Associated production of a heavy quark pair and a heavy boson in NNLO QCD

Luca Buonocore

in collaboration with S. Devoto, M. Grazzini, S. Kallweit, J. Mazzitelli, L. Rottoli and C. Savoini

[Phys.Rev.D 107 (2023) 7, 074032, arXiv:2212.04954]
[Phys.Rev.Lett. 131 (2023) 23, 231901, arXiv:2306.16311]

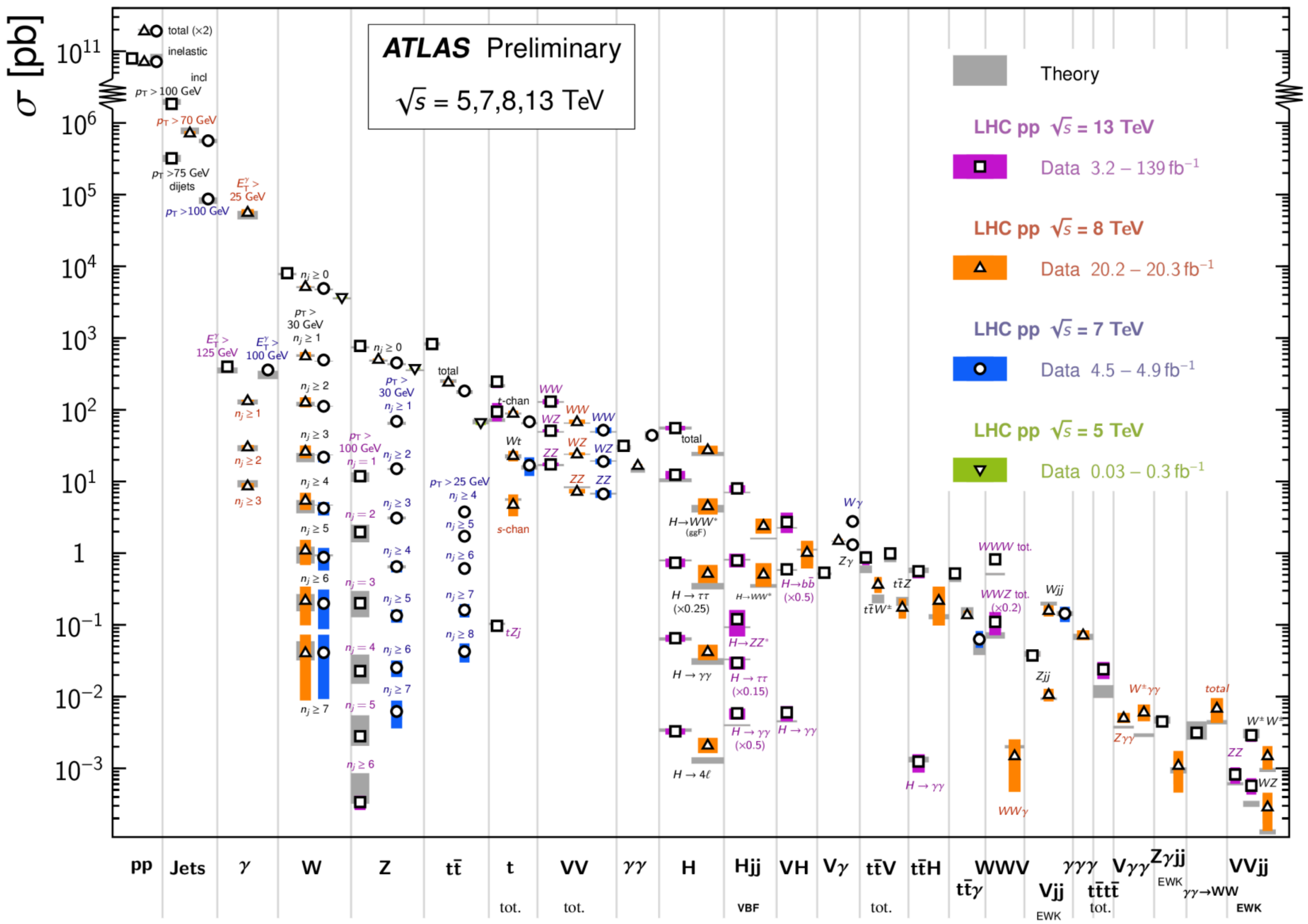
THEORY SEMINAR

Nikhef - 15 February 2024

Introduction

Precision era @ LHC

- astonishing measurements of many SM processes spanning across several order of magnitudes
- so far, agreement with accurate theoretical predictions
- great opportunity for advancing our (experimental and theory) understanding and possibly discover hints of NP



[ATL-PHYS-PUB-2022-009, February 2022]

Introduction

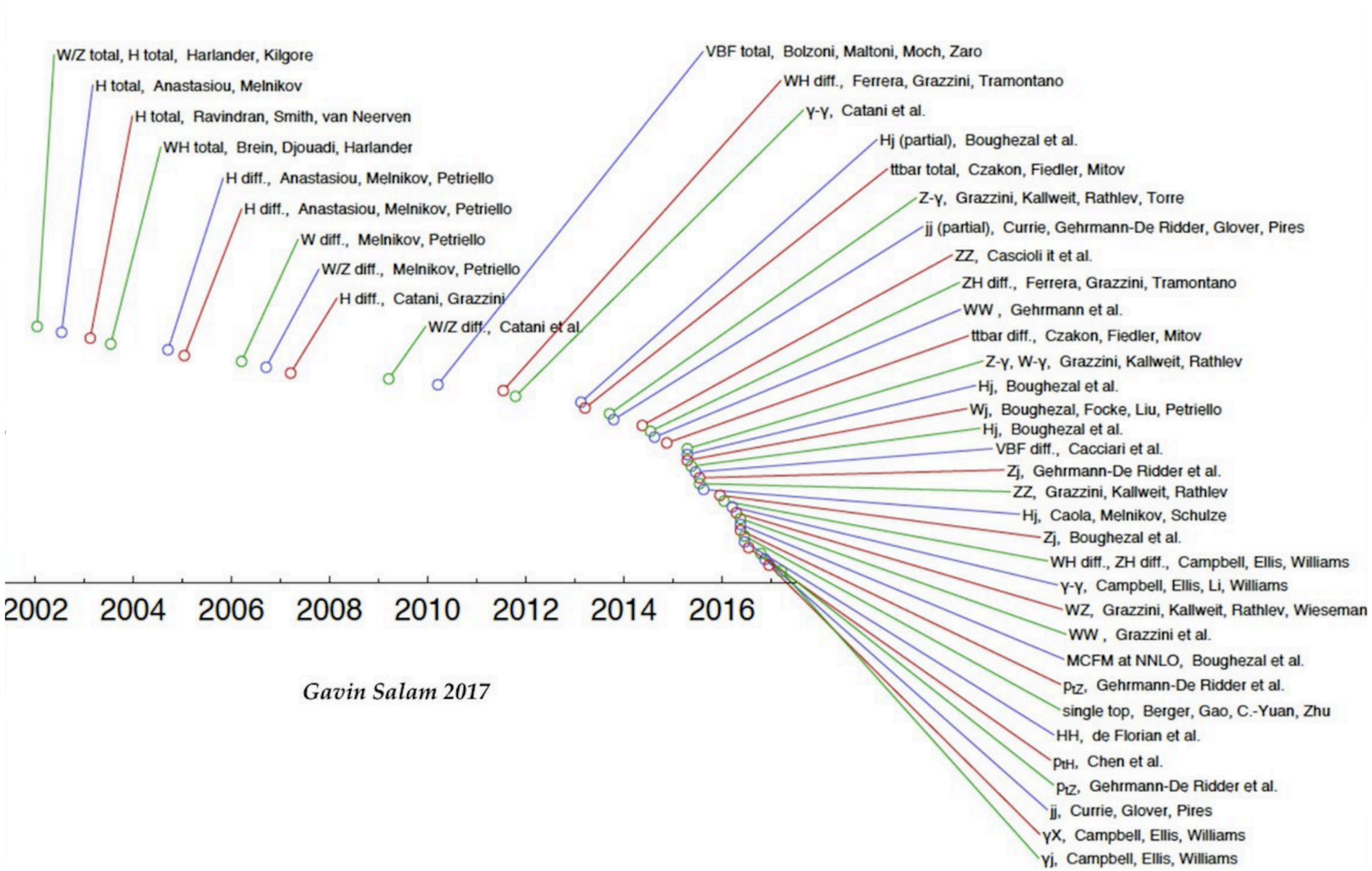
NNLO QCD calculations: challenging but important!

Status of NNLO QCD @ LHC

- great progress in techniques for amplitude calculation and subtraction methods
- available for many 2 → 2 processes

Current frontier

- 2 → 3 processes: jjj, Wjj, Zjj, γjj, Wbb (massless b), ttH …
- 2 → 2 with many scales



Gavin Salam 2017

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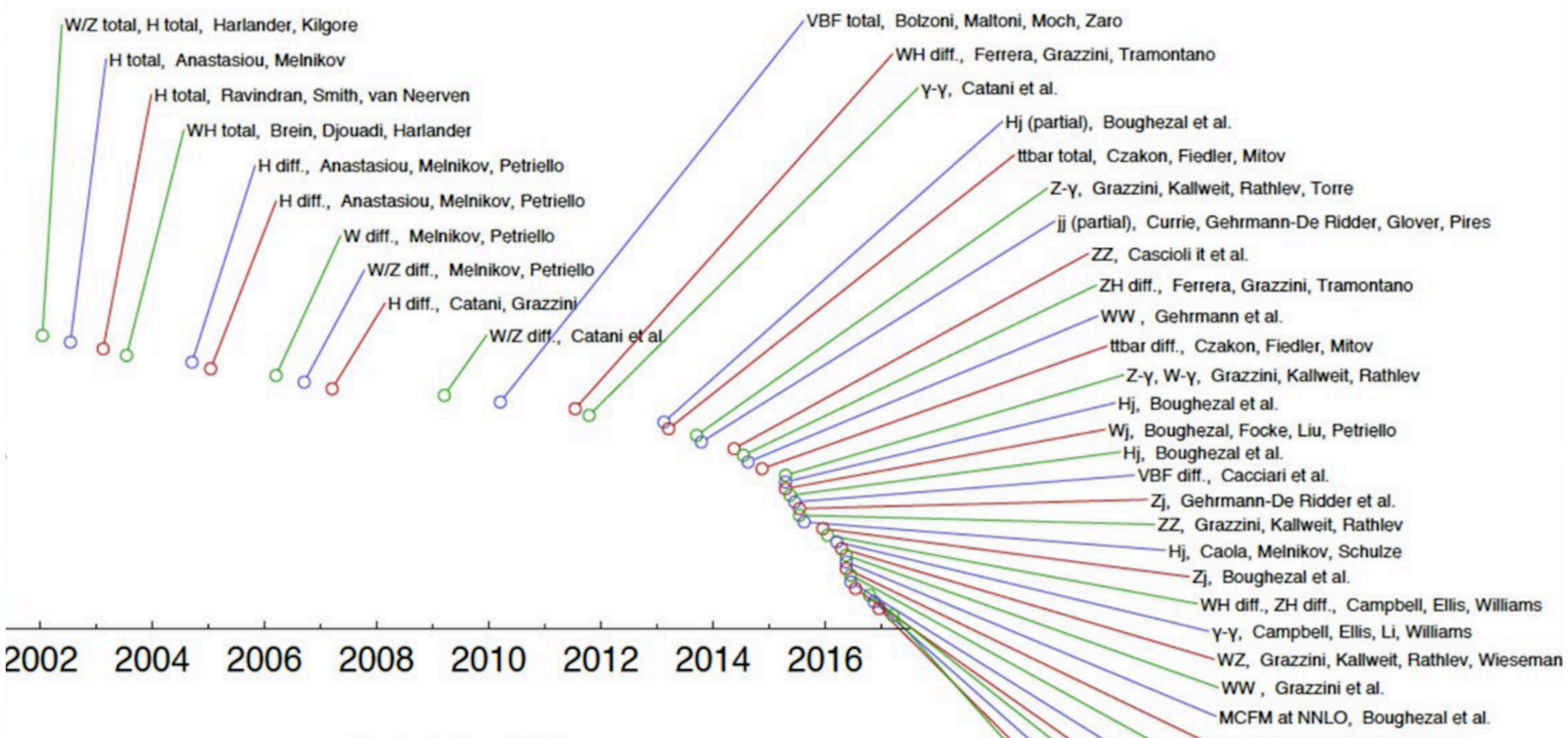

Gavin Salam 2017

This TALK: $Q\bar{Q}W$

$2 \to 3$ processes with masses

Outline

- Motivations
- Methodology I: slicing formalism
- Methodology II: two-loop virtual amplitude
- Phenomenological results
- Conclusions

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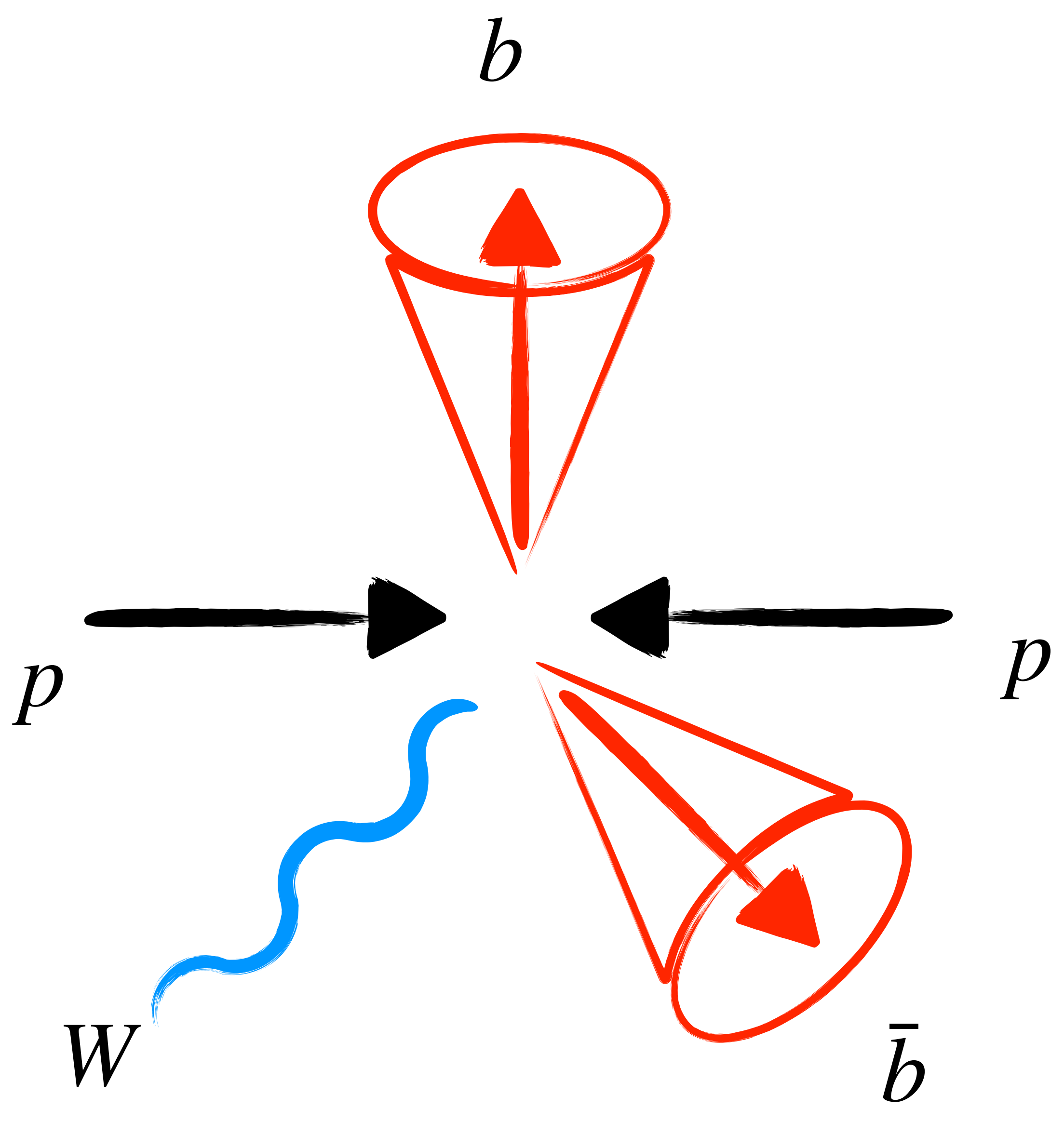
$b\bar{b}W$



Motivations

W+1bj and W+2bj interesting signatures

- tests of QCD at LHC
- background to $WH(H \to b\bar{b})$ and single top $\bar{b}t(t \to Wb)$
- **bottom quarks modelling:** massive effects, bottom in the PDF, flavour tagging

Interesting things happen going to higher order!

from VH(->bb) analysis [CMS:arXiv:1808.08242]

Large normalisation corrections with respect to SM simulation

Postfit normalisation corrections

Process	$Z(\nu\nu)H$	$W(\ell\nu)H$	$Z(\ell\ell)H$ low-p_T	$Z(\ell\ell)H$ high-p_T
$W + udscg$	1.04 ± 0.07	1.04 ± 0.07	–	–
$W + b$	2.09 ± 0.16	2.09 ± 0.16	–	–
$W + b\bar{b}$	1.74 ± 0.21	1.74 ± 0.21	–	–
$Z + udscg$	0.95 ± 0.09	–	0.89 ± 0.06	0.81 ± 0.05
$Z + b$	1.02 ± 0.17	–	0.94 ± 0.12	1.17 ± 0.10
$Z + b\bar{b}$	1.20 ± 0.11	–	0.81 ± 0.07	0.88 ± 0.08
$t\bar{t}$	0.99 ± 0.07	0.93 ± 0.07	0.89 ± 0.07	0.91 ± 0.07

State of the art

NLO corrections (massless bottom quarks)

[Ellis, Veseli, 1999]

NLO corrections (massive bottom quarks)

[Febres Cordero, Reina, Wackeroth, 2006, 2009]

NLO corrections (4FS+5FS)

[Campbell, Ellis, Febres Cordero, Maltoni, Reina, Wackeroth, Willenbrock, 2009] [Campbell, Caola, Febres Cordero, Reina, Wackeroth,2011]

NLO+PS

[Oleari, Reina,2011] [Frederix, Frixione, Hirschi, Maltoni, Pittau, Torrielli, 2011]

POWHEG+MiNLO

[Luisoni, Oleari, Tramontano, 2015]

Wbb + up to 3 jets

[Anger, Febres Cordero, Ita, Sotnikov, 2018]

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Analytical Two-loop W+4 partons amplitude in Leading Colour Approximation (LCA)

[Badger, Hartanto, Zoia, 2021] [Abreu, Febres Cordero, Ita, Klinkert, Page, Sotnikov, 2021]

NNLO corrections (massless bottom quarks)

[Hartanto, Poncelet, Popescu, Zoia, 2022]

First NNLO QCD calculation for massless bottom quarks!

$Wb\bar{b}$ @ NNLO with massless b quarks

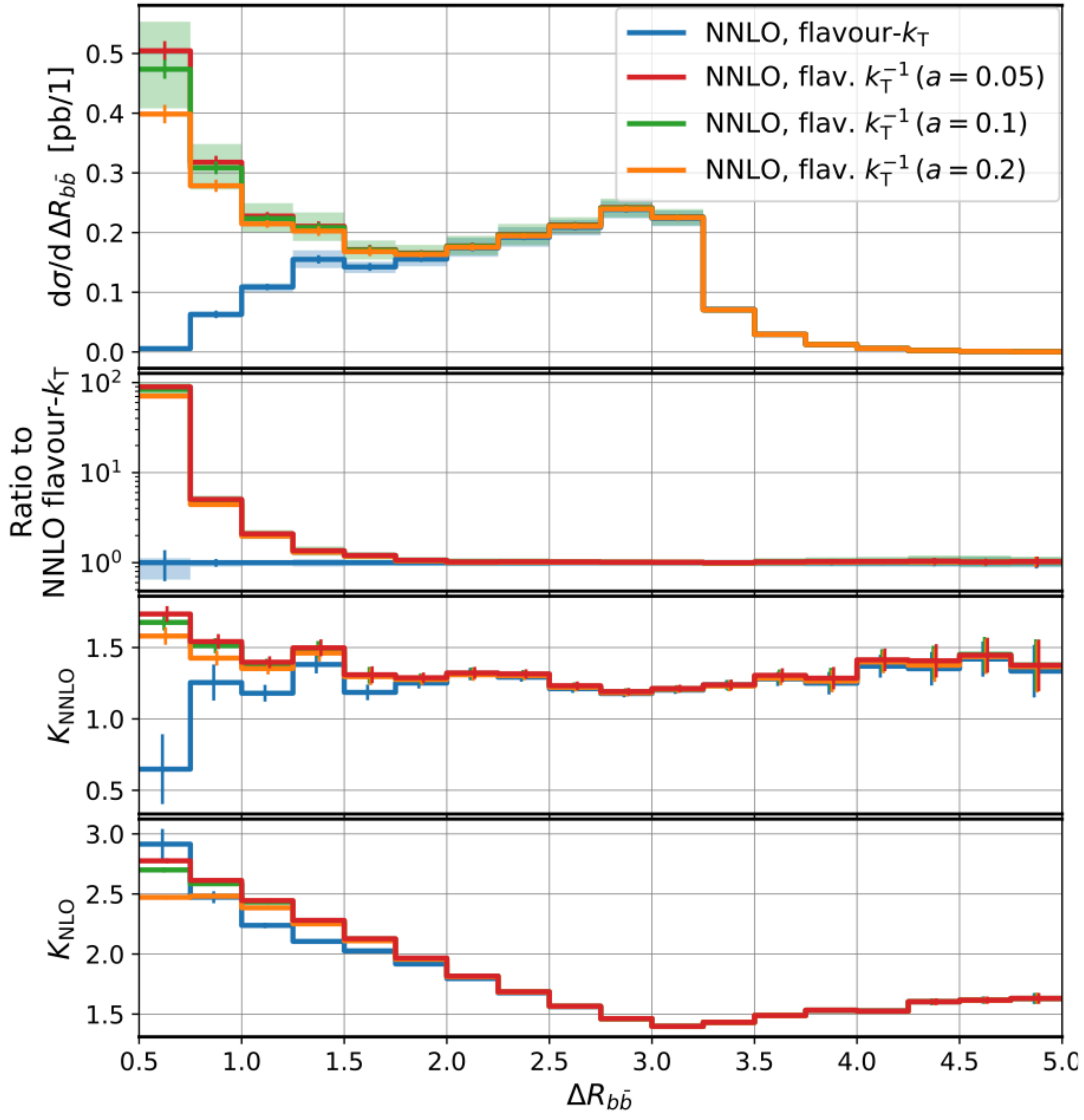
[Hartanto, Poncelet, Popescu, Zoia, 2022]

First computation for Wbb @ NNLO with massless b quarks recently performed

But, massless calculations are subject to ambiguities related to flavor tagging

Jet algorithm	σ_{NNLO} [fb]	K_{NNLO}
flavour-k_{T}	$445(5)^{+6.7\%}_{-7.0\%}$	1.23
flavour anti-k_{T} $(a = 0.05)$	$690(7)^{+10.9\%}_{-9.7\%}$	1.38
flavour anti-k_{T} $(a = 0.1)$	$677(7)^{+10.4\%}_{-9.4\%}$	1.36
flavour anti-k_{T} $(a = 0.2)$	$647(7)^{+9.5\%}_{-8.9\%}$	1.33

$\mathcal{O}(50\%)$ difference when using flavour k_T algorithm



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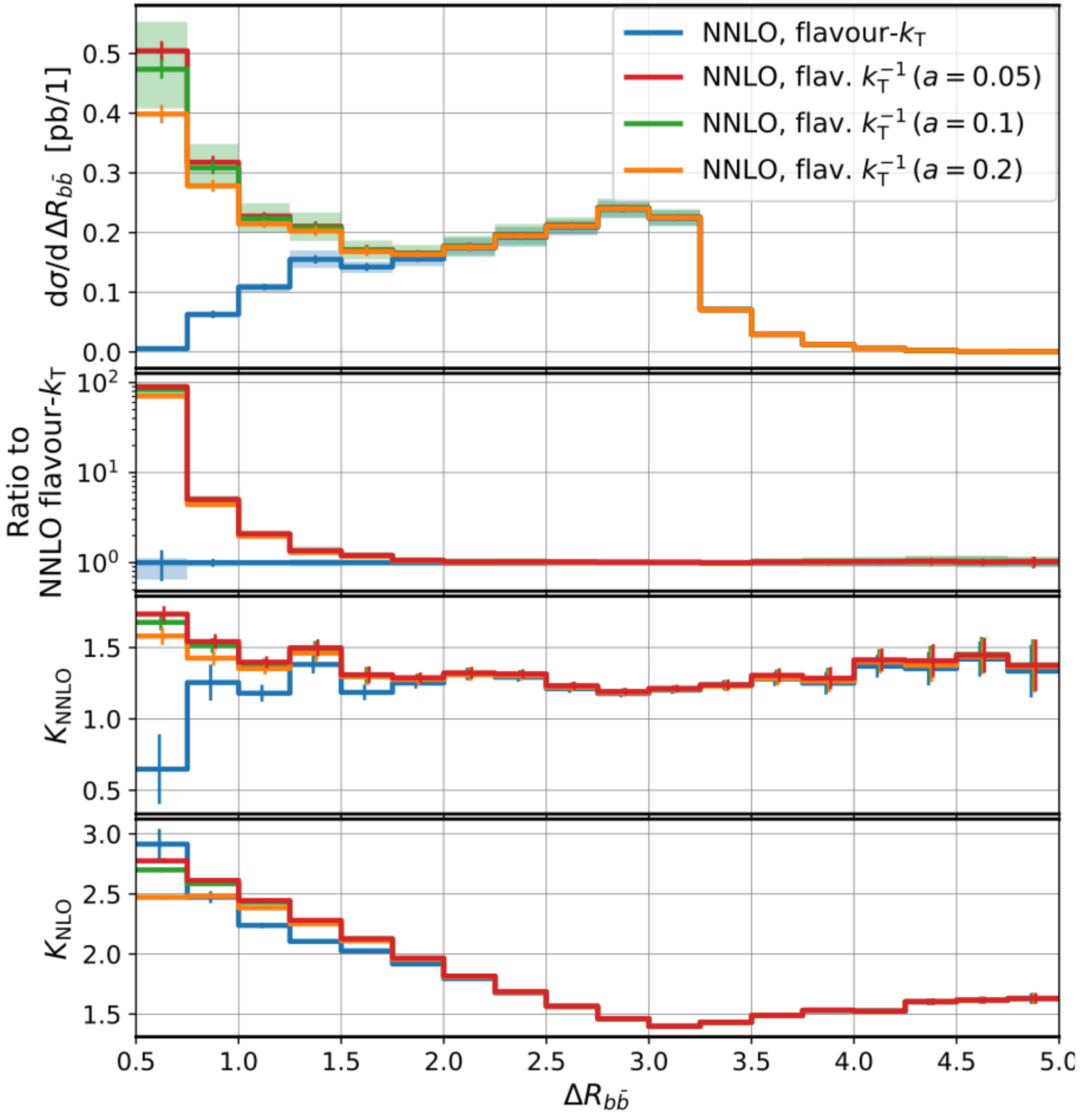
Uncertainties relate to the ambiguities reduced when using flavour-aware anti-k_T



[Czakon, Mitov, Poncelet, 2022]

Infrared safety and flavour tagging

Jet clustering algorithms consist in a sequence of two-to-one recombination steps. They are then completely defined once the binary distance d_{ij} and the beam distance d_{iB} are given. For the family of k_T algorithms

$$d_{ij} = \min\left(k_{T,i}^{2\alpha}, k_{T,j}^{2\alpha}\right)\frac{R_{ij}^2}{R^2}, \quad d_{iB} = k_{T,i}^{2\alpha} \qquad R_{ij}^2 = (y_i - y_j)^2 + (\phi_i - \phi_j)^2$$

For parton level calculation (fixed order), **infrared safety** is a crucial requirement

IRC observables, qualitatively

An observable is **infrared and collinear (IRC) safe** if its value is not altered abruptly by multiple soft and collinear emissions

An IRC observable is **inclusive** in the sense that it does not spoil the cancellation of singularities between real and virtual contributions

Observables defined at the parton level for massless parton in the final state are usually IRC unsafe, must be replaced by suitably defined jet (or hadrons in the non perturbative regime)

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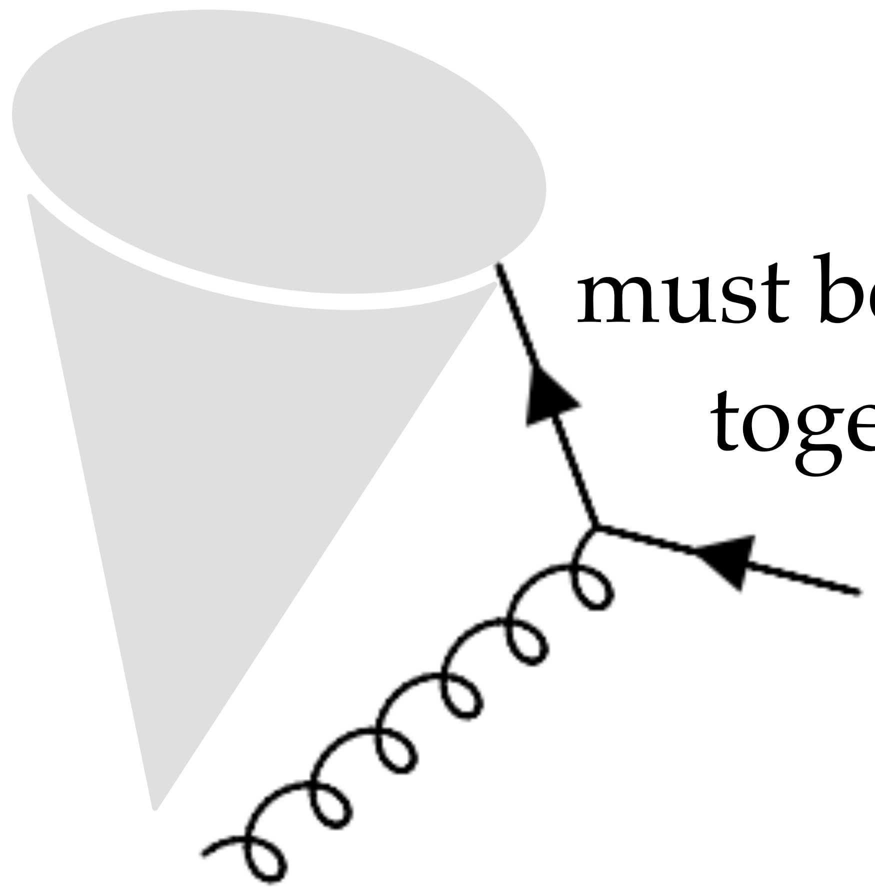
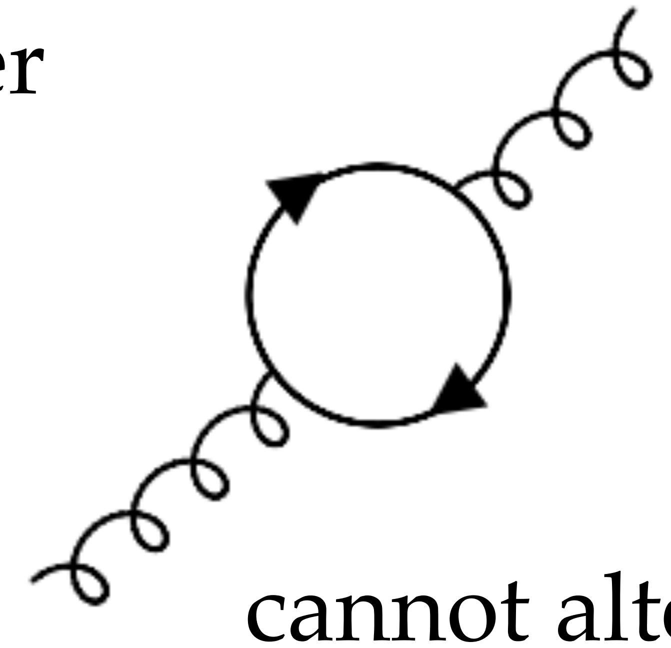
For observable sensitive to the flavour assignment, **infrared safety can be an issue**, usually associated **to gluon splitting to quarks in the double soft limit** (the problem starts at NNLO)





this may lead to a flavour configuration different from the corresponding virtual one, spoiling KLN cancellation

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To ensure infrared safety, two necessary conditions must hold for a wide-angle double-soft limit of two opposite flavoured parton i and j **[Czakon, Mitov, Poncelet, 2022]**

1. d_{ij} vanishes for every R_{ij}

2. d_{ij} vanishes faster than the distance of either i or j to the remaining (hard) pseudojets

Flavour aware jet algorithms: flavour k_T

[Banfi, Salam, Zanderighi, 2006]

Theoretically sounded but problematic for data/theory comparison

- experimentally, jet reconstruction and flavour assignment are performed **at the particle level** (not at the parton level)
- **anti-k_T is de-facto the jet algorithm** used in all analysed for its properties

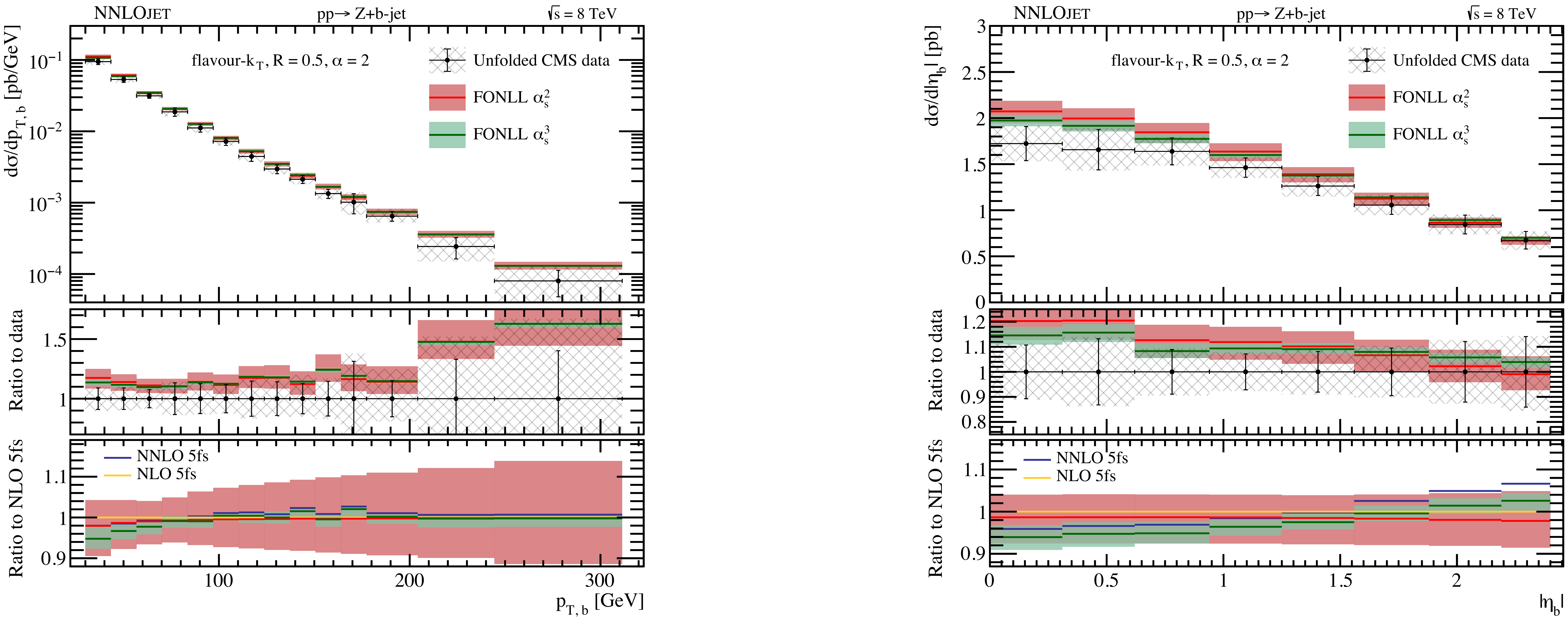
Flavour aware jet algorithms: flavour k_T

[Banfi, Salam, Zanderighi, 2006]

Theoretically sounded but problematic for data/theory comparison

- requires to unfold the experimental data to the theory calculation performed with the flavour k_T algorithm
- **unfolding corrections** can be **sizeable:** $\sim 12\,\%$ Z + b jet as estimated at NLO+PS accuracy

[Gauld, Gehrmann–De Ridder, Glover, Huss, Majer, 2020]



Flavour aware jet algorithms: flavour anti-k_T

[Czakon, Mitov, Poncelet, 2022]

Standard anti-k_T algorithm

$$d_{ij} = \min\left(k_{T,i}^{-2}, k_{T,j}^{-2}\right) R_{ij}^2, \quad d_{iB} = k_{T,i}^{-2}$$

does not vanish in the double soft limit

Flavour anti-k_T algorithm

$$d_{ij}^{(F)} = d_{ij} \times \begin{cases} \mathcal{S}_{ij}, & \text{if both } i \text{ and } j \text{ have non-zero flavour of opposite sign} \\ 1, & \text{otherwise} \end{cases}$$

$$\mathcal{S}_{ij} = 1 - \theta(1-\kappa)\cos\left(\frac{\pi}{2}\kappa\right), \qquad \kappa = \frac{1}{a}\frac{k_{T,i}^2 + k_{T,j}^2}{2k_{T,max}^2}$$

$$\mathcal{S}_{ij} \sim E^4 \implies d_{ij}^{(F)} \sim E^2$$

the suppression factor overcompensates the divergent behavior of d_{ij} in the double soft limit

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The parameter a controls the turning on of the suppression factor: in the limit $a \to 0$, the standard anti-k_T algorithm is recovered. The best choice of the parameter a is taken from comparisons performed at NLO+PS (aiming at minimizing unfolding)

Flavour-dependent metric still needs some (possibly small) unfolding

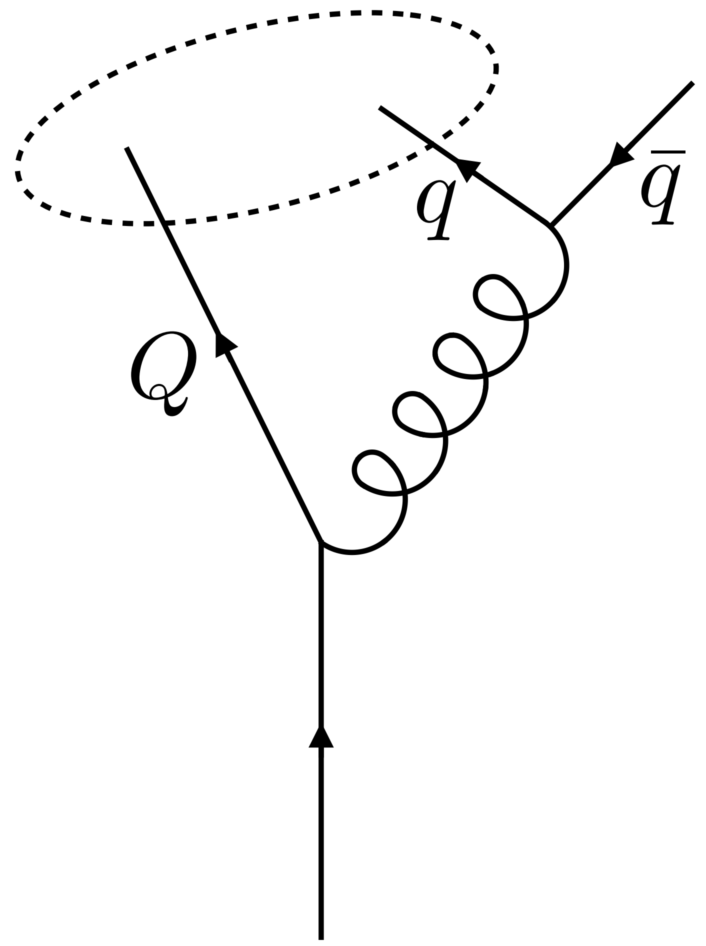
Flavour aware jet algorithms: new ideas

Renewed interest in flavor tagging (just some examples ...)

Use **Soft Drop** to remove soft quarks

No unfolding needed

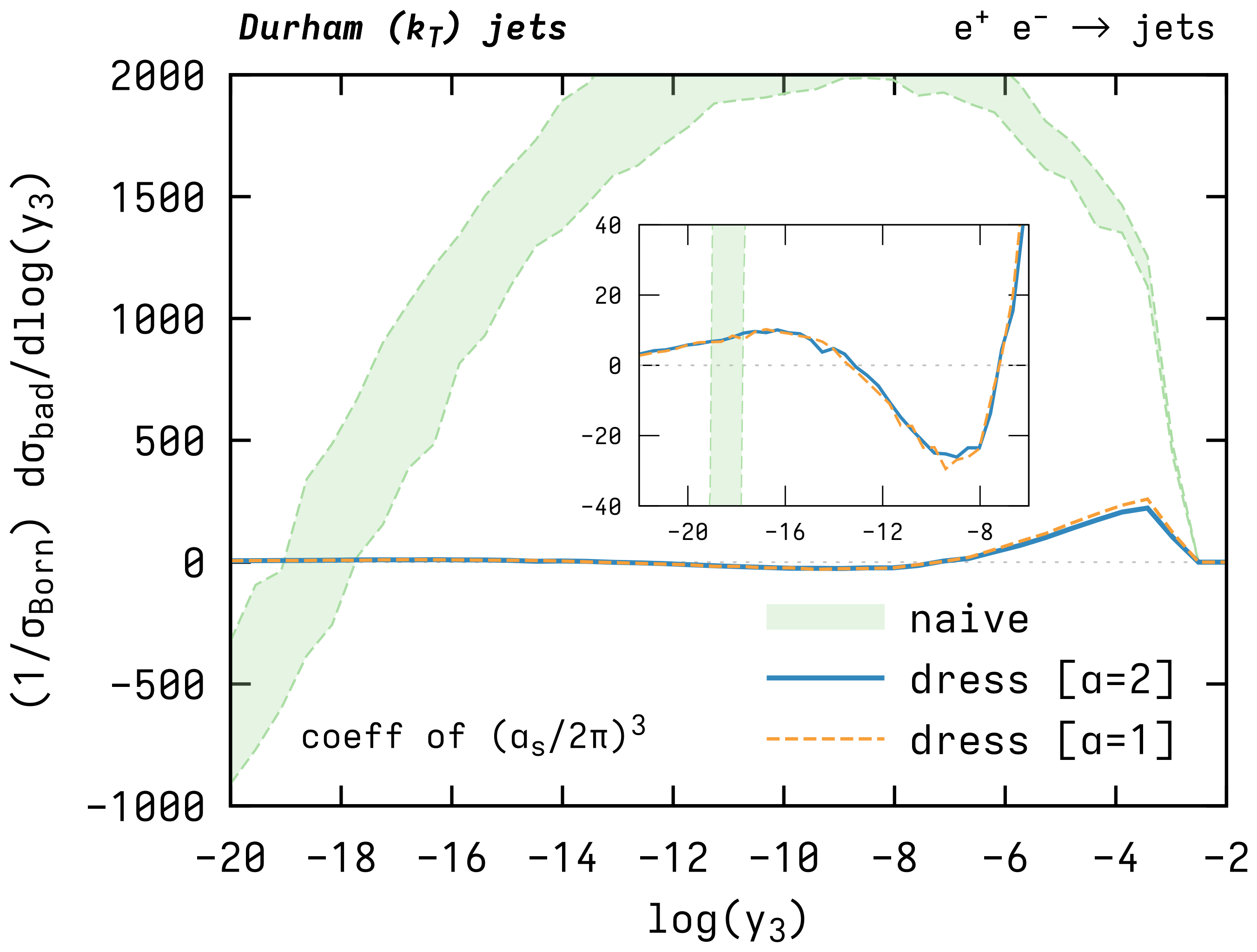
Requires reclustering with JADE (issue with IRC safety beyond NNLO)



[Caletti, Larkoski, Marzani, Reichelt, 2022]

Assign a **flavour dressing** to jets reconstructed with any IRC flavour-blind jet algorithms

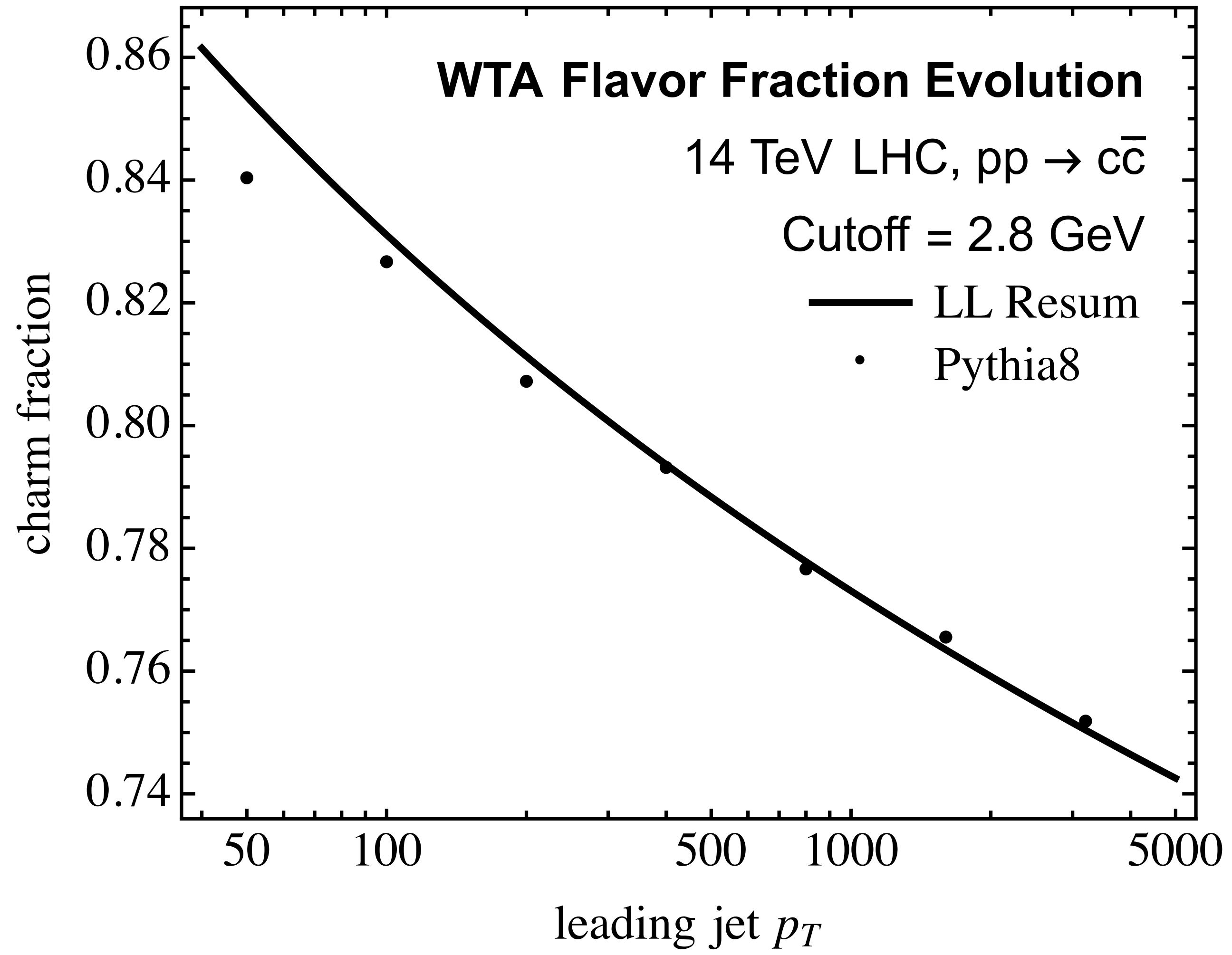
Requires flavour information of many particles in the event



[Gauld, Huss, Stagnitto, 2022]

Recluster using the flavour aware **Winner-Take-All** (WTA) recombination scheme (**soft-safe**)

Requires fully perturbative WTA flavour fragmentation function (for **collinear safety**)



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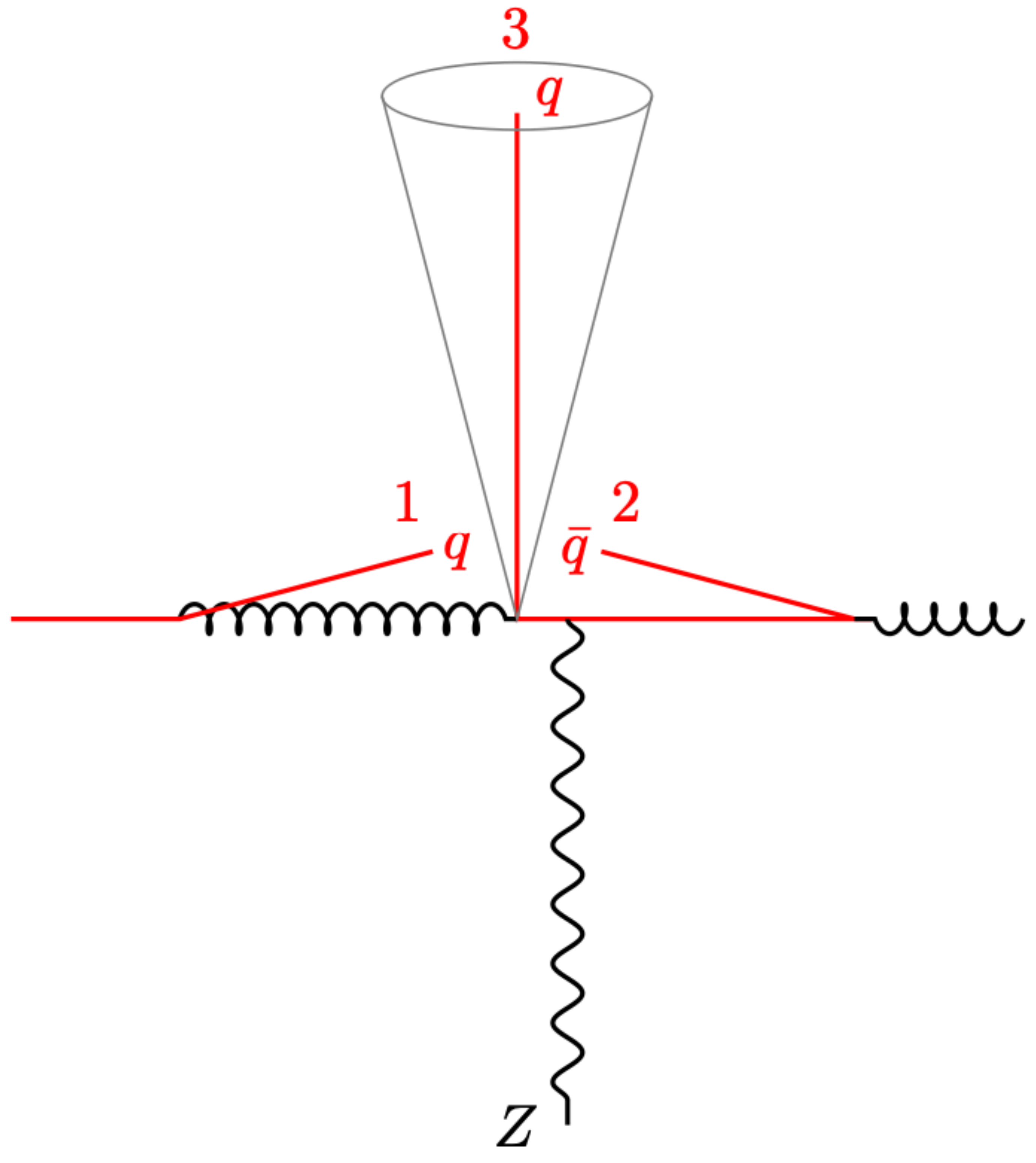
Flavour aware jet algorithms: new ideas and IRC safety

Testing IRC safety to all orders in perturbation theory is a highly non-trivial task

New proposal for a flavour-aware jet-clustering algorithm IRC safe up to $\mathcal{O}(\alpha_S^6)$, thanks to the development of a dedicated **testing framework**

[Caola, Grabarczyk, Hutt, Salam, Scyboz, Thaler 2023]

Example of IRC issue in flavour anti k_T



Configuration with two collinear initial-state emissions

Expectation: the algorithm should assign particle 1 and particle 2 to the beams leaving untouched the project 3

However, given the definition of distance

$$d_{ij}^{(F)} = d_{ij} \times \begin{cases} \mathcal{S}_{ij}, & \text{if both } i \text{ and } j \text{ have non-zero flavour of opposite sign} \\ 1, & \text{otherwise} \end{cases}$$

$$\mathcal{S}_{ij} = 1 - \theta(1-\kappa)\cos\left(\frac{\pi}{2}\kappa\right), \qquad \kappa = \frac{1}{a}\frac{k_{T,i}^2 + k_{T,j}^2}{2k_{T,max}^2}$$

particle 1 and particle 2 cluster together!

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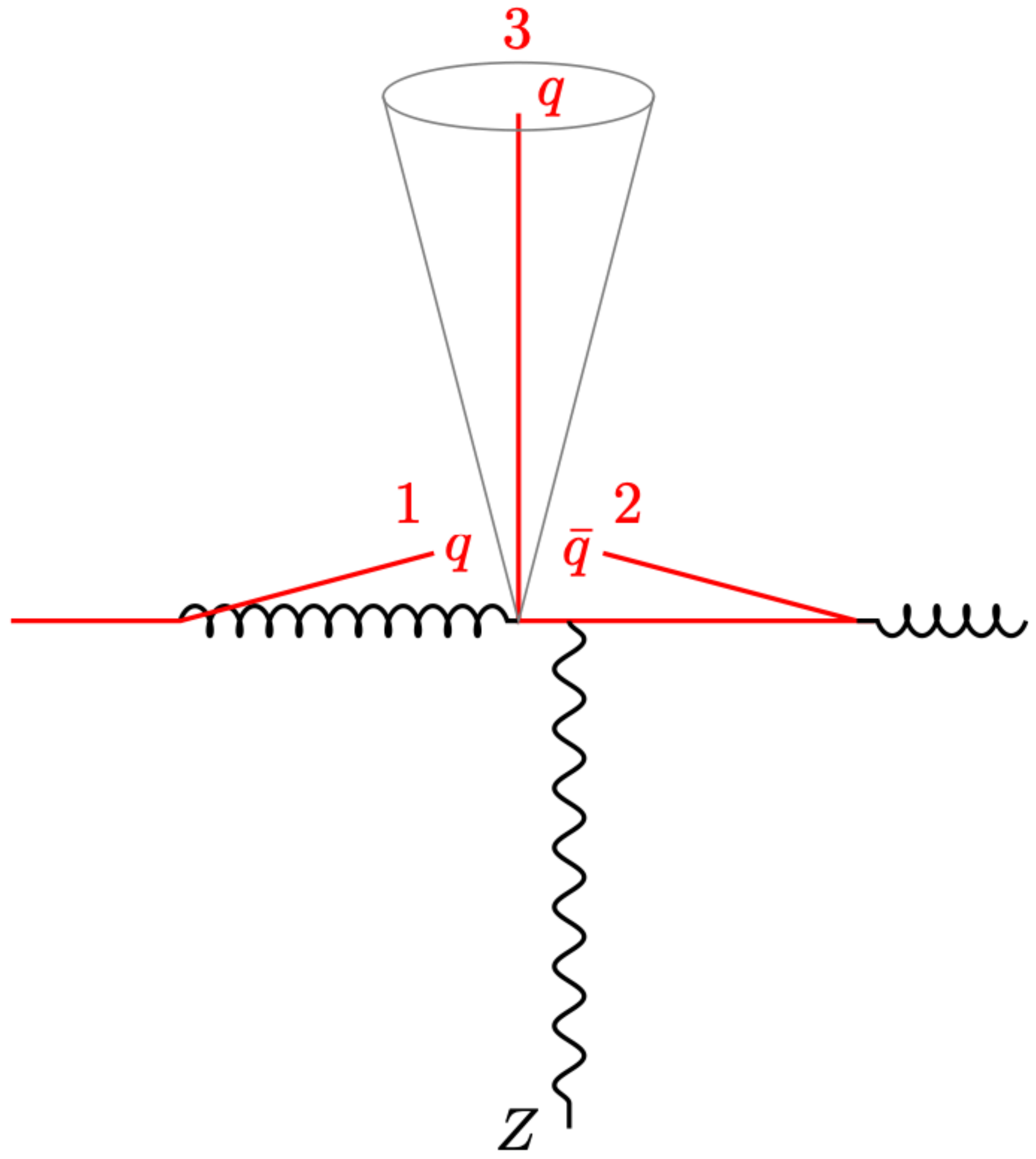


Configuration with two collinear initial-state emissions

Expectation: the algorithm should assign particle 1 and particle 2 to the beams leaving untouched the project 3

Flavourless protojet (12) can be, then, clustered with protojet 3, changing substantially its momentum -> IRC unsafe!

$$R \sim \alpha_S^2 \int_{\Lambda_{IR}} \frac{dk_{T1}}{k_{T1}} \int_{\Lambda_{IR}} \frac{dk_{T2}}{k_{T2}} \approx \alpha_S^2 \ln^2 \Lambda_{IR}$$

Flavour aware jet algorithms: massive calculation

Massive bottom quarks

- quark mass is the physical IR regulator: physical suppression in the double-soft limit
- No requirement for flavour-aware jet algorithms: any **flavour-blind algorithm** can be used, in particular **anti** k_T

Direct comparison with experimental data possible
(unfolding corrections limited to non-perturbative modelling and hadronisation)

Caveat

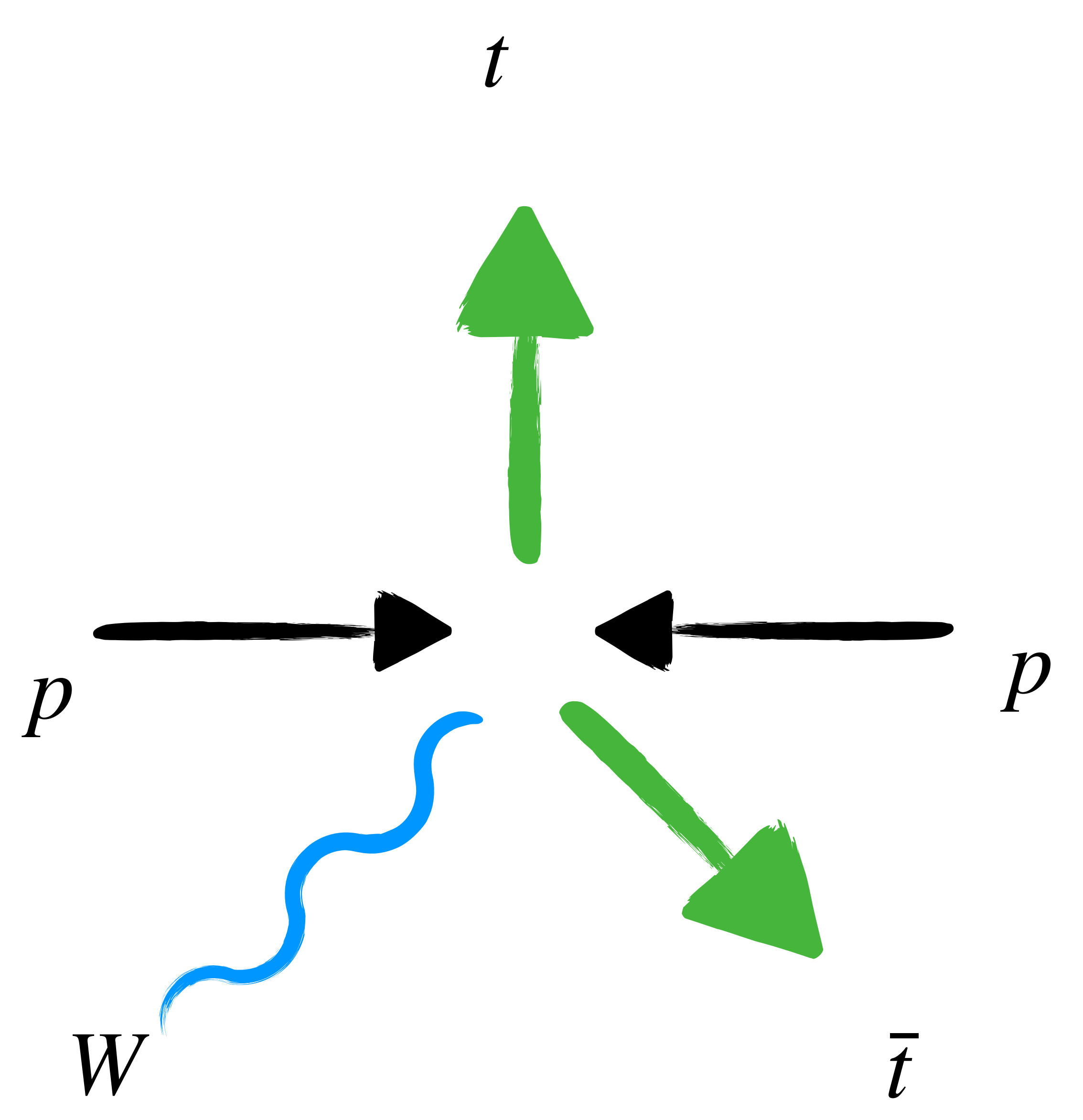
- left over IR sensitivity in the form of logarithms of the heavy quark mass at each order in perturbative theory
- Calculation with massive quarks is challenging

$$\alpha_S^2 \ln \frac{p_{T,jet}}{m_Q}$$

Outline

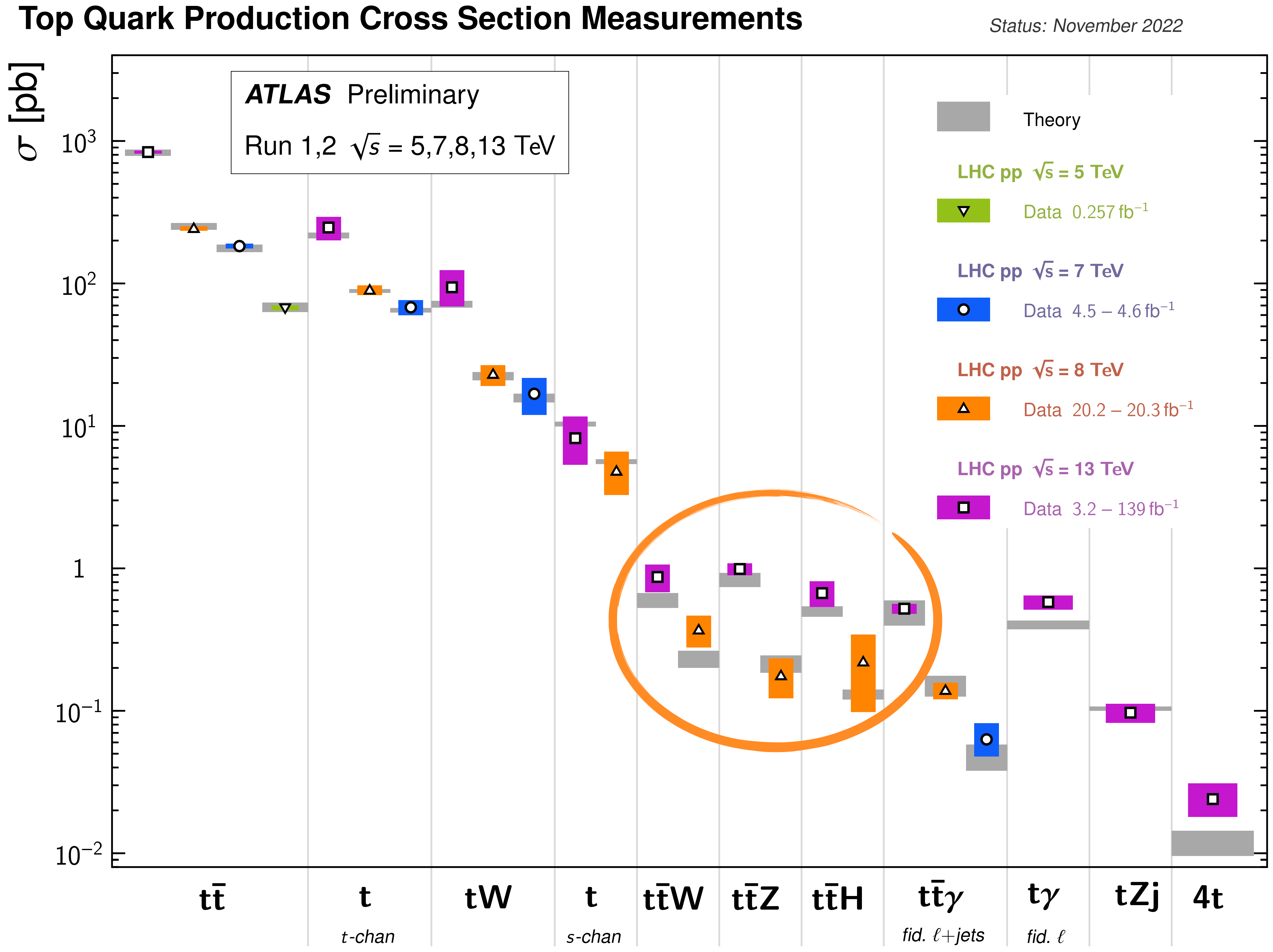
- WQQ: motivations
- Methodology: infrared subtraction and two-loop virtual amplitude
- Phenomenological results
- Conclusions

$t\bar{t}W$ (stable tops)



Introduction

The production of a top-quark pair together with a vector or Higgs boson is among **the most massive SM signatures** at hadron colliders



Small cross sections, but already observed and **measured with** $10 - 20\,\%$ **uncertainties**

Crucial to characterise the top-quark interactions, in particular with the Higgs boson

Introduction

Among the other $t\bar{t}X$ processes, the $t\bar{t}W$ process is **rather peculiar**

- Complex final-state signature characterised by two b-jets and three W bosons: **irreducible SM source of same sign dilepton pairs**

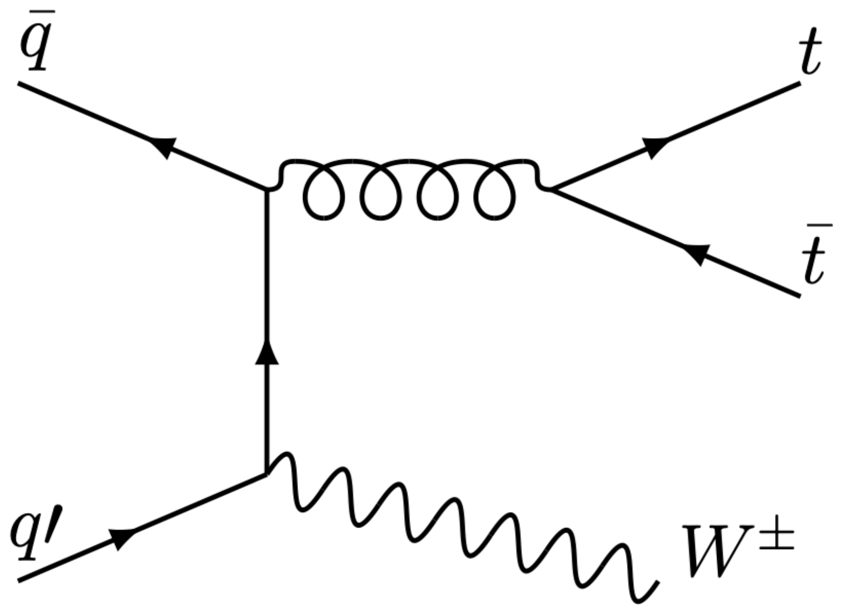
→ Relevant for BSM searches in **multi-lepton signature**

- It represents a **relevant background** also for SM processes like $t\bar{t}H$ and $t\bar{t}t\bar{t}$ production

Introduction

Among the other $t\bar{t}X$ processes, the $t\bar{t}W$ process is **rather peculiar**

- The W boson can only be emitted off an initial-state light quark: **no gluon fusion channel at LO**



Different pattern of radiative corrections

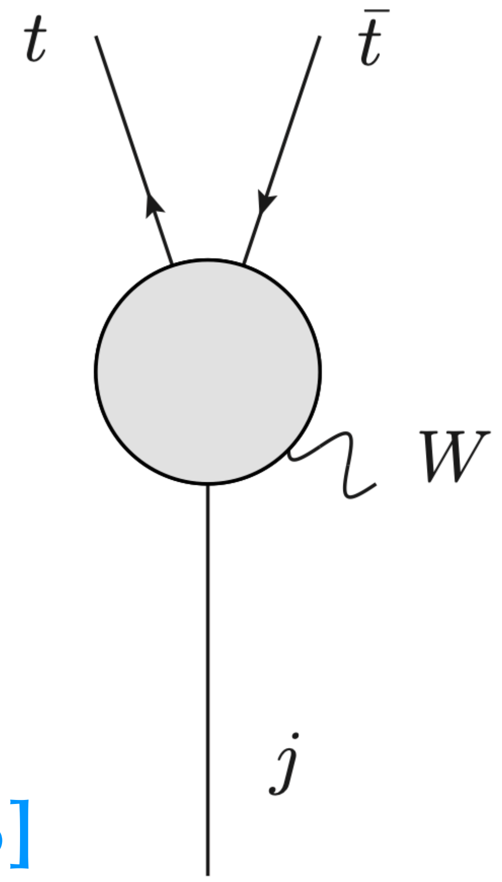
$\alpha_S^2\alpha$ LO QCD | ~~$\alpha_S\alpha^2$~~ | α^3

$\alpha_S^3\alpha$ NLO QCD | $\alpha_S^2\alpha^2$ | $\alpha_S\alpha^3$ | α^4

Large NLO QCD corrections: $\mathcal{O}(50\%)$
Giant K-factor in the region of high transverse momenta of the top-quark pair, which recoils against a hard jet while the W boson is relatively soft

quark-gluon channel opening

[Maltoni, Pagani, Tsinikos, 2015]



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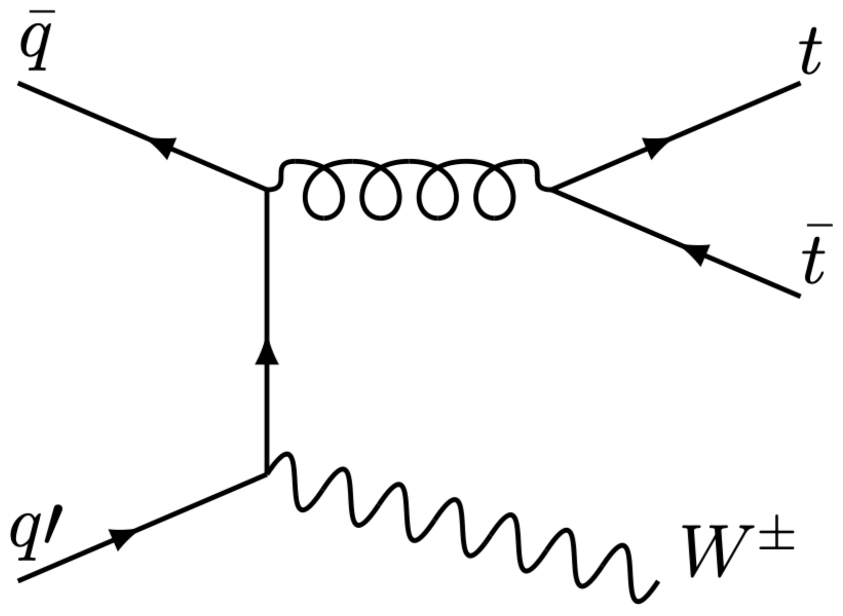


Different pattern of radiative corrections

$\alpha_S^2\alpha$
LO QCD

~~$\alpha_S\alpha^2$~~

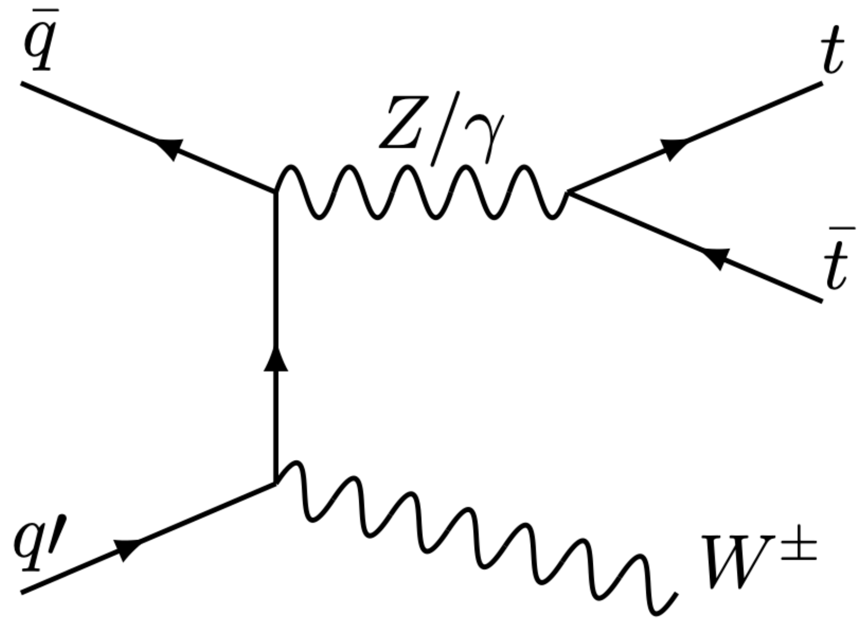
α^3

$\alpha_S^3\alpha$
NLO QCD

$\alpha_S^2\alpha^2$
NLO EW

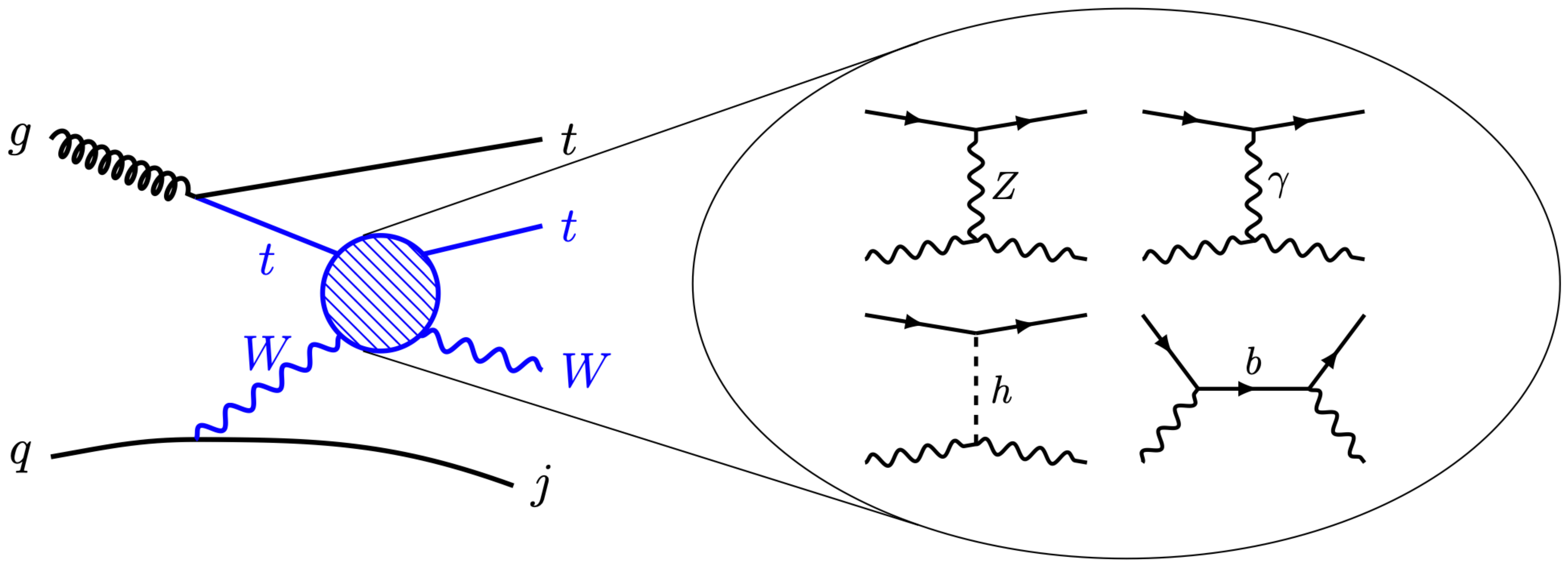
$\alpha_S\alpha^3$

α^4



Subleading EW

[Frederix, Pagani, Zaro, 2017]



Large **positive** subleading EW $\mathcal{O}(+10\%)$ (at the LHC) which partially cancels against the **negative** NLO EW $\mathcal{O}(-5\%)$
Dominated by configurations involving the $tW \to tW$ scattering process and enhanced by the gluon luminosity

State of the art: theory

NLO QCD corrections

[Badger, Campbell, Ellis, 2010] [Campbell, Ellis, 2012]

NLO QCD + EW corrections (on-shell top quarks and *W*)

[Frixione, Hirschi, Pagani, Shao, Zaro, 2015] [Frederix, Pagani, Zaro, 2017]

inclusion of soft gluon resummation at NNLL

[Li, Li, Li, 2014] [Broggio, Ferroglia, Ossola, Pecjak, 2016] [Kulesza, Motyka, Schwartlaender, Stebel, Theeuwes, 2019]

NLO QCD corrections (full off-shell process, three charged lepton signature)

[Bevilacqua, Bi, Hartanto, Kraus, Nasuti, Worek, 2020-2021] [Denner, Pellicciolі, 2020]

combined NLO QCD + EW corrections (full off-shell process, three charged lepton signature)

[Denner, Pellicciolі, 2020]

NLO QCD + EW (on-shell) predictions supplemented with multi-jet merging as la FxFx

[Frixione, Frederix, 2012] [Frederix, Tsinikos, 2021]

Current theory reference in comparison with data

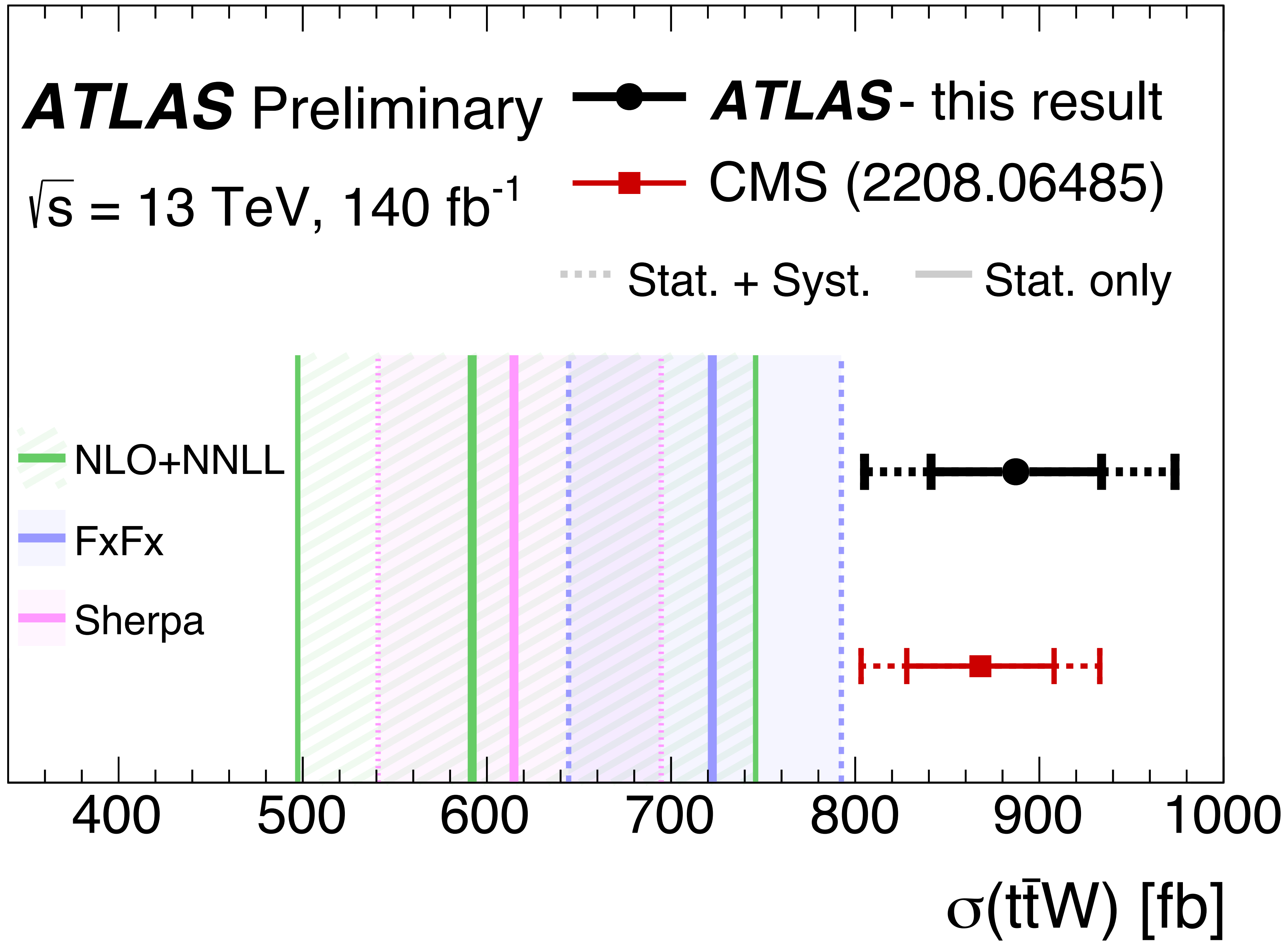
State of the art: data-theory comparison

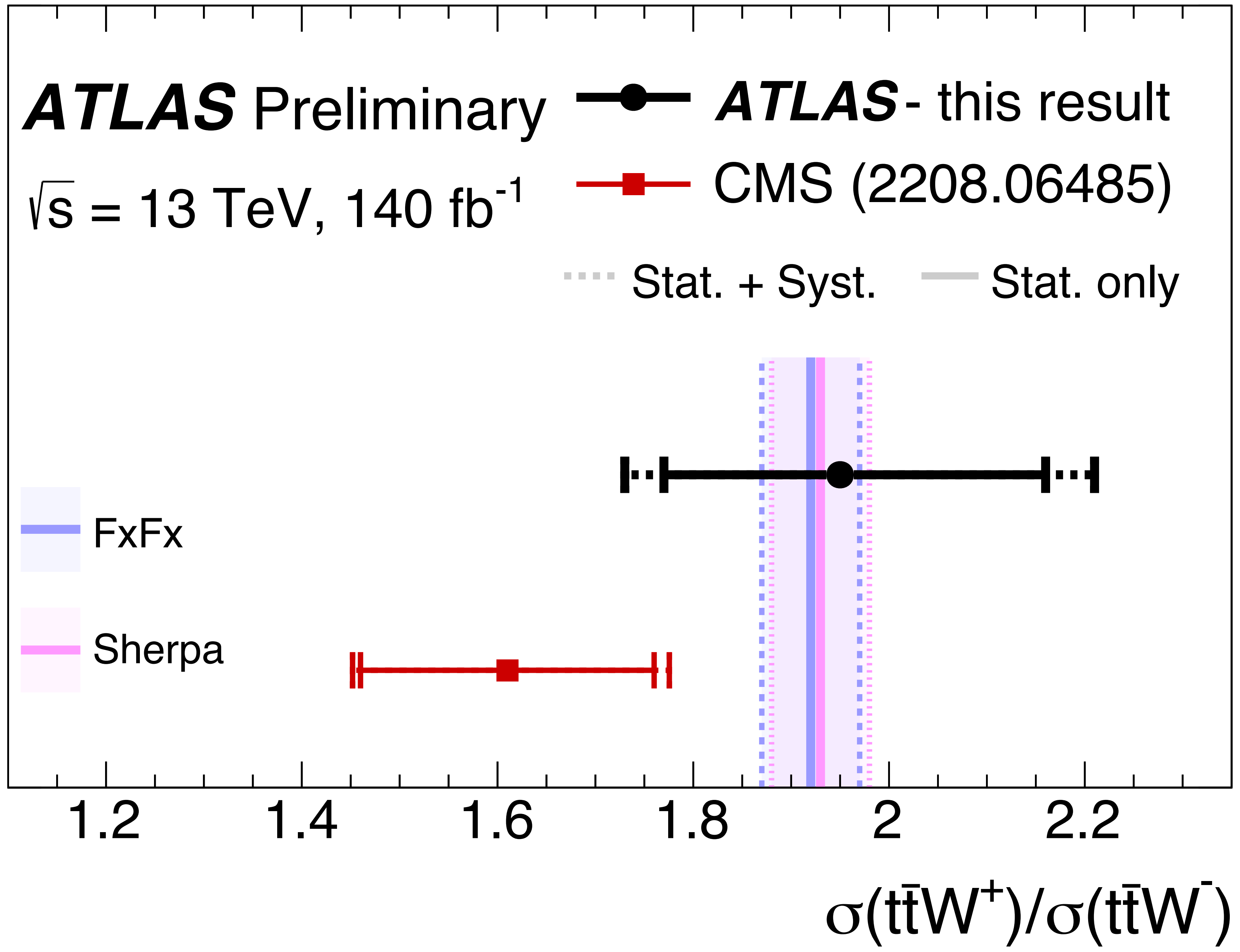
[CMS, 2208.06485, 2022]
[ATLAS-CONF-2023-019, 2023]

- FxFx multi-jet merging (including NLO QCD corrections to $t\bar{t}Wj$) and EW corrections increase the NLO QCD cross sections

- Nonetheless, measured $t\bar{t}W$ rates by ATLAS and CMS at $\sqrt{s} = 8$ TeV and $\sqrt{s} = 13$ TeV are consistently higher than the SM predictions. This tension is also confirmed by indirect measurements of $t\bar{t}W$ in the context of $t\bar{t}H$ and $t\bar{t}t\bar{t}$ analyses

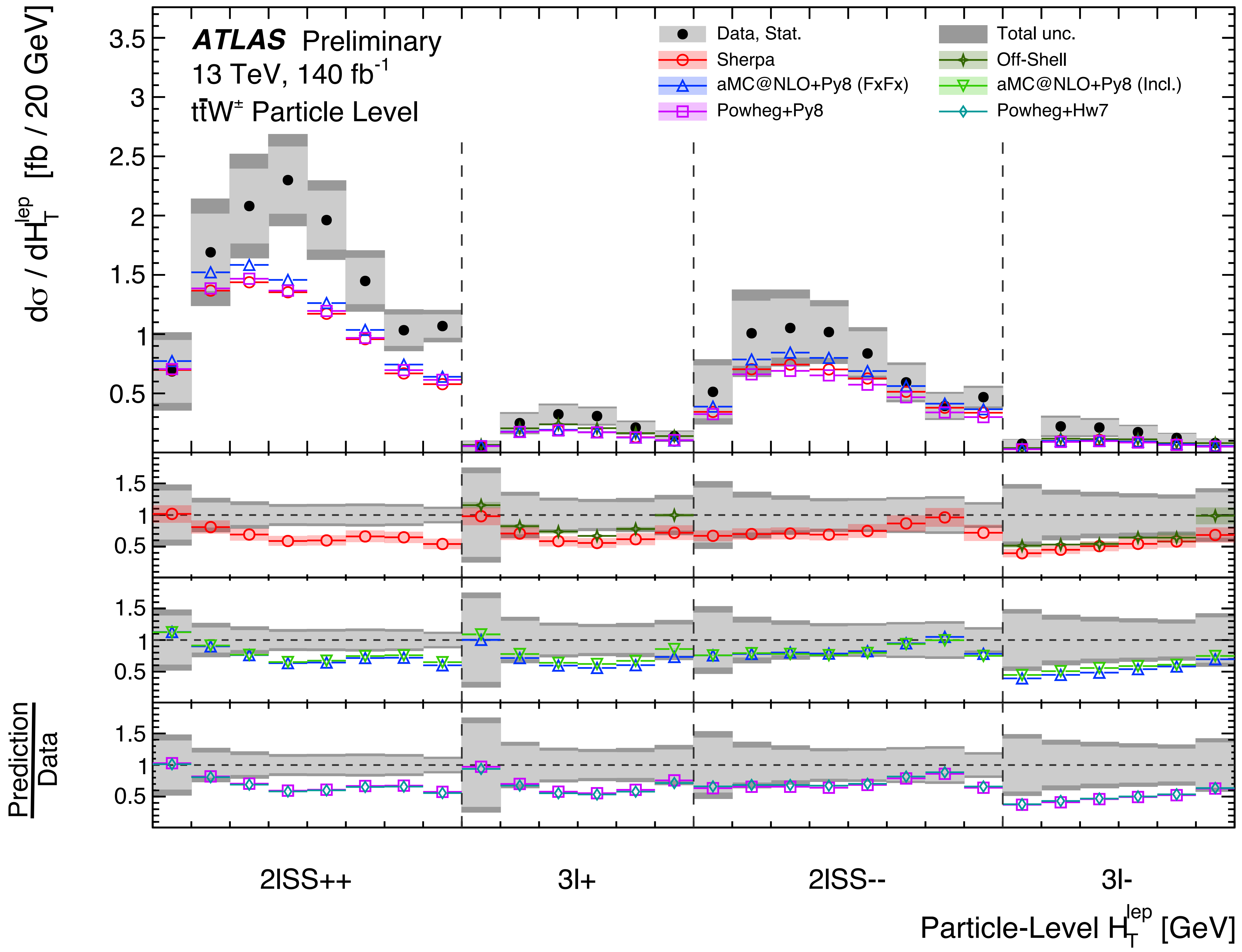
- **The most recent measurements confirm this picture with a slightly excess at the $1\sigma - 2\sigma$ level**

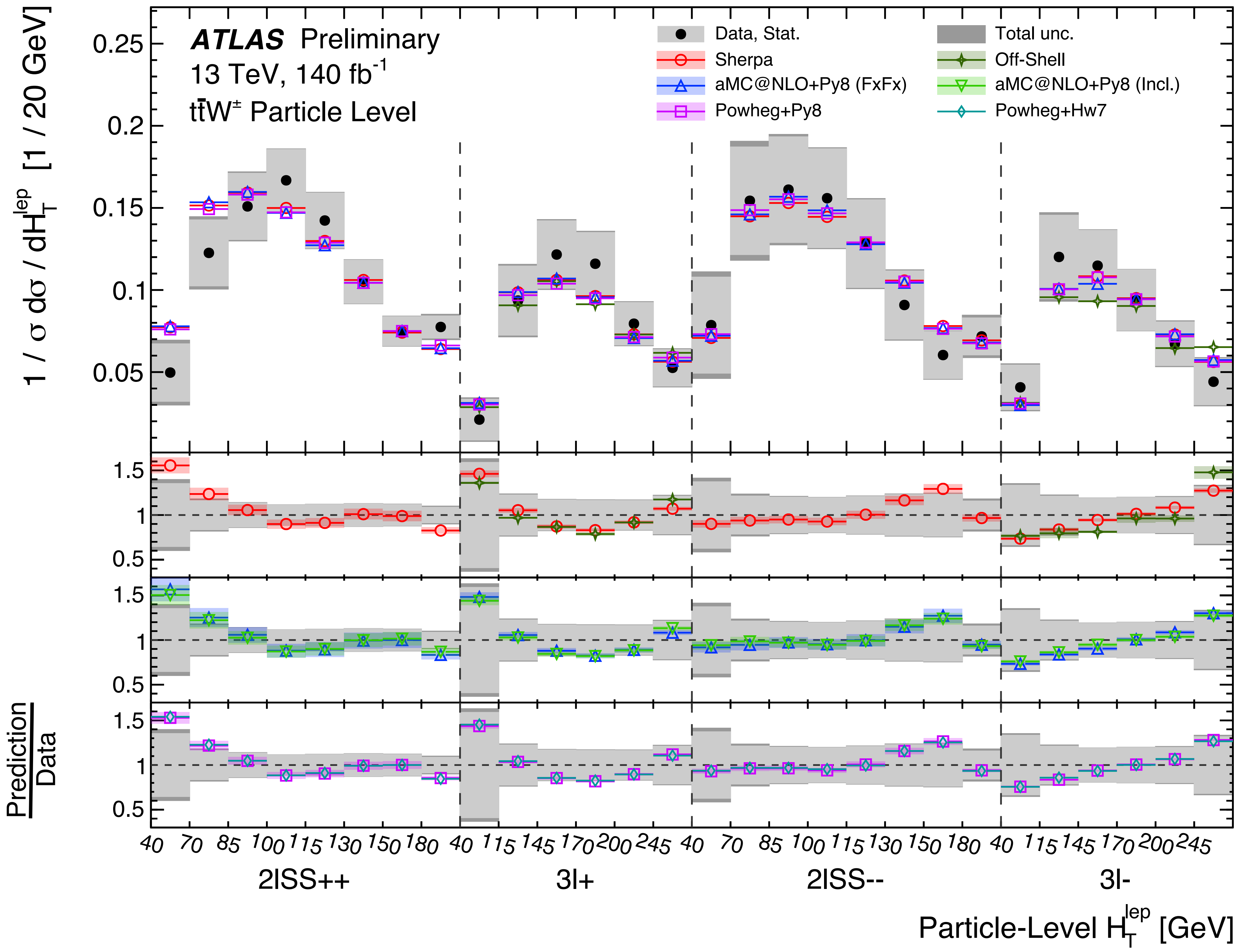




State of the art: data-theory comparison

- ATLAS measured also **differential distributions**, finding a disagreement in the overall normalisation consistent with the inclusive measurement result
- The latest off-shell fixed-order predictions give indications that this disagreement **is not predominantly due to missing singly-resonant contributions** which are not included in the reference on-shell predictions





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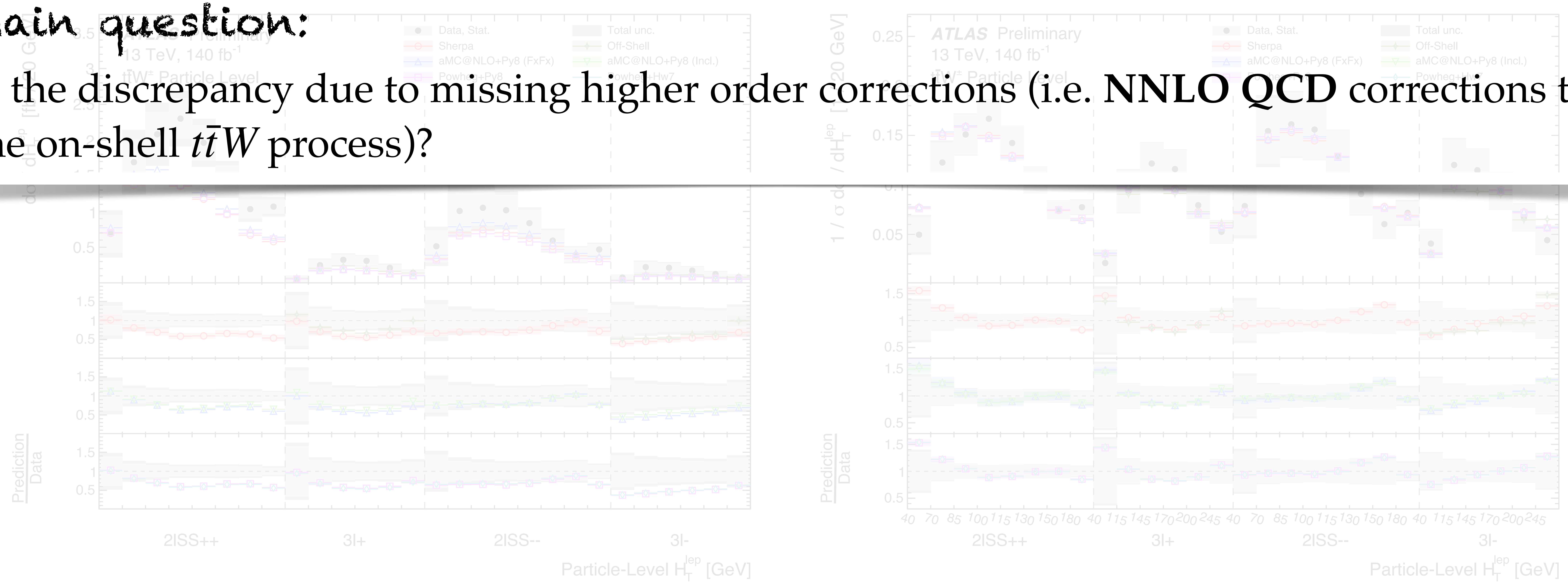

Main question:

Is the discrepancy due to missing higher order corrections (i.e. **NNLO QCD** corrections to the on-shell $t\bar{t}W$ process)?

Outline

- Motivations
- Methodology I: slicing formalism
- Methodology II: two-loop virtual amplitude
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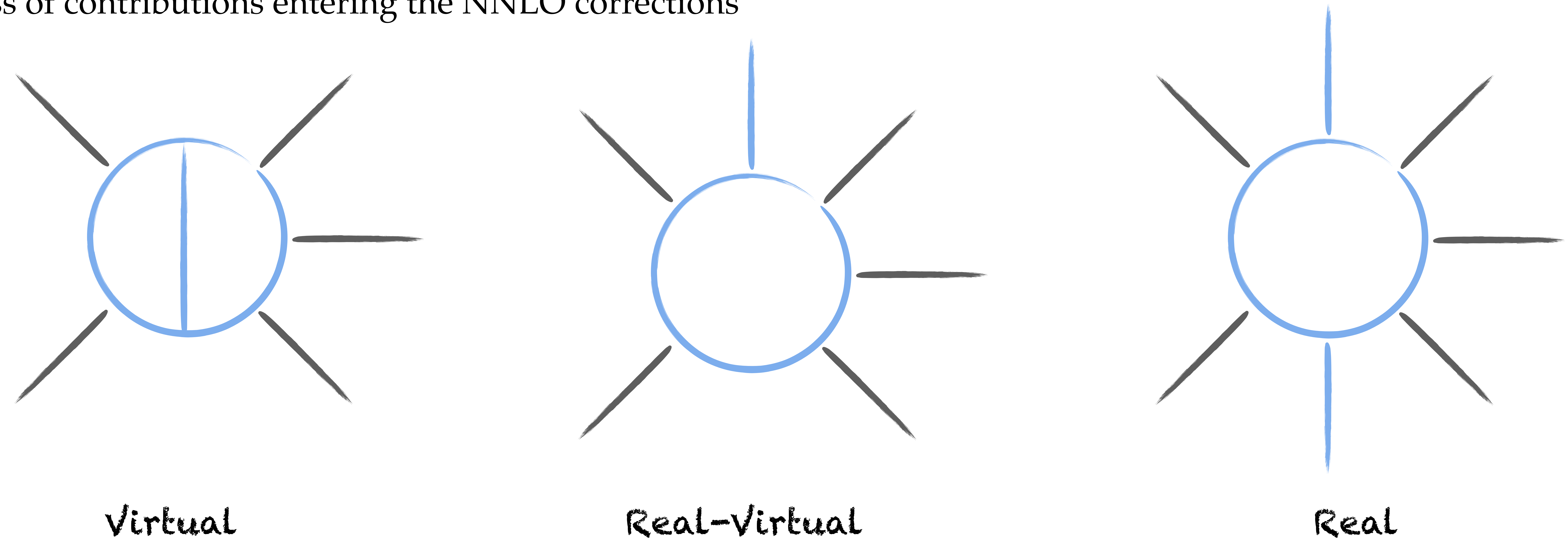
Infrared singularities

Class of contributions entering the NNLO corrections



KLN theorem and collinear factorisation ensure the cancellation of singularities for any infrared safe observables, but virtuals, real-virtual and reals live on different phase spaces and are separately divergent …

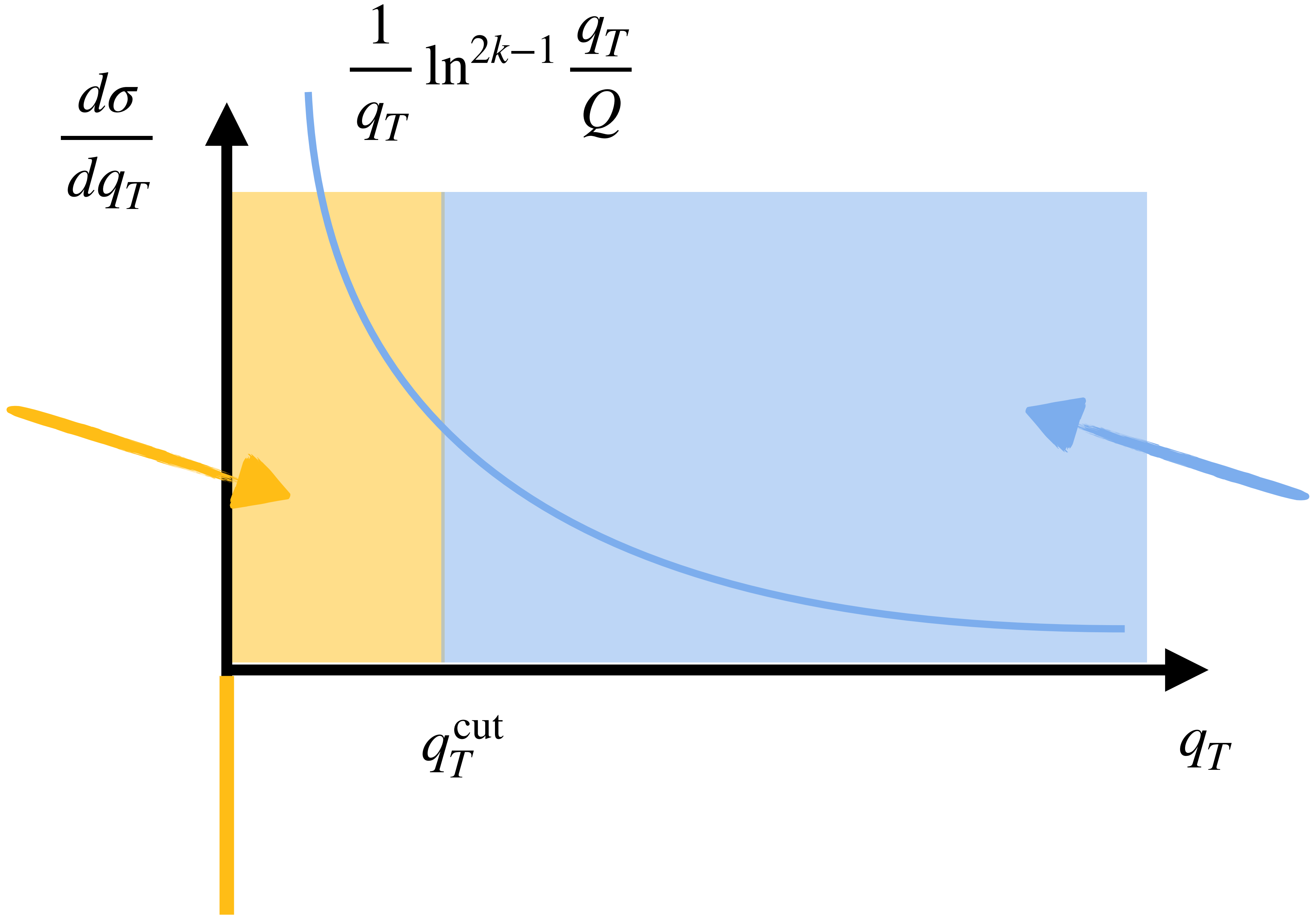
Subtraction/Slicing scheme required!

q_T-subtraction formalism

[Catani, Grazzini, 2007]

Cross section for the production of a triggered final state F at N^{k}LO

All emission unresolved; approximate the cross section with its singular part in the soft and/or collinear limits



1 emission always resolved

$F + j$ @ N^{k-1}LO

complexity of the calculation reduced by one order!

q_T resummation

- expand to fixed order
- $\mathcal{O}(\alpha_s^k)$ ingredient required

$$\int d\sigma_{N^kLO} = \mathcal{H} \otimes d\sigma_{LO} + \int \left[d\sigma^{R}_{N^{k-1}LO} - d\sigma^{CT}_{N^kLO} \right]_{q_T > q_T^{\text{cut}}} + \mathcal{O}\left((q_T^{\text{cut}})^{\ell} \right)$$

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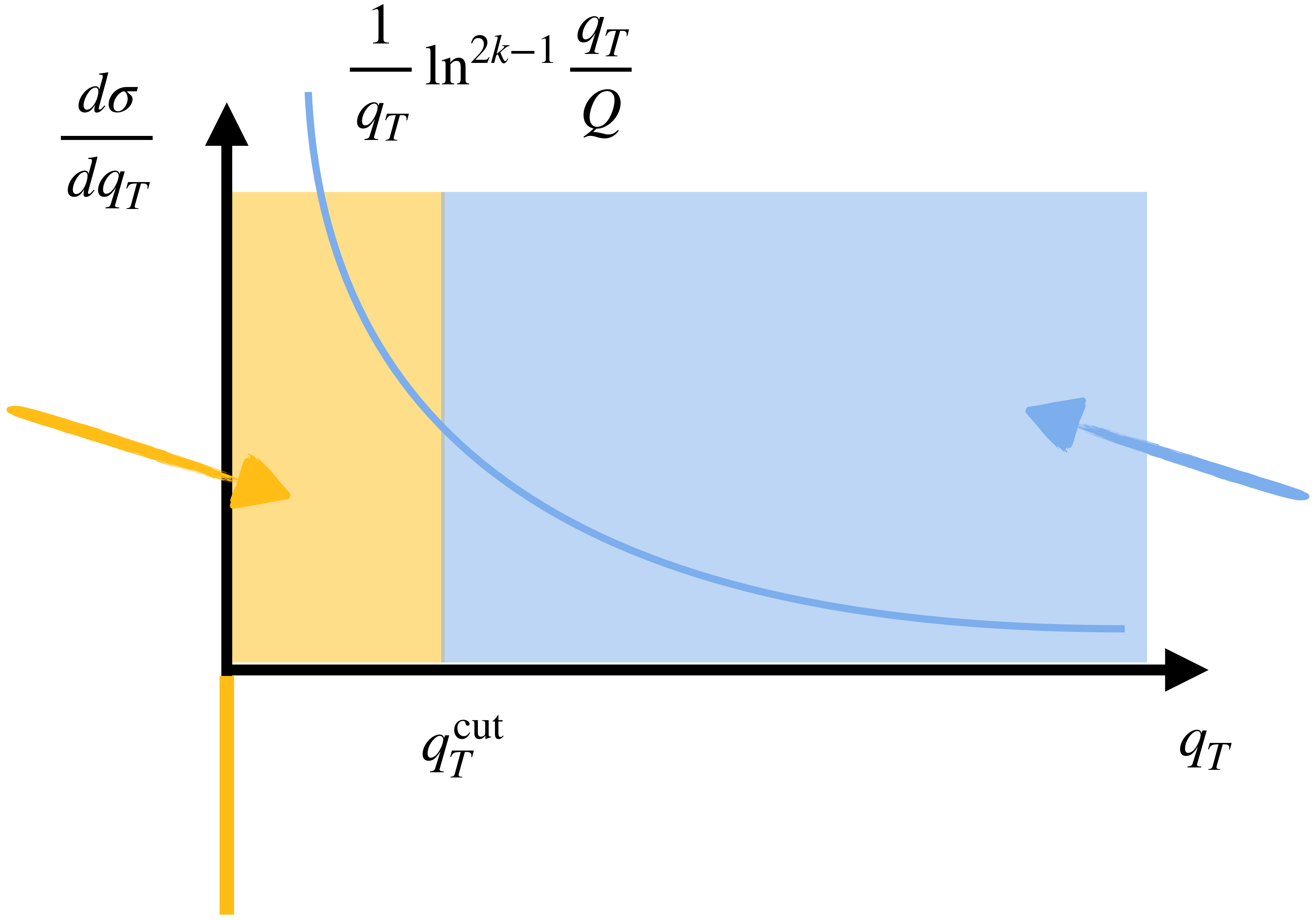

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residual power corretions

q_T-subtraction formalism: extension to massive final states

$$\int d\sigma_{NNLO} = \mathcal{H} \otimes d\sigma_{LO} + \int \left[d\sigma^{R}_{NLO} - d\sigma^{CT}_{NNLO}\right]_{q_T > q_T^{\rm cut}} + \mathcal{O}\left((q_T^{\rm cut})^{\ell}\right)$$

All ingredients for $Q\bar{Q}W + j$ @ NLO available:

Required matrix elements implemented in public libraries such as OpenLoops2

[Buccioni, Lang, Lindert, Maierhöfer, Pozzorini, Zhang, Zoller '19]

General end efficient NLO local subtraction schemes available, for example dipole subtraction

[Catani, Seymour, '98] [Catani, Dittmaier, Seymour, Trocsanyi '02]

Automatised implementation in the **MATRIX framework**, which relies on the efficient multi-channel Monte Carlo integrator MUNICH

[Grazzini, Kallweit, Wiesemann '17] [Kallweit in preparation]

q_T-subtraction formalism: extension to massive final states

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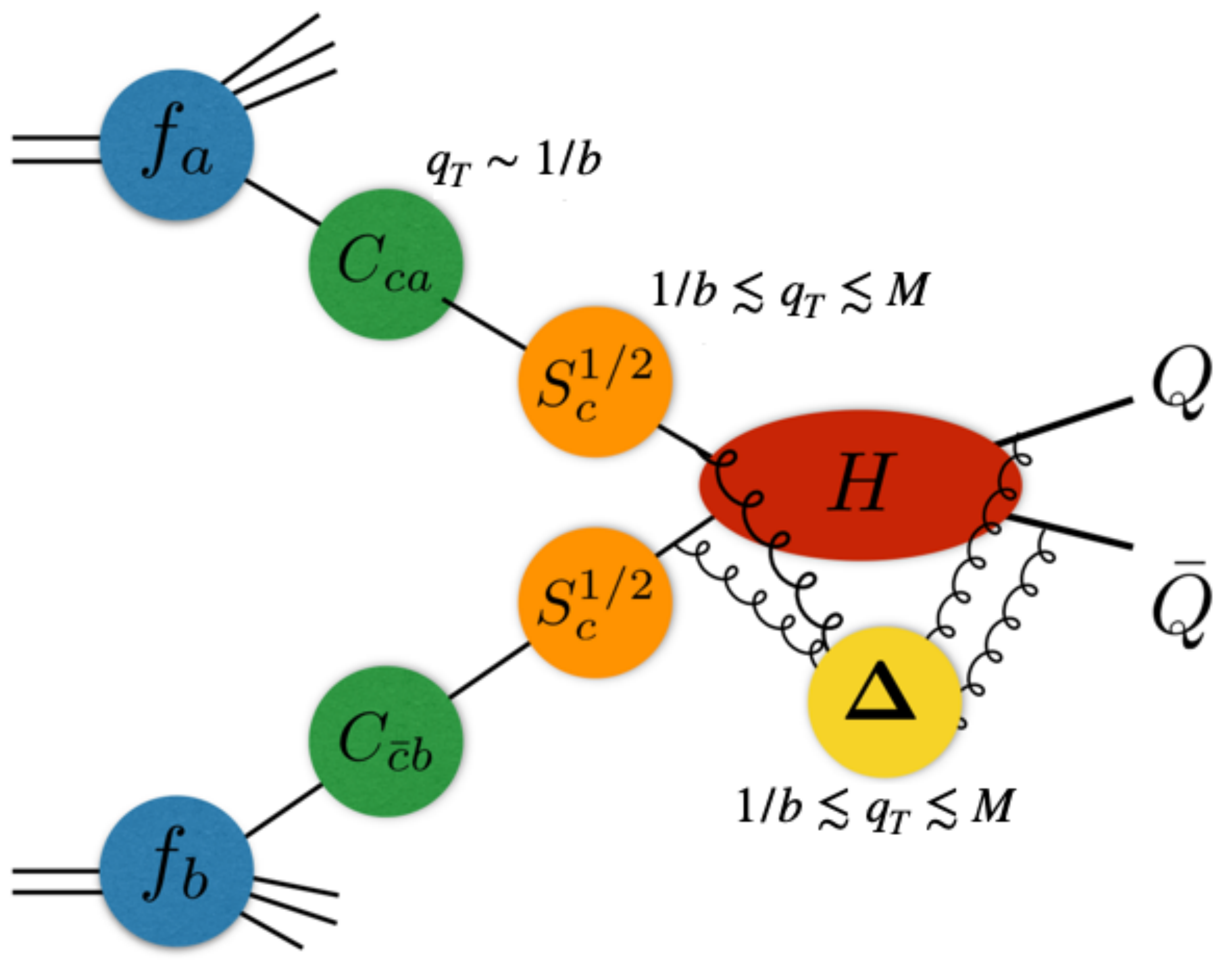
$\mathscr{H}$ contains virtual correction after subtraction of IR singularities and contribution of soft/collinear origin

- Beam functions ✓
- Soft function

[Catani, Cieri, de Florian, Ferrera, Grazzini '12]
[Gehrmann, Luebbert, Yang '14]
[Echevarria, Scimemi, Vladimirov '16]
[Luo, Wang, Xu, Yang, Yang, Zhu '19]
[Ebert, Mistlberger, Vita]



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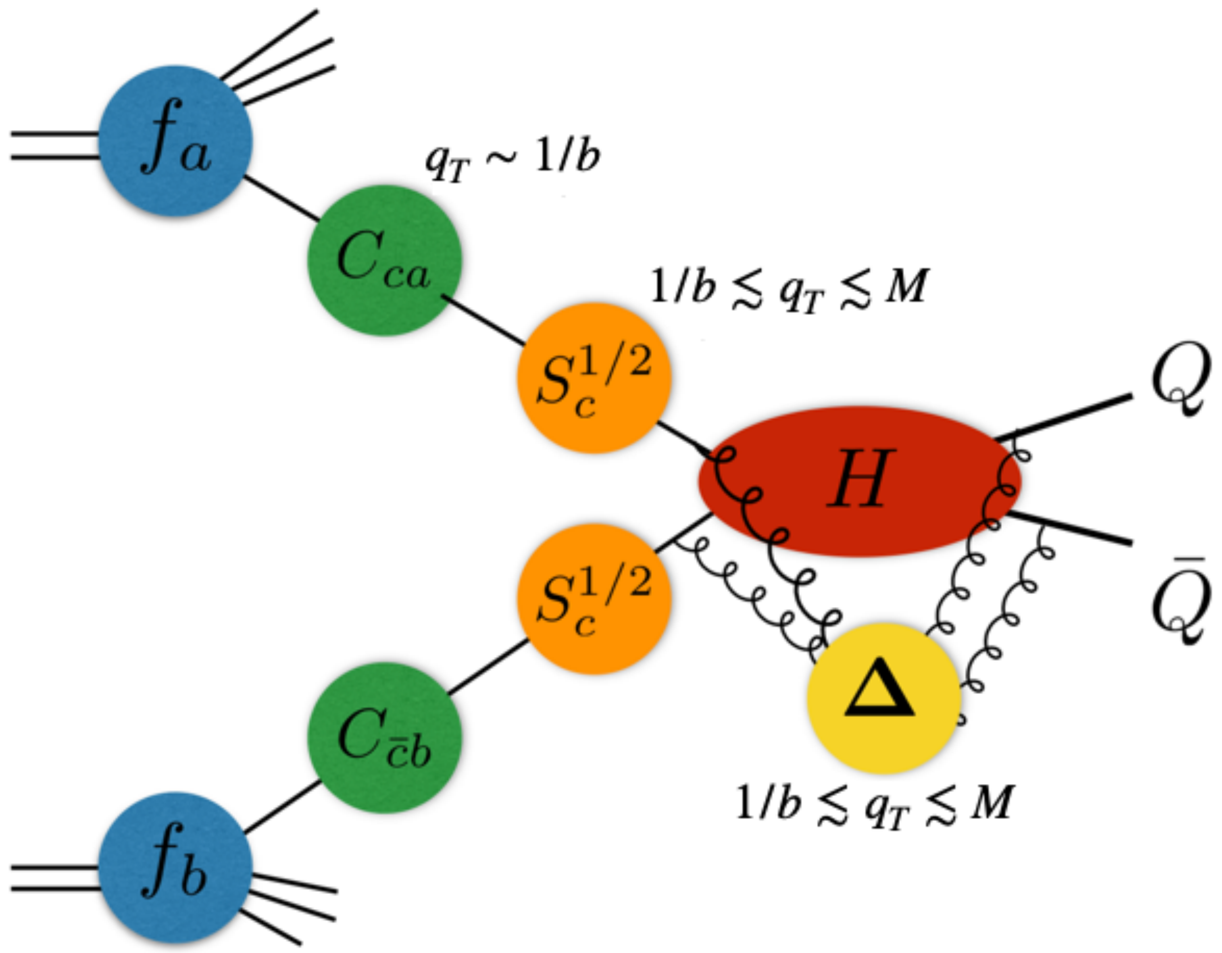

The resummation formula shows a **richer structure** because of additional soft singularities

- Soft logarithms controlled by the **transverse momentum anomalous dimension** $\mathbf{\Gamma}_t$ known up to NNLO **[Mitov, Sterman, Sung, 2009], [Neubert, et al 2009]**
- Hard coefficient gets a **non-trivial** colour structure (matrix in colour-space)
- Non trivial azimuthal correlations

q_T-subtraction formalism: extension to massive final states

$$\int d\sigma_{NNLO} = \mathscr{H} \otimes d\sigma_{LO} + \int \left[d\sigma^{R}_{NLO} - d\sigma^{CT}_{NNLO}\right]_{q_T > q_T^{\rm cut}} + \mathcal{O}\left((q_T^{\rm cut})^{\ell}\right)$$

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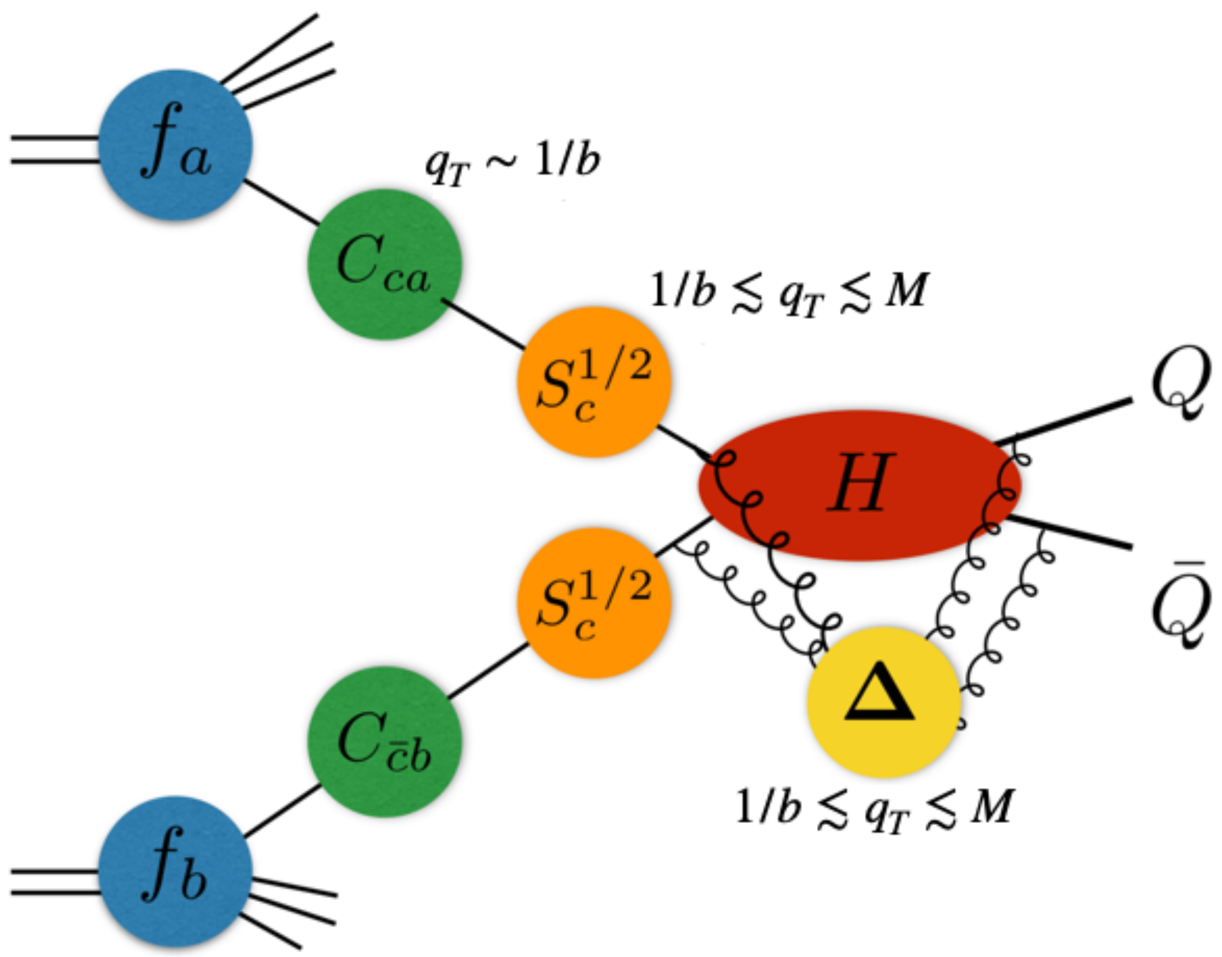

The resummation formula shows a **richer structure** because of additional soft singularities

q_T subtraction formalism extended to the case of **heavy quarks** production [Catani, Grazzini, Torre, 2014]

Successful employed for the computation of NNLO QCD corrections to the production of

- a **top pair** [Catani, Devoto, Grazzini, Kallweit, Mazzitelli, Sargsyan 2019]
- a **bottom pair** production [Catani, Devoto, Grazzini, Kallweit, Mazzitelli, 2021]

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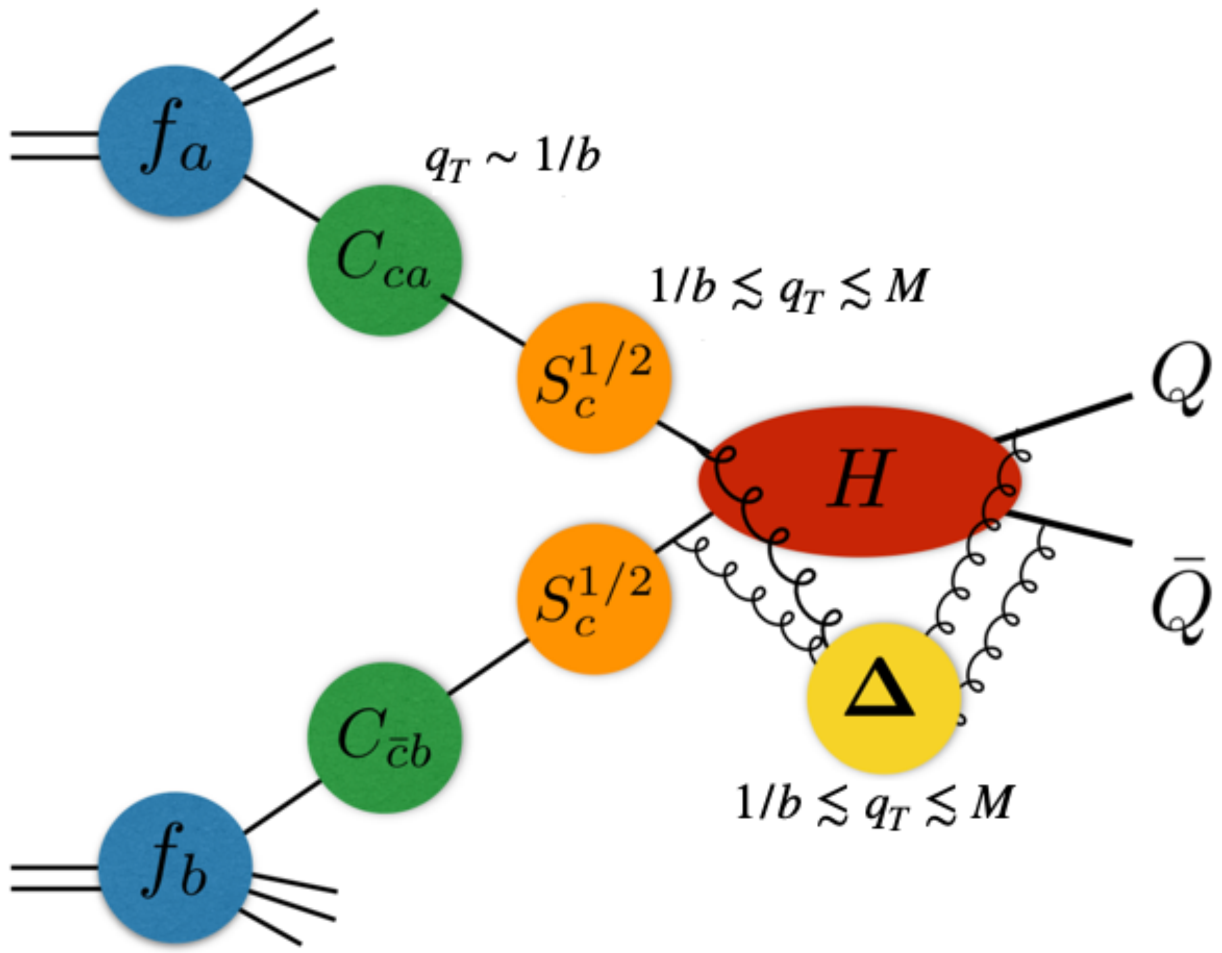

The resummation formula shows a **richer structure** because of additional soft singularities

Non trivial ingredient

- **Two-loop soft function** for heavy-quark (back-to-back Born kinematic) **[Catani, Devoto, Grazzini, Mazzitelli,2023]**
- Recently generalised to **arbitrary kinematics** **[Devoto, Mazzitelli in preparation]**

q_T-subtraction formalism: hard-virtual coefficient

All the ingredients are available and implemented in MATRIX **except for the two-loop virtual amplitude** entering $\mathscr{H}$

$$\mathscr{H} = H\delta(1-z_1)\delta(1-z_1) + \delta H(z_1, z_2)$$

in terms of the perturbatively computable **hard-virtual function**

$$H = 1 + \frac{\alpha_S(\mu_R)}{2\pi} H^{(1)} + \left(\frac{\alpha_S(\mu_R)}{2\pi}\right)^2 H^{(2)} + \ldots$$

$$H^{(n)} = \frac{2\Re < \mathscr{M}^{(n)}_{\text{fin}} | \mathscr{M}^{(0)} >}{|\mathscr{M}^{(0)}|^2}$$

$$|\mathscr{M}_{\text{fin}}(\mu_{\text{IR}}) > = Z^{-1}(\mu_{\text{IR}}) | \mathscr{M} >$$

IR subtraction at the subtraction scale μ_{IR}
[Ferroglia, Neubert, Pecjak, Yang, 2008]

At NNLO, the only missing ingredient is then contained in the $H^{(2)}$ contribution

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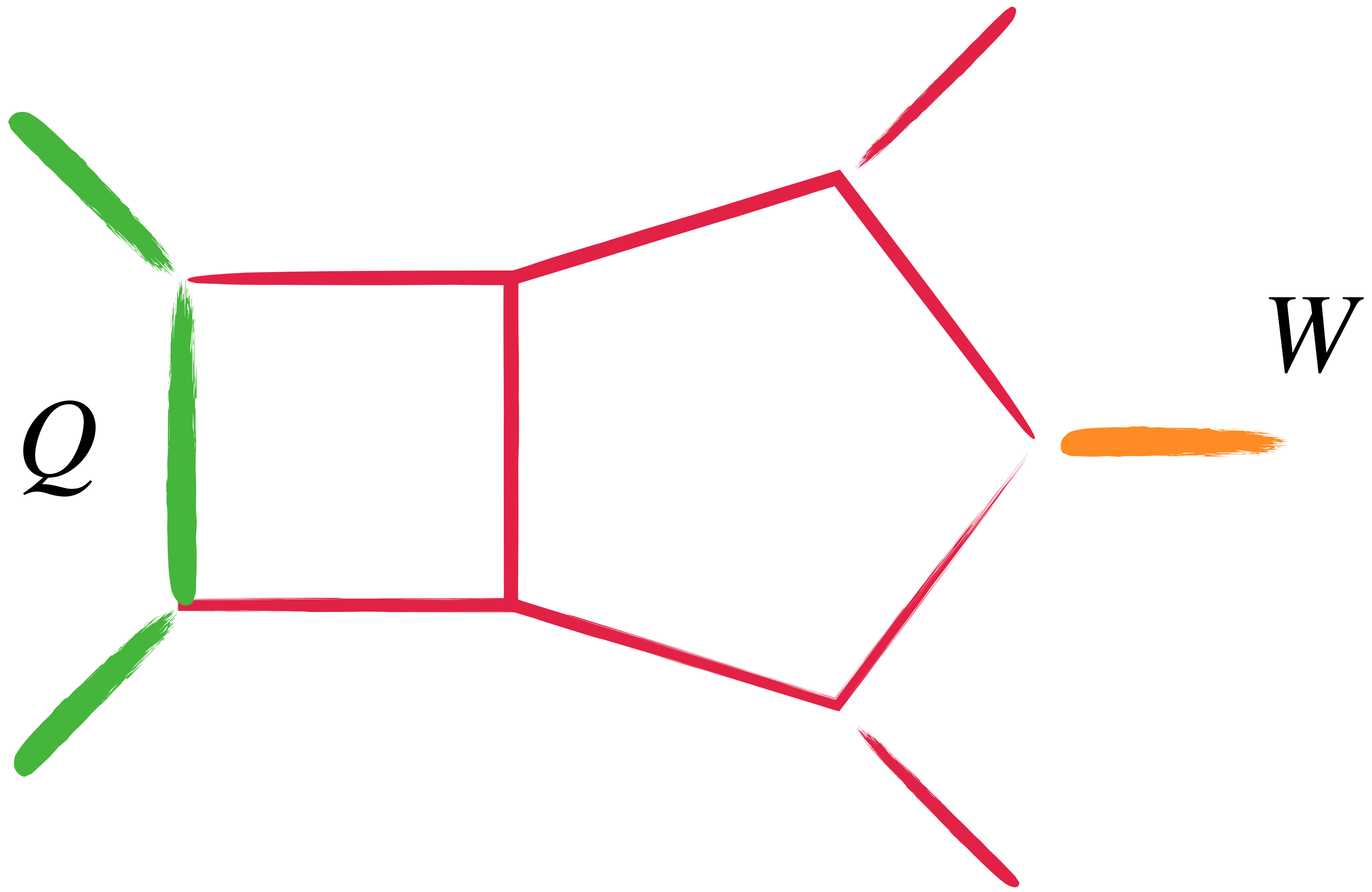
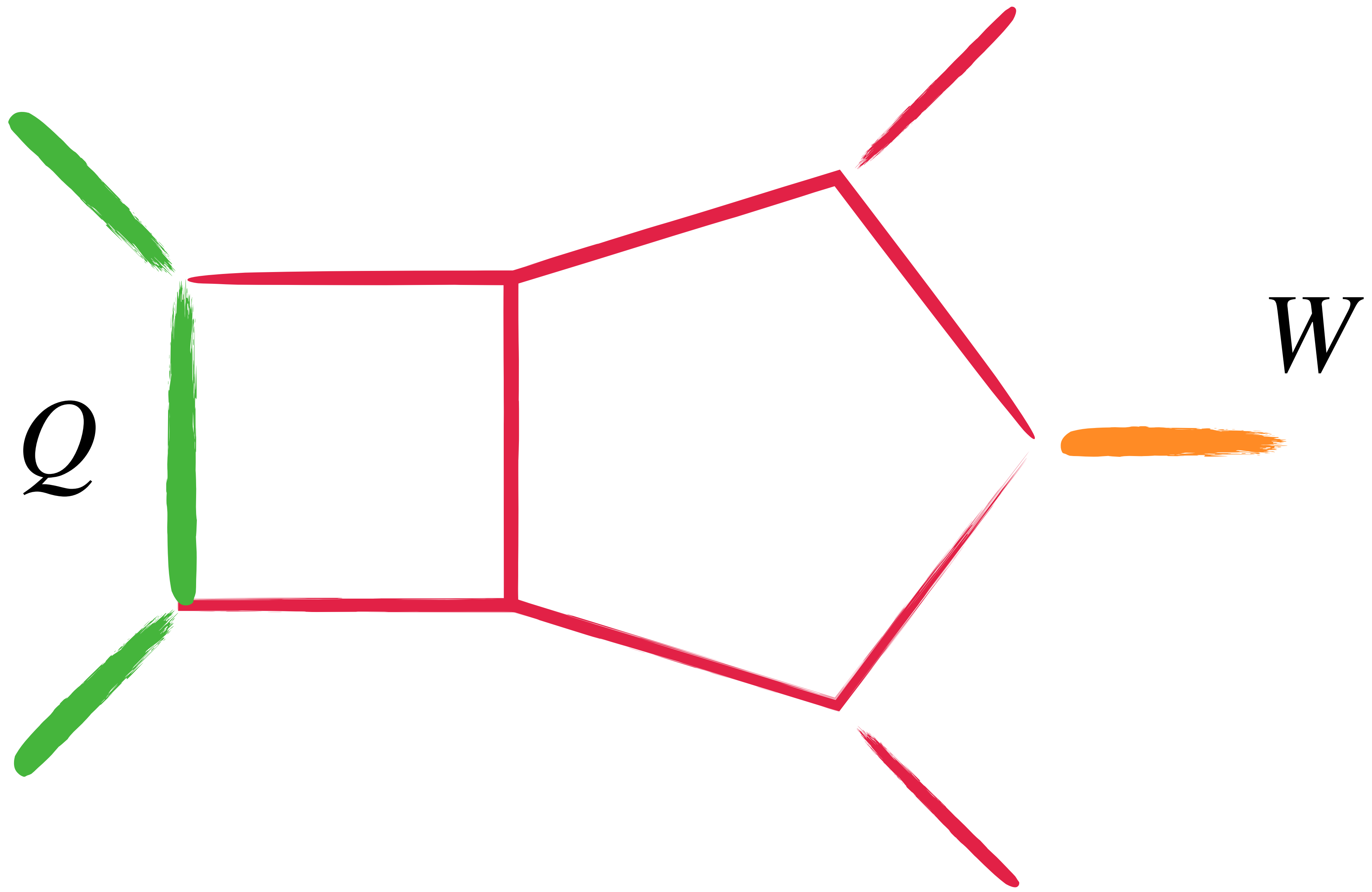
Two-loop virtual amplitude



Leading color 5-point amplitude with 1 massive particle current state of the art, more massive legs out of reach!

[Badger, Hartanto, Zoia, 2021]
[Abreu, Febres Cordero, Ita, Klinkert, Page, Sotnikov, 2021]

Two-loop virtual amplitude



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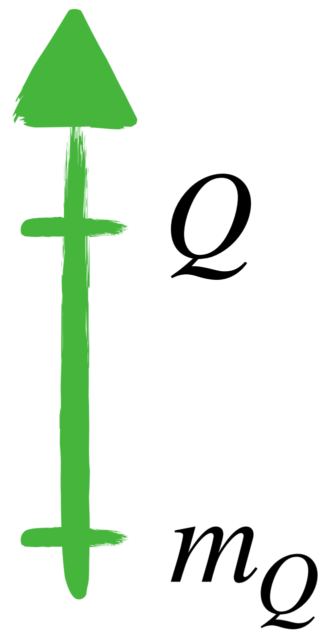
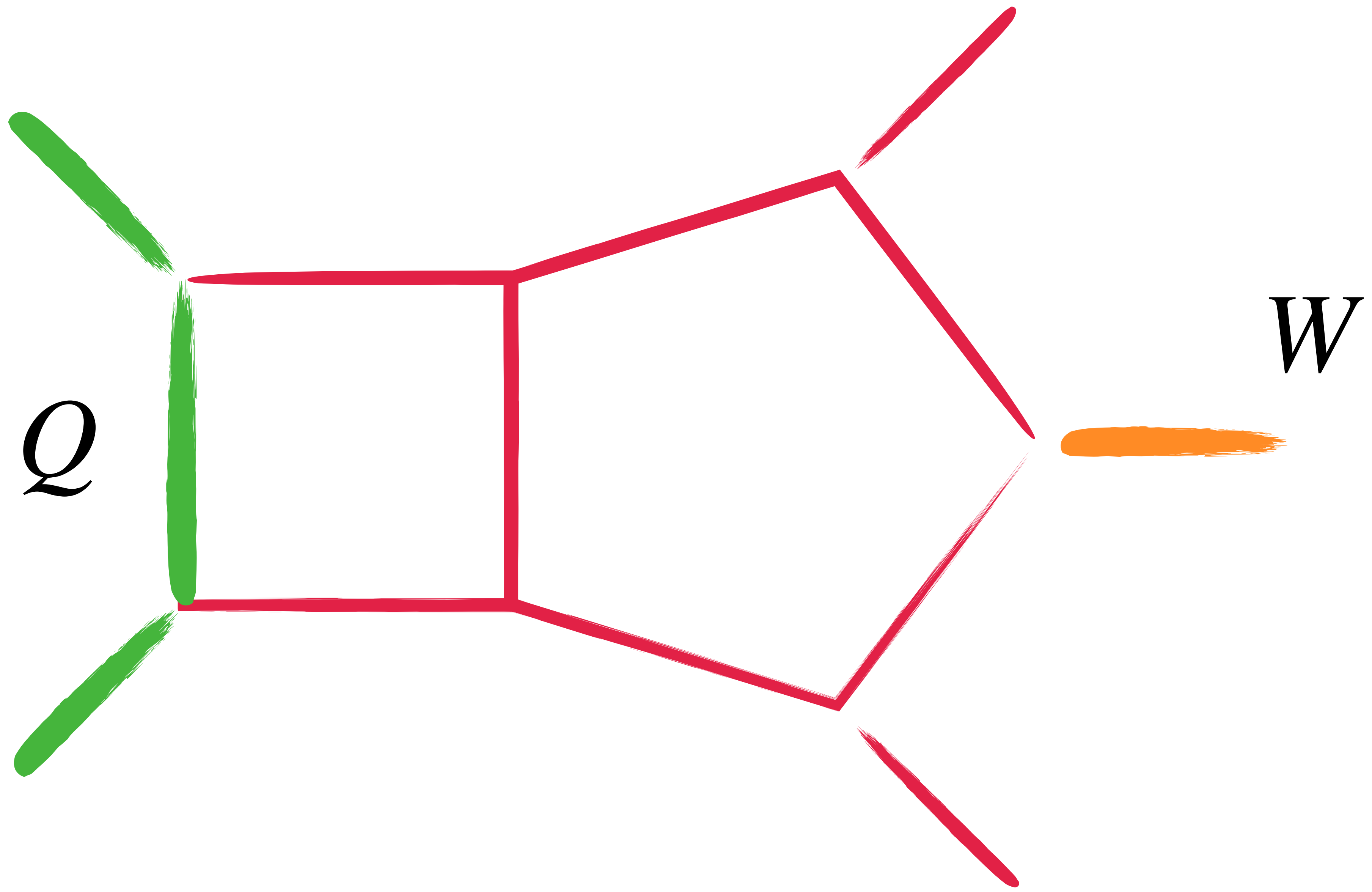
Smart idea: look for reliable approximation(s) based on **factorisation theorems**

In some kinematical regimes, the amplitude "**factorises**" into a *calculable factor* and a *simpler (available) amplitude*

- the mass of the heavy quark is negligible compared to its energy and other relevant hard scales (ultra relativistic quarks)
  massification



Two-loop virtual amplitude



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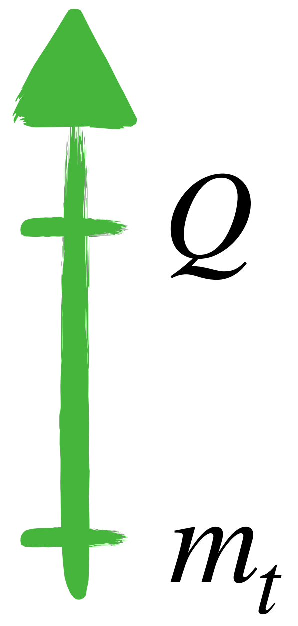
Remark: reasonable approximation for the case of bottom quarks!



Massification procedure in a nutshell

[Mitov, Moch, 2007]

Amplitude factorisation in massless QCD

[Catani, 1998][Sterman, Tejeda-Yeomans, 2003]

$$|\mathscr{M}^{[p]}> = \mathscr{J}^{[p]}\left(\frac{Q^2}{\mu^2}, \alpha_S(\mu^2), \epsilon\right) \times \mathscr{S}^{[p]}\left(\{k_i\}\frac{Q^2}{\mu^2}, \alpha_S(\mu^2), \epsilon\right) \times |\mathscr{H}^{[p]}>$$

Jet function: collinear contributions

Soft function: coherent soft radiation

Hard function: short-distance dynamics

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Amplitude factorisation in QCD with a **massive** parton of mass $m^2 \ll Q^2$

$$|\mathcal{M}^{[p],(m)}> = \mathcal{J}^{[p]}\left(\frac{Q^2}{\mu^2}, \frac{m_i^2}{\mu^2}\alpha_S(\mu^2), \epsilon\right) \times \mathcal{S}^{[p]}\left(\{k_i\}\frac{Q^2}{\mu^2}, \alpha_S(\mu^2), \epsilon\right) \times |\mathcal{H}^{[p]}> + \mathcal{O}\left(\frac{m^2}{Q^2}\right)$$

$$\mathcal{J}^{[p]}\left(\frac{Q^2}{\mu^2}, \frac{m_i^2}{\mu^2}\alpha_S(\mu^2), \epsilon\right) = \prod_i \mathcal{J}^i\left(\frac{Q^2}{\mu^2}, \frac{m_i^2}{\mu^2}\alpha_S(\mu^2), \epsilon\right) = \prod_i \left(\mathcal{F}^i\left(\frac{Q^2}{\mu^2}, \frac{m_i^2}{\mu^2}\alpha_S(\mu^2), \epsilon\right)\right)^{1/2}$$

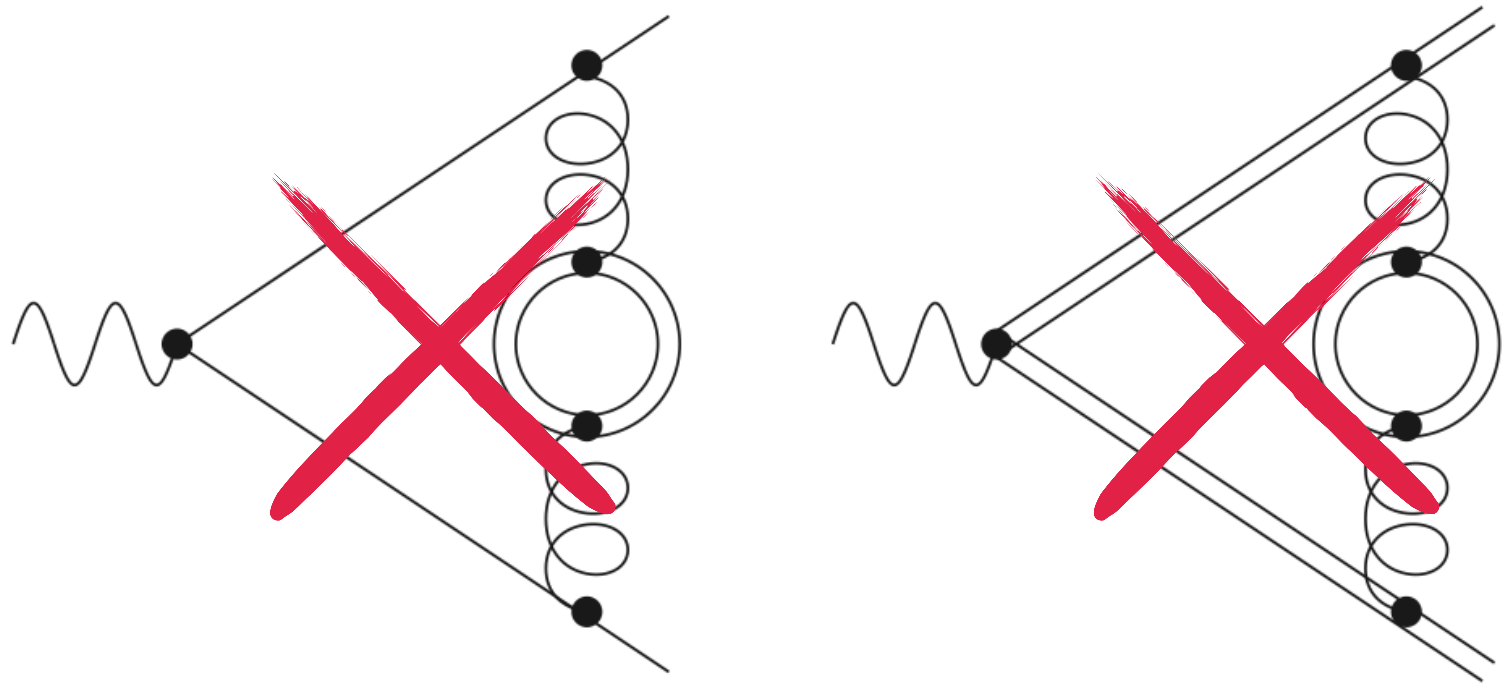
space-like massive form factor

Massification procedure in a nutshell

[Mitov, Moch, 2007]

Caveat: starting from NNLO, heavy quark loop insertions **break** this simple "collinear" factorisation picture

We estimate that they have a negligible impact by inspecting the tree-level emission process of four tops and by removing heavy quark loop diagrams from the real-virtual contribution



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Massification procedure in a nutshell

[Mitov, Moch, 2007]

Master formula of "massification"

$$|\mathcal{M}^{[p],(m)}> = \prod_i \left[Z_{[i]}\left(\frac{m^2}{\mu^2}, \alpha_s(\mu^2), \epsilon\right)\right]^{1/2} \times |\mathcal{M}^{[p]}> + \mathcal{O}\left(\frac{m^2}{Q^2}\right)$$

$$Z_{[i]}\left(\frac{m^2}{\mu^2}, \alpha_S(\mu^2), \epsilon\right) = \mathcal{F}^i\left(\frac{Q^2}{\mu^2}, \frac{m_i^2}{\mu^2}, \alpha_S(\mu^2), \epsilon\right)\left[\mathcal{F}^i\left(\frac{Q^2}{\mu^2}, 0, \alpha_S(\mu^2), \epsilon\right)\right]^{-1}$$

History & Remarks

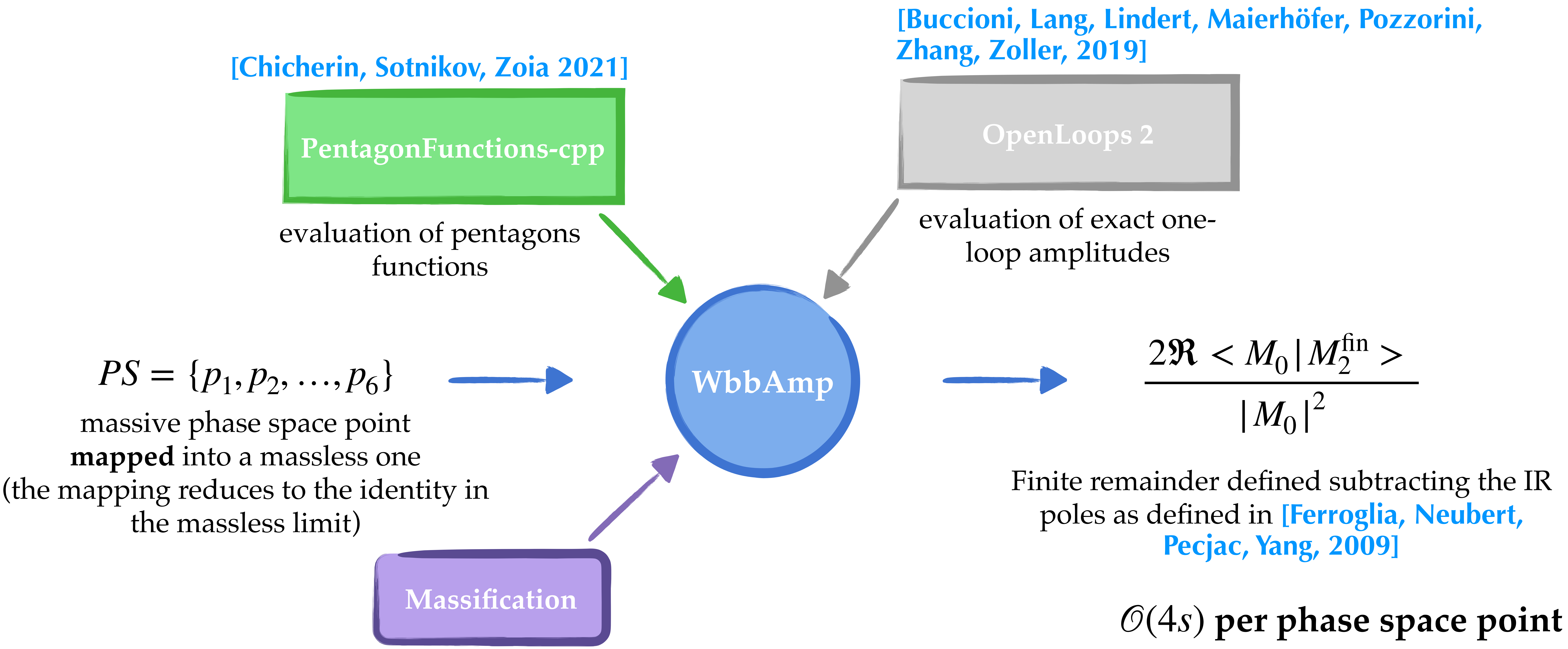
- Neglecting heavy quark insertions, the formula retrieves **mass logarithms** and **constant terms**
- Consistent with previous results for NNLO QED correction to Bhabha scattering [Glover, TauskandJ, VanderBij, 2001] [Penin 2005-2006]
- Successfully employed to derive and cross check results for $q\bar{q} \to Q\bar{Q}$ and $gg \to Q\bar{Q}$ amplitudes [Czakon, Mitov, Moch, 2007]
- Recently extended to the case of two different external masses ($M \gg m$)

[Engel, Gnendiger, Signer, Ulrich 2019]

WQQAmp: a massive C++ implementation

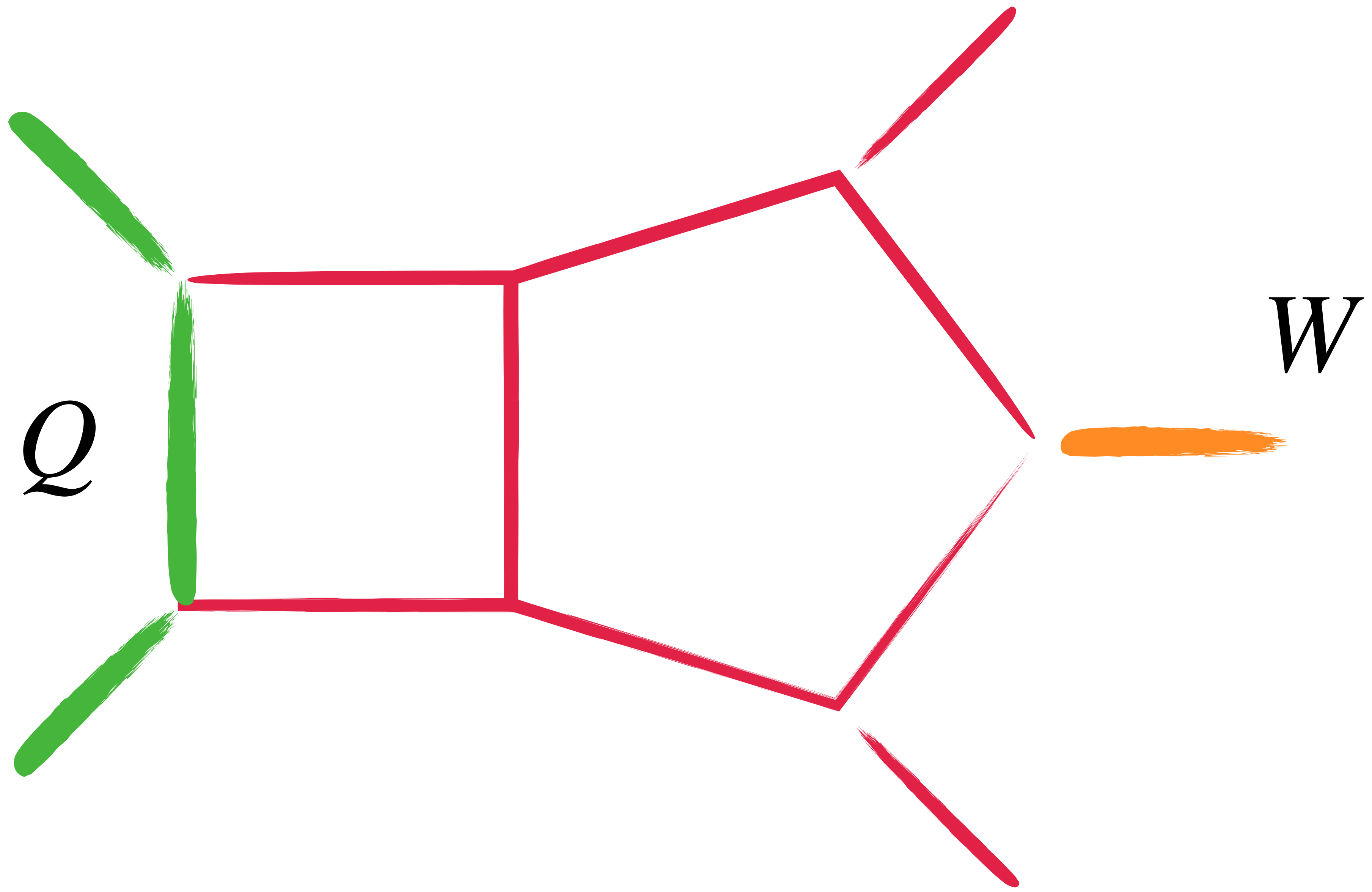
[Buonocore, Rottoli, Savoini, https://gitlab.com/lrottoli/WQQAmp]

We have implemented the one-loop and two-loop **leading colour** amplitudes of [Abreu et al, 2022] in a **C++ library** for the efficient numerical evaluation of the **massive amplitudes**



$\mathcal{O}(4s)$ **per phase space point**

Two-loop virtual amplitude



5-point amplitude with 1 massive particle
current state of the art, more massive legs out of reach!

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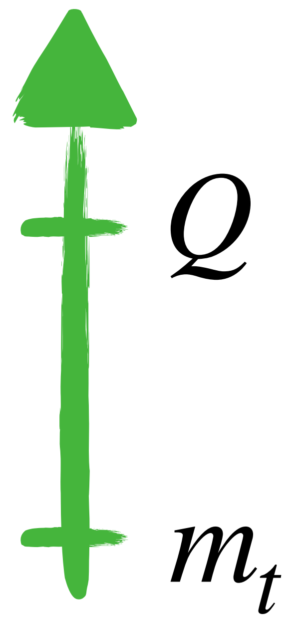
In some kinematical regimes, the amplitude "**factorises**" into a *calculable factor* and a *simpler (available) amplitude*

- the mass of the heavy quark is negligible compared to its energy and other relevant hard scales (ultra relativistic quarks)

Remark: in principle, not so good for top quarks …



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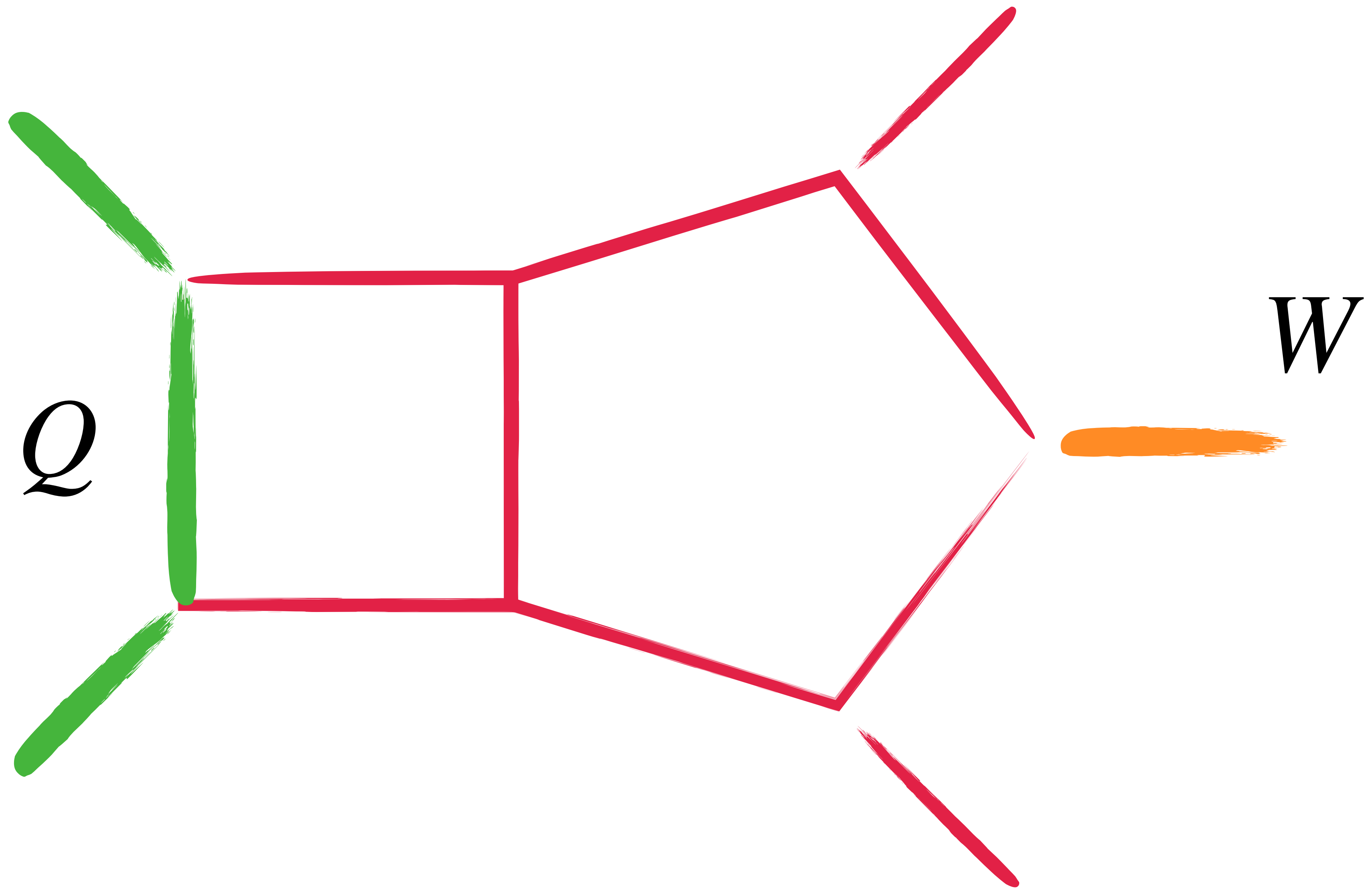

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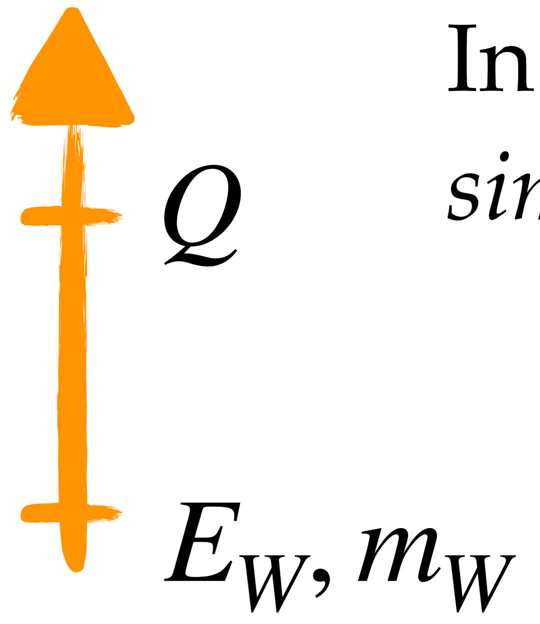
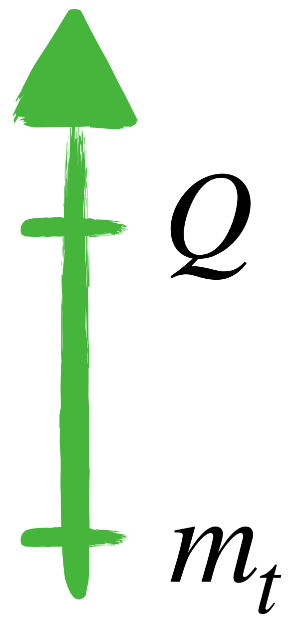


In some kinematical regimes, the amplitude "**factorises**" into a *calculable factor* and a *simpler (available) amplitude*

- the mass of the heavy quark is negligible compared to its energy
  massification
- the energy and mass of the *W* boson are smaller than the other relevant scales
  soft W approximation



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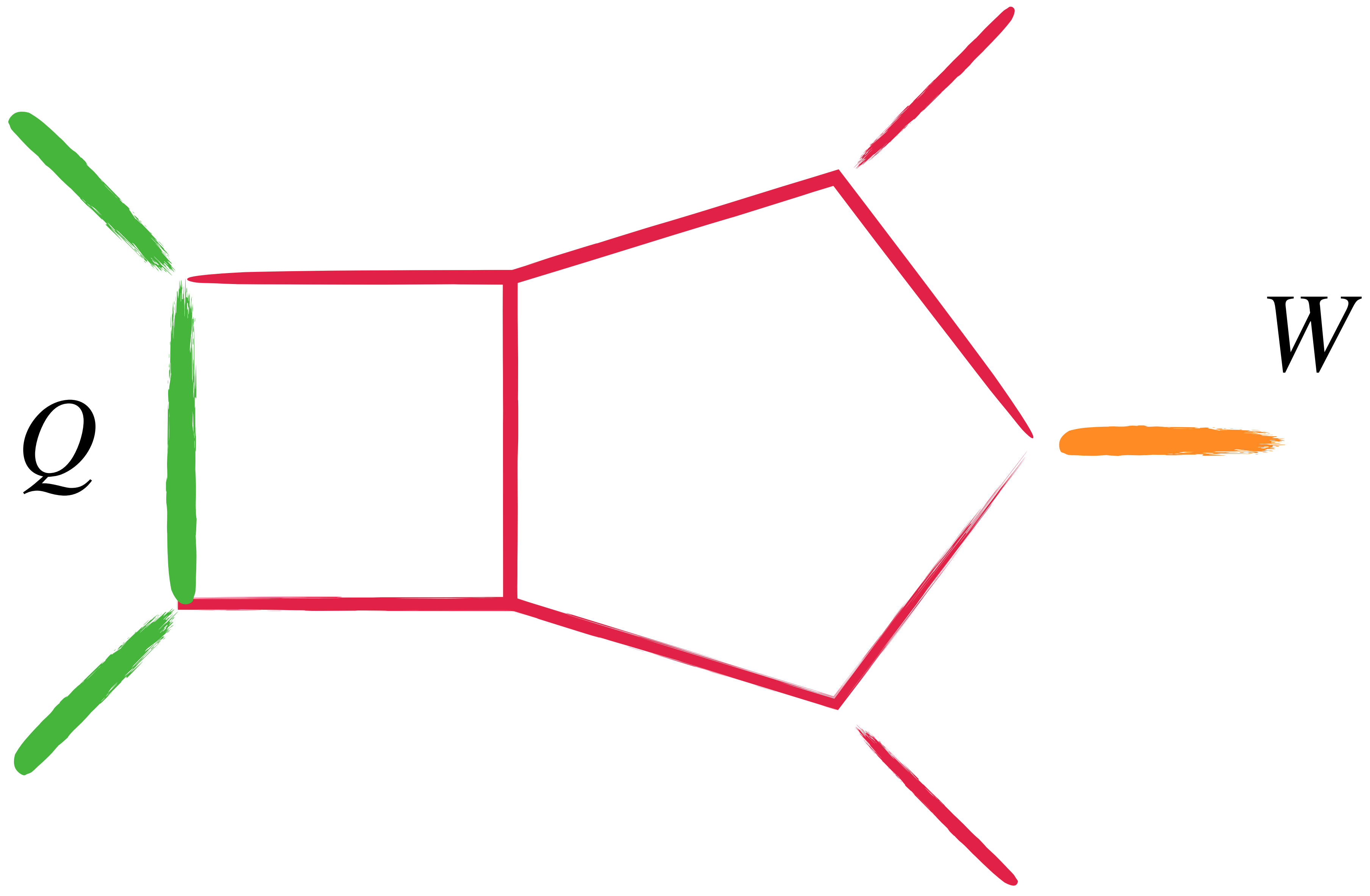

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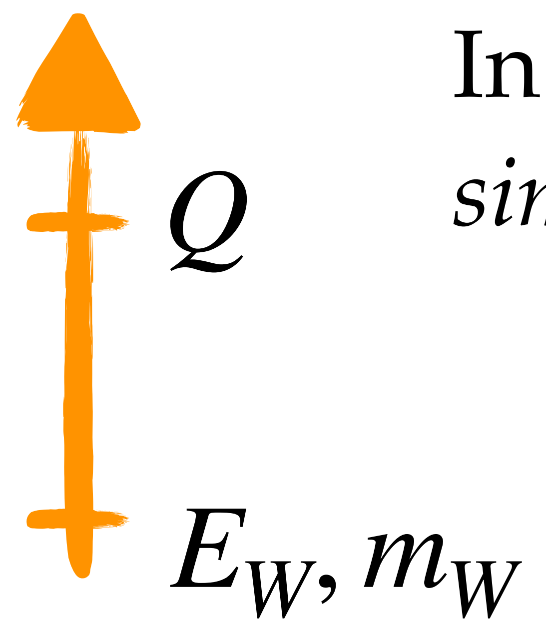
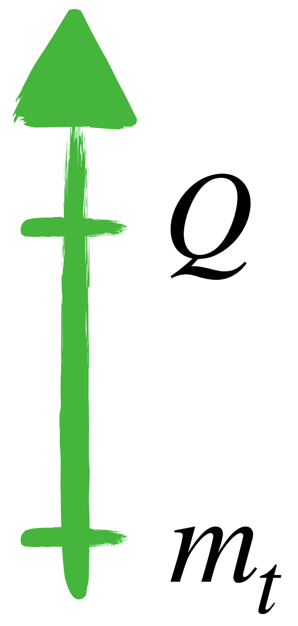


In some kinematical regimes, the amplitude "**factorises**" into a *calculable factor* and a *simpler (available) amplitude*

Disclaimer: None of the two regimes is reasonable for the case of top quarks. The quality of the approximation **must be carefully assessed**

Good starting point: two largely complementary approximations!



Soft approximation

In the limit in which the incoming $q\bar{q}'$ pair emits a soft W, the multi-loop QCD amplitude factorises as

$$|\mathcal{M}^{[p,k]}_{q\bar{q}'\to t\bar{t}W}> \simeq \frac{g}{\sqrt{2}}\left(\frac{p_2\cdot\varepsilon^*(k)}{p_2\cdot k}-\frac{p_1\cdot\varepsilon^*(k)}{p_1\cdot k}\right)\times|\mathcal{M}^{[p]}_{q_L\bar{q}'_R\to t\bar{t}}>$$

Eikonal factor
(analogous to soft photon/gluon)

"reduced" polarised $t\bar{t}$ amplitude

Remarks

- the soft W emission **selects a particular helicity configuration**
- the required NNLO QCD $q\bar{q}'\to t\bar{t}$ amplitude is **available** [Bärnreuther, Czakon, Fiedler, 2013] [Chen, Czakon, Poncelet, 2017] [Mandal, Mastrolia, Ronca, Bobadilla Torres, 2022]
- the use of the formula for a generic phase point required a **momentum mapping**: we adopt a recoil scheme in which the momentum of the W is absorbed by the top quark pair preserving the invariant mass of the event

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Remarks

- We apply the approximation for estimating the hard-virtual coefficient

$$H^{(n)} = \frac{2\Re < \mathscr{M}^{(n)}_{\text{fin}}|\mathscr{M}^{(0)}>}{|\mathscr{M}^{(0)}|^2}$$

both on numerator and denominator: in this way we are effectively reweighing by the exact LO result!

Outline

- Motivations
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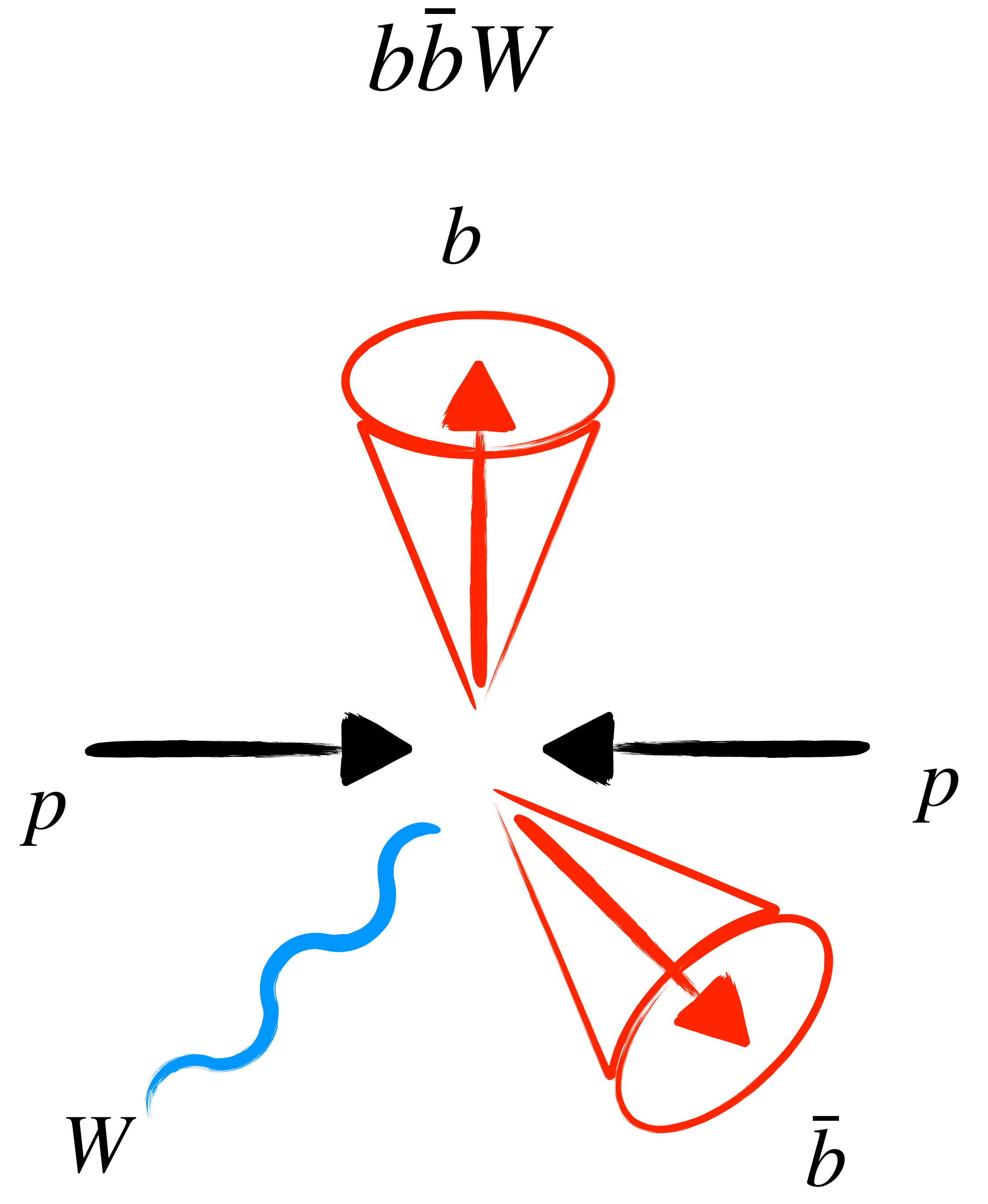

Comparison with HPPZ (flavor anti-k_T algorithm)

$$W + 2\ b_{jet} + X\ \textbf{(inclusive)}\ @\ \sqrt{s} = 8\,\text{TeV}$$

[CMS:arXiv:1608.07561]

Selection cuts

$$p_{T,\ell} > 30\ \text{GeV} \qquad |\eta_\ell| < 2.1$$

$$n_b = 2 : p_{T,b} > 25\ \text{GeV} \qquad |\eta_\ell| < 2.4$$

$$p_{T,j} > 25\ \text{GeV} \qquad |\eta_\ell| < 2.4$$

Reference scale

$$H_T = E_T(\ell\nu) + p_T(b_1) + p_T(b_2)$$

$$E_T(\ell\nu) = \sqrt{M^2(\ell\nu) + p_T^2(\ell\nu)}$$

	HPPZ	**This work**
α_s and PDF scheme	5FS	4FS
Jet clustering algorithm	flavour k_T and flavour anti-k_T algorithm (R=0.5)	k_T and anti-k_T algorithm (R=0.5)
pdf sets	`NNPDF31_as_0118` (LO, NLO, NNLO)	`NNPDF30_as_0118_nf_4` (LO) `NNPDF31_as_0118_nf_4` (NLO, NNLO)

Comparison with HPPZ: fiducial cross sections

order	σ^{4FS} [fb]	$\sigma^{\mathrm{5FS}}_{a=0.05}$ [fb]	$\sigma^{\mathrm{5FS}}_{a=0.1}$ [fb]	$\sigma^{\mathrm{5FS}}_{a=0.2}$ [fb]
LO	$210.42(2)^{+21.4\%}_{-16.2\%}$	$262.52(10)^{+21.4\%}_{-16.1\%}$	$262.47(10)^{+21.4\%}_{-16.1\%}$	$261.71(10)^{+21.4\%}_{-16.1\%}$
NLO	$468.01(5)^{+17.8\%}_{-13.8\%}$	$500.9(8)^{+16.1\%}_{-12.8\%}$	$497.8(8)^{+16.0\%}_{-12.7\%}$	$486.3(8)^{+15.5\%}_{-12.5\%}$
NNLO	$649.9(1.6)^{+12.6\%}_{-11.0\%}$	$690(7)^{+10.9\%}_{-9.7\%}$	$677(7)^{+10.4\%}_{-9.4\%}$	$647(7)^{+9.5\%}_{-9.4\%}$

Remarks

- The parameter a of the flavour anti k_T algorithm plays a role similar to m_b in our massive calculation
- Uncertainty estimated by varying $a \in [0.05,0.2]$ amounts to 7 % ; **smaller** uncertainty estimated by varying $m_b \in [4.2,4.92]$, at the 2% level
- General **agreement within scale variations**, but the massive calculation performed in the 4FS **systematically below due to the different flavour scheme**

Comparison with HPPZ: fiducial cross sections

order	σ^{4FS} [fb]	$\sigma^{5FS}_{a=0.05}$ [fb]	$\sigma^{5FS}_{a=0.1}$ [fb]	$\sigma^{5FS}_{a=0.2}$ [fb]
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Remarks

Change of scheme @NLO [Cacciari, Greco, Nason, 1998]

1. Use same running coupling and PDF set of the 5FS calculation
2. Add the extra factor (due to the conversion between $\overline{MS}$ and decoupling schemes) : $-\alpha_s \frac{2T_R}{3\pi} \ln \frac{\mu_R^2}{m^2} \sigma^{LO}_{q\bar{q}}$

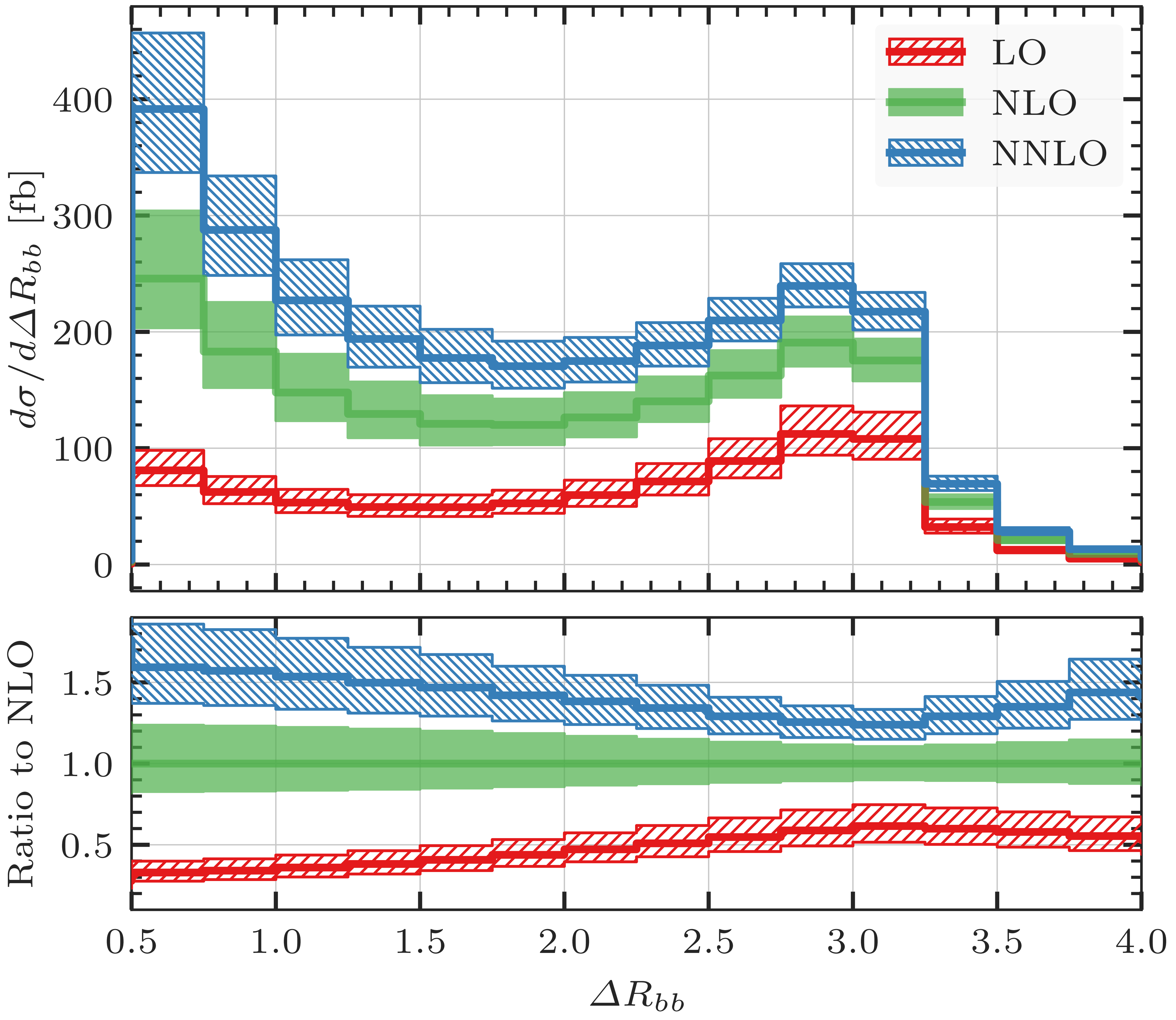
   No corrective term for pdfs at this order
3. Take the massless limit $m_b \to 0$

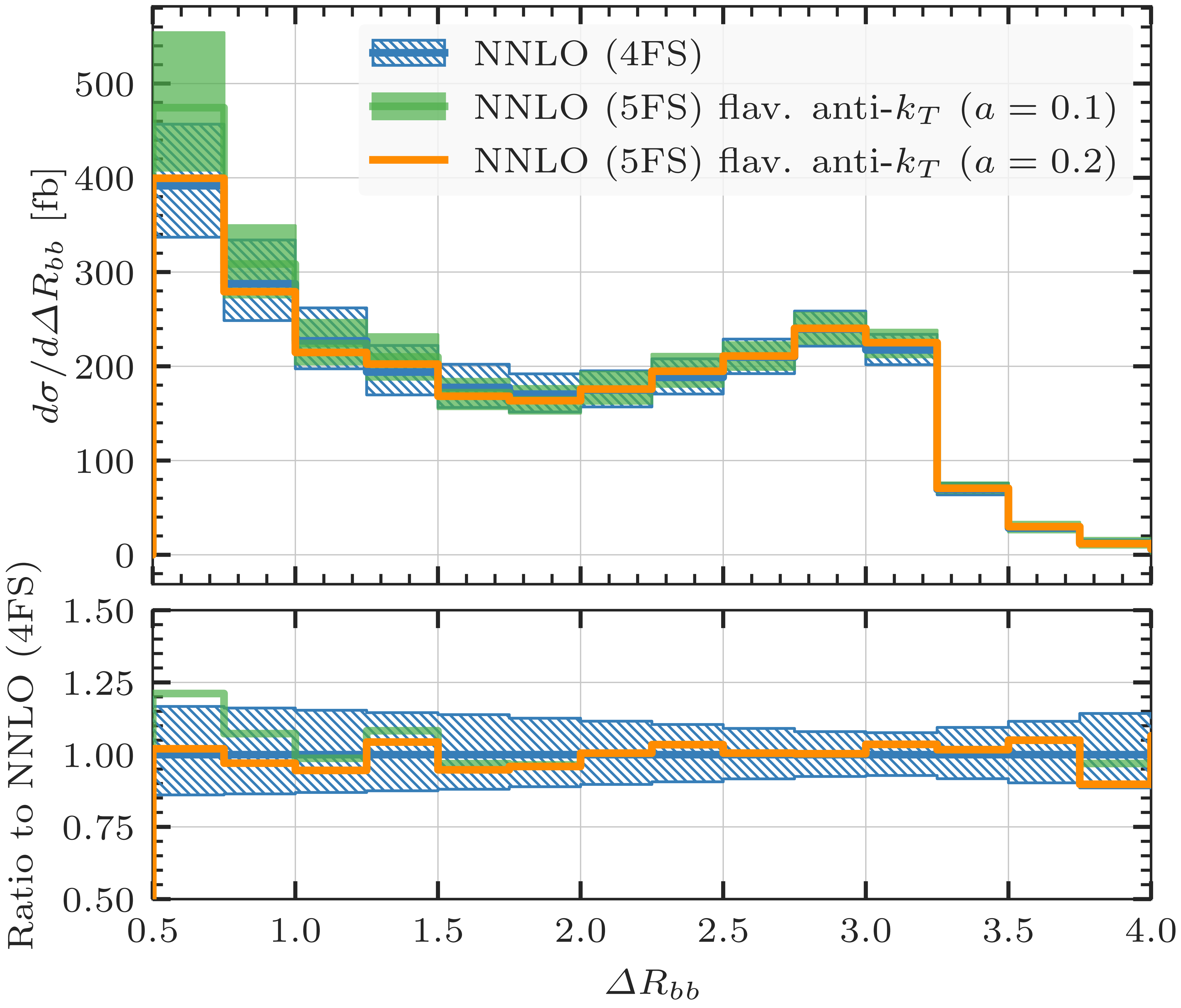
NLO 4FS: 468 fb $\xrightarrow{1,2}$ 481 fb $\xrightarrow{3}$ 493 fb

Comparison with HPPZ: jet clustering algorithms

Sizeable NNLO corrections which lead to a steeper slope at small ΔR_{bb} (where scale uncertainties are larger)

Good agreement between flavour and standard anti-k_T for the largest value $a = 0.2$





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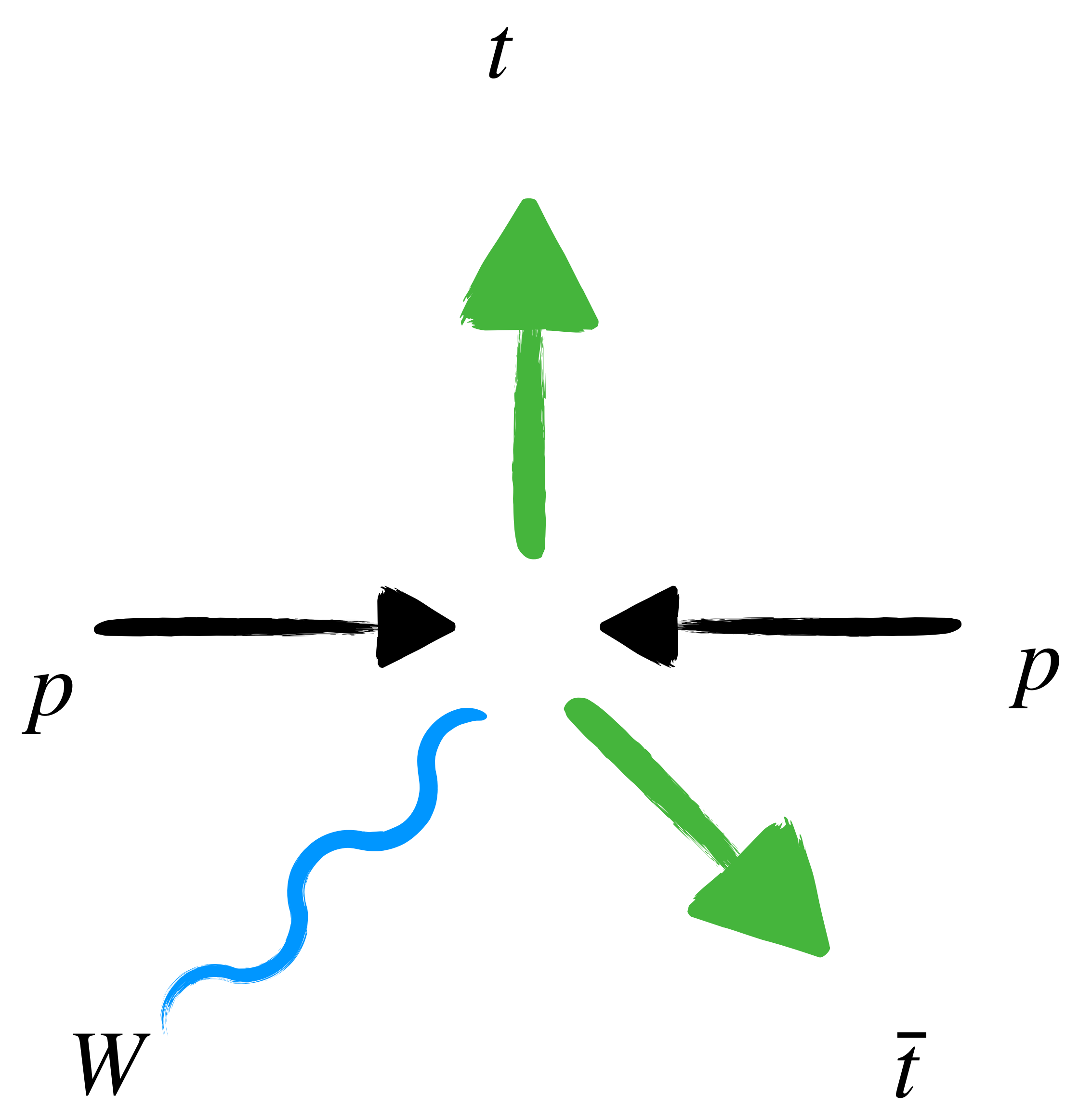
$t\bar{t}W$ (stable tops)



Quality of the approximations for $t\bar{t}W$

Observations

- Soft approximation first applied in $t\bar{t}H$ production: relatively large uncertainty but the corresponding hard virtual contribution represents a small fraction of the full NNLO QCD correction

  but the approximation works better for the $q\bar{q}$ channel!

- massification approach fully justified for $b\bar{b}W$

  does it still work for a very heavy quark as the top?

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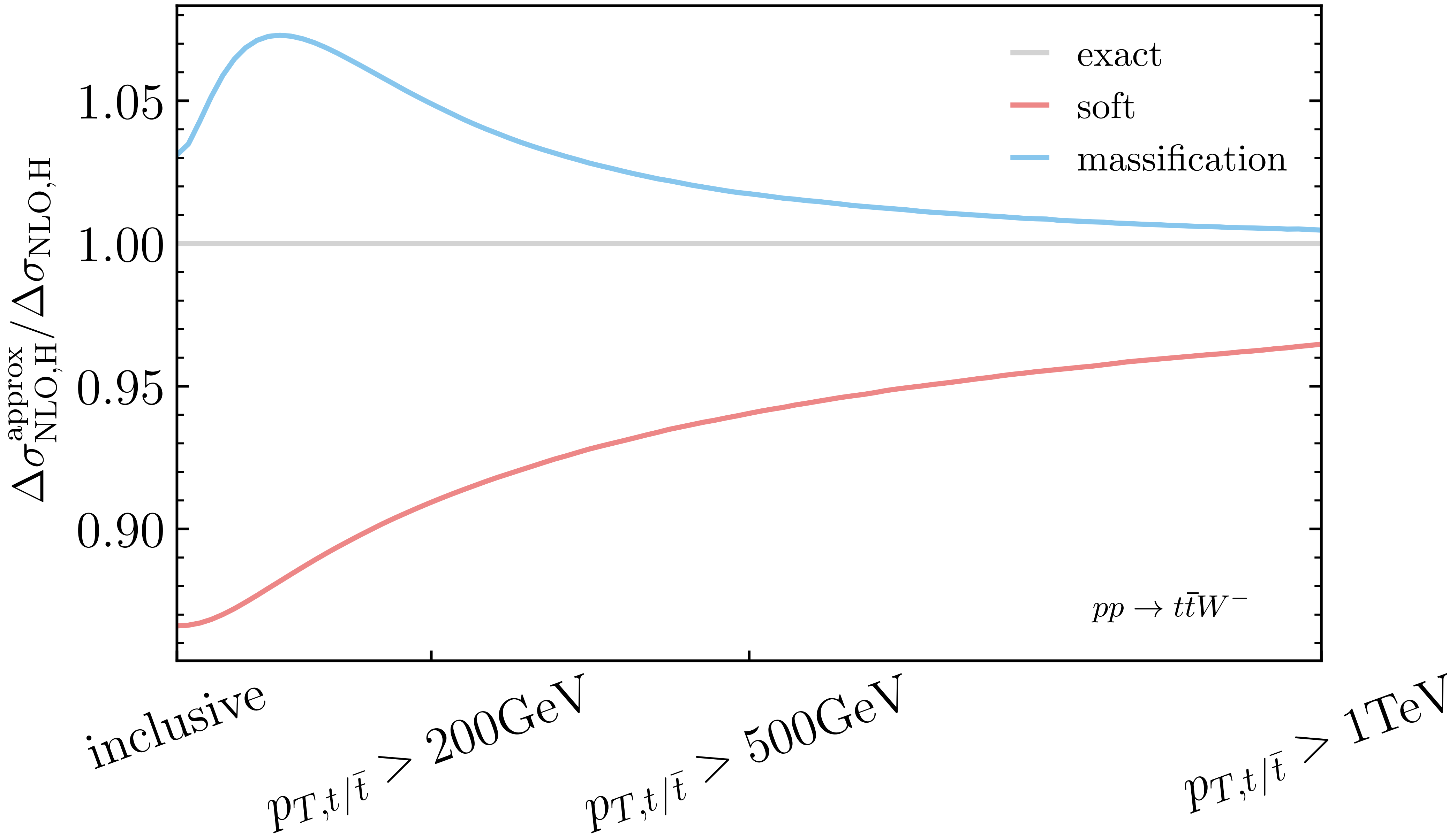
  does it still work for a very heavy quark as the top?

Analysis at NLO (comparison with the exact result!)



- **Both** approximations **provide a good estimate** of the exact one-loop contribution!

- Clear pattern: soft approximation tends to undershoot the exact result while massification tends to overshoot it

- Convergence in the asymptotic limit for high p_T top quarks where both approximation are expected to work

Quality of the approximations for $t\bar{t}W$

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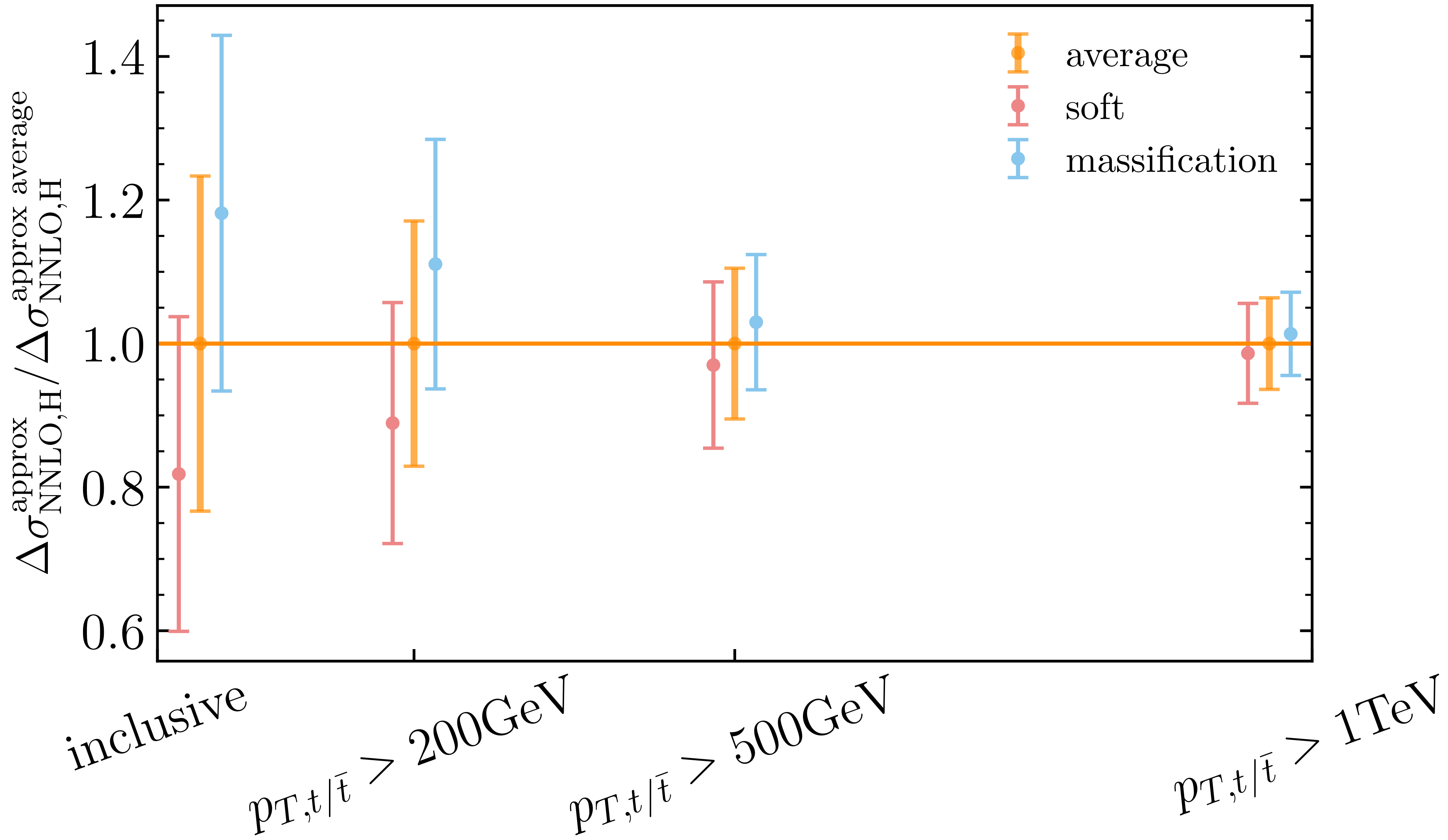

- **Similar pattern** as at NLO
- **Uncertainties** estimated as the maximum between what we obtain varying the subtraction scale $1/2 \le \mu_{\text{IR}}/Q \le 2$ and twice the NLO deviation
- Soft approximation and massification are consistent within their uncertainties!

Quality of the approximations for $t\bar{t}W$

Observations

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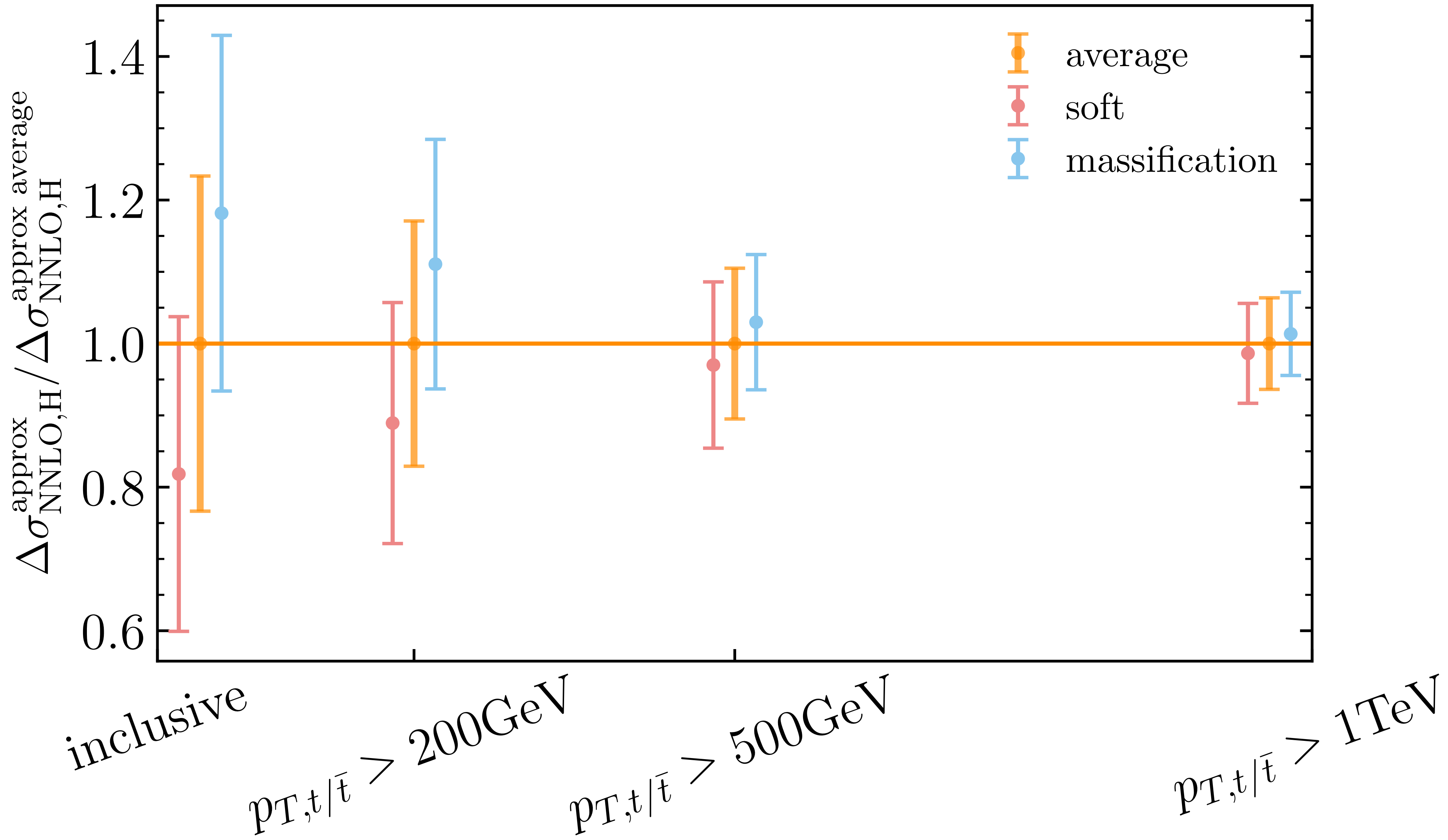
Analysis at NNLO



Best prediction obtained as average of the two with linear combination of uncertainties

Relatively large impact of two-loop virtual contribution: $\sim 7\,\%$ of NNLO cross section

FINAL UNCERTAINTY:

$\pm 1.8\,\%$ on σ_{NNLO}, $\pm 25\,\%$ on $\Delta\sigma_{\text{NNLO,H}}$

similar to what obtained in recent $2 \to 3$ in leading colour approximation

see e.g. [Abreu, De Laurentis, Ita, Klinkert, Page, Sotnikov 2023]

Setup

$$t\bar{t}W + X \ @ \sqrt{s} = 13\,\text{TeV}$$

EW	G_μ-scheme, CKM diagonal
pdf sets	`NNPDF31_nnlo_as_0118_luxqed`
α_s	3-loop running with $n_f = 5$ light quarks
scale variations	7-point $(1/2 < \mu_R/\mu_F < 2)$

Main input values

$$m_t = 172.2 \text{ GeV}$$

$$m_W = 80.385 \text{ GeV}$$

$$m_Z = 91.1876 \text{ GeV}$$

$$G_\mu = 1.6639 \times 10^{-5} \text{ GeV}^{-2}$$

Reference scale

$$\mu_0 = m_t + \frac{m_W}{2} \equiv \frac{M}{2}$$

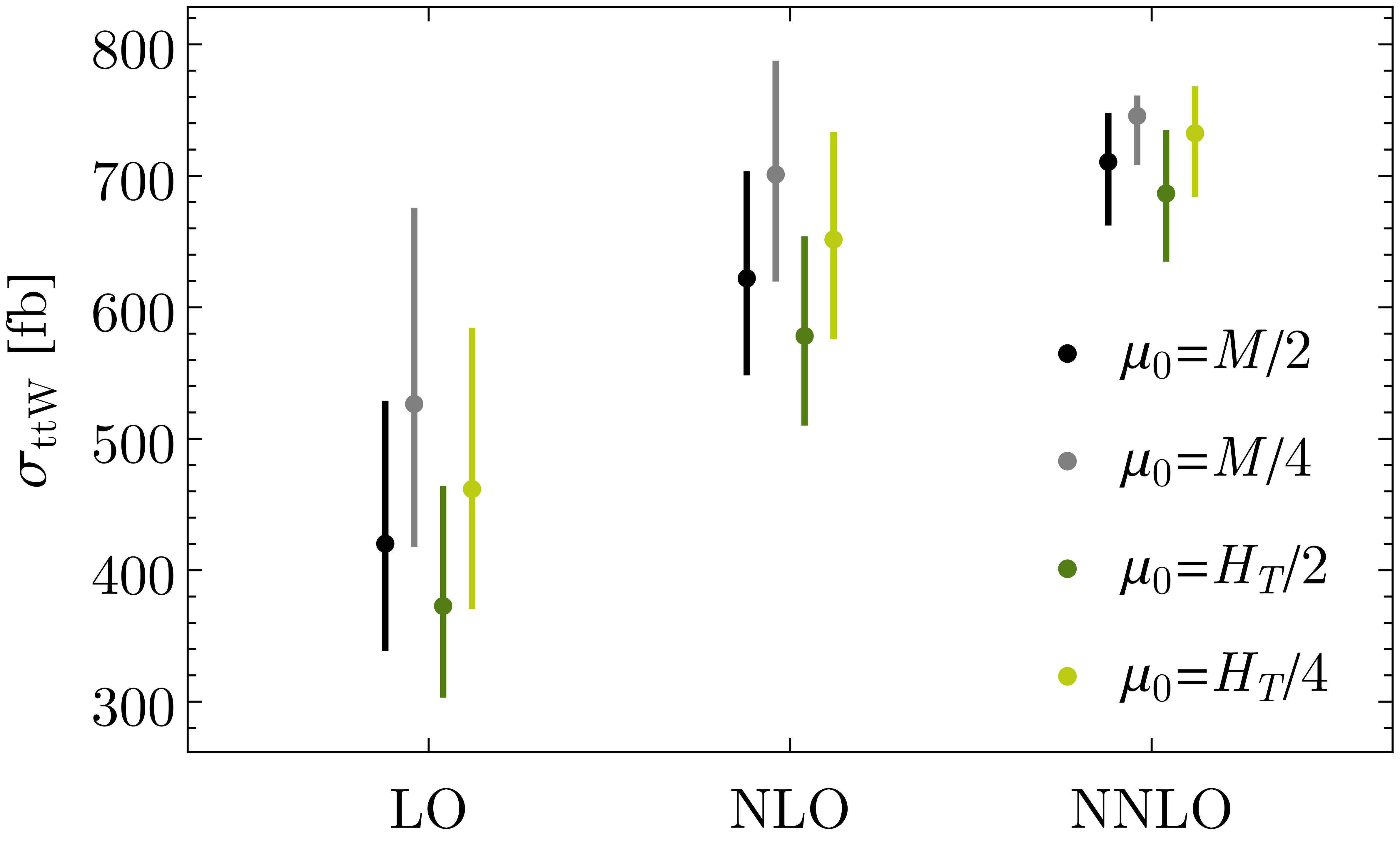
Other scales

$$\mu_0 = \frac{m_T(W) + m_T(t) + m_T(\bar{t})}{2} \equiv \frac{H_T}{2}$$

Scale variations and perturbative uncertainties

We estimate the **perturbative uncertainties** (due to missing higher order corrections) on the basis of

- scale variations
- behaviour of the perturbative series
- different scale choices: $M/2$, $M/4$, $H_T/2$, $H_T/4$
- breakdown of the corrections in different channels



First evidence of the convergence of the perturbative expansion starts at NNLO. Preference for smaller scale choices

The four predictions are fully consistent within their uncertainties

Scale variations and perturbative uncertainties

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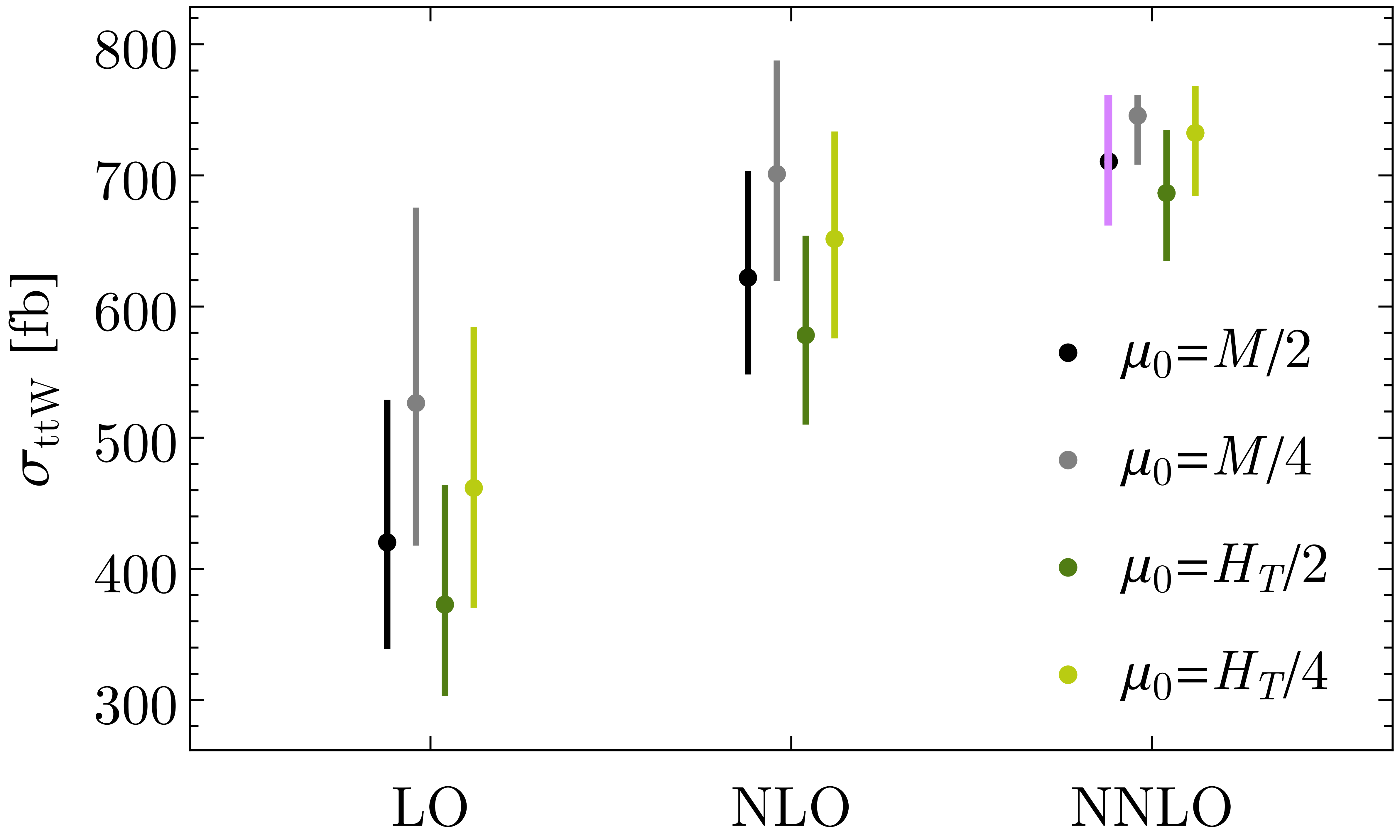


First evidence of the convergence of the perturbative expansion starts at NNLO. Preference for smaller scale choices

Using the predictions with $\mu_0 = M/2$ and **symmetrising its scale uncertainty**, we obtain an interval that almost encompasses also the predictions obtained with $\mu_0 = M/4$ and $\mu_0 = H_T/4$.

Scale variations and perturbative uncertainties

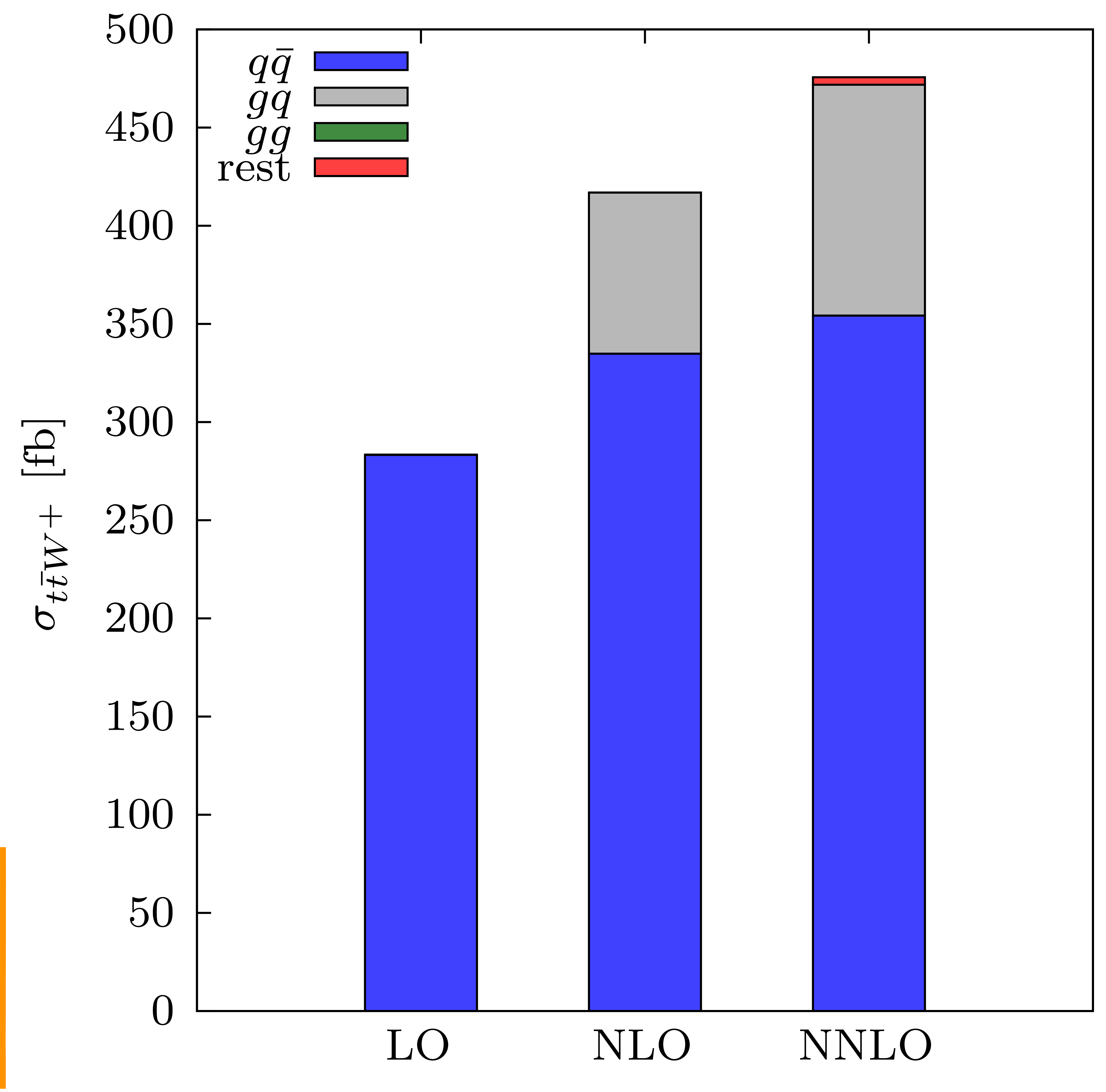
We estimate the **perturbative uncertainties** (due to missing higher order corrections) on the basis of

- scale variations
- behaviour of the perturbative series
- different scale choices: $M/2$, $M/4$, $H_T/2$, $H_T/4$
- **breakdown** of the corrections in **different channels**

No new large contribution from channels opening up at NNLO

NNLO corrections dominated by virtual and real correction to the gq channel (NLO accurate)

→ We use the central scale $\mu_0 = M/2$ and estimate perturbative uncertainties through **symmetrised scale variations**



$t\bar{t}W$: inclusive cross sections

	$\sigma_{t\bar{t}W^+}$ [fb]	$\sigma_{t\bar{t}W^-}$ [fb]	$\sigma_{t\bar{t}W}$ [fb]	$\sigma_{t\bar{t}W^+}/\sigma_{t\bar{t}W^-}$
$\mathrm{LO_{QCD}}$	$283.4^{+25.3\%}_{-18.8\%}$	$136.8^{+25.2\%}_{-18.8\%}$	$420.2^{+25.3\%}_{-18.8\%}$	$2.071^{+3.2\%}_{-3.2\%}$
$\mathrm{NLO_{QCD}}$	$416.9^{+12.5\%}_{-11.4\%}$	$205.1^{+13.2\%}_{-11.7\%}$	$622.0^{+12.7\%}_{-11.5\%}$	$2.033^{+3.0\%}_{-3.4\%}$
$\mathrm{NNLO_{QCD}}$	$475.2^{+4.8\%}_{-6.4\%} \pm 1.9\%$	$235.5^{+5.1\%}_{-6.6\%} \pm 1.9\%$	$710.7^{+4.9\%}_{-6.5\%} \pm 1.9\%$	$2.018^{+1.6\%}_{-1.2\%}$
$\mathrm{NNLO_{QCD}+NLO_{EW}}$	$497.5^{+6.6\%}_{-6.6\%} \pm 1.8\%$	$247.9^{+7.0\%}_{-7.0\%} \pm 1.8\%$	$745.3^{+6.7\%}_{-6.7\%} \pm 1.8\%$	$2.007^{+2.1\%}_{-2.1\%}$
ATLAS	$585^{+6.0\%+8.0\%}_{-5.8\%-7.5\%}$	$301^{+9.3\%+11.6\%}_{-9.0\%-10.3\%}$	$890^{+5.6\%+7.9\%}_{-5.6\%-7.9\%}$	$1.95^{+10.8\%+8.2\%}_{-9.2\%\ -6.7\%}$
CMS	$553^{+5.4\%+5.4\%}_{-5.4\%-5.4\%}$	$343^{+7.6\%+7.3\%}_{-7.6\%-7.3\%}$	$868^{+4.6\%+5.9\%}_{-4.6\%-5.9\%}$	$1.61^{+9.3\%+4.3\%}_{-9.3\%-3.1\%}$

Best prediction

Uncertainty associated to the approximation of the 2-loop virtual amplitude

Impact of radiative corrections

- Large positive NLO QCD corrections: $+50\,\%$
- Moderate positive NNLO QCD corrections: $+14-15\,\%$
- Relatively sizeable positive corrections from all LO and NLO contributions at $O(\alpha^3)$, $O(\alpha_S^2\alpha^2)$, $O(\alpha\alpha^3)$, $O(\alpha^4)$: $+5\,\%$
- The ratio $\sigma_{t\bar{t}W^+}/\sigma_{t\bar{t}W^-}$ is rather stable and only slightly decreases increasing the perturbative order

$t\bar{t}W$: inclusive cross sections

Best prediction

	$\sigma_{t\bar{t}W^+}$ [fb]	$\sigma_{t\bar{t}W^-}$ [fb]	$\sigma_{t\bar{t}W}$ [fb]	$\sigma_{t\bar{t}W^+}/\sigma_{t\bar{t}W^-}$
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Uncertainty associated to the approximation of the 2-loop virtual amplitude

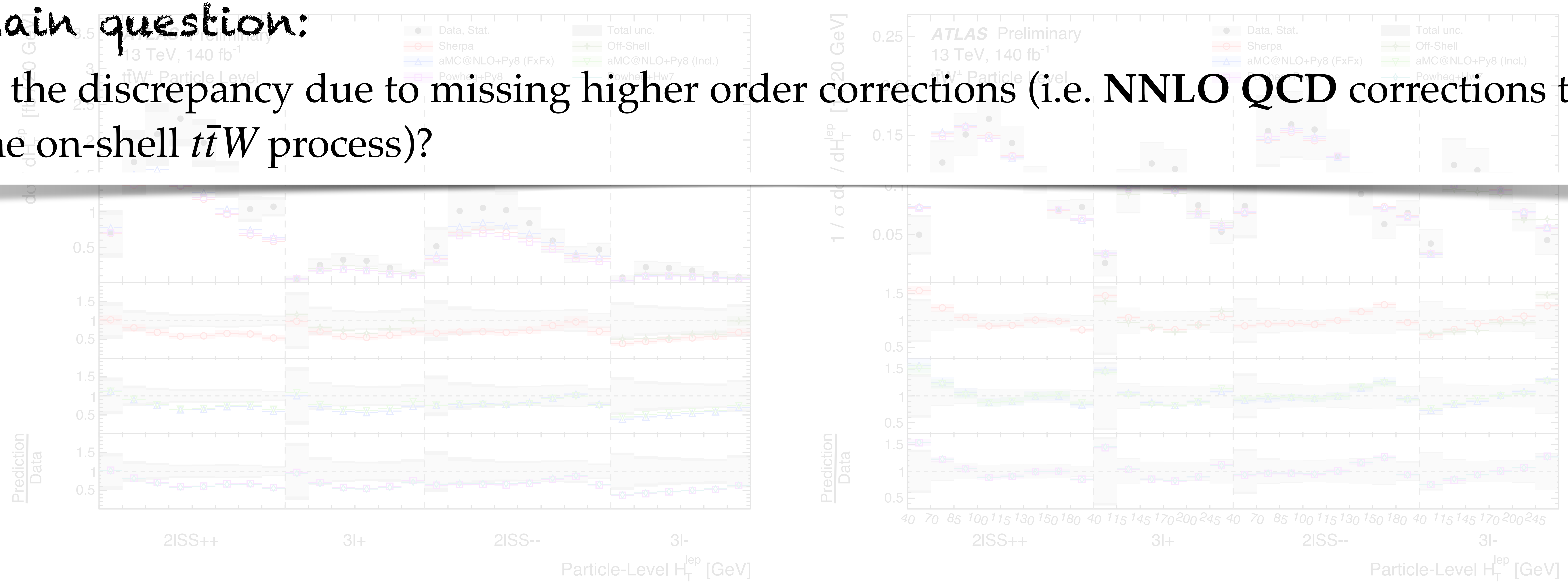
Other uncertainties

- PDF uncertainties: $\pm 1.8\,\%$ ($\pm 1.8\,\%$ ratio) computed with new MATRIX+PINEAPPL implementation [S. Devoto, T. Jezo, S. Kallweit and C. Schwan in preparation]
- α_s uncertainties (half the difference between pdf sets for $\alpha_s(m_Z) = 0.118 \pm 0.001$) $\pm 1.8\,\%$ (negligible for ratio)
- Systematics of the q_T-subtraction method ($r_{\mathrm{cut}} \to 0$ extrapolation) are negligible

State of the art: data-theory comparison

- ATLAS measured also **differential distributions**, finding a disagreement in the overall normalisation consistent with the inclusive measurement result

- The latest off-shell fixed-order predictions give indications that this disagreement **is not predominantly due to missing singly-resonant contributions** which are not included in the reference on-shell predictions



Main question:

Is the discrepancy due to missing higher order corrections (i.e. **NNLO QCD** corrections to the on-shell $t\bar{t}W$ process)?

$t\bar{t}W$: updated comparison with data

The inclusion of newly computed NNLO QCD corrections leads to

- moderately higher rates
- reduction of perturbative uncertainties

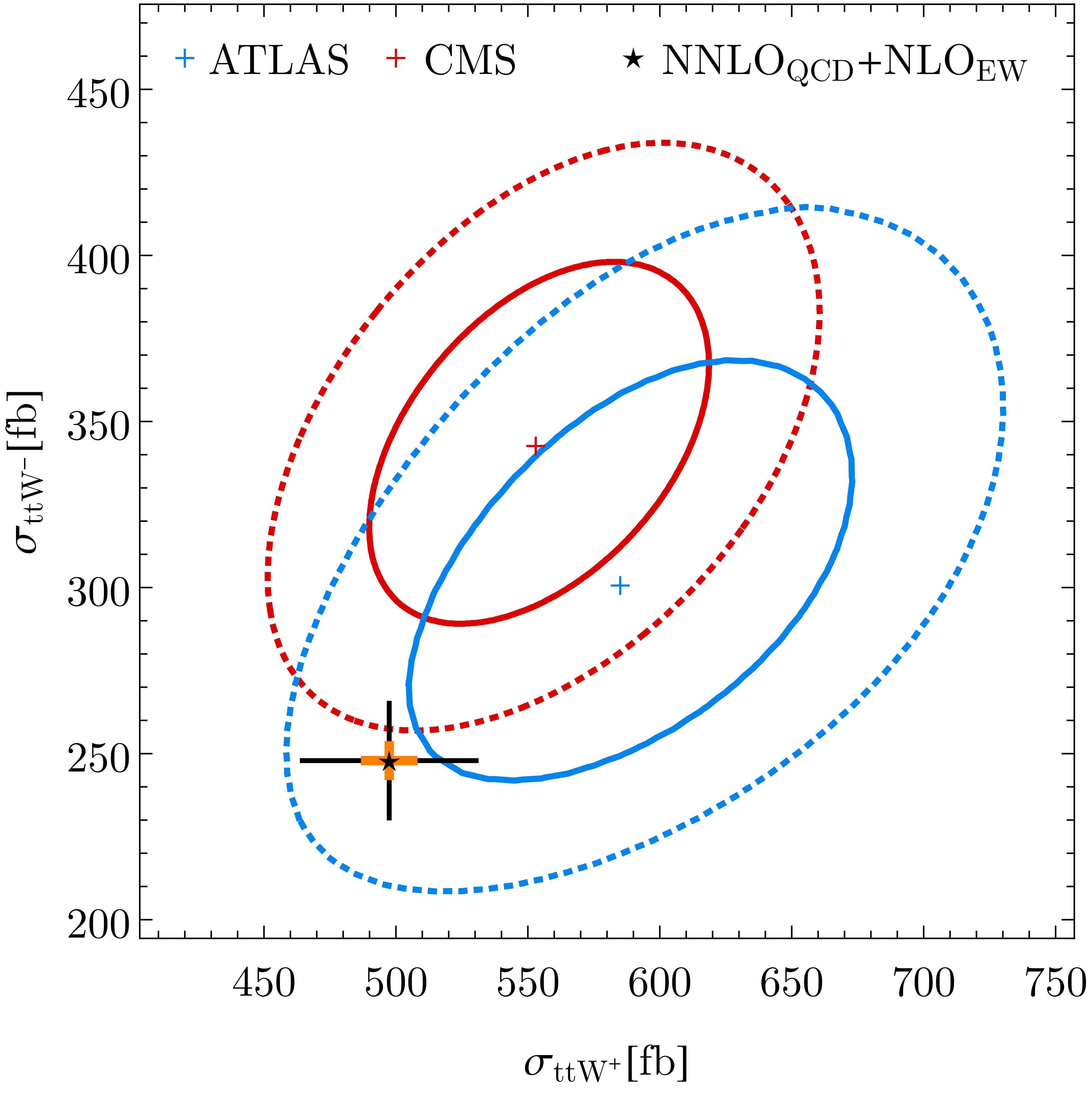
Comparing to the NLO QCD + EW prediction supplemented with FxFx multijet merging, we find good agreement within the quoted uncertainties

$$\sigma_{t\bar{t}W} = 745.3^{+6.7\%}_{-6.7\%}$$ Our best prediction

$$\sigma^{FxFx}_{t\bar{t}W} = 722.3^{+9.7\%}_{-10.8\%}$$

Tension stays at the level of

1σ (ATLAS) - 2σ (CMS)



Conclusions

We have presented the first calculation of the NNLO QCD radiative corrections to $b\bar{b}W$ with massive bottom quark and to (on-shell) $t\bar{t}W$ based on

- the q_T subtraction formalism for the production of **a colored massive final state + a color singlet system** (thanks to the progress in the calculation of the corresponding soft function)
- a **reliable approximation of the missing two-loop virtual amplitude** based on two factorization approaches: the massification procedure and the soft W boson approximation.

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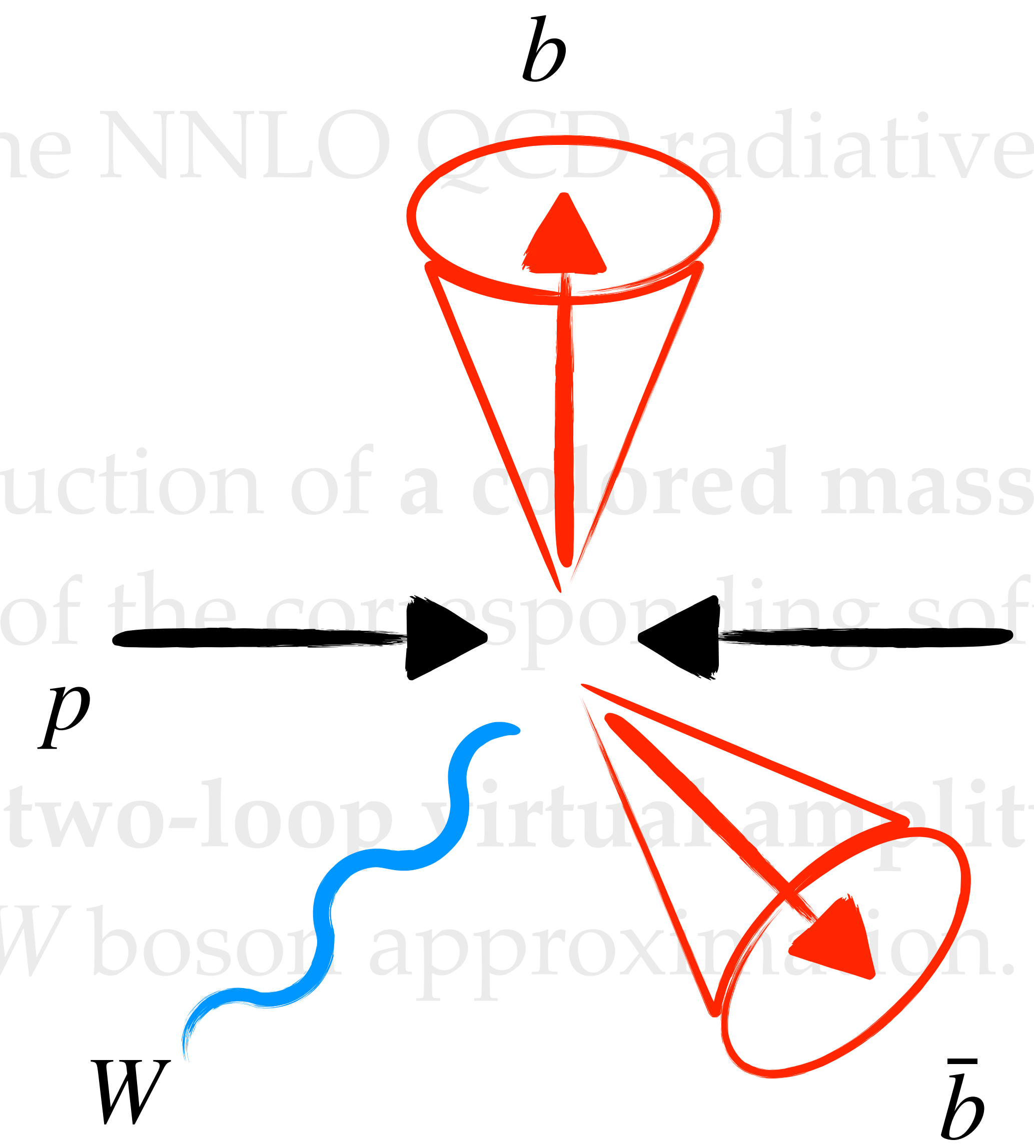

$b\bar{b}W$: flavor tagging is non-trivial when including higher-order corrections in perturbation theory

- thanks to the bottom mass, we can build flavored jets adopting the standard anti-k_T algorithm, reducing unfolding corrections for data-theory comparisons
- good agreement with the 5-flavor massless calculation
- our massive calculation can be matched to a parton shower within the MiNNLO$_{\text{PS}}$ formalism

[Monni, Nason, Re, Wiesemann, Zanderighi 2020]
[Mazzitelli, Monni, Nason, Re, Wiesemann, Zanderighi 2020]

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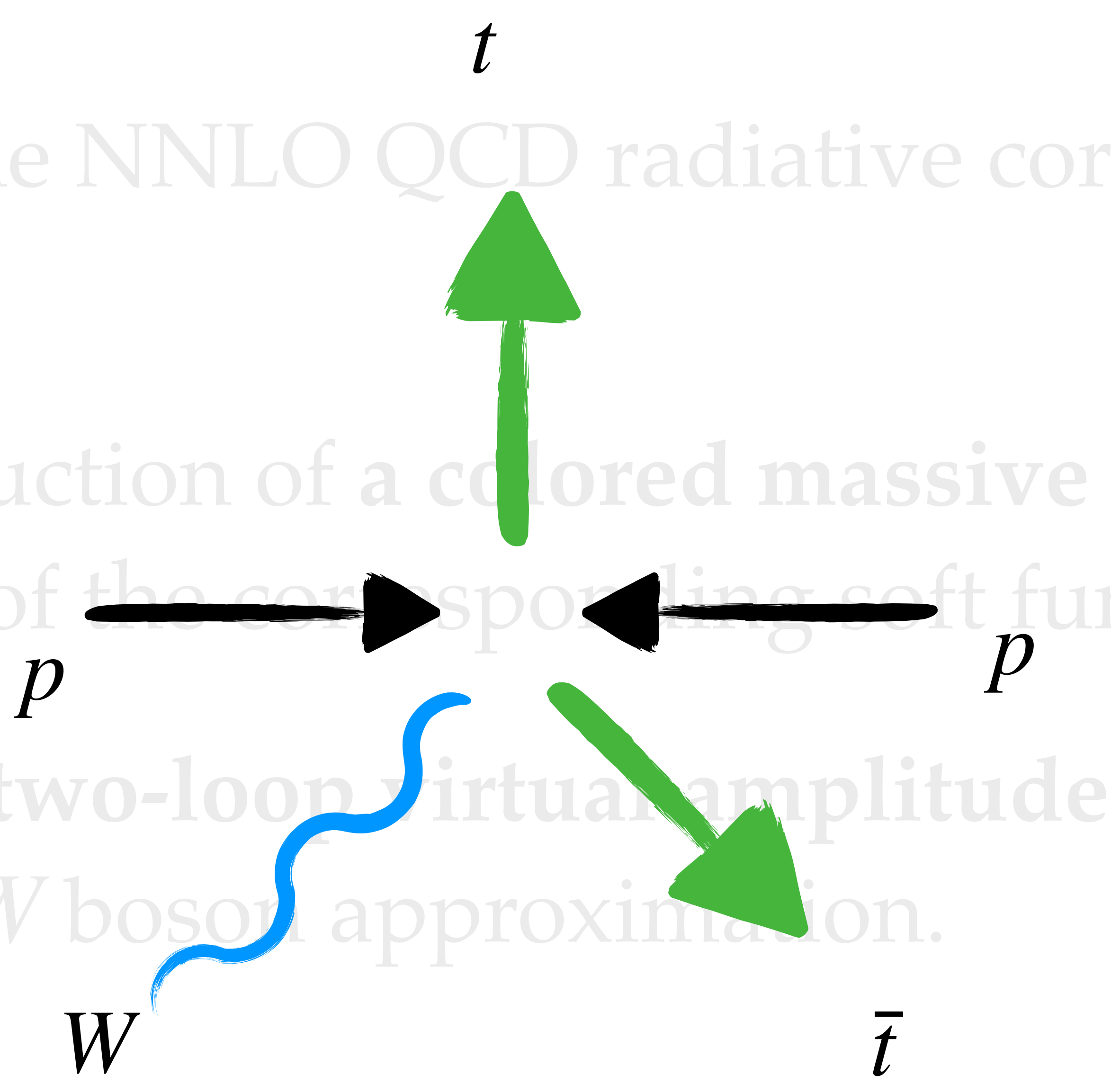

$t\bar{t}W$ rates @NNLO QCD+NLO EW at the LHC

- The two-loop virtual contribution is **not negligible** (7% of σ_{NNLO}), and it is estimated with an uncertainty of 25%. This translates into an uncertainty of 1.8% on the NNLO fiducial cross section, which is substantially smaller than the perturbative uncertainties
- NNLO QCD radiative corrections lead to **moderately higher rates** (around +15%) and **reduce the perturbative uncertainties** (from 13% to 7%)
- **the tension with data stays at the $1\sigma - 2\sigma$ level**

BACKUP

Application of soft approximation: $t\bar{t}H$

[Catani, Devoto, Grazzini, Kallweit, Mazzitelli, Savoini, 2022]

In the case of soft H emission, we have a similar factorisation formula (for soft scalars)

$$|\mathscr{M}^{[p,k]}_{t\bar{t}H}> \simeq F(\alpha_s(\mu)R); m_t/\mu_R) \times J(k) \times |\mathscr{M}^{[p]}_{t\bar{t}}>$$

Normalisation correction factor beyond LO factorisation Calculable in perturbation theory

Eikonal factor

Application of soft approximation: $t\bar{t}H$

[Catani, Devoto, Grazzini, Kallweit, Mazzitelli, Savoini, 2022]

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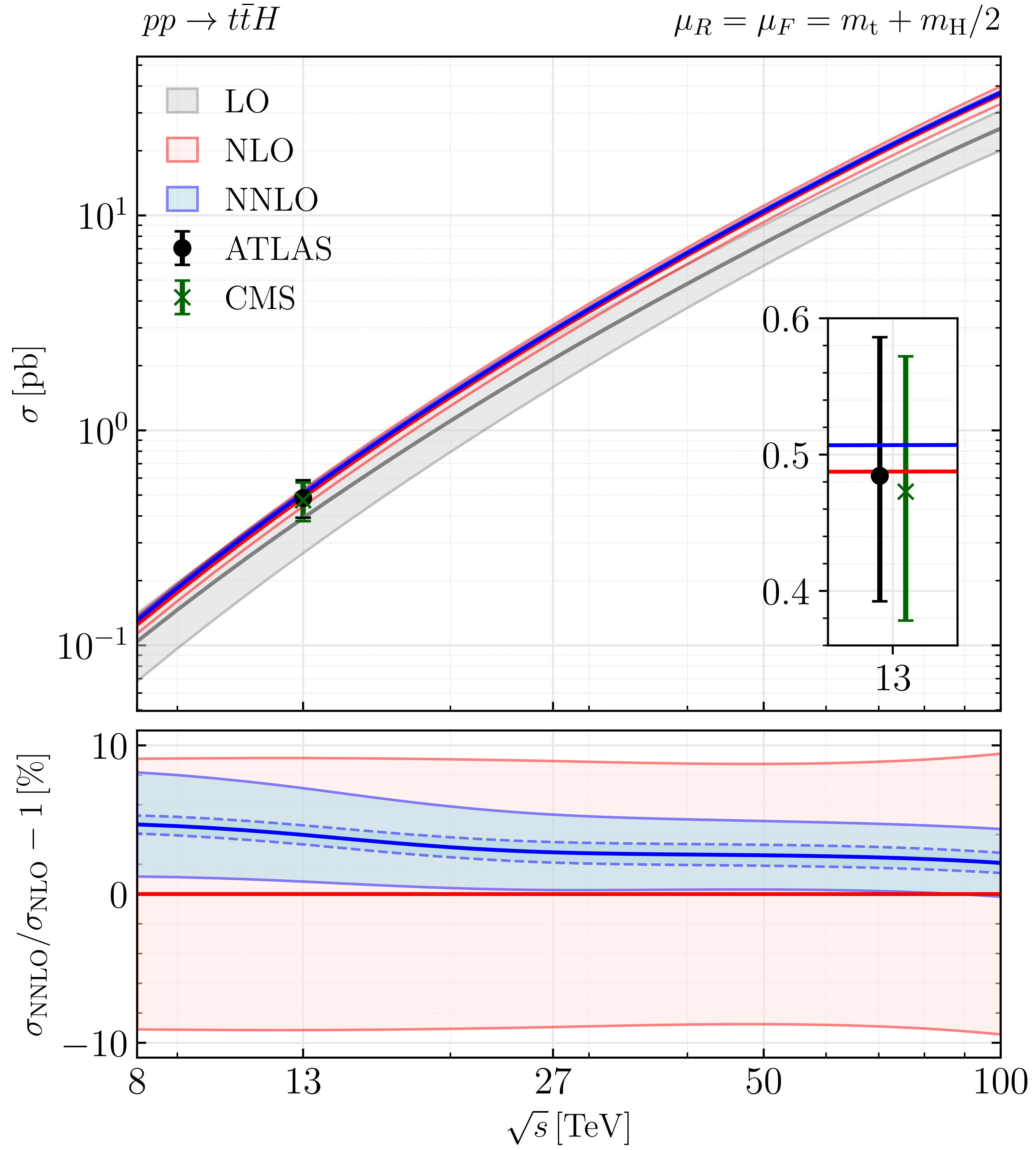
Successfully applied to $t\bar{t}H$ production at hadron colliders

- Careful assessment of the uncertainties associated to the soft approximation
  $\sim 100\,\%$ uncertainty in gg, $\sim 15\,\%$ uncertainty in $q\bar{q}$
  it works better for the $q\bar{q}$ channel

- Relative size of the hard contribution $\Delta\sigma_{\mathrm{NNLO,H}}$ wrt the σ_{LO}
  $\sim 1\,\%$ in gg, $\sim 3\,\%$ in $q\bar{q}$

FINAL UNCERTAINTY:
$\pm 0.6\,\%$ on σ_{NNLO}, $\pm 15\,\%$ on $\Delta\sigma_{\mathrm{NNLO}}$

subdominant wrt scale variations!



Soft H approximation

$$|\mathcal{M}^{[p,k]}_{t\bar{t}H} > \simeq F(\alpha_s(\mu)R); m_t/\mu_R) \times J(k) \times |\mathcal{M}^{[p]}_{t\bar{t}} >$$

$$J(k) = \sum_i \frac{m_t}{v}\frac{m_t}{p_i \cdot k}$$

The perturbative function $F\left(\alpha_S(\mu_R); m_t/\mu_R\right)$ can be extracted from the soft limit of the scalar form factor of the heavy quark

[Bernreuther et al, 2005] [Blümlein et al, 2017]

$$F(\alpha_s(\mu)R); m_t/\mu_R) = 1 + \frac{\alpha_S}{2\pi}(-3C_F) + \left(\frac{\alpha_S}{2\pi}\right)^2 \left(\frac{33}{4}C_F^2 - \frac{185}{12}C_F C_A + \frac{13}{6}C)F(n_l+1) - 6C_F\beta_0 \ln\frac{\mu_R^2}{m_t^2}\right) + \mathcal{O}\left(\alpha_S^3\right)$$

Alternatively, it can be derived by using Higgs low-energy theorems

see e.g. [Kniehl, Spira, 1995]

$t\bar{t}H$: quality of the soft H approximation

At LO, the soft H approximation overestimates the exact result by

- gg channel: a factor of 2.3 at $\sqrt{s} = 13$ TeV and a factor of 2 at $\sqrt{s} = 100$ TeV
- $q\bar{q}$ channel: a factor of 1.11 at $\sqrt{s} = 13$ TeV and a factor of 1.06 at $\sqrt{s} = 100$ TeV

	$\sqrt{s} = 13$ TeV		$\sqrt{s} = 100$ TeV	
σ [fb]	gg	$q\bar{q}$	gg	$q\bar{q}$
σ_{LO}	261.58	129.47	23055	2323.7
$\Delta\sigma_{\mathrm{NLO,H}}$	88.62	7.826	8205	217.0
$\Delta\sigma_{\mathrm{NLO,H}}\vert_{\mathrm{soft}}$	61.98	7.413	5612	206.0
$\Delta\sigma_{\mathrm{NNLO,H}}\vert_{\mathrm{soft}}$	$-2.980(3)$	2.622(0)	$-239.4(4)$	65.45(1)

At NLO, the approximation performs better than at LO because of the LO re-weighting

$t\bar{t}H$: quality of the soft H approximation & uncertainties

Uncertainties estimates by

- varying the momentum mapping used to absorb the recoil of the H boson
- varying the infrared μ_{IR} subtraction scale at which the $H^{(2)}$ is evaluated from the central value $m_{t\bar{t}H}$ to $m_{t\bar{t}H}/2$ and $2m_{t\bar{t}H}$
  When evaluating $H^{(2)}$ at a subtraction scale different from the central value, we added the contribution stemming from the running from the μ_{IR} to $m_{t\bar{t}H}$ using the exact matrix elements

Uncertainties estimated by multiplying by a **tolerance factor of 3** the deviations found at NLO:
30% for the gg channel and 5% for the $q\bar{q}$ channel.
This encompasses the uncertainties associated to the variations above

Finally uncertainties obtained by combining linearly the gg and the $q\bar{q}$ channel
0.6% on σ_{NNLO}

Flavour aware jet algorithms: flavour k_T

[Banfi, Salam, Zanderighi, 2006]

Standard k_T algorithm

$$d_{ij} = \min\left(k_{T,i}^2, k_{T,j}^2\right) R_{ij}^2, \quad d_{iB} = k_{T,i}^2$$

condition 1 automatically satisfied

Flavour aware k_T algorithm (usually $\alpha = 2$):

flavour information available at each step of the clustering procedure

$$d_{ij}^{(F)} = R_{ij}^2 \times \begin{cases} \left[\max\left(k_{T,i}^2, k_{T,j}^2\right)\right]^{\alpha} \left[\min\left(k_{T,i}^2, k_{T,j}^2\right)\right]^{2-\alpha}, & \text{if softer of } i,j \text{ is flavoured} \\ \min\left(k_{T,i}^2, k_{T,j}^2\right), & \text{if softer of } i,j \text{ is flavourless} \end{cases}$$

this ensures condition 2 among final state protojets, as soft flavoured quark-anti-quark pair clusters first

Flavour aware jet algorithms: flavour k_T

[Banfi, Salam, Zanderighi, 2006]

Standard k_T algorithm

$$d_{ij} = \min\left(k_{T,i}^2, k_{T,j}^2\right) R_{ij}^2, \quad d_{iB} = k_{T,i}^2$$

Flavour aware k_T algorithm (usually $\alpha = 2$):

flavour information available at each step of the clustering procedure

Also beam distance problematic:

a soft flavoured parton can be identified as a protojet and removed from the list)

$$d_{iB(\bar{B})}^{(F)} = R_{ij}^2 \times \begin{cases} \left[\max\left(k_{T,i}^2, k_{T,B(\bar{B})}^2\right)\right]^{\alpha} \left[\min\left(k_{T,i}^2, k_{T,B(\bar{B})}^2\right)\right]^{2-\alpha}, & \text{if } i \text{ is flavoured} \\ \min\left(k_{T,i}^2, k_{T,B(\bar{B})}^2\right), & \text{if } i \text{ is flavourless} \end{cases}$$

$$k_{T,B}(y) = \sum_i k_{T,i}\left(\Theta(y_i - y) + \Theta(y - y_i)e^{y_i - y}\right) \qquad k_{T,\bar{B}}(y) = \sum_i k_{T,i}\left(\Theta(y - y_i) + \Theta(y_i - y)e^{y - y_i}\right)$$

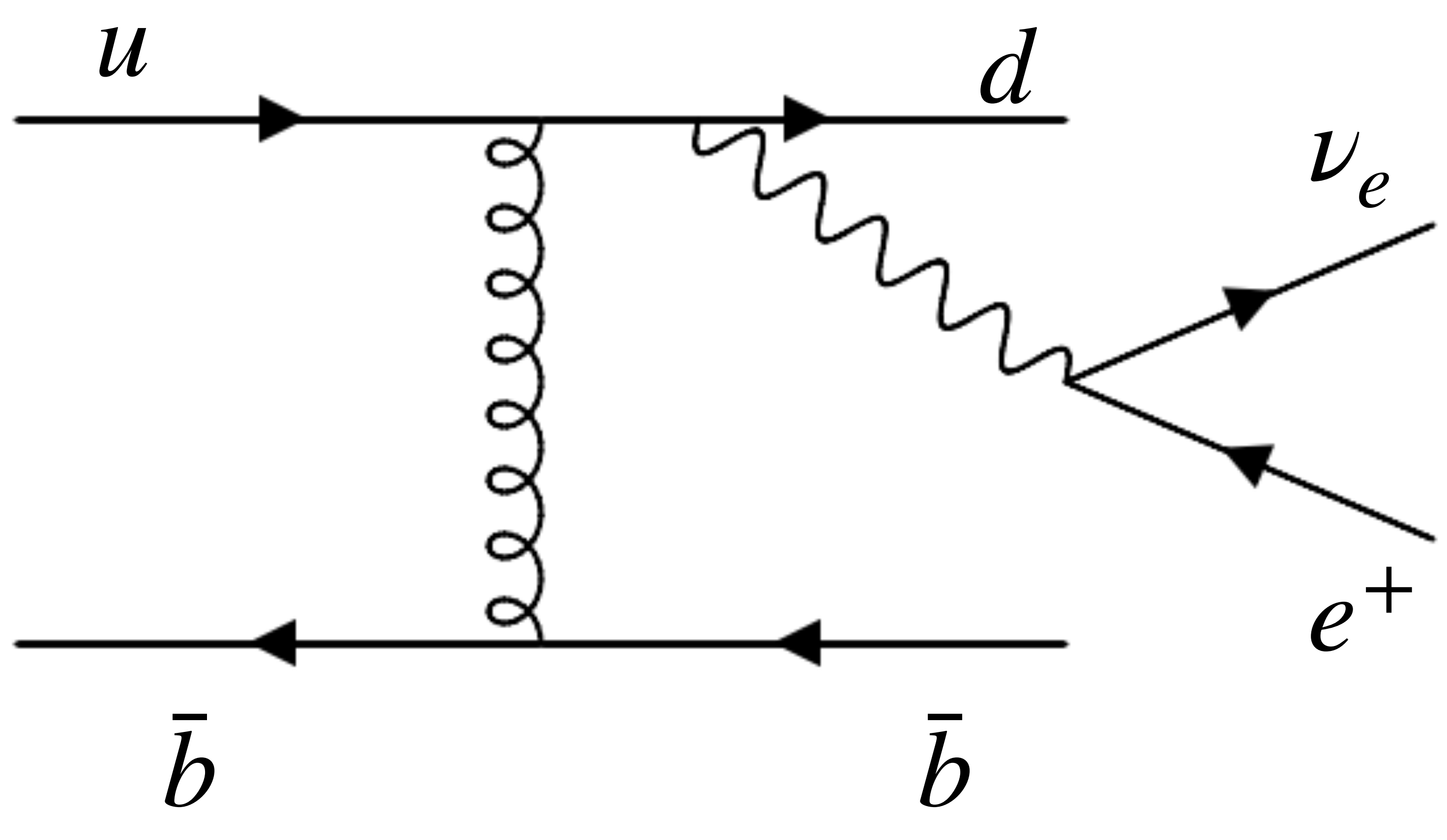
Ingredients: two-loop massless amplitudes [Abreu, Febres-Cordero, Ita, Klinkert, Page, Sotnikov, 2022]

Two-loop helicity virtual amplitudes for **W boson and four partons available in the Leading-colour approximation (LCA)**

- analytical expressions obtained within the framework of numerical unitary (using numerical samples)
- the results are expressed in terms of a basis of **one-mass pentagon functions** [Chicherin, Sotnikov, Zoia 2021]
- **off-shell W boson** including its leptonic decay
- publicly available http://www.hep.fsu.edu/~ffebres/W4partons
- **analytical expressions of the one-loop amplitudes up to** $\mathcal{O}(\epsilon^2)$ available in LCA

Some complications

- Amplitudes provided as analytical expressions that can be processed in Mathematica; **this is not suitable for on-the-fly numerical evaluation** for Monte Carlo integration
- Rather long algebraic expressions akin to numerical round-off errors
- Reference process is $u\bar{b} \to \bar{b}de^+\nu_e$. Initial-final state crossing involves in general **analytic continuation**



WQQAmp: a massive C++ implementation

[Buonocore, Rottoli, Savoini, https://gitlab.com/lrottoli/WQQAmp]

LCA and Massification

- we have carried out the massification procedure in LCA to explicitly check the cancellation of the poles
- however, in this way we are artificially introducing **spurious miscancellation** between real and virtual contributions
- moreover, the terms introduced with the massification, being enhanced by large logarithms of μ^2/m^2, are generally the dominant contributions and the difference between Full Colour and Leading Colour can be sizeable $C_F/(N_C/2) \sim 0.89$ and $(C_F/(N_C/2))^2 \sim 0.8$

Retain massification contributions at full colour whenever possible!

$$\mathcal{M}_{(2)}^{Wbb,(m)} = \mathcal{M}_{(2)}^{Wbb,(m=0)} + Z_{[q]}^{(1)}\mathcal{M}_{(1)}^{Wbb,(m=0)} + Z_{[q]}^{(2)}\mathcal{M}_{(0)}^{Wbb,(m=0)}$$

$$Z_{[q]}^{(1),2}M_{(1)}^{Wbb,(m=0),-2} + Z_{[q]}^{(1),1}M_{(1)}^{Wbb,(m=0),-1} + Z_{[q]}^{(1),0}M_{(1)}^{Wbb,(m=0),0} + Z_{[q]}^{(1),-1}M_{(1)}^{Wbb,(m=0),1} + Z_{[q]}^{(1),-2}M_{(1)}^{Wbb,(m=0),2}$$

with **OpenLoops2**

these contributions cancel in the final remainder

WQQAmp: a massive C++ implementation

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Dealing with the complications

One-Loop amplitudes: $\mathcal{O}(1000)$ source files of small-moderate size (< 100 Kb)

- algebraic expressions (rational function of the invariants) simplified using MultiVariate Apart [Heller, von Manteuffel, 2021] at the level of Mathematica before exporting them
- automatised generation of C++ source files from the Mathematica expressions; very simple optimisation introducing abbreviations (https://github.com/lecopivo/OptimizeExpressionToC)

Two-Loop amplitudes: $\mathcal{O}(3000)$ source files of moderate size (< 250 Kb)

- algebraic expressions **too long and complex**; no pre-simplification step
- breakdown of each expression in small blocks (we found this step to be crucial)
- automatised generation of C++ source files for each block
- handling of **numerical instabilities a posteriori with a simple rescue system** (at integration stage)

Crossing

- simple permutation of the momenta in the algebraic coefficients
- the action of the permutation transforms the **pentagon functions** into each others, no need for analytic continuation. All permutations available in a Mathematica script [Chicherin, Sotnikov, Zoia 2021]

WQQAmp: a massive C++ implementation

[Buonocore, Rottoli, Savoini, https://gitlab.com/lrottoli/WQQAmp]

Validation and checks

- two-loop massless amplitudes (stability)
  the C++ (double precision) code reproduces the massless results obtained with (quad precision) Mathematica for different phase space points and crossing of the amplitudes within the single floating-precision (7-9 digits), apart for some points where it badly fails (simple **rescue system**)

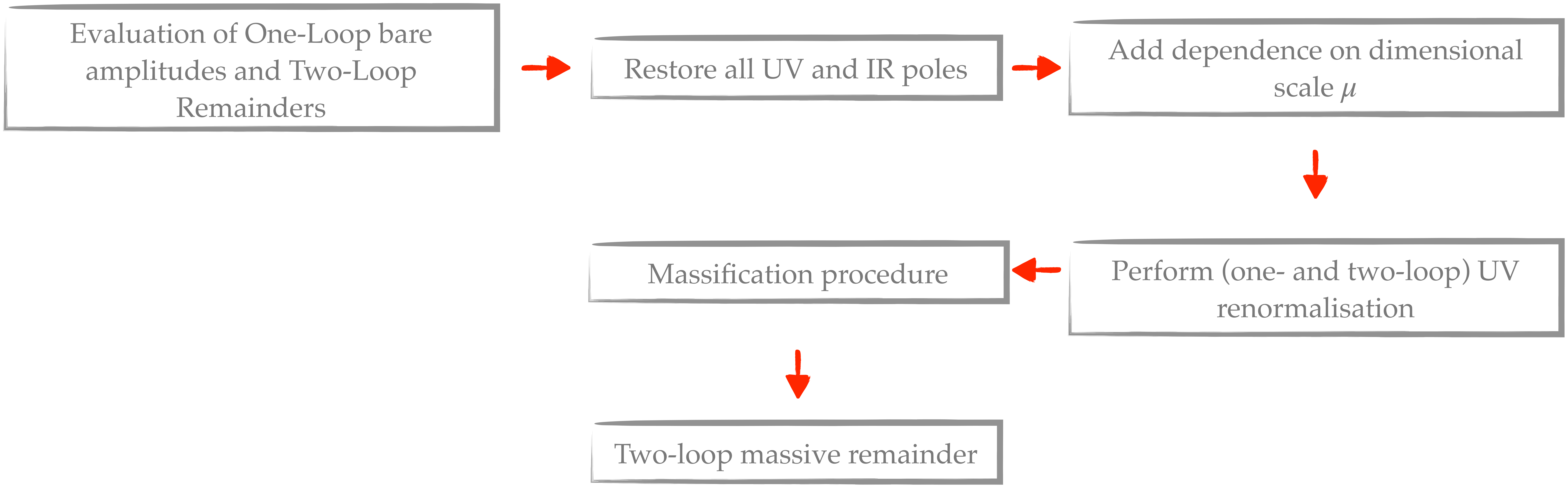
- one-loop amplitudes in LCA
  we have tested both the **massless and massive** amplitudes against the **independent implementation available in MCFM**, which allows to extract the LCA

- Poles cancelled!
  the IR singularities of the massive amplitude agree with the ones predicted in [Ferroglia, Neubert, Pecjac, Yang, 2009] (in LCA)

WQQAmp: a massive C++ implementation

[Buonocore, Rottoli, Savoini, https://gitlab.com/lrottoli/WQQAmp]

WORKFLOW in a NUTSHELL



$\mathcal{O}(4s)$ **for phase space**

Setup

$$W + 2\, b_{(\text{jet})} + X \;@\; \sqrt{s} = 13.6\,\text{TeV}$$

α_s and PDF scheme	4-flavour scheme (4FS), m_b=4.92 GeV
EW	G_μ-scheme, CKM diagonal
Jet clustering algorithm	anti-k_T (and k_T) algorithm with R = 0.4
pdf sets	`NNPDF30_as_0118_nf_4` (LO) `NNPDF31_as_0118_nf_4` (NLO, NNLO)

SETUP

- **fiducial**: inspired by ATLAS $VH(\to b\bar{b})$ **boosted** analysis [ATLAS:arXiv:2007.02873]

$p_{T,\ell} > 25$ GeV $\quad |\eta_\ell| < 2.5 \quad p_T^W > 150\,\text{GeV}$

Jet selection

$p_{T,j} > 20$ GeV and $|\eta_\ell| < 2.5$ or

$p_{T,j} > 30$ GeV and $2.5 < |\eta_\ell| < 4.5$

Requirements on b-tagged jets

$n_b = 2, \quad p_{T,b_1} > 45$ GeV, $\quad 0.5 < \Delta R_{bb} < 2$

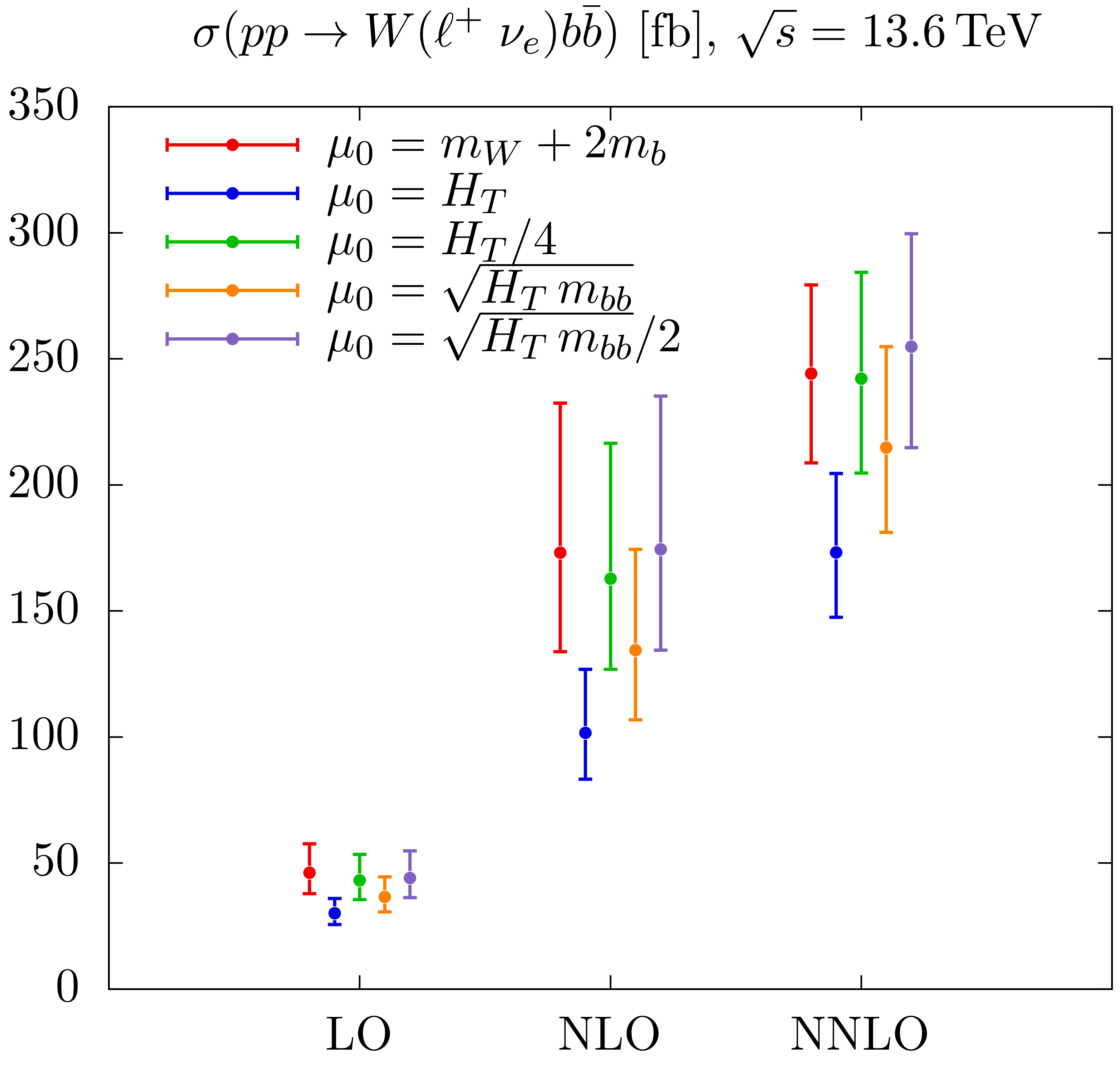
$bin\ I: 150 < p_T^W < 250\,\text{GeV}$

$bin\ II: p_T^W > 250\,\text{GeV}$

Wbb phenomenology (**bin I+bin II**): scale choice

Behaviour of the perturbative series and scale choice

- A priori, the use of a fixed scale is physically **not very well motivated**



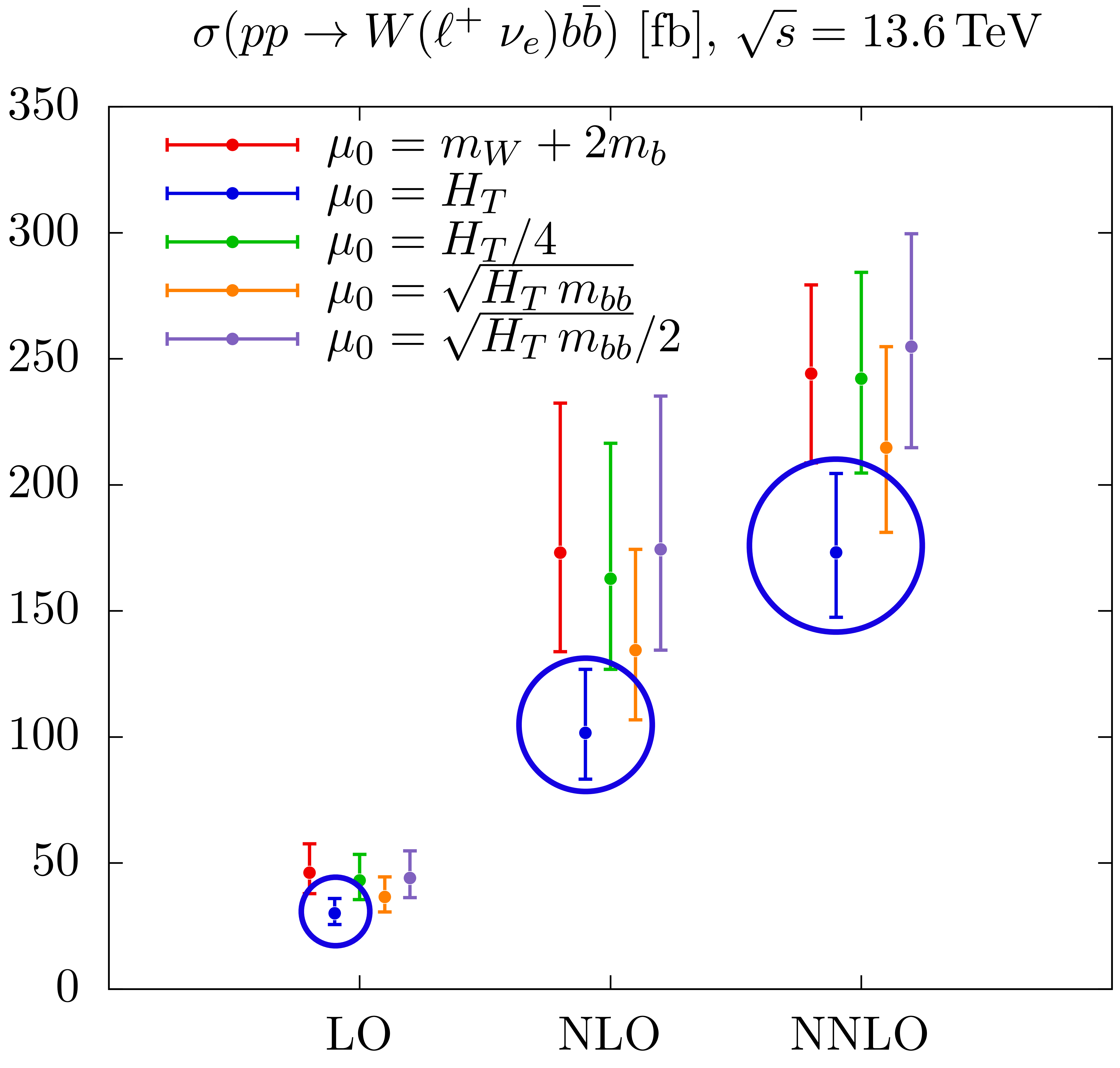
Wbb phenomenology (**bin I+bin II**): scale choice

Behaviour of the perturbative series and scale choice

- A priori, the use of a fixed scale is physically not very well motivated
- Naively, a dynamic scale as H_T would be a better choice. However, it leads to **a poor perturbative convergence with no overlap between NLO and NNLO** within their uncertainties bands

$$H_T = E_T(\ell\nu) + p_T(b_1) + p_T(b_2)$$

$$E_T(\ell\nu) = \sqrt{M^2(\ell\nu) + p_T^2(\ell\nu)}$$



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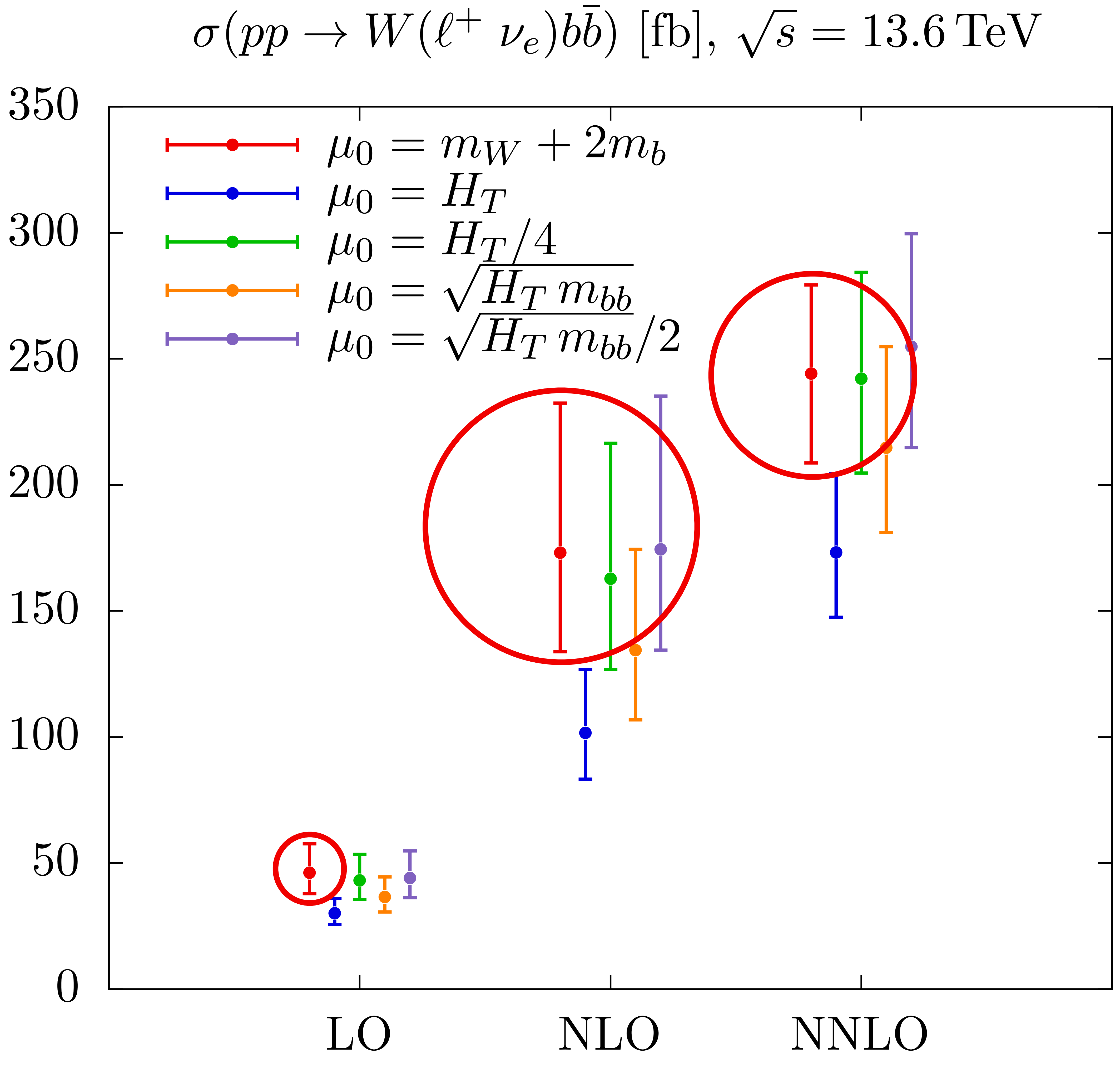

Wbb phenomenology (**bin I+bin II**): scale choice

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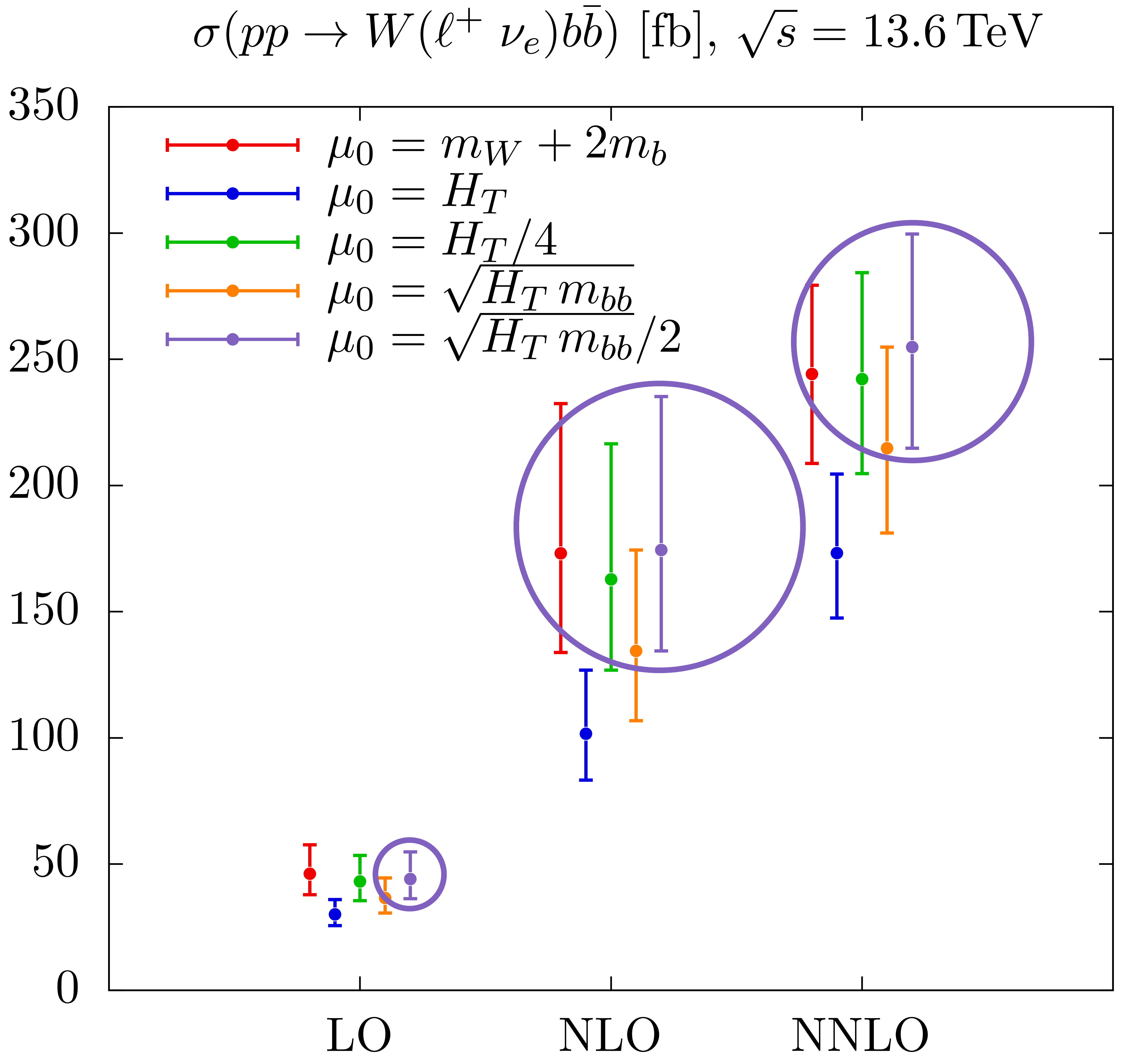
- On the contrary, the choice of a fixed scale leads to a better perturbative convergence, suggesting a preference for smaller scales
- A more detailed analysis should take into account the **“multi-scale” nature** of the process



H_T high-p_T kinematics
m_{bb} gluon splitting kinematics
→ $\sqrt{H_T \cdot m_{bb}}$

possibly divided by a factor of 2

Wbb phenomenology: fiducial cross sections

Results

- Reference scale: $\sqrt{H_T \cdot m_{bb}}/2$
- Large NLO K-factors $K_{\text{NLO}} \gtrsim 3$
- **Relative large positive NNLO corrections**, $K_{\text{NNLO}} \sim 1.5$
- **More reliable** theory uncertainties estimated by scale variations with a reduction to the $15 - 20\,\%$ level

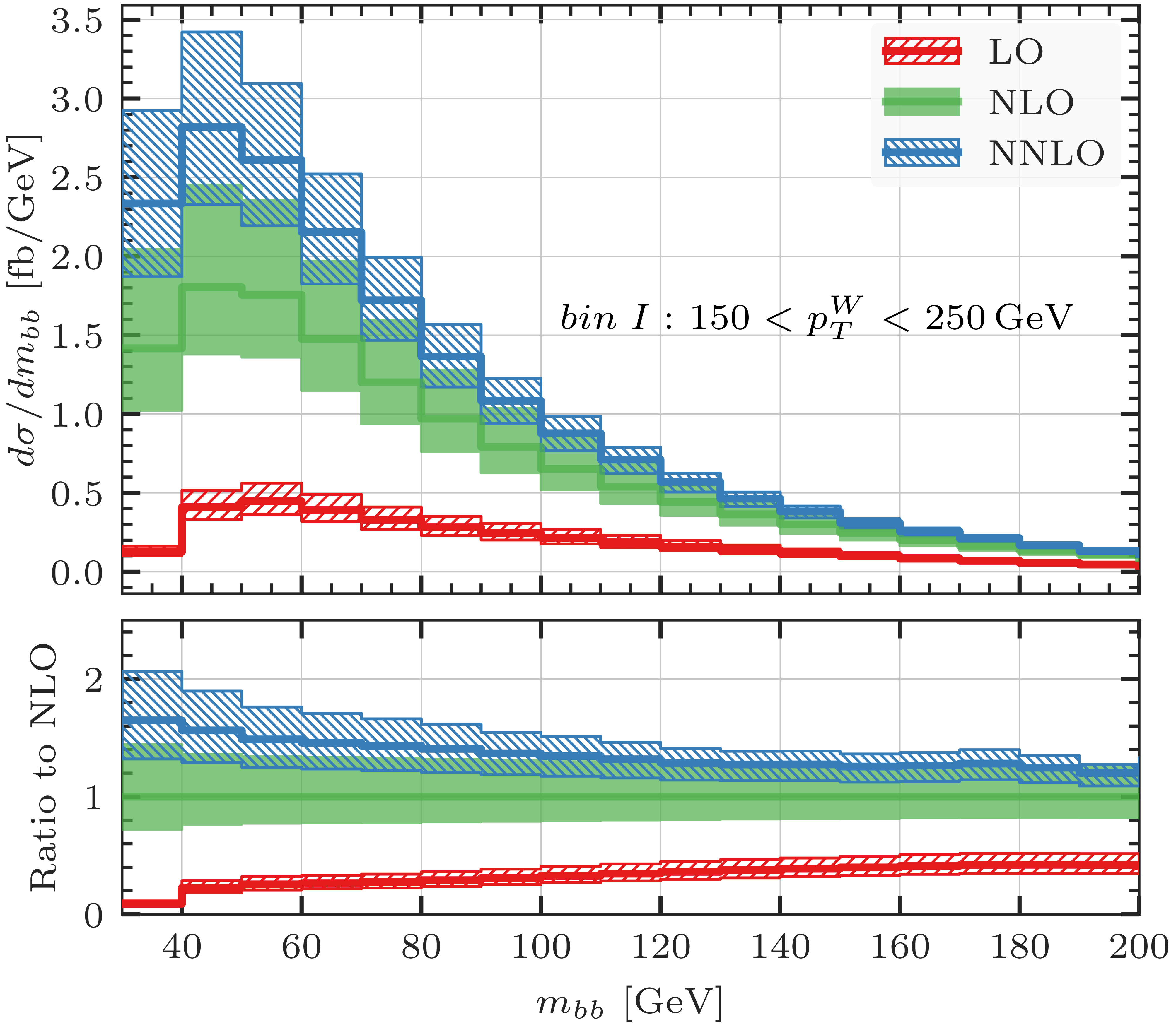
order	$\sigma_{\text{fid}}^{bin\ I}$ [fb]	$\sigma_{\text{fid}}^{bin\ II}$ [fb]
LO	$35.49(1)^{+25\%}_{-18\%}$	$8.627(1)^{+25\%}_{-18\%}$
NLO	$137.20(5)^{+34\%}_{-23\%}$	$37.24(1)^{+38\%}_{-24\%}$
NNLO	$198.9(8)^{+17\%}_{-15\%}$	$55.90(7)^{+19\%}_{-17\%}$

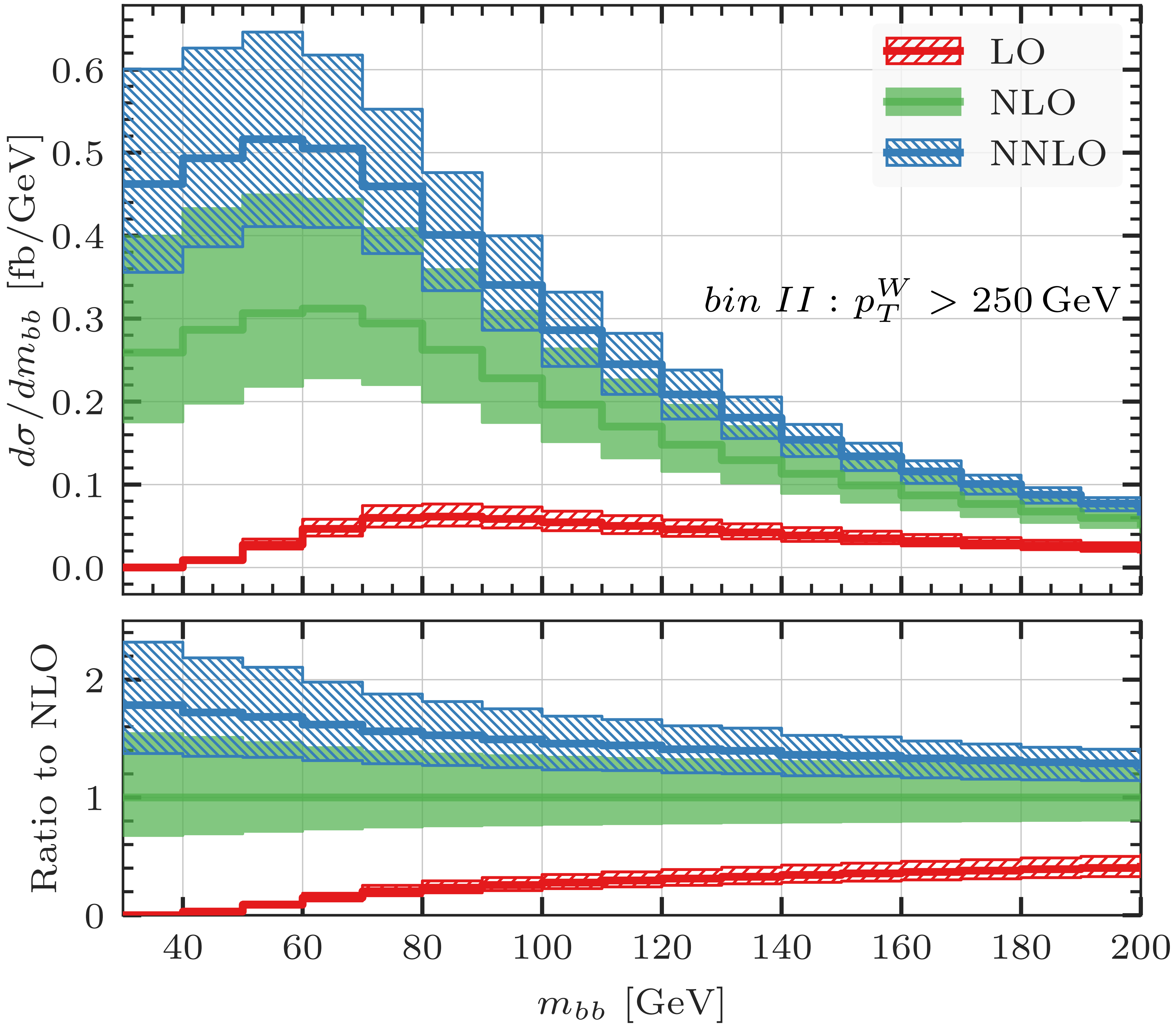
Other theoretical uncertainties are subdominant:

- Variation of bottom mass: $m_b = 4.2\,\text{GeV} \implies \delta\sigma_{\text{NNLO}}/\sigma_{\text{NNLO}} = +\,2\,\%$
- Impact of massification estimated at NLO: $|\delta(\Delta\sigma_{\text{NLO}})/\Delta\sigma_{\text{NLO}}^{exact}| = 3\,\%$
- The part of the two-loop virtual amplitude computed in LCA contributes at the 2% level of the full NNLO correction

Wbb phenomenology: m_{bb} differential distribution

- Similar pattern of NNLO corrections for the two considered p_T^W bins
- NNLO corrections **not uniform**, larger for smaller invariant-mass values
- **Reduction** of scale uncertainties, **partial overlap** with the NLO bands

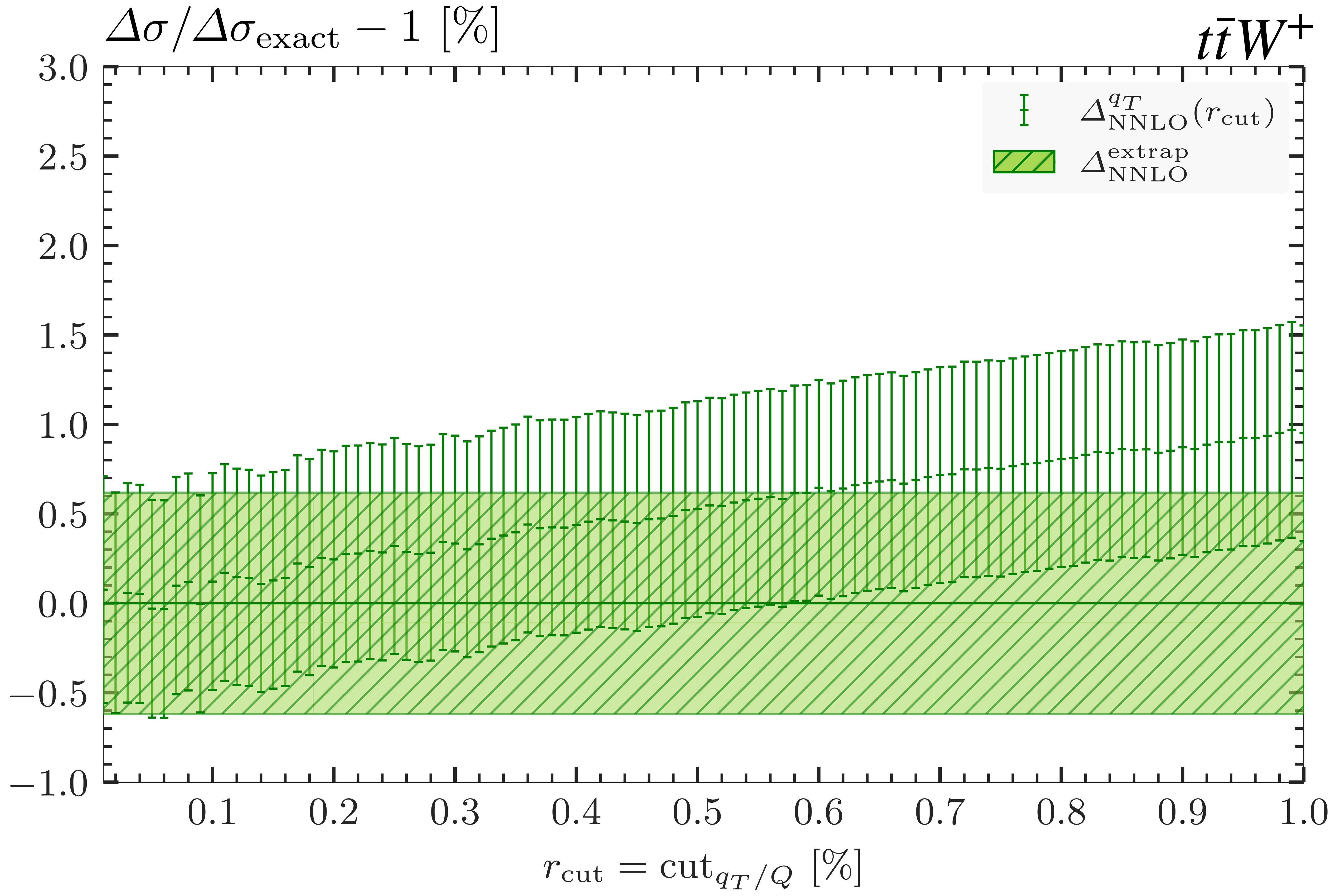




q_T subtraction systematics

$$d\sigma_{N^kLO} = \mathscr{H} \otimes d\sigma_{LO} + \left[d\sigma^{R}_{N^{k-1}LO} - d\sigma^{CT}_{N^kLO} \right]_{q_T/Q > r_{\text{cut}}} + \mathcal{O}(r^{\ell}_{\text{cut}}) \qquad r_{\text{cut}} = \frac{q_{T,\text{cut}}}{m_{t\bar{t}W}}$$

residual power corrections



Behaviour of the power corrections compatible with a **linear scaling** as expected from processes with massive final state

Overall very mild power corrections

Control of the NNLO correction at $\mathcal{O}(0.6\%)$
→ sub permille effect at the level of the total cross section