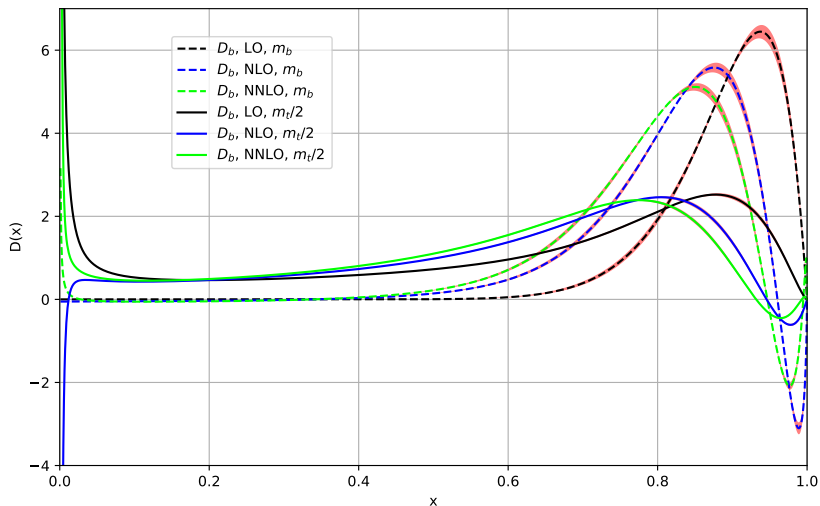
$$D_i^B(x) = \sum_j (Z_{ij} \otimes D_j)(x), \quad (f \otimes g)(x) = \int_x^1 \frac{dz}{z} f\left(\frac{x}{z}\right) g(z)$$

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

## 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"

## A Fragmentation Function Through NNLO



# 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

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

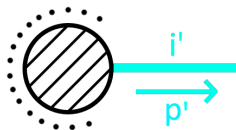
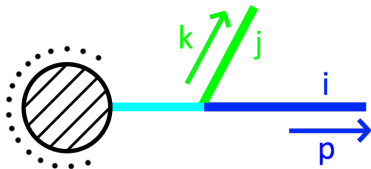
- Idea: subtract divergences differentially (subtraction terms), add them in integrated form (integrated subtraction terms):

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

## Introduction to Subtraction Schemes

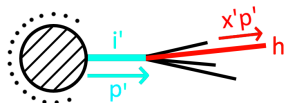
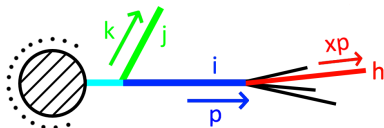
$$\bullet \sigma = \underbrace{\int_0^1 \left( \frac{f_\epsilon(x)}{x^{1-a\epsilon}} - \frac{f_\epsilon(0)}{x^{1-a\epsilon}} \right) dx}_{\text{expand in } \epsilon \text{ around } d=4} + \frac{f_\epsilon(0)}{a\epsilon}$$

- 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  $q(p_1) + \bar{q}(p_2)$  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

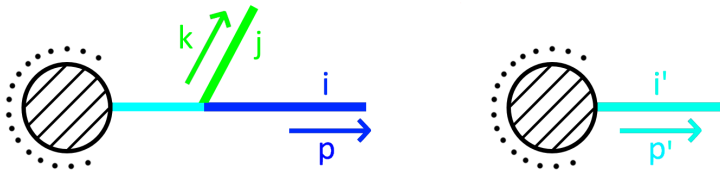
$$\mathcal{V}_{ij}(\epsilon) = \int_0^1 d\tilde{z}_i (\tilde{z}_i(1 - \tilde{z}_i))^{-\epsilon} \int_0^1 \frac{dy}{y} (1 - y)^{1-2\epsilon} y^{-\epsilon} \frac{\langle \mathbf{V}_{ij,k}(\tilde{z}_i; y) \rangle}{8\pi\alpha_S\mu^{2\epsilon}}$$

with  $\downarrow$  fragmentation

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

# 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



# Sector-Improved Residue Subtraction Scheme

- Implemented in C++ library STRIPPER
- Many NNLO firsts over the years. Recently:
  - 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, T.G., Mitov, Poncelet (2021)*
  - W + c-jet at the LHC *Czakon, Mitov, Pellen, Poncelet (2020)*
  - ...
- Edge over competitors due to minimisation of analytic integration
- First implementation of fragmentation in a general NNLO subtraction scheme
- Fully general implementation; not limited to cases presented in this talk

# Tests of the Implementation

- Implementation has been tested in several ways
- Cancellation of divergences
- A sum rule for top-decay:

$$\Gamma = \int_0^1 x \frac{d\Gamma}{dx} dx \quad \text{if} \quad \int_0^1 z D_{i \rightarrow h}(z) dz = 1$$

- Comparison of  $e^+e^- \rightarrow B + X$  to an analytic calculation
- All tests confirm the implementation is correct

# Cross-Check: B-Hadrons at LEP

