Monte Carlo simulation of top spin correlations

Eleni Vryonidou

Quantum Observables for Collider Physics

10/11/23, GGI Florence

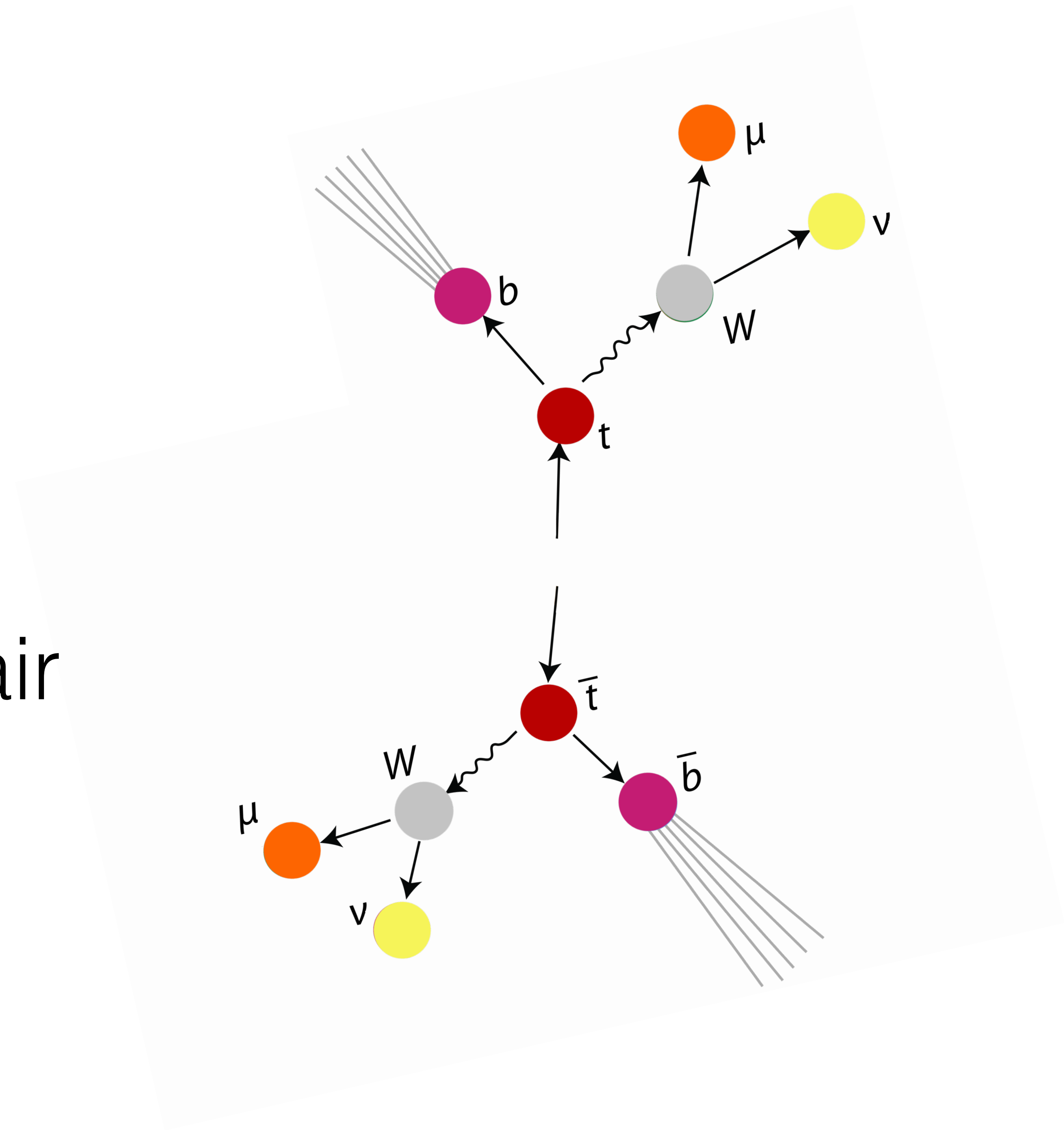
Spin density matrix (again)

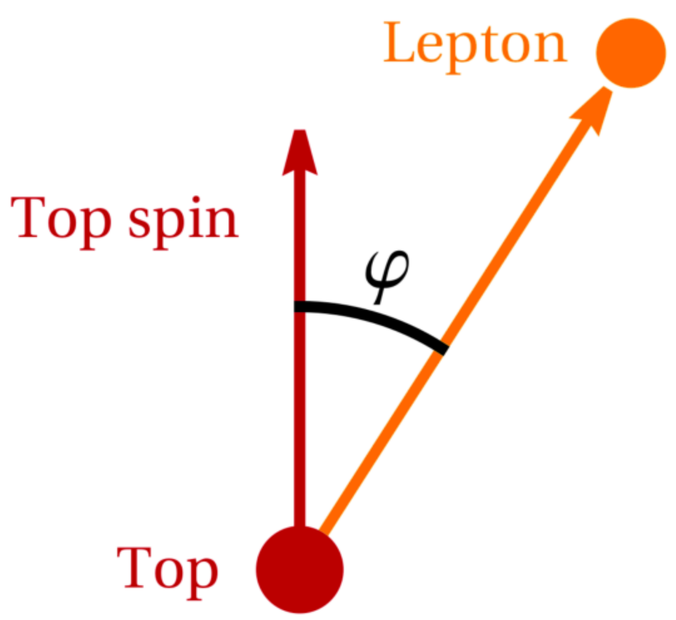
Tops produced in pairs have their spins S_i, S_j correlated

Spin density matrix:

$$\boxed{\rho = \frac{1}{4}\left(\mathbb{1} \otimes \mathbb{1} + \sum_{i=1}^{3} B_i\, \sigma_i \otimes \mathbb{1} + \sum_{i=j}^{3} \bar{B}_j\, \mathbb{1} \otimes \sigma_j + \sum_{i=1}^{3}\sum_{j=1}^{3} C_{ij}\, \sigma_i \otimes \sigma_j\right)}$$

15 parameters describe the quantum state of the top pair





$$\langle S_i \rangle = B_i, \quad \langle \bar{S}_i \rangle = \bar{B}_j, \quad \langle S_i \bar{S}_j \rangle = C_{ij}$$

Extracted by measuring angular distributions of decay products

Spin correlation observables

15 observables are independent and can all be measured by defining a set of axes
Based on lepton decay angles

Observable	Coefficient	Coefficient function
$\cos\theta_1^k$	B_1^k	b_k^+
$\cos\theta_2^k$	B_2^k	b_k^-
$\cos\theta_1^r$	B_1^r	b_r^+
$\cos\theta_2^r$	B_2^r	b_r^-
$\cos\theta_1^n$	B_1^n	b_n^+
$\cos\theta_2^n$	B_2^n	b_n^-
$\cos\theta_1^k \cos\theta_2^k$	C_{kk}	c_{kk}
$\cos\theta_1^r \cos\theta_2^r$	C_{rr}	c_{rr}
$\cos\theta_1^n \cos\theta_2^n$	C_{nn}	c_{nn}
$\cos\theta_1^r \cos\theta_2^k + \cos\theta_1^k \cos\theta_2^r$	$C_{rk}+C_{kr}$	c_{rk}
$\cos\theta_1^r \cos\theta_2^k - \cos\theta_1^k \cos\theta_2^r$	$C_{rk}-C_{kr}$	c_n
$\cos\theta_1^n \cos\theta_2^r + \cos\theta_1^r \cos\theta_2^n$	$C_{nr}+C_{rn}$	c_{nr}
$\cos\theta_1^n \cos\theta_2^r - \cos\theta_1^r \cos\theta_2^n$	$C_{nr}-C_{rn}$	c_k
$\cos\theta_1^n \cos\theta_2^k + \cos\theta_1^k \cos\theta_2^n$	$C_{nk}+C_{kn}$	c_{kn}
$\cos\theta_1^n \cos\theta_2^k - \cos\theta_1^k \cos\theta_2^n$	$C_{nk}-C_{kn}$	$-c_r$
$\cos\varphi$	D	$-(c_{kk}+c_{rr}+c_{nn})/3$
$\cos\varphi_{\text{lab}}$	$A^{\text{lab}}_{\cos\varphi}$	—
$\lvert\Delta\phi_{\ell\ell}\rvert$	$A_{\lvert\Delta\phi_{\ell\ell}\rvert}$	—
$\lvert\Delta\eta_{\ell\ell}\rvert$	$\lvert\Delta\eta_{\ell\ell}\rvert$	—

Boost to top rest Frames:
Need to reconstruct the top and anti-top

Lab observables

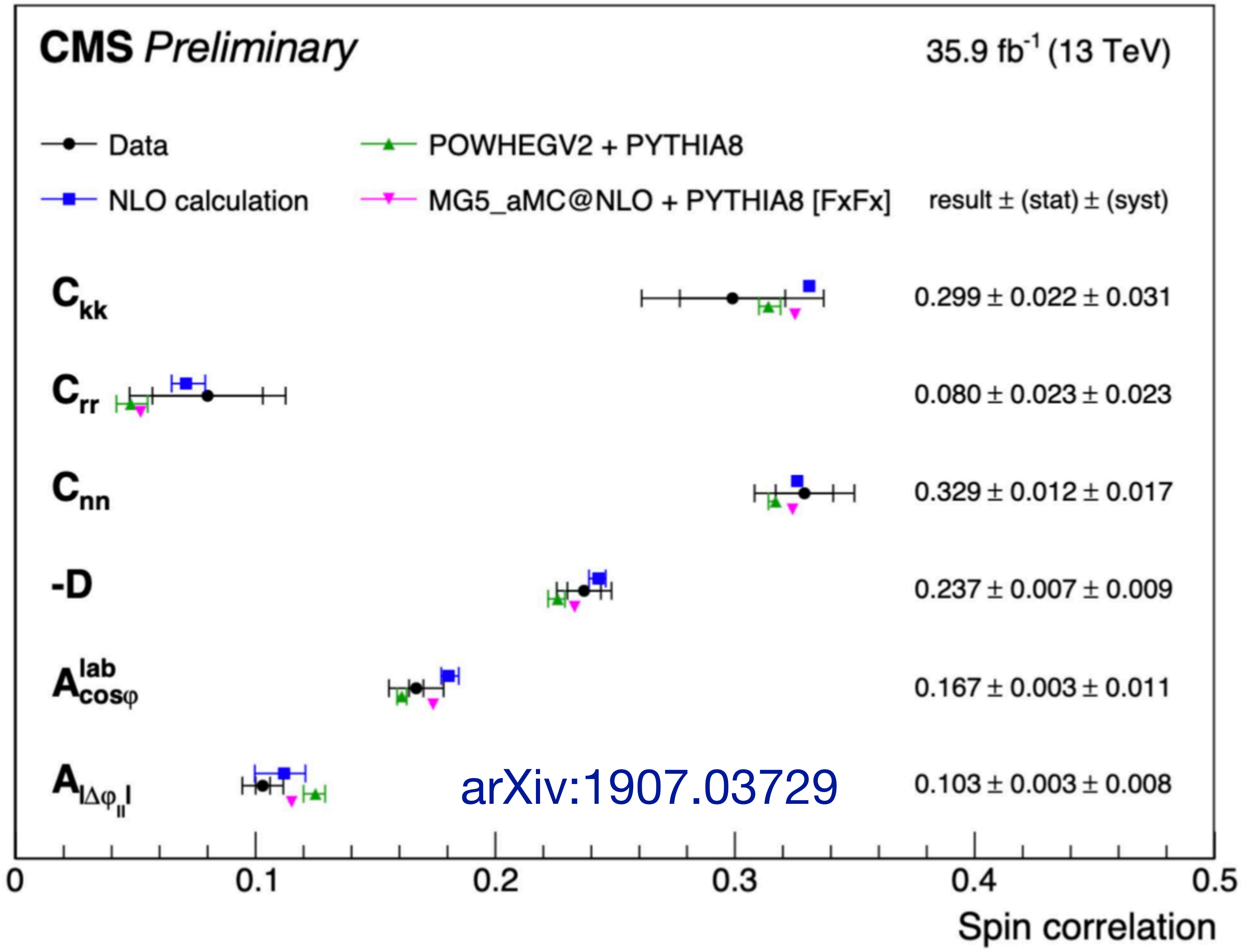
CMS: FTR-18-034-pas

$$\Delta = |C_{kk} + C_{rr}| - C_{nn} - 1 > 0$$

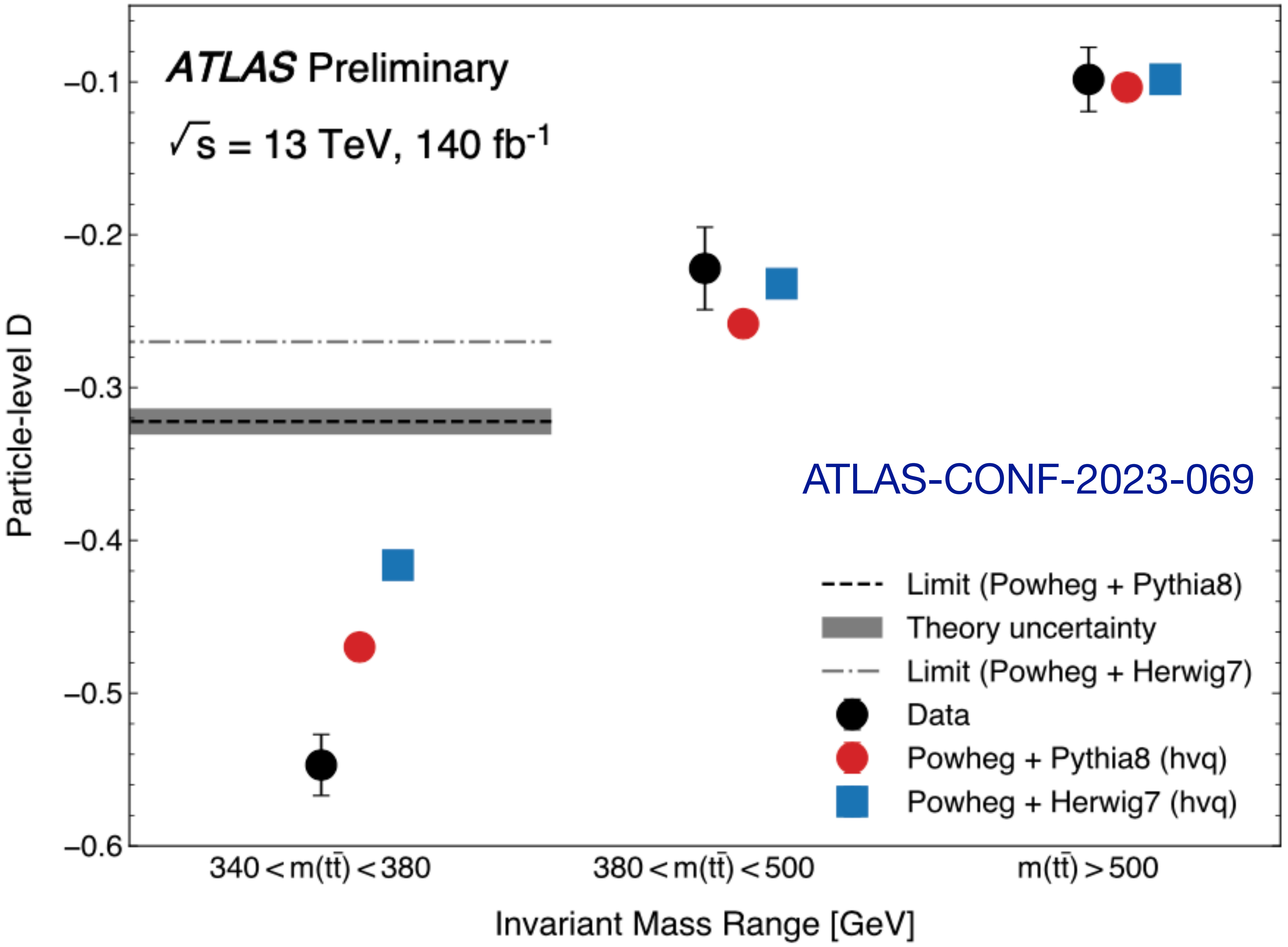
$$\mathcal{C}[\rho] = \begin{cases} \Delta/2, & \Delta > 0 \quad \text{Entangled} \\ 0 & \Delta \leq 0 \quad \text{Classical} \end{cases}$$

Latest experimental measurements

What has been measured?



Full density matrix measured inclusively by CMS



Entanglement observation by ATLAS

What do we need from the Monte Carlo?

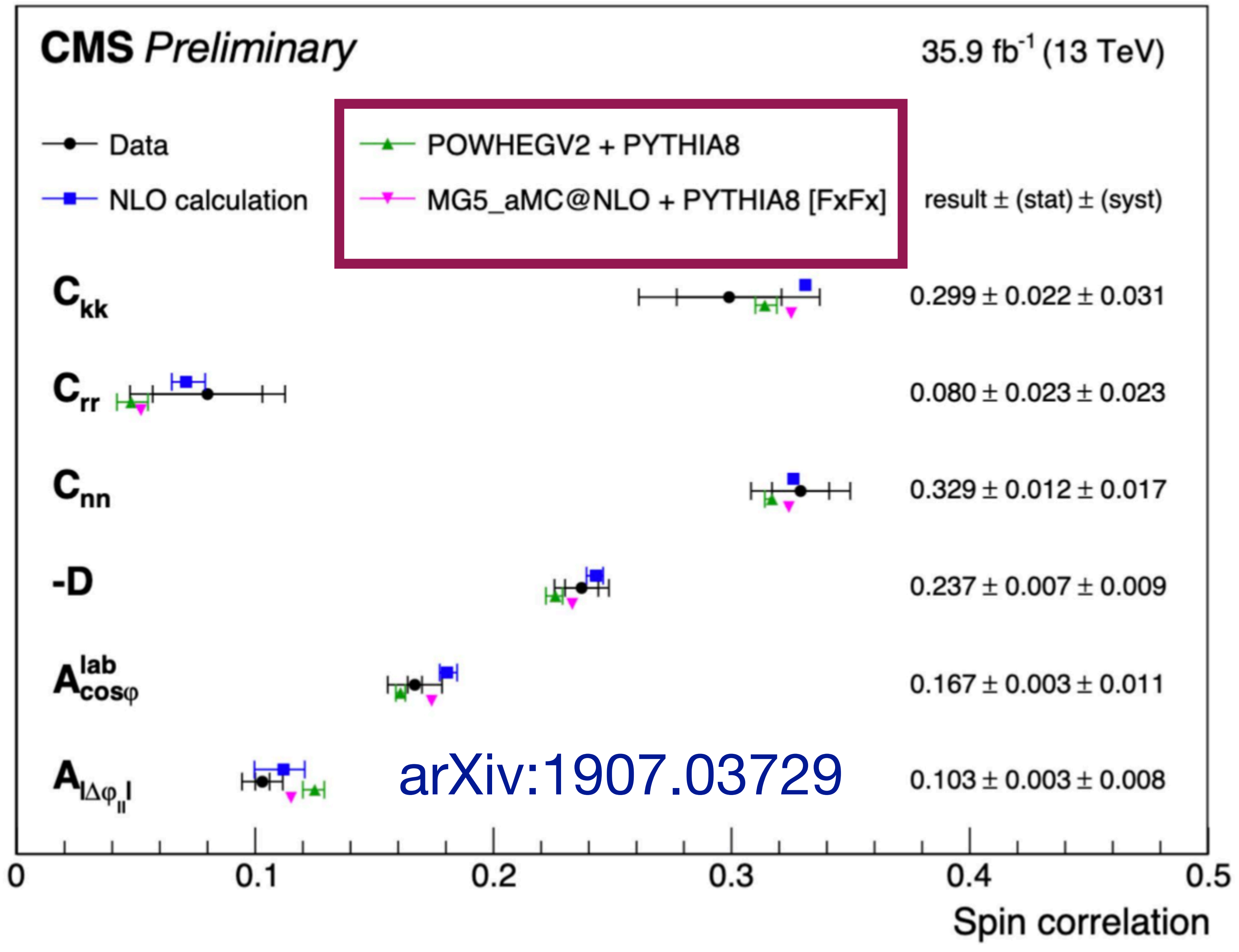
Measurements are always compared to SM predictions provided by MC generators
MC also needed for calibration

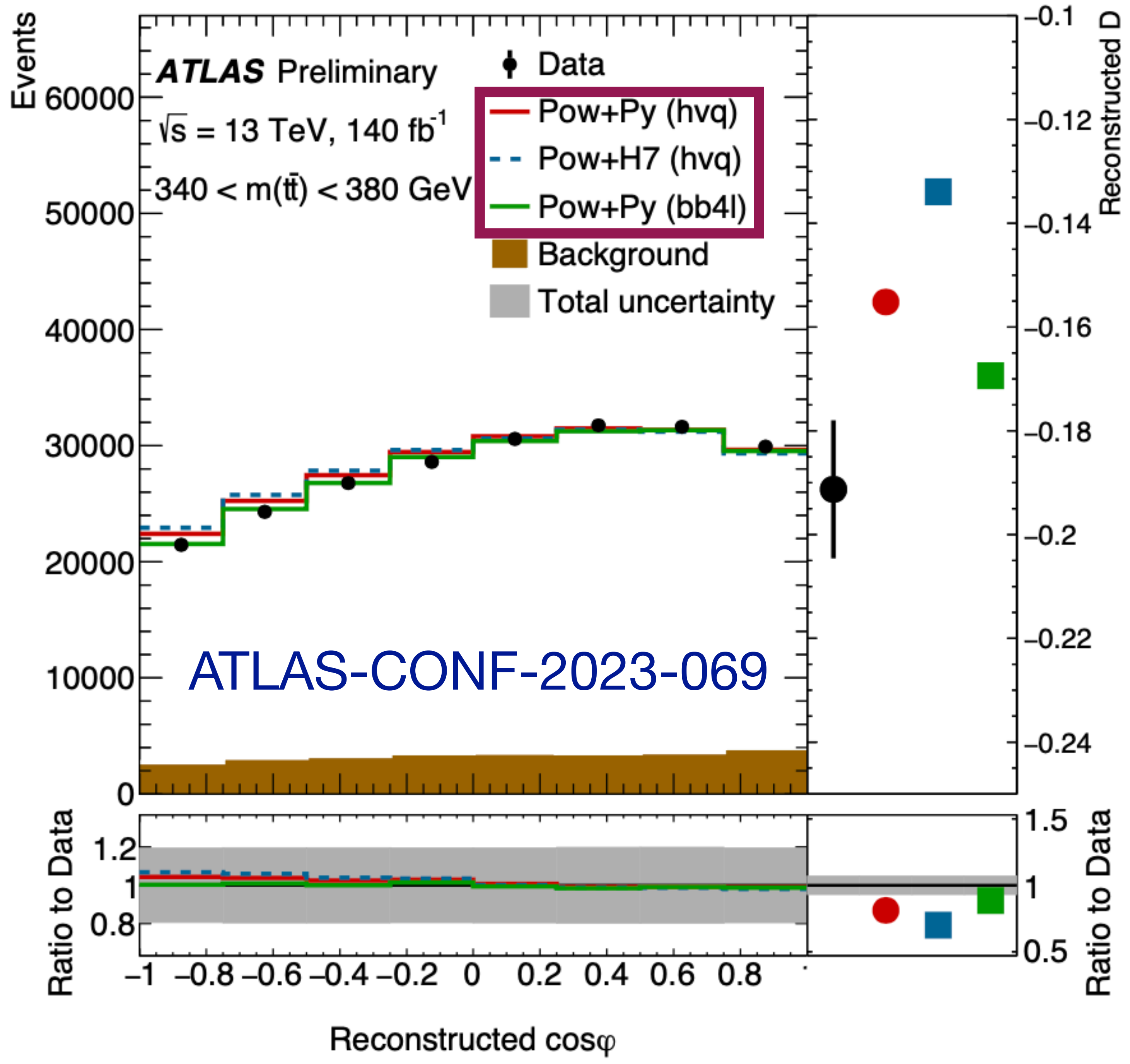
- Preserves the spin information
- Higher order predictions
  - QCD corrections
  - EW corrections
  - Corrections to decays
- Off-shell effects
- Threshold effects/bound state effects
- Matching to the Parton Shower

We can't have all!
Let's try to see what matters

Current Monte Carlo

hvq/MG5_aMC+MadSpin/bb4l





Used Monte Carlo:
- hvq
- MG5_aMC@NLO+FxFx
- bb4l

Used shower:
- Pythia8
- HW7

NLO Monte Carlo for top+anti-top (2->2) with spin correlations & LO decays
bb4l includes 2->6 amplitudes (without demanding two tops)

NLO generators

Label	$t\bar{t}$	$b\bar{b}4\ell$
Generator	hvq [20]	bb4l
Framework	POWHEG-BOX	POWHEG-BOX-RES
NLO matrix elements	$t\bar{t}$	$\ell^+\nu_\ell l^-\bar{\nu}_l b\bar{b}$
Decay accuracy	LO+PS	NLO+PS
NLO radiation	Single	Multiple
Spin correlations	Approx.	Exact
Off-shell $t\bar{t}$ effects	BW smearing	Exact
Wt and non-resonant effects	No	Exact
b Quark massive	Yes	Yes

Jezo et al arXiv:1607.04538

Same for MG5_aMC+MadSpin
FxFx is also allowing extra jet multiplicities

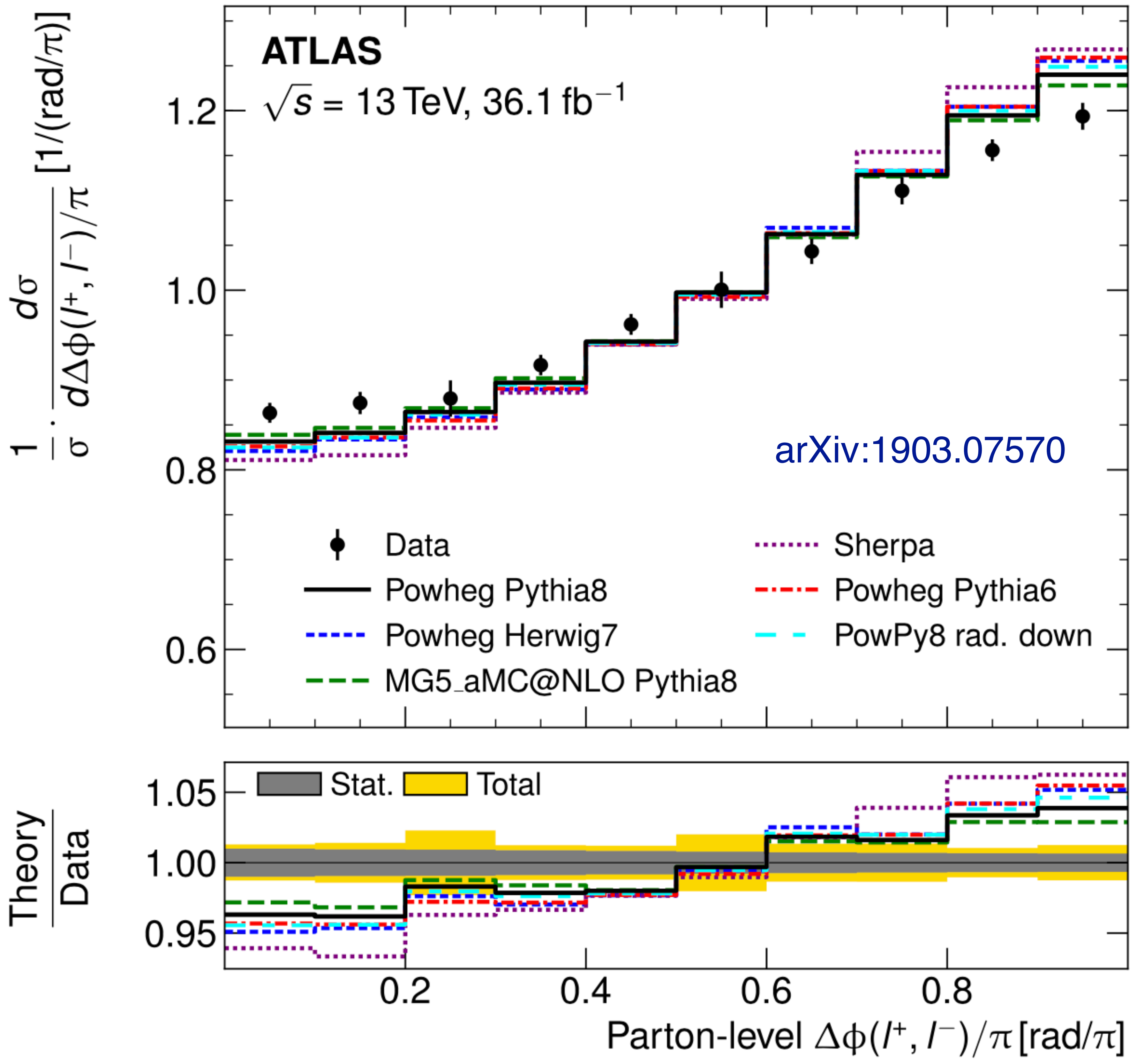
Includes single top backgrounds, which are removed for top pair production samples

Decays in hvq and MadSpin are based on the same algorithm for preserving spin information from:
Frixione, Laenen, Motylinski and Webber, JHEP 0704, 081 (2007) [hep-ph/0702198]

	LO QCD	NLO QCD	
		Real emission	Virtual corrections
$t\,\bar{t}$ kinematics	✓	✓	✓
$t\,\bar{t}$ spin state	✓	✓	Approximate

How well does NLO MC describe the data?

Example 1: Δϕ distribution



Disagreement with NLO Monte Carlo at inclusive/parton-level

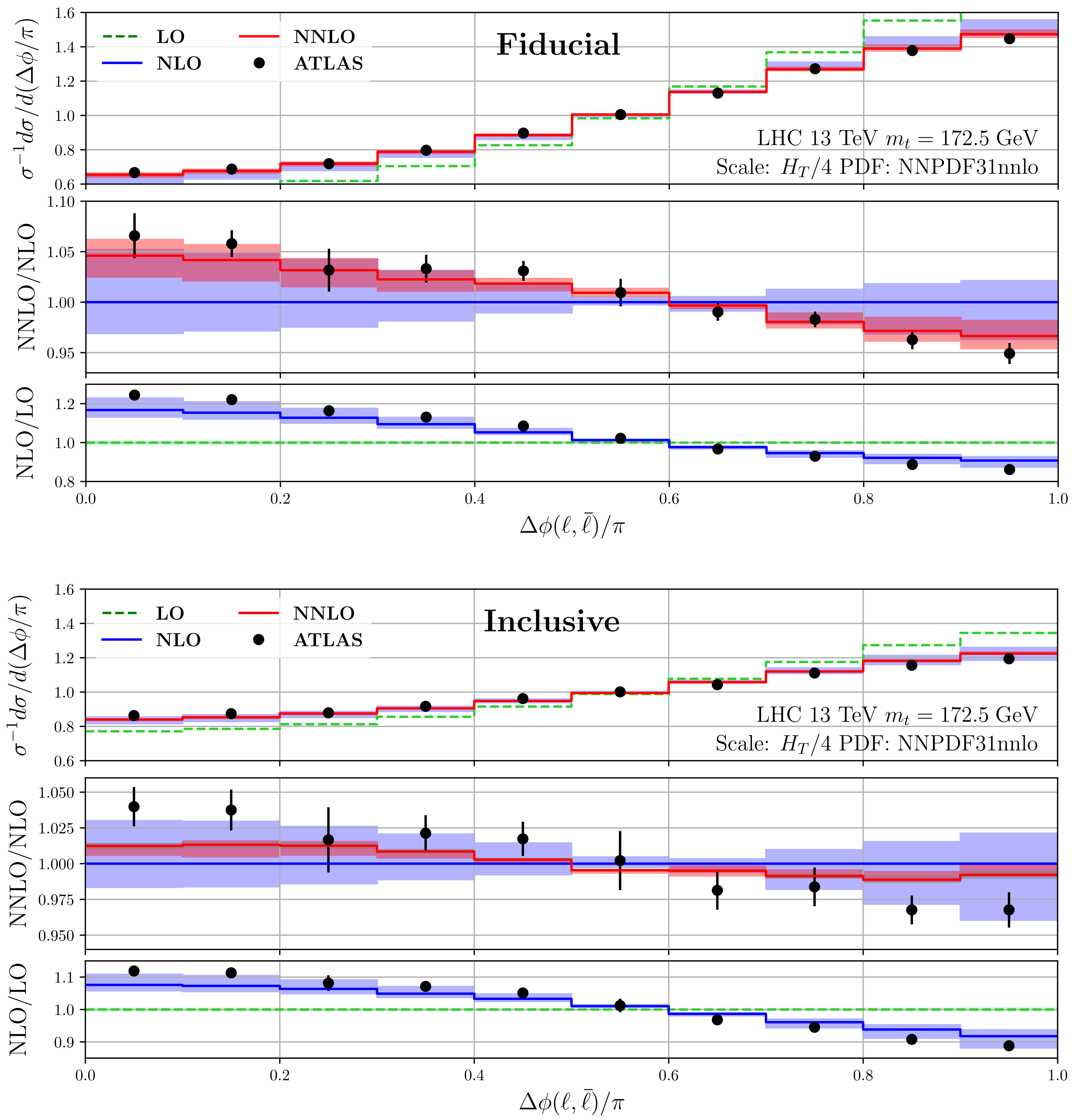
Systematic shape difference

Has this been fixed by NNLO?

Or is this something else?

NNLO results

Δϕ@NNLO



Behring at al arXiv:1901.05407

NNLO production+ NNLO decay

$$
\begin{aligned}
d\sigma^{\mathrm{NNLO}} &= d\sigma^{\mathrm{NNLO}\times\mathrm{LO}} + d\sigma^{\mathrm{LO}\times\mathrm{NNLO}} + d\sigma^{\mathrm{NLO}\times\mathrm{NLO}} \\
&- \frac{2\Gamma_t^{(1)}}{\Gamma_t^{(0)}} d\sigma^{\mathrm{NLO}} - \frac{\left(\Gamma_t^{(1)}\right)^2 + 2\Gamma_t^{(0)}\Gamma_t^{(2)}}{\left(\Gamma_t^{(0)}\right)^2} d\sigma^{\mathrm{LO}}\,.
\end{aligned}
$$

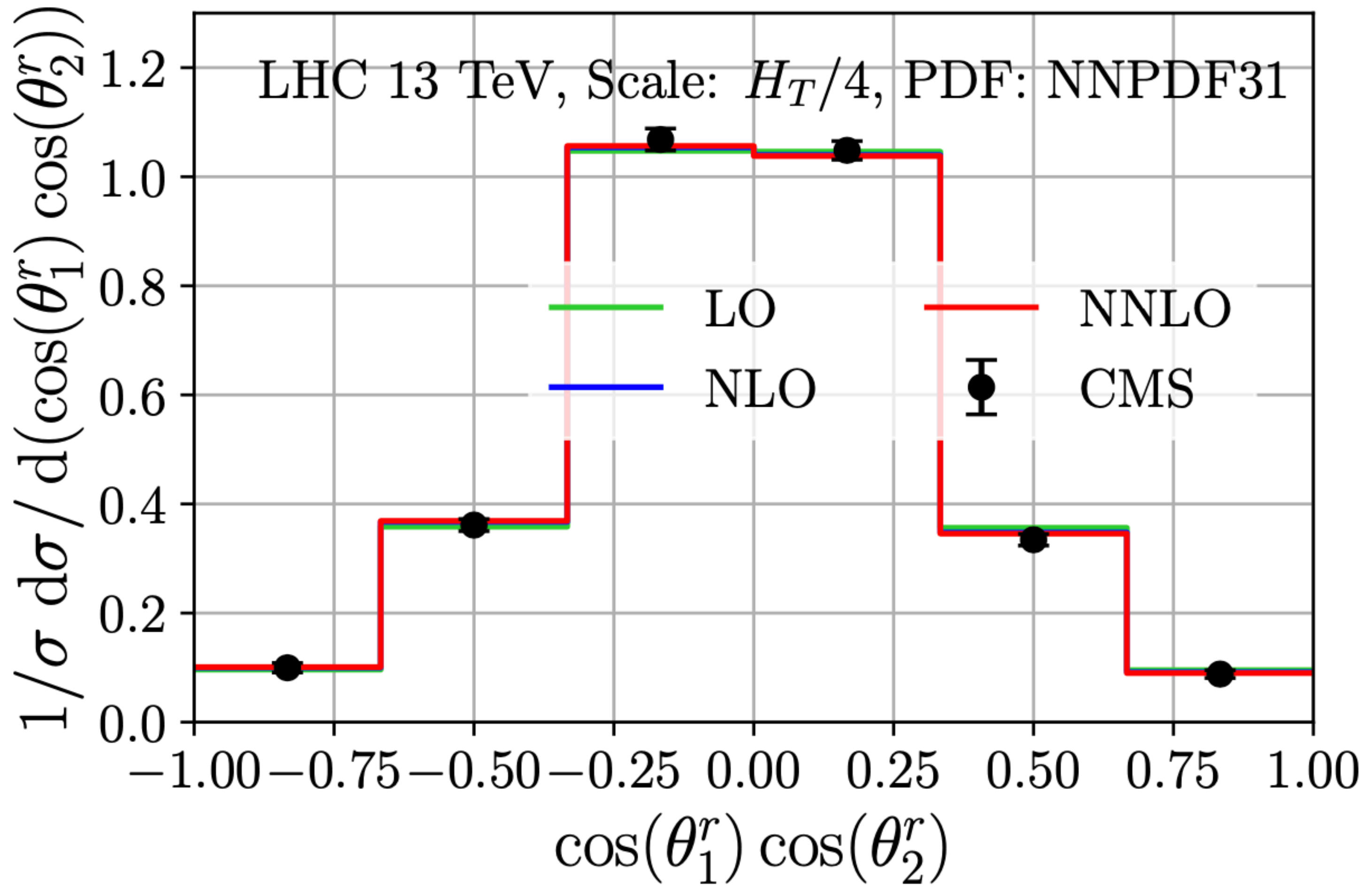
An important finding of the present work is that data extrapolation to full phase space with existing event generators seems not to be compatible with the direct NNLO QCD calculation. We believe that thanks to the very high precision of both theory predictions and experimental measurements we begin to see clear evidence that top quark measurements begin to resolve and constrain such delicate modeling effects.

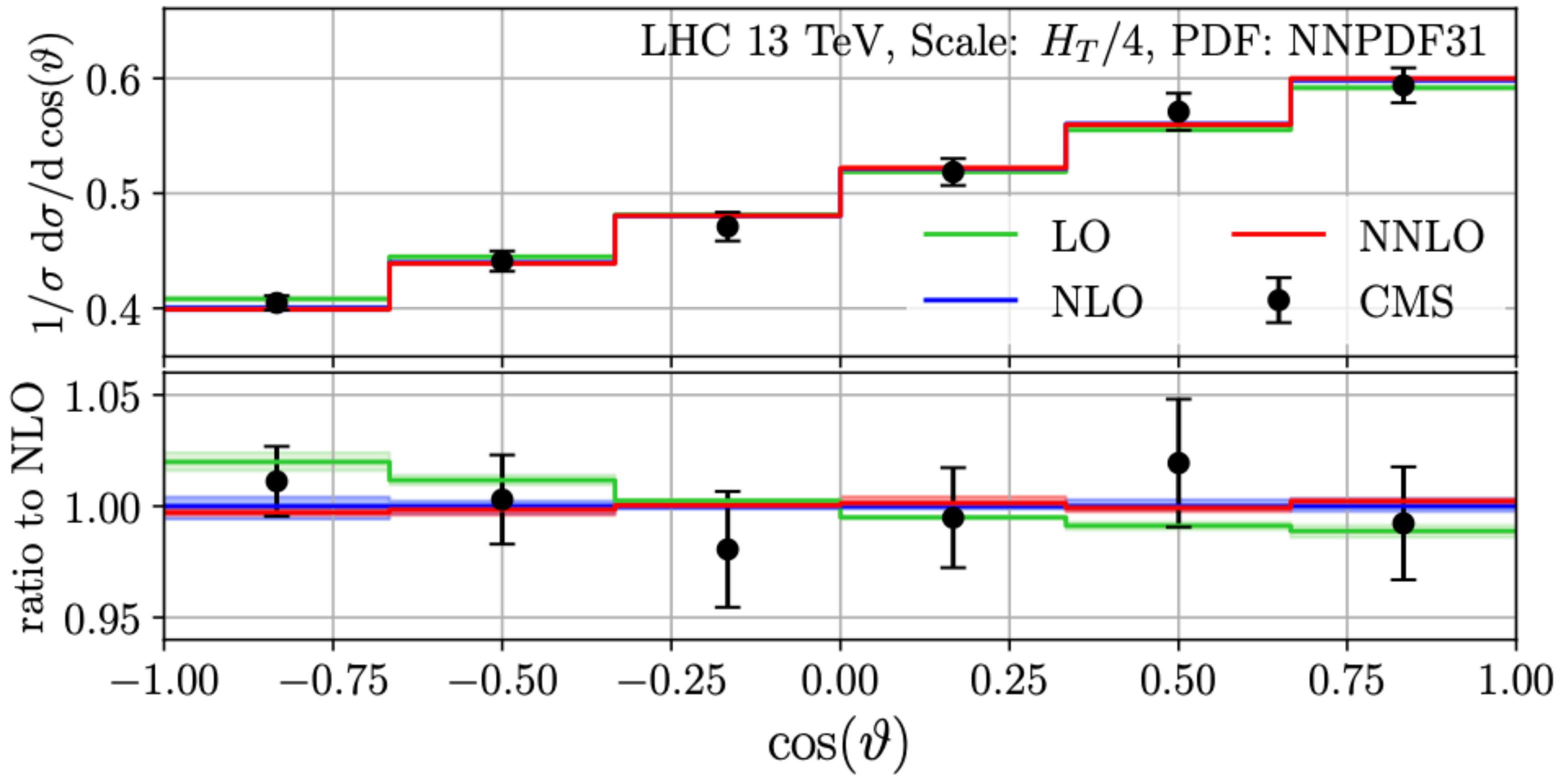
Behring at al arXiv:1901.05407

Spin density matrix@NNLO

Coefficient	LO ($\times 10^3$)	NLO ($\times 10^3$)	NNLO ($\times 10^3$)	CMS ($\times 10^3$)
B_1^k	1^{+0}_{-0} [sc] ± 1 [mc]	1^{+0}_{-1} [sc] ± 2 [mc]	-1^{+0}_{-1} [sc] ± 4 [mc]	5 ± 23
B_1^r	0^{+0}_{-0} [sc] ± 1 [mc]	0^{+1}_{-0} [sc] ± 2 [mc]	0^{+1}_{-2} [sc] ± 2 [mc]	-23 ± 17
B_1^n	0^{+0}_{-0} [sc] ± 1 [mc]	3^{+1}_{-1} [sc] ± 1 [mc]	4^{+1}_{-0} [sc] ± 3 [mc]	6 ± 13
B_2^k	0^{+0}_{-0} [sc] ± 1 [mc]	0^{+0}_{-1} [sc] ± 1 [mc]	-5^{+2}_{-3} [sc] ± 3 [mc]	7 ± 23
B_2^r	0^{+0}_{-0} [sc] ± 1 [mc]	0^{+2}_{-0} [sc] ± 1 [mc]	-2^{+0}_{-1} [sc] ± 2 [mc]	-10 ± 20
B_2^n	0^{+0}_{-0} [sc] ± 1 [mc]	-2^{+0}_{-1} [sc] ± 1 [mc]	-3^{+1}_{-0} [sc] ± 3 [mc]	17 ± 13
C_{kk}	324^{+7}_{-7} [sc] ± 1 [mc]	330^{+2}_{-2} [sc] ± 3 [mc]	323^{+2}_{-5} [sc] ± 6 [mc]	300 ± 38
C_{rr}	6^{+5}_{-5} [sc] ± 1 [mc]	58^{+18}_{-12} [sc] ± 2 [mc]	69^{+8}_{-7} [sc] ± 3 [mc]	81 ± 32
C_{nn}	332^{+1}_{-0} [sc] ± 1 [mc]	330^{+1}_{-1} [sc] ± 2 [mc]	326^{+1}_{-1} [sc] ± 4 [mc]	329 ± 20
$C_{nr} + C_{rn}$	1^{+0}_{-0} [sc] ± 1 [mc]	-1^{+1}_{-0} [sc] ± 3 [mc]	-4^{+4}_{-0} [sc] ± 6 [mc]	-4 ± 37
$C_{nr} - C_{rn}$	0^{+0}_{-1} [sc] ± 1 [mc]	-1^{+1}_{-0} [sc] ± 2 [mc]	2^{+4}_{-2} [sc] ± 8 [mc]	-1 ± 38
$C_{nk} + C_{kn}$	0^{+0}_{-0} [sc] ± 1 [mc]	2^{+1}_{-0} [sc] ± 1 [mc]	3^{+4}_{-1} [sc] ± 3 [mc]	-43 ± 41
$C_{nk} - C_{kn}$	1^{+0}_{-0} [sc] ± 1 [mc]	1^{+1}_{-1} [sc] ± 2 [mc]	6^{+0}_{-2} [sc] ± 7 [mc]	40 ± 29
$C_{rk} + C_{kr}$	-229^{+4}_{-4} [sc] ± 1 [mc]	-203^{+9}_{-7} [sc] ± 2 [mc]	-194^{+8}_{-6} [sc] ± 7 [mc]	-193 ± 64
$C_{rk} - C_{kr}$	1^{+0}_{-0} [sc] ± 1 [mc]	1^{+0}_{-1} [sc] ± 4 [mc]	-1^{+1}_{-3} [sc] ± 5 [mc]	57 ± 46

Czakon, Mitov, Poncelet arXiv:2008.11133





Czakon, Mitov, Poncelet arXiv:2008.11133

- Perturbative series (QCD) under control
- Very small corrections at the inclusive level
- NNLO results within scale uncertainties of NLO results
- Agreement with CMS measurement

NNLO+PS

MINNLOps

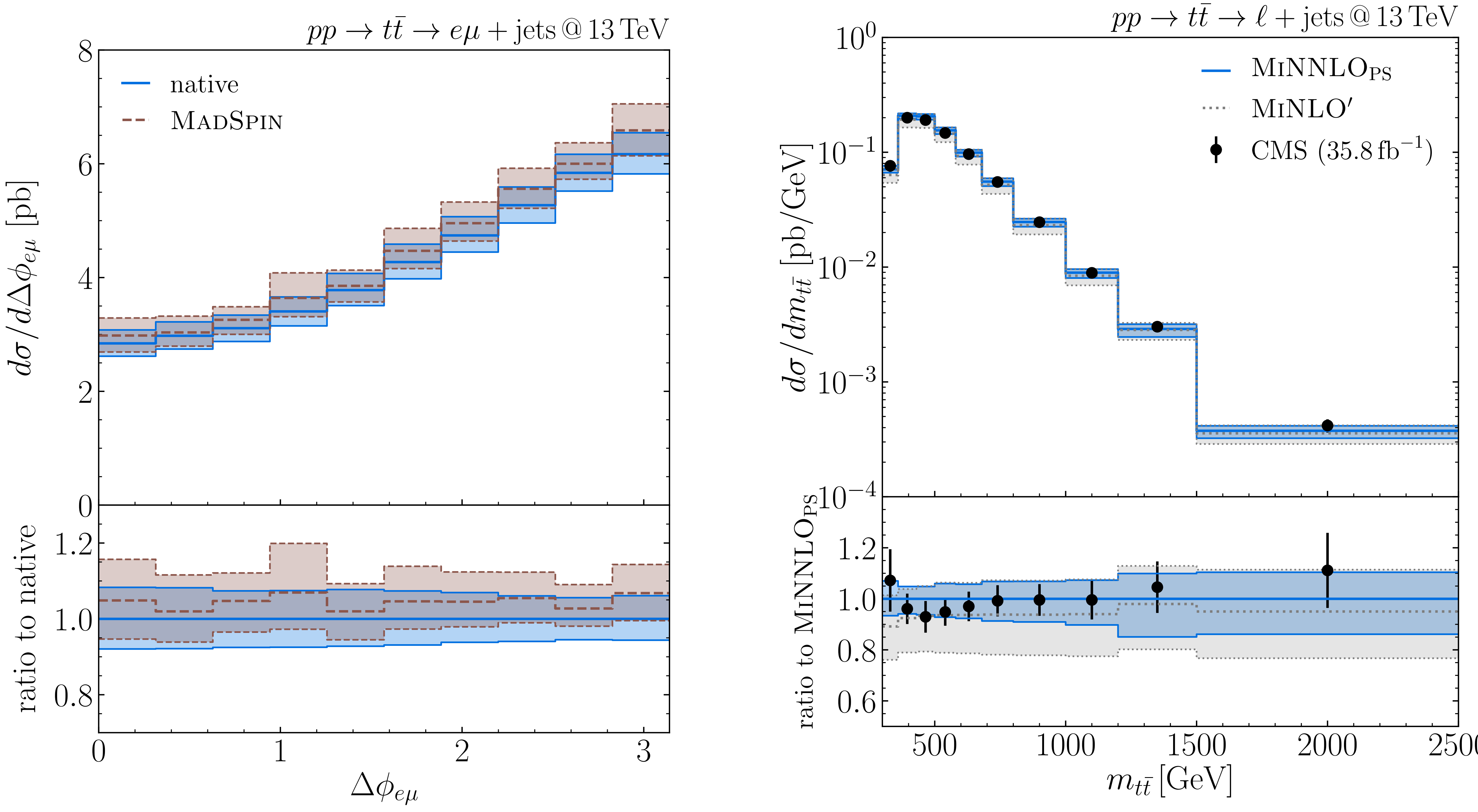
A new computation:

- NNLO accuracy for tt observables
- NLO for tt+j
- LO for tt+2j

Mazzitelli et al, arXiv:2112.12135

Tree-level decay as in hvq

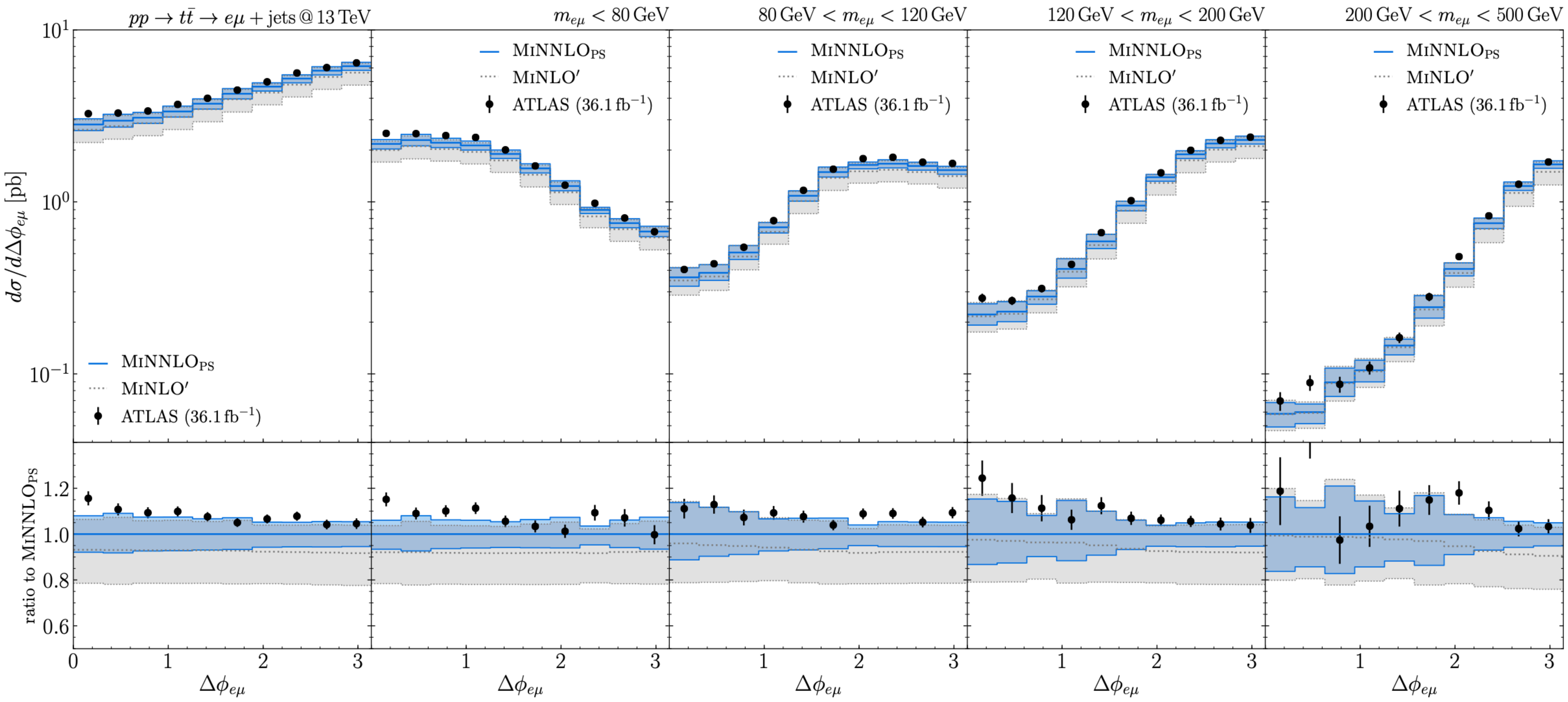
Decay implementation validated against MadSpin



Mazzitelli et al, arXiv:2112.12135

NNLO+PS

MiNNLOps



Better agreement with data
Implementation publicly available

Mazzitelli et al, arXiv:2112.12135

NLO EW

How about EW corrections?

$$\Sigma_{\rm LO}(\alpha,\alpha_S)=\underbrace{\alpha_S^2\Sigma_{2,0}}_{\rm LO_1}+\underbrace{\alpha_S\alpha\Sigma_{1,1}}_{\rm LO_2}+\underbrace{\alpha^2\Sigma_{0,2}}_{\rm LO_3}$$

$$\Sigma_{\rm NLO}(\alpha,\alpha_S)=\underbrace{\alpha_S^3\Sigma_{3,0}}_{\rm NLO_1}+\underbrace{\alpha_S^2\alpha\Sigma_{2,1}}_{\rm NLO_2}+\underbrace{\alpha_S\alpha^2\Sigma_{1,2}}_{\rm NLO_3}+\underbrace{\alpha^3\Sigma_{0,3}}_{\rm NLO_4}$$

$$\mathscr{O}=\frac{\sigma_{\mathscr{O}}}{\sigma}=\frac{\sigma^{\rm QCD+EW}_{\mathscr{O},\rm NLO}}{\sigma^{\rm QCD+EW}_{\rm NLO}} \qquad \mathscr{O}^{\rm QCD}_{\rm NLO}=\frac{N^{\rm QCD}_{\rm NLO}}{D^{\rm QCD}_{\rm NLO}}$$

unexpanded

$$\tilde{\mathscr{O}}^{\rm QCD+EW}_{\rm NLO}=K^{\rm QCD}_{\rm NLO}\,\mathscr{O}^{\rm QCD+EW}_{\rm NLO}+(1-K^{\rm QCD}_{\rm NLO})\frac{N^{\rm QCD}_{\rm LO}}{D^{\rm QCD}_{\rm LO}}$$

expanded

		Unexpanded		Expanded	
Asymmetry	LO QCD [%]	NLO QCD [%]	NLO QCD+EW [%]	NLO QCD [%]	NLO QCD+EW [%]
A_C^{tt}	0	$0.453(5)^{+28.2\%}_{-20.5\%}{}^{+3.4\%}_{-3.4\%}$	$0.546(6)^{+25.1\%}_{-18.0\%}{}^{+2.4\%}_{-2.4\%}$	$0.62(2)^{+18.1\%}_{-14.8\%}{}^{+3.3\%}_{-3.3\%}$	$0.73(3)^{+13.8\%}_{-11.5\%}{}^{+2.3\%}_{-2.3\%}$
$A_C^{\ell\ell}$	0	$0.27(2)^{+29.3\%}_{-21.4\%}{}^{+3.8\%}_{-3.8\%}$	$0.33(3)^{+25.0\%}_{-17.8\%}{}^{+3.8\%}_{-3.8\%}$	$0.36(3)^{+19.3\%}_{-15.9\%}{}^{+3.7\%}_{-3.7\%}$	$0.45(4)^{+14.6\%}_{-12.0\%}{}^{+3.9\%}_{-3.9\%}$
$A_{\Delta\Phi}$	$17.51(1)^{+3.2\%}_{-2.8\%}{}^{+0.4\%}_{-0.4\%}$	$12.65(2)^{+8.3\%}_{-14.8\%}{}^{+0.4\%}_{-0.4\%}$	$12.42(3)^{+8.7\%}_{-15.5\%}{}^{+0.4\%}_{-0.4\%}$	$10.88(3)^{+7.2\%}_{-10.1\%}{}^{+0.3\%}_{-0.3\%}$	$10.58(4)^{+7.4\%}_{-10.5\%}{}^{+0.4\%}_{-0.4\%}$
$A_{\Delta\theta}$	$14.63(1)^{+4.0\%}_{-4.6\%}{}^{+1.5\%}_{-1.5\%}$	$16.03(2)^{+4.0\%}_{-2.2\%}{}^{+1.4\%}_{-1.4\%}$	$16.24(2)^{+4.1\%}_{-2.2\%}{}^{+1.4\%}_{-1.4\%}$	$16.54(3)^{+2.9\%}_{-1.7\%}{}^{+1.3\%}_{-1.3\%}$	$16.83(4)^{+2.8\%}_{-1.5\%}{}^{+1.3\%}_{-1.3\%}$

Frederix, Tsinikos, Vitos arXiv:2105.11478

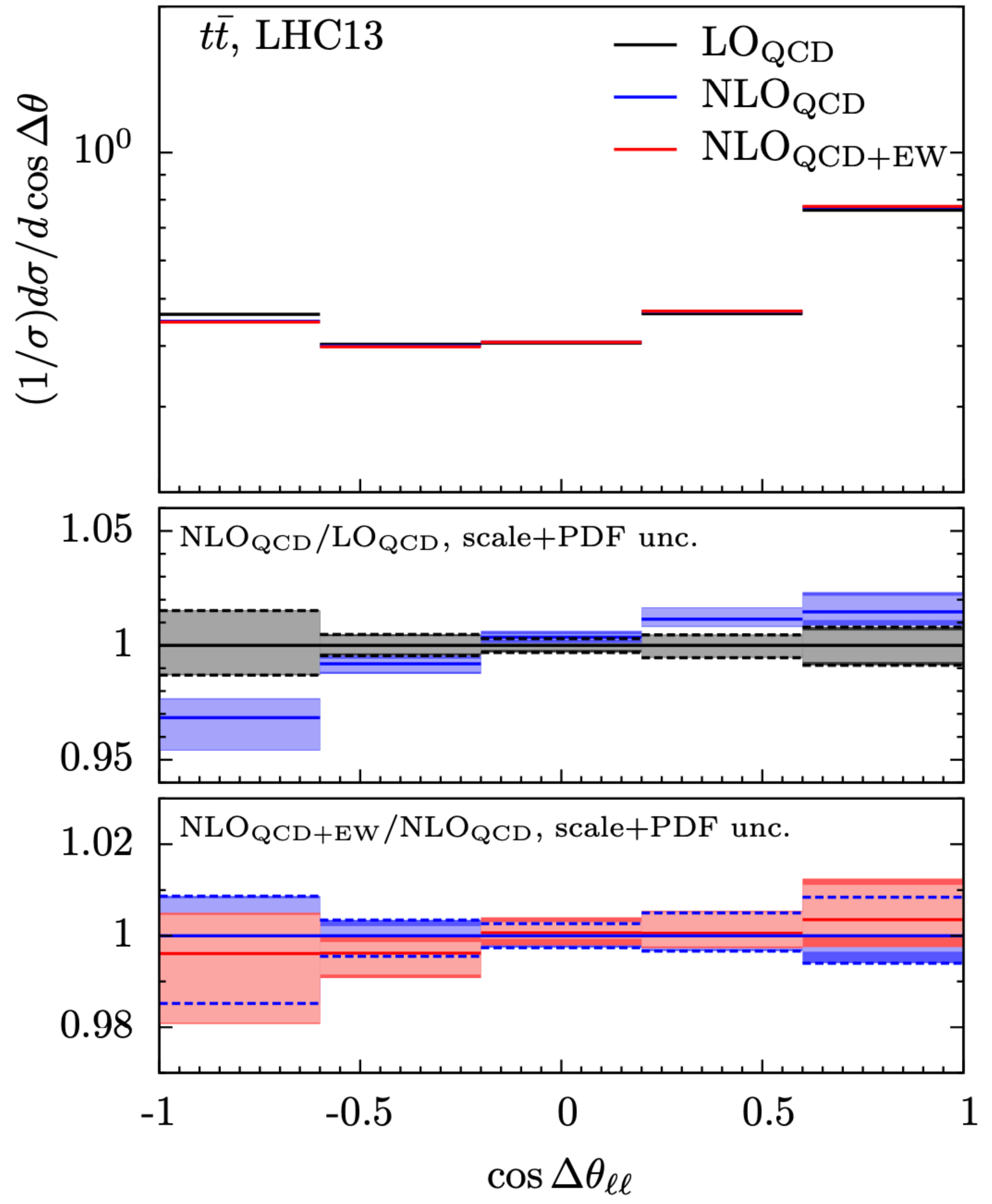
Small EW corrections to the asymmetries

NLO EW

How about EW corrections?

		Unexpanded		Expanded	
	LO QCD [%]	NLO QCD [%]	NLO QCD+EW [%]	NLO QCD [%]	NLO QCD+EW [%]
C_{kk}	$32.68(3)^{+1.5\%}_{-1.7\%}{}^{+0.8\%}_{-0.8\%}$	$32.88(3)^{+1.3\%}_{-0.4\%}{}^{+0.7\%}_{-0.7\%}$	$32.69(5)^{+1.1\%}_{-0.4\%}{}^{+0.7\%}_{-0.7\%}$	$32.96(7)^{+1.7\%}_{-0.8\%}{}^{+0.6\%}_{-0.6\%}$	$32.65(9)^{+1.5\%}_{-0.6\%}{}^{+0.6\%}_{-0.6\%}$
C_{nn}	$33.01(3)^{+0.3\%}_{-0.5\%}{}^{+0.2\%}_{-0.2\%}$	$31.97(3)^{+0.9\%}_{-1.1\%}{}^{+0.2\%}_{-0.2\%}$	$31.89(5)^{+0.9\%}_{-1.3\%}{}^{+0.2\%}_{-0.2\%}$	$31.59(7)^{+0.6\%}_{-0.5\%}{}^{+0.2\%}_{-0.2\%}$	$31.49(9)^{+0.7\%}_{-0.6\%}{}^{+0.2\%}_{-0.2\%}$
C_{rr}	$0.71(3)^{+45.1\%}_{-51.5\%}{}^{+3.2\%}_{-3.2\%}$	$4.80(3)^{+28.9\%}_{-19.2\%}{}^{+2.8\%}_{-2.8\%}$	$4.83(5)^{+29.4\%}_{-19.4\%}{}^{+2.5\%}_{-2.5\%}$	$6.28(7)^{+12.6\%}_{-8.3\%}{}^{+1.9\%}_{-1.9\%}$	$6.33(9)^{+11.6\%}_{-8.1\%}{}^{+1.7\%}_{-1.7\%}$
$C_{nr}+C_{rn}$	$-0.02(4)^{+18.4\%}_{-18.8\%}{}^{+1.0\%}_{-1.0\%}$	$0.002(50)^{+0\%}_{-0\%}{}^{+0\%}_{-0\%}$	$0.08(7)^{+60.6\%}_{-59.7\%}{}^{+3.8\%}_{-3.8\%}$	$0.01(10)^{+0\%}_{-0\%}{}^{+0\%}_{-0\%}$	$0.1(1)^{+45.2\%}_{-48.4\%}{}^{+3.6\%}_{-3.6\%}$
$C_{nr}-C_{rn}$	$0.02(4)^{+10.5\%}_{-12.0\%}{}^{+1.8\%}_{-1.8\%}$	$-0.05(4)^{+29.9\%}_{-53.6\%}{}^{+4.0\%}_{-4.0\%}$	$-0.08(7)^{+34.1\%}_{-54.3\%}{}^{+8.3\%}_{-8.3\%}$	$-0.07(9)^{+22.1\%}_{-31.6\%}{}^{+2.4\%}_{-2.4\%}$	$-0.1(1)^{+23.0\%}_{-28.3\%}{}^{+7.5\%}_{-7.5\%}$
$C_{nk}+C_{kn}$	$-0.02(4)^{+13.1\%}_{-10.3\%}{}^{+3.3\%}_{-3.3\%}$	$-0.004(60)^{+0\%}_{-0\%}{}^{+0\%}_{-0\%}$	$-0.14(9)^{+30.8\%}_{-40.6\%}{}^{+5.1\%}_{-5.1\%}$	$0.001(100)^{+0\%}_{-0\%}{}^{+0\%}_{-0\%}$	$-0.2(2)^{+28.6\%}_{-30.3\%}{}^{+5.7\%}_{-5.7\%}$
$C_{nk}-C_{kn}$	$-0.004(40)^{+54.1\%}_{-59.2\%}{}^{+3.3\%}_{-3.3\%}$	$-0.03(6)^{+79.7\%}_{-80.1\%}{}^{+13.9\%}_{-13.9\%}$	$0.12(9)^{+13.7\%}_{-11.4\%}{}^{+4.0\%}_{-4.0\%}$	$-0.04(10)^{+78.4\%}_{-83.5\%}{}^{+9.3\%}_{-9.3\%}$	$0.2(2)^{+6.5\%}_{-8.3\%}{}^{+4.1\%}_{-4.1\%}$
$C_{rk}+C_{kr}$	$-22.87(4)^{+1.5\%}_{-1.5\%}{}^{+0.4\%}_{-0.4\%}$	$-20.51(6)^{+3.8\%}_{-2.8\%}{}^{+0.4\%}_{-0.4\%}$	$-20.48(9)^{+4.1\%}_{-2.9\%}{}^{+0.4\%}_{-0.4\%}$	$-19.7(1)^{+2.3\%}_{-1.4\%}{}^{+0.3\%}_{-0.3\%}$	$-19.6(1)^{+2.2\%}_{-1.5\%}{}^{+0.4\%}_{-0.4\%}$
$C_{rk}-C_{kr}$	$0.02(4)^{+17.2\%}_{-15.7\%}{}^{+5.1\%}_{-5.1\%}$	$-0.13(6)^{+18.1\%}_{-30.7\%}{}^{+2.2\%}_{-2.2\%}$	$0.09(9)^{+52.4\%}_{-29.4\%}{}^{+4.7\%}_{-4.7\%}$	$-0.2(1)^{+10.2\%}_{-13.1\%}{}^{+2.2\%}_{-2.2\%}$	$0.1(2)^{+36.8\%}_{-25.0\%}{}^{+4.8\%}_{-4.8\%}$

Frederix, Tsinikos, Vitos arXiv:2105.11478



Frederix, Tsinikos, Vitos arXiv:2105.11478

Small corrections to the Spin Correlation coefficients
NLO EW results fall with the uncertainties of the NLO QCD predictions

Modelling the decay

NLO in the decay?

Most currently used MC e.g. hvq, MG5_aMC have LO decays
Could corrections in the decays have an impact?

QCD order / [%]	C_{kk}	C_{nn}	C_{rr}	C_{rk+kr}
NLO × NLO 2008.11133	33.0(3)	33.0(2)	5.8(2)	-20.3(2)
NLO × LO (MCFM)	33.04(4)	33.09(4)	5.96(4)	-20.71(7)

Small impact on Spin Correlation coefficients relevant for entanglement measurement

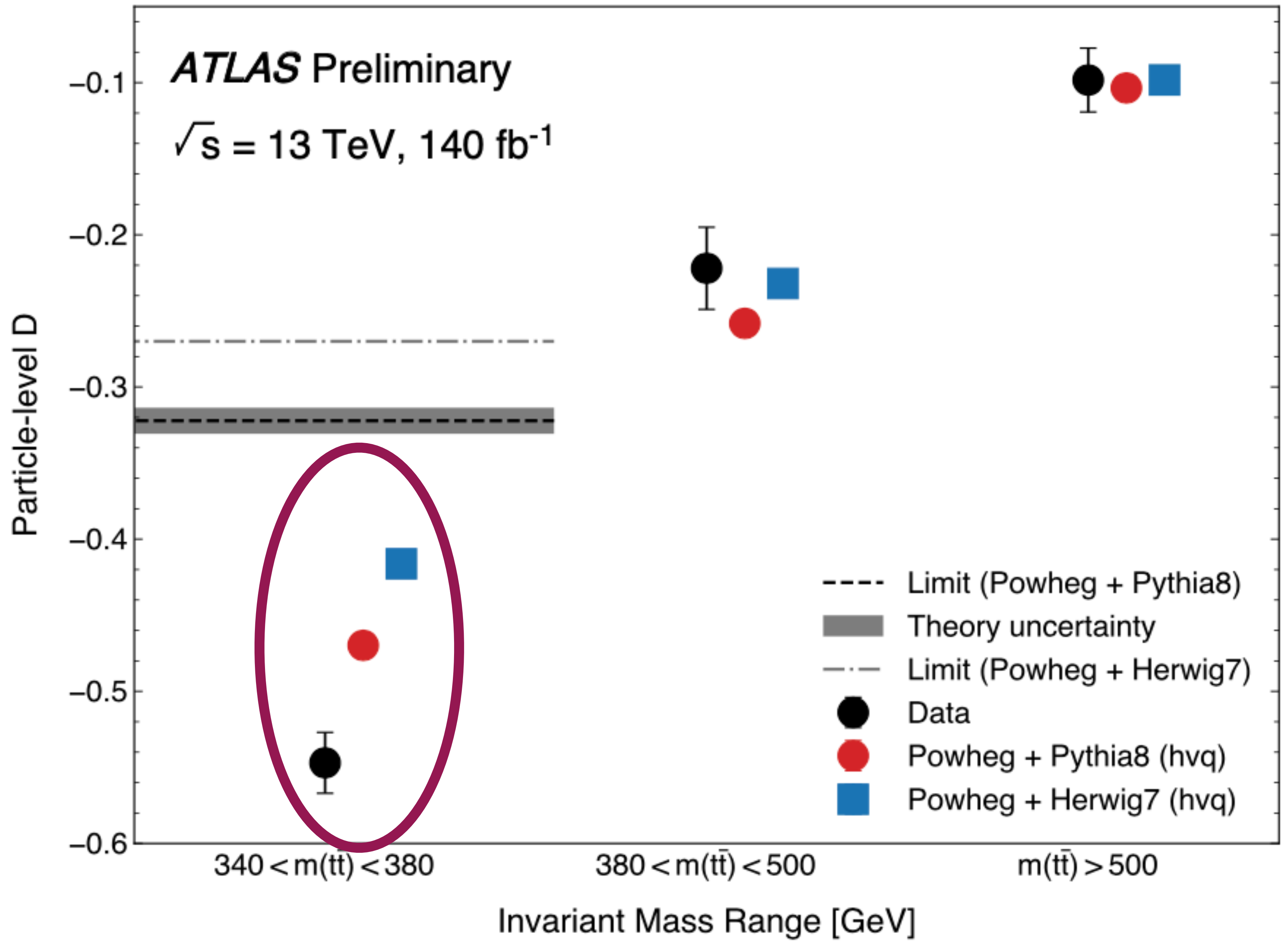
How about the virtual corrections?

	LO QCD [%]	NLO QCD [%]
C_{kk}	$32.68(3)^{+1.5\%}_{-1.7\%}\,^{+0.8\%}_{-0.8\%}$	$32.88(3)^{+1.3\%}_{-0.4\%}\,^{+0.7\%}_{-0.7\%}$
C_{nn}	$33.01(3)^{+0.3\%}_{-0.5\%}\,^{+0.2\%}_{-0.2\%}$	$31.97(3)^{+0.9\%}_{-1.1\%}\,^{+0.2\%}_{-0.2\%}$
C_{rr}	$0.71(3)^{+45.1\%}_{-51.5\%}\,^{+3.2\%}_{-3.2\%}$	$4.80(3)^{+28.9\%}_{-19.2\%}\,^{+2.8\%}_{-2.8\%}$

Frederix, Tsinikos, Vitos arXiv:2105.11478

25% difference between the value of C_rr due to approximation of virtual corrections (in MadSpin and Hvq)
Relevant?

Parton shower dependence



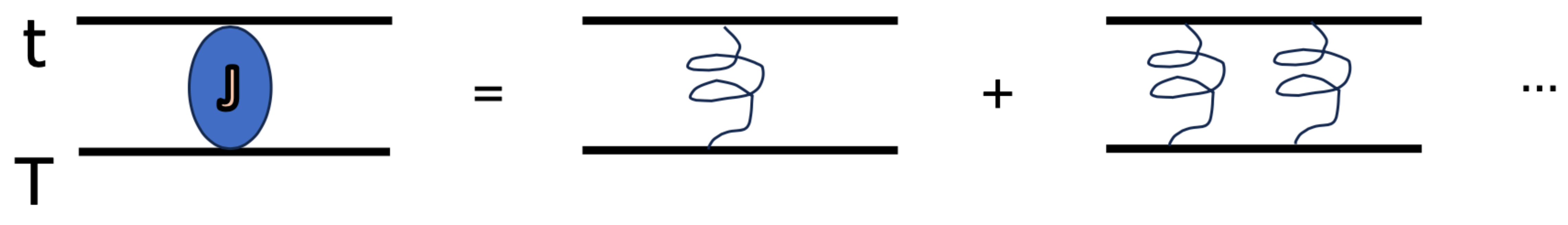
ATLAS-CONF-2023-069

Big difference in low mass region

- Does this happen for other spin observables?
- Why is this region affected by the shower ordering?
- Does this go away with vetoing additional radiation?

Threshold issues?

Bound state



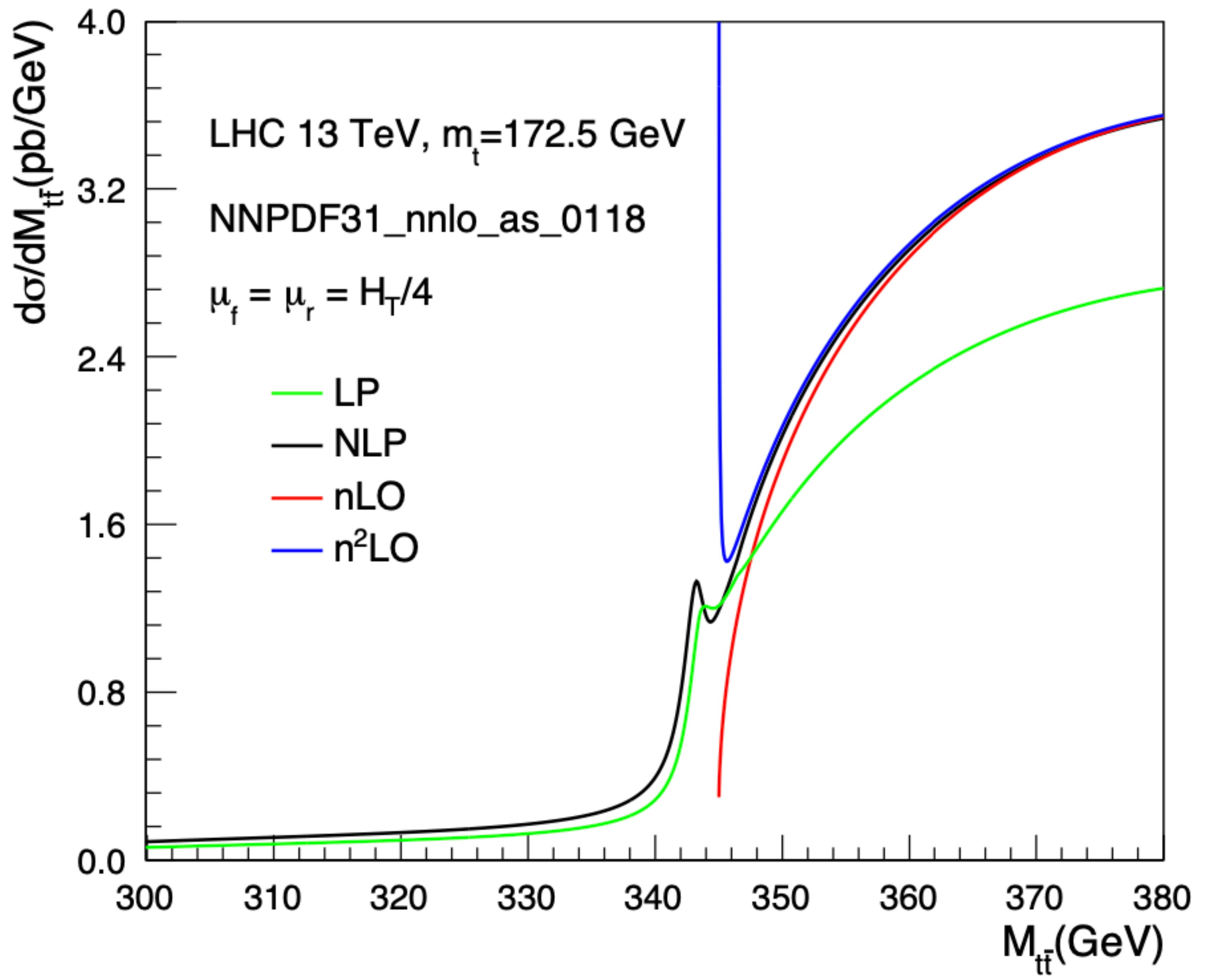
We can sum up:

leading power (LP) $\left(\frac{\alpha_s}{\beta}\right)^n$

next to leading power (NLP) $\alpha_s\left(\frac{\alpha_s}{\beta}\right)^n$

This results in a complicated function (Sommerfeld factor): $J \sim \frac{\alpha_s/\beta}{e^{\pi\frac{\alpha_s}{\beta}}-1} = 1 + \frac{\alpha_s}{\beta} + \ldots$

From A. Mitov@top2023



Ju, Wang, Wang, Xu, Xu and Li Lin Yang arXiv:2004.03088

Not included in current MC but a very localised effect
Split 340-380 GeV interval? Approximate effect by reweighting?

Conclusions

- Significant advances in theory calculations of spin correlation observables over the last years
- Important to evaluate impact of higher order effects as well as approximations in existing Monte Carlo
- Eventually MC should include more physics effects, interesting to see if any of these will resolve the difference between MC and data

Thank you for your attention