

# NNLL resummation with PB using the effective soft-gluon coupling & $N_f$ studies

Cascade developer meeting

Mees van Kampen,  
Lissa Keersmaekers, Ola Lelek

September 29, 2022

# The CSS approach

[Nuclear Physics B250 (1985) 199-224]

Well-established formalism that provides an analytical expression for inclusive processes:

$$h_1(p_1) + h_2(p_2) \rightarrow F(M, \mathbf{q}_\perp^2) + X$$

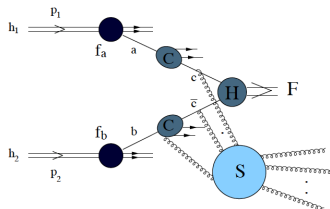
The differential cross section is given by:

$$\begin{aligned} \frac{d\sigma}{dQ^2 dy d\mathbf{q}_\perp^2} &= \left[ \frac{d\sigma^{(\text{res.})}}{dQ^2 dy d\mathbf{q}_\perp^2} \right]_{q_T \ll Q} + \left[ \frac{d\sigma^{(\text{fin.})}}{dQ^2 dy d\mathbf{q}_\perp^2} \right]_{q_T \gg Q} \\ &= \int d^2\mathbf{b} e^{i\mathbf{b} \cdot \mathbf{q}_\perp} \frac{\sigma^{(0)}(Q^2)}{s} H(\alpha_s(Q^2)) \sum_{a,b} \mathcal{F}_{a/A}(\mathbf{b}; Q, \xi_a, \mu) \mathcal{F}_{b/B}(\mathbf{b}; Q, \xi_b, \mu) \\ &\quad + Y(\mathbf{q}_\perp; Q, x_a, x_b) \end{aligned}$$

TMDs from CSS are factorized:

$$\mathcal{F}_{q/i} \sim f_{q/i} \otimes C_{jq} \otimes \sqrt{S}$$

- parton distributions:  $f_{q/i}(x, b_0/b)$
- coefficient functions:  $C_{jq}(\alpha_s(b_0/b), z)$
- Sudakov form factor:  $\sqrt{S(Q, b)}$



Schematic representation of factorized TMDs of low- $q_T$  contribution to  $\sigma$   
[Catani, de Florian, Grazzini  
arXiv:0008184v2]

# The CSS approach - Sudakov

- Soft-gluon resummation by coefficient functions  $C_{ab}$  and Sudakov form factor  $\sqrt{S}$
- Perturbative part
- Non-negligible non-perturbative part  $S_{NP}$

$$\sqrt{S(Q, b)} = \exp \left\{ -\frac{1}{2} \int_{b_0/b}^{Q^2} \frac{d\mu^2}{\mu^2} \left[ \ln \frac{Q^2}{\mu^2} A_a(\alpha_s(\mu^2)) + B_a(\alpha_s(\mu^2)) \right] \right\} \times S_{NP}(b)$$

Perturbatively calculable coefficients:

$$A_a(\alpha_s) = \sum_{n=1}^{\infty} \left( \frac{\alpha_s}{\pi} \right)^n A_a^{(n)},$$

$$B_a(\alpha_s) = \sum_{n=1}^{\infty} \left( \frac{\alpha_s}{\pi} \right)^n B_a^{(n)},$$

$$C_{ab}(\alpha_s, z) = \delta_{ab} \delta(1-z) + \sum_{n=1}^{\infty} \left( \frac{\alpha_s}{\pi} \right)^n C_{ab}^{(n)}(z),$$

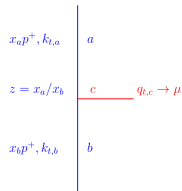
$$H(\alpha_s) = 1 + \sum_{n=1}^{\infty} \left( \frac{\alpha_s}{\pi} \right)^n H^{(n)}$$

# The Parton Branching (PB) method

JHEP 01 (2018) 070 [arXiv:1708.03279]

**PB evolution equation for TMDs**  $\tilde{\mathcal{A}}_a(x, k_t^2, \mu^2)$  can be solved iteratively with the Monte Carlo method:

$$\begin{aligned} \tilde{\mathcal{A}}_a(x, k_t^2, \mu^2) = & \Delta_a(\mu^2) \tilde{\mathcal{A}}_a(x, k_{t,0}^2, \mu_0^2) + \\ & + \sum_b \left[ \int \frac{d^2 \mu'}{\pi \mu'^2} \int_x^{z_M(\mu')} dz \Theta(\mu^2 - \mu'^2) \Theta(\mu'^2 - \mu_0^2) \right. \\ & \times \left. \frac{\Delta_a(\mu^2)}{\Delta_a(\mu'^2)} P_{ab}^{(R)}(\alpha_s(q_\perp), z) \tilde{\mathcal{A}}_b\left(\frac{x}{z}, \underbrace{k_{t,b} - q_{t,c}}_{k_{t,a}}, \mu'^2\right) \right] \end{aligned}$$



Kinematics in each branching governed by momentum conservation:  $k_{t,b} = k_{t,a} + q_{t,c}$

DGLAP splitting functions:

$$\begin{aligned} P_{ab}(\alpha_s, z) &= d_a(\alpha_s) \delta_{ab} \delta(1-z) + \frac{k_a(\alpha_s) \delta_{ab}}{(1-z)_+} + R_{ab}(\alpha_s, z) \\ P_{ab}^{(R)}(\alpha_s, z) &= \frac{k_a(\alpha_s) \delta_{ab}}{1-z} + R_{ab}(\alpha_s, z) \quad \text{resolvable emission probability} \end{aligned}$$

Sudakov form factor (**non-resolvable / no-emission probability**):

$$\Delta_a^{(PB)}(\mu, \mu_0) = \exp \left\{ - \sum_b \int_{\mu_0^2}^{\mu^2} \frac{d\mu'^2}{\mu'^2} \int_0^{z_M(\mu')} dz \, z \, P_{ba}^{(R)}(\alpha_s(q_t), z) \right\}$$

# The Parton Branching (PB) method

Angular ordering condition:  $q_t^2 = (1 - z)^2 \mu'^2$

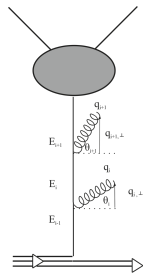
$$\begin{aligned} \tilde{\mathcal{A}}_a(x, k_t^2, \mu^2) = & \Delta_a(\mu^2) \tilde{\mathcal{A}}_a(x, k_{t,0}^2, \mu_0^2) + \\ & + \sum_b \int \frac{d^2 \mu'}{\pi \mu'^2} \int_x^{1 - \frac{q_0}{\mu'}} dz \Theta(\mu^2 - \mu'^2) \Theta(\mu'^2 - \mu_0^2) \frac{\Delta_a(\mu^2)}{\Delta_a(\mu'^2)} \\ & \times P_{ab}^{(R)}(\alpha_s((1 - z)\mu'), z) \tilde{\mathcal{A}}_b\left(\frac{x}{z}, k_{t,b} - (1 - z)\mu', \mu'^2\right) \end{aligned}$$

Dynamical soft-gluon resolution scale, avoid Landau pole  $\Lambda_{\text{QCD}}$ .  
Hautmann, Keersmaekers, Lelek, MvK [arXiv:1908.08524]

- Sum over all transverse momenta:  $k_t = k_{t,0} - \sum_i q_{t,i}$
- Intrinsic  $k_t$  in non-perturbative part:  $\tilde{\mathcal{A}}_a(x, k_{t,0}, \mu_0)$   
e.g. collinear with Gaussian  $f_a(x, \mu_0) e^{-k_t^2/2\sigma^2} \rightarrow f_a(x, \mu_0)$  and  $\sigma$  fitted to data

PB implemented in the Monte Carlo event generator CASCADE3 [arXiv:2101.10221]:

- associate  $k_t$  to partons in the hard process according to the TMD
- for exclusive observables: perform backward evolution with TMD parton shower (unfolding the TMD)



# Analytical comparison CSS and PB: logarithmic accuracy

CSS Sudakov (with scale  $\mu = q_t$ ):

$$S(Q^2, b^2) = \exp \left( - \int_{1/b^2}^{Q^2} \frac{dq_t^2}{q_t^2} \left[ \ln \left( \frac{Q^2}{q_t^2} \right) A_a(\alpha_s(q_t^2)) + B_a(\alpha_s(q_t^2)) \right] \right)$$

PB Sudakov (*twice in the cross section!*) rewritten with angular ordering and virtual splitting functions:

$$\Delta_a^{(PB)}(Q^2, q_0^2) = \exp \left( - \int_{q_0^2}^{Q^2} \frac{dq_t^2}{q_t^2} \left[ \frac{1}{2} \ln \left( \frac{Q^2}{q_t^2} \right) k_a(\alpha_s(q_t^2)) - d_a(\alpha_s(q_t^2)) \right] \right)$$

Logarithmic accuracy	Terms	Single log	Double log	
Leading log (LL)	$\alpha_s^n \ln^{n+1}(Q^2/q_t^2)$		$A_a^{(1)} = k_a^{(0)}$	✓
Next-to-leading log (NLL)	$\alpha_s^n \ln^n(Q^2/q_t^2)$	$B_a^{(1)} = -2d_a^{(0)}$	$A_a^{(2)} = k_a^{(1)}$	✓
Next-to-next-to-leading log (NNLL)	$\alpha_s^n \ln^{n-1}(Q^2/q_t^2)$	$B_q^{(2)} = -2d_q^{(1)}$ $+16\pi C_F \beta_0 (\zeta_2 - 1)$ $\Downarrow$ <i>Resummation scheme dependence</i>	$A_q^{(3)} = k_q^{(2)}$ $+2\beta_0 C_F d_2^{q*}$ $\Downarrow$ <i>Effective <math>\alpha_s</math></i>	✓/✗

Soft-gluon effective coupling: Banfi et al. [arXiv:1807.11487] & Catani et al. [arXiv:1904.10365]  $*d_2^q = C_F C_A \left( \frac{808}{27} - 28\zeta_3 \right) - \frac{112}{27} C_F N_f$

$$B_q^{(2)} - (-2) \cdot d_q^{(1)} = 16\pi C_F \beta_0 (\zeta_2 - 1)$$

- In PB, we use universal splitting functions  $P_{ab}$ . These are independent of any scheme choice. So  $d_q^{(1)}$  is fixed.
- In CSS, certain perturbative coefficients can mix via renormalization group transformations:

$$\frac{\partial \ln H^F(\alpha_s(\mu^2))}{\partial \ln \mu^2} = \gamma_H(\alpha_s(\mu^2))$$
$$H^F(\alpha_s(c_1 Q^2)) = \exp \left\{ \int_{c_0/b^2}^{c_1 Q^2} \frac{d\mu^2}{\mu^2} \gamma_H(\alpha_s(\mu^2)) \right\} H^F(\alpha_s(c_0/b^2)).$$

- Parts of  $H$  can mix with the  $B$  in the Sudakov with a different *resummation scheme*

$$B^F(\alpha_s(\mu^2)) = B(\alpha_s(\mu^2)) - (-\beta_0 \alpha_s^2 - \beta_1 \alpha_s^3 + \mathcal{O}(\alpha_s^4)) \left( \frac{H^{F(1)}}{\pi} + \frac{2\alpha_s}{\pi^2} H^{F(2)} + \mathcal{O}(\alpha_s^2) \right).$$

The difference we found is equal to the first term of this expansion of  $\gamma_H$ , the term with  $\alpha_s^2$

## Double logarithmic part

$$A_i^{(3)} - k_i^{(2)} = C_i(\beta_0\pi) \left[ C_A \left( \frac{808}{27} - 28\zeta_3 \right) - N_f \frac{112}{27} \right]$$

- $K$  part from splitting functions is *cusplike anomalous dimension*, in other words: *soft-gluon coupling*
- Intensity of soft-gluon radiation is  $C_i\alpha_s/\pi$ . **To get NLL**, replace it by:

$$C_i \frac{\alpha_s}{\pi} \rightarrow \mathcal{A}_i^{CMW}(\alpha_s(q_T^2)) = C_i \frac{\alpha_s(q_T^2)}{\pi} \left( 1 + \frac{\alpha_s(q_T^2)}{2\pi} K \right)$$

- **To go to NNLL** (or higher), use the *effective soft-gluon coupling*:

$$\alpha_s^{\text{eff}} = \alpha_s \left( 1 + \sum_n \left( \frac{\alpha_s}{2\pi} \right)^n K^{(n)} \right).$$

Banfi et al. [arXiv:1807.11487] & Catani et al. [arXiv:1904.10365]

- $A_i^{(3)}$  of CSS is obtained by taking  $n = 2$  and multiplication with  $C_i/\pi$
- NNLL resummation in PB? implement the effective coupling up to  $n = 2$  in TMD evolution



# Implementation effective soft-gluon coupling in TMD evolution

A start has been made in the implementation of  $\alpha_s^{eff}$  into UPDFEVOLV.

Use within:

- $\Delta_a(\mu^2, \mu_0^2, \alpha_s^{eff})$
- $P_{ab}^{(R)}(z, \alpha_s^{eff})$

We have already NLO splitting functions (so  $k_1$  is there) and the CMW coupling for NLL resummation. Only need for  $K^{(2)}$ !

In the code:

$$\alpha_s \rightarrow \alpha_s \cdot \left(1 + \alpha_s^2 K^{(2)}\right)$$

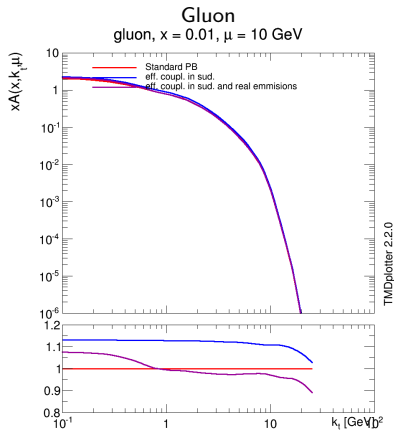
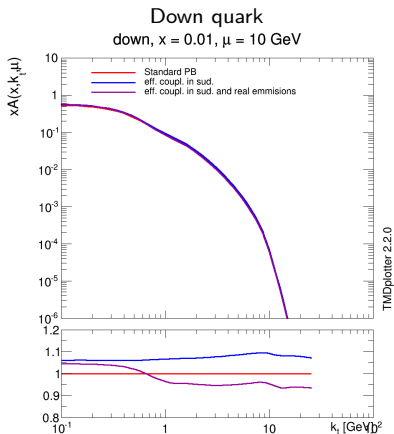
with

$$\begin{aligned} K^{(2)} = & C_A^2 \left( \frac{245}{24} - \frac{67}{9} \zeta_2 + \frac{11}{6} \zeta_3 + \frac{11}{5} \zeta_2^2 \right) + C_F N_f \left( -\frac{55}{24} + 2\zeta_3 \right) \\ & + C_A N_f \left( -\frac{209}{108} + \frac{10}{9} \zeta_2 - \frac{7}{3} \zeta_3 \right) - \frac{1}{27} N_f^2 + \frac{\pi\beta_0}{2} \left( C_A \left( \frac{808}{27} - 28\zeta_3 \right) - \frac{224}{54} N_f \right). \end{aligned}$$

Open question: what should  $N_f$  be? It depends on the evolution scale  $\mu'$ .

However:  $\alpha_s(q_t)$ !

# First numerical results: TMDs

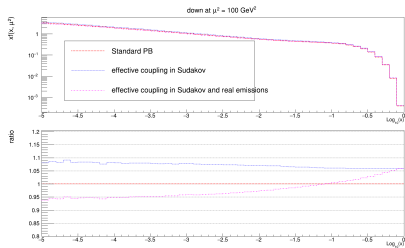


test: PB TMD

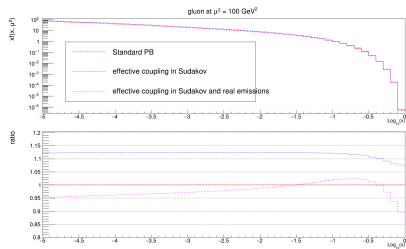
test1:  $\alpha_s^{eff}$  in Sudakov

test2:  $\alpha_s^{eff}$  in Sudakov and splitting functions

# First numerical results: iTMDs



Down quark



Gluon

# Number of active flavors $N_f$

- The number of active flavors  $N_f$  depends on a certain scale.
- Branching scale  $\mu'$  or the emitted transverse momentum  $q_T$

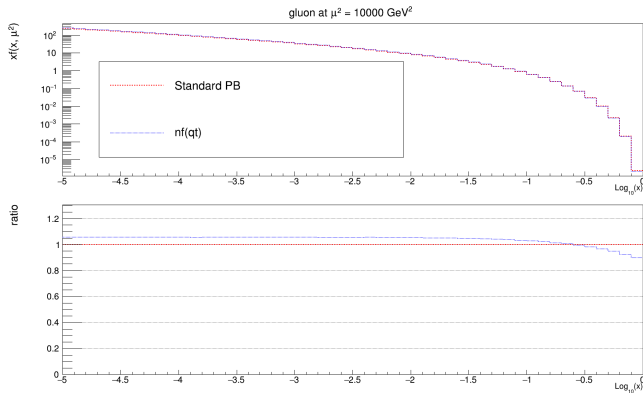
$N_f$  appears in the evolution in:

- Splitting function  $P_{ab}(\alpha_s, z, N_f)$
- $\alpha_s(N_f)$  (and later also  $K^{(2)}(N_f)$ )

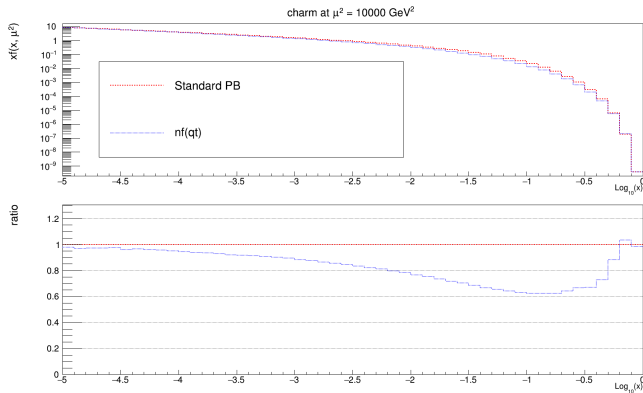
→ we investigated the numerical effect on (i)TMDs of varying the scale of  $N_f$  in the following scenarios, without implementation of the effective soft-gluon coupling:

- Standard evolution:  $P_{ab}(\alpha_s(q_T), N_f(\mu')), \alpha_s(N_f(q_T))$
- $q_T$  in all functions where  $N_f$  appears

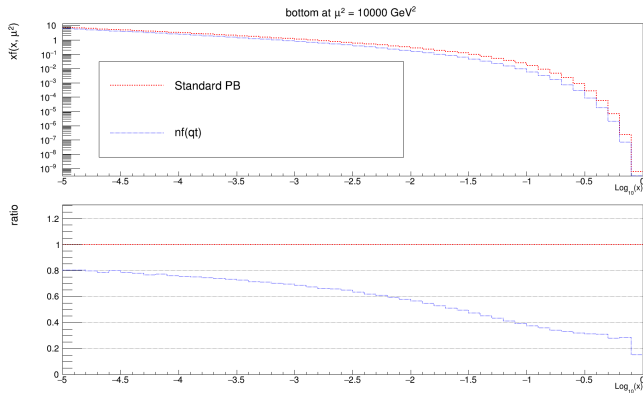
# Number of active flavors $N_f$ - gluon distribution



# Number of active flavors $N_f$ - charm distribution



# Number of active flavors $N_f$ - bottom distribution



Efforts have been put in the systematical comparison of the PB and CSS approaches to Sudakov resummation for DY  $p_T$  spectra.

- PB and CSS Sudakov form factors coincide at LL and NLL
- Differences at NNLL tracked down to **resummation scheme dependence** (single log) and **effective soft-gluon coupling** (double log)

Open issues and future steps:

- Number of light quarks  $N_f$  in  $K^{(2)}$  not the same as in calculation  $\alpha_s$
- Numerical comparison with CSS; e.g. generate DY  $p_T$  spectrum with MC@NLO+CASCADE3. For this, integrated TMDs are necessary.



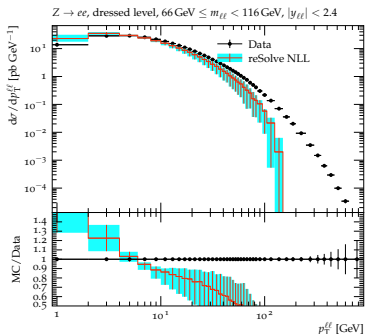
# Backup

# Inclusive Z boson $p_T$ spectrum @LHC using reSolve

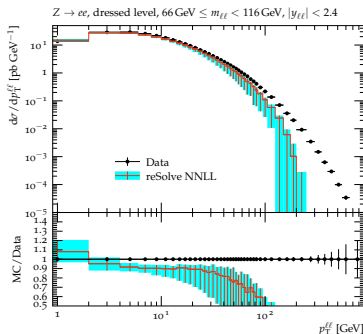
reSOLVE [Coradeschi, Cridge arXiv:1711.02083] provides a numerical implementation of CSS

- Resummation  $d\sigma^{(\text{res.})}/dp_T^2 dQ^2 dy$  up to NNLL
- No matching with finite Y-terms yet (no NLO for Z+0)

## Z boson $p_T$ spectrum at $\sqrt{s} = 8$ TeV



NLL prediction with scale uncertainties

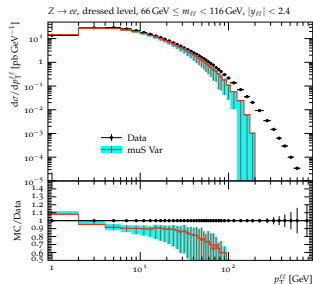


NNLL prediction with scale uncertainties

# Estimation of theoretical uncertainties

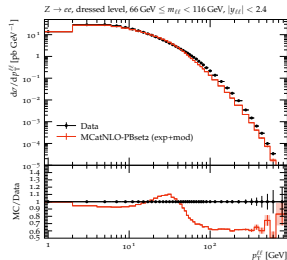
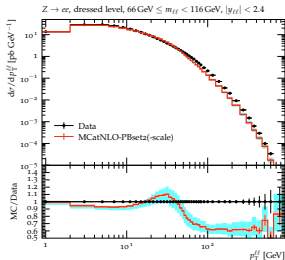
CSS:

- $\mu_S$  resummation/matching scale  $\longrightarrow$
- $\mu_R$  variation mostly influences small  $p_T$
- $\mu_F$  variation both at small and large  $p_T$
- 9-point scale variation
  - Vary  $\mu_R$  and  $\mu_F$  with factor 2 and  $1/2$  (9 combinations)
  - Constraint  $1/2 \leq \mu_R/\mu_F \leq 2$  (leaves 7 combinations)
  - Vary  $\mu_S$  factor 2 and  $1/2$  with central value of  $\mu_R, \mu_F$



PB:

- Scale variations:  $\mu_F, \mu_R$  (9-point)
- Matching scale not varied yet
- TMD variations included but small uncertainties in LHC region around  $M_Z$



Comparisons of theoretical uncertainty bands with different resummation approaches by LHC electroweak working group: <https://twiki.cern.ch/twiki/bin/view/LHCPhysics/EWWG1>

# Parameterization of non-perturbative physics

Gaussian smearing factor in reSOLVE for non-perturbative physics:

$$S_{NP} = \exp(-g_{NP}b^2)$$

Commonly  $g^{NP}$  [0.5 – 2.5]

In the PB method intrinsic  $k_t$ :

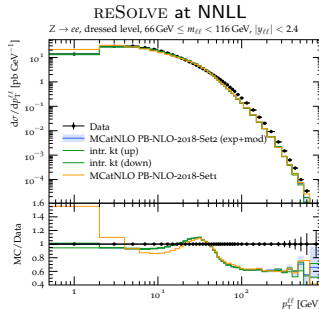
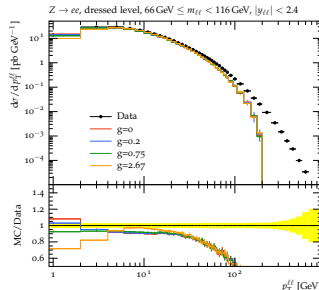
$$\tilde{A}_a(x, k_{t,0}, \mu_0) \sim f_a(x, \mu_0) e^{-\frac{k_t^2}{2\sigma^2}} \quad (\sigma \sim 350 \text{ MeV})$$

- subject to (perturbative) evolution!
- describe effects in a few GeV range

Width of PB Gaussian is small compared to the one used in reSolve and also compared to parton shower event generators.

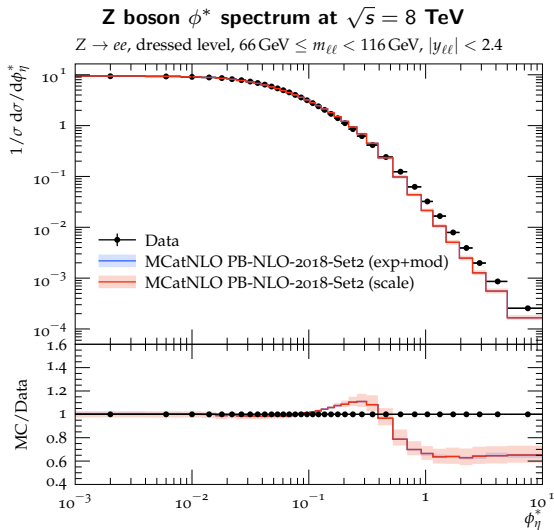
$$\int e^{-k_t^2/2\sigma^2} e^{ik_t b} dk_t \sim e^{-b^2\sigma^2/4}$$

$$\rightarrow \sigma \sim 350 \text{ MeV} \Leftrightarrow g_i^{NP} \sim 0.03$$



PB at NLO

# Z boson $\phi^*$ distribution with PB



[arXiv:1906.00919]

# Rewrite PB Sudakov

PB Sudakov:

$$\Delta_a^{(PB)}(\mu, \mu_0) = \exp \left\{ - \sum_b \int_{\mu_0^2}^{\mu^2} \frac{d\mu'^2}{\mu'^2} \int_0^{z_M} dz \, z \, P_{ba}^{(R)}(\alpha_s(a(z)\mu'), z) \right\}.$$

Real part of the splitting functions:

$$P_{ab}^{(R)}(\alpha_s, z) = K_{ab}(\alpha_s) \frac{1}{1-z} + R_{ab}(\alpha_s, z)$$

Virtual part of the splitting functions:

$$P_{ab}^{(V)}(\alpha_s, z) = \delta_{ab} \frac{k_a(\alpha_s)}{(1-z)_+} + \delta(1-z) \delta_{ab} d_a(\alpha_s)$$

Use:

- **angular ordering** condition:  $q_t = (1-z)\mu'$  and
- **virtual splitting functions**:  $P_{ab}^{(R)} = P_{ab} - P_{ab}^{(V)}$  and
- **momentum sum rule**:  $\sum_b \int_0^1 dz \, z \, P_{ab}(z, \mu'^2) = 0$

$$\Delta_a^{(PB)}(Q^2, q_0^2) \simeq \exp \left\{ - \int_{q_0^2}^{Q^2} \frac{dq_t^2}{q_t^2} \left[ \frac{1}{2} \ln \left( \frac{\mu^2}{q_t^2} \right) k_a(\alpha_s(q_t^2)) - d_a(\alpha_s(q_t^2)) \right] \right\}$$

[de Florian, Grazzini; Phys.Rev.Lett. 85 (2000) 4678-4681]  
[Hautmann et al.; JHEP 01 (2018) 070]

- LL':

$$A_q^{(1)} = C_F,$$

$$k_q^{(0)} = 2C_F$$

- NLL':

$$A_q^{(2)} = \frac{1}{2} C_F C_A \left( \frac{67}{18} - \frac{\pi^2}{6} \right) - \frac{5}{18} N_f C_F$$

$$B_q^{(1)} = -\frac{3}{2} C_F$$

$$k_q^{(1)} = 2C_F C_A \left( \frac{67}{18} - \frac{\pi^2}{6} \right) - \frac{10}{9} N_f C_F$$

$$d_q^{(0)} = \frac{3}{2} C_F$$

# Scale variations reSolve

