Spin Correlations in ttbar Production and Decay at the LHC in pQCD

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Introduction and take-home messages

- Both ATLAS and CMS have reported, over the past years, an excess in the ttbar production cross-section near threshold. This deviation from the “baseline Standard Model prediction” is often interpreted as a bound-state contribution, commonly referred to as “toponium.”

- This talk: results from arXiv:2505.00096, in collaboration with L. Rottoli and P. Nason. There’s ongoing work on this topic together with G. Pelliccioli too.

- We’ve found that the tensions between LHC results and MC generators can be alleviated **taking into account threshold corrections properly**.
  Including N3LO terms (that include (not only) bound state terms) helps, but **it is not crucial**.

Introduction and take-home messages

- The main intuitive point is that, since Mtt bins (so far) aren't very narrow, x-sections and observables therein can be reliably estimated keeping only the first few terms in the expansion α_S/v, with contributions due to bound states being rather small.

- At N3LO there's certainly a contribution to the x-section due to "toponium".

  ⇒ Our point is not that this contribution is not there, but that it is premature to claim that the observed TH-EXP tension requires necessarily bound-state formation to be explained.

- Relevant literature: M.Braun (1968), 1109.1536 [Beneke, Falgari, Klein, Schwinn] 1402.5690 [Melnikov, Vainshtein, Voloshin], 1606.02434 [Beneke, Ruiz-Femenia].

Spin correlations in threshold region

- Threshold production: interesting per se in QCD and for entanglement in ttbar.

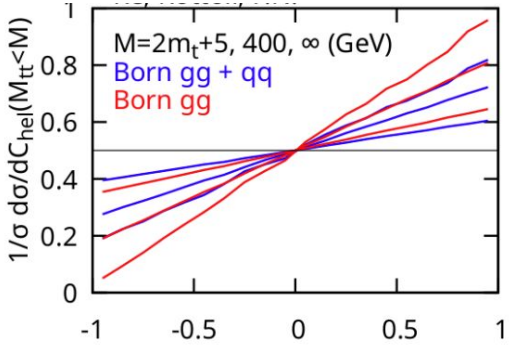
- Threshold dominated by s-wave ttbar states:
  → angular momentum from spin: singlet or triplet ttbar state.
- spin triplet: mixed state
  spin singlet: pure state → $\frac{|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle}{\sqrt{2}}$ → entanglement studies

- At threshold: qqbar→ ttbar is spin-triplet dominated (offshell s-channel gluon)
  gg→ ttbar is spin-singlet dominated (Landau-Yang)
- c_{hel}=scalar product of leptons directions (in ttbar rest frame): $c_{hel} = \hat{p}_+ \cdot \hat{p}_-$

- If spin singlet: $\frac{1}{\sigma}\frac{d\sigma}{dc_{hel}} = \frac{1+c_{hel}}{2}$

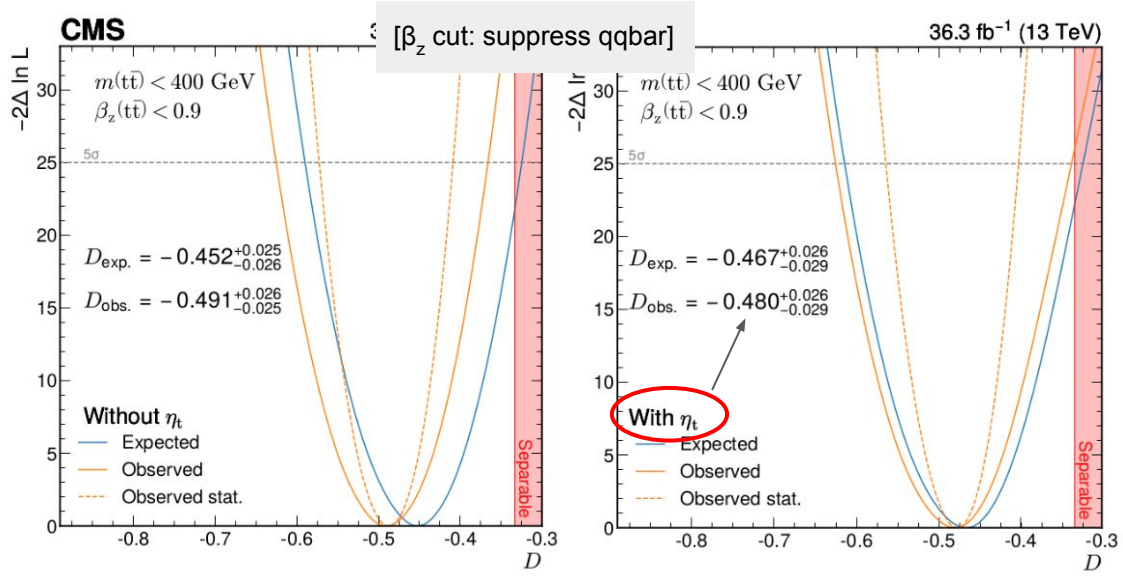
- D=-3<c_{hel}>. D=-1 for pure spin singlet.

  D<-⅓ entanglement condition.



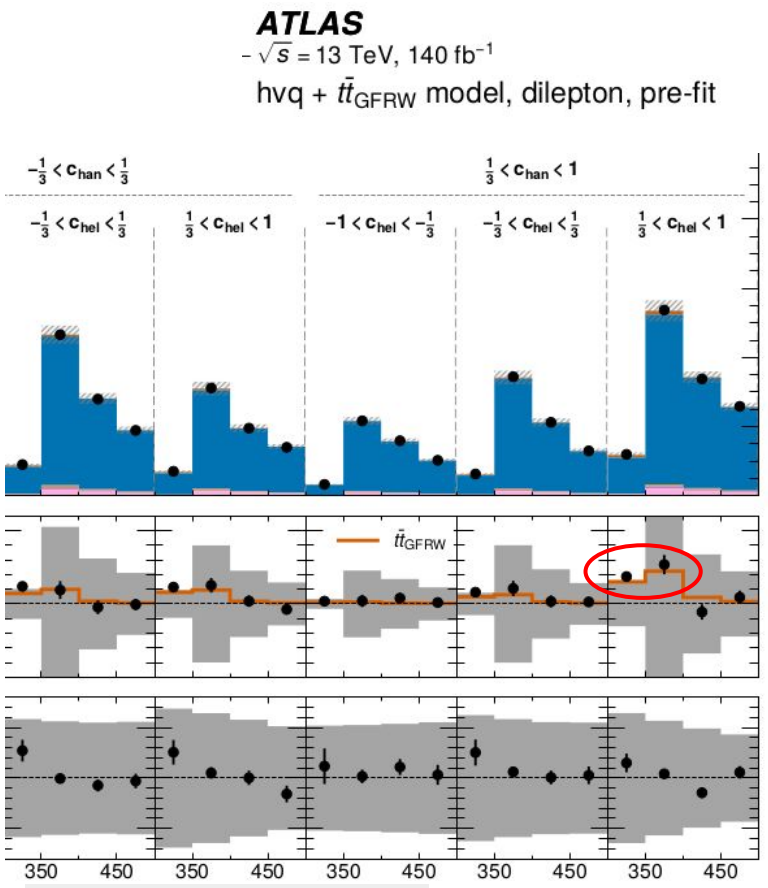
Measurements & physics case

- BSM (pseudo)-scalar coupled to tops would enhance signal
- entanglement at the LHC, new physics, …
- toponium?



[β_z cut: suppress qqbar]

EXP results seem to support contribution from pseudoscalar contribution ($\eta_{t,}$ toponium).



[large c_{han}: favour color singlet]

Threshold enhancement & bound states

- Coulomb exchange in non-relativistic limit: $(\alpha_S/v)^n$ enhancement. [v=speed of t in ttbar frame]

- Represented by “ladder diagram”.

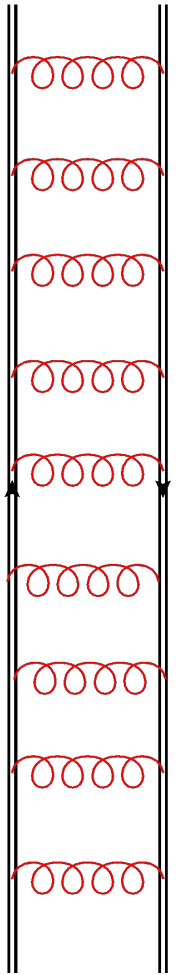
- a_S = [col. factor] x α_S

  [col. factor] → {C_F, $-1/(2N_C)$} if {singlet, octet}

- Each ladder → (α_s/v)
- Potential energy: (a_s/r)
- Momentum: $|\mathbf{p}| \approx 1/r$
- Bound state: $\mathbf{p}^2/m \approx (a_s/r)$

⇒ $v \approx a_s$

⇒ close to bound state regime: need to resum $(\alpha_S/v)^n$ terms.



Threshold enhancement & spin correlation

- Coulomb exchange:
- Attractive if ttbar in colour singlet, repulsive if color octet
- qqbar→ttbar@thr: LO | gg→ttbar@thr: LO

$$\sigma_{q\bar{q}}^{(8)} \approx \frac{\alpha_s^2}{m^2}\frac{\pi v}{9} \qquad \sigma_{gg} \approx \frac{\alpha_s^2}{m^2}\frac{\pi v}{192}\left[\underbrace{2}_{\text{singlet}} + \underbrace{5}_{\text{octet}}\right]$$

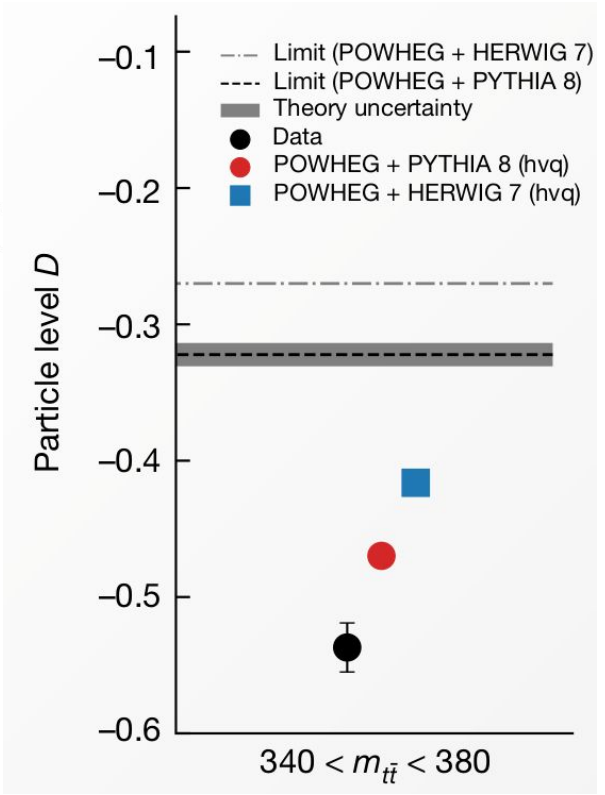
- Coulomb enhancement: singlet: C_F, octet: $-1/(2N_C)$

$$\left[2 \times \frac{4}{3} + 5 \times \left(-\frac{1}{6}\right)\right] = \left[\frac{8}{3} - \frac{5}{6}\right] > 0$$

⇒ 1st order overall correction to gg positive

- Cross-section: enhanced close to threshold.

- Spins: gg@thr → spin singlet, qqbar@thr→ spin triplet
  ⇒ (a_S/v) correction leads to enhanced correlation.



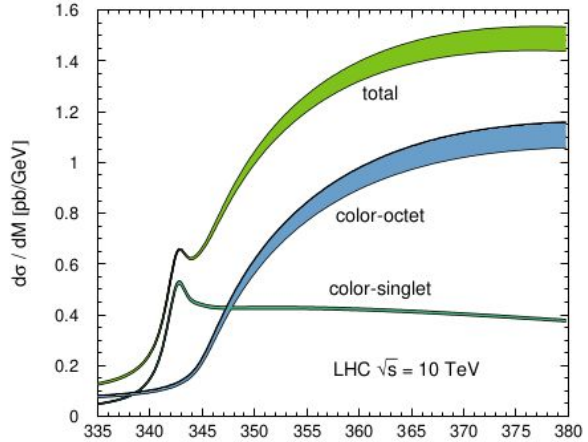
[ATLAS '23]

Cross-section, bound states & counting

- Near threshold: possible to form Coulomb-like bound states.
- $v \approx a_S$ (as hydrogen atom).
- Size of system: $r_b \approx 1/(m\, a_S)$, time to orbit ~ size/v ~ $1/(m\, a_S^2)$

  $\Rightarrow |\Psi(0)|^2 \approx (1/r_b)^3 \approx (m\, a_S)^3$
  $\Rightarrow$ using $a_S = \alpha_S$ x $[C_F]$:
  time to orbit ~ top lifetime ($a_S \sim 0.16$) $\rightarrow$ bump

[Kiyo, Kühn, Moch, Steinhauser, Uwer, '09; see also Hagiwara et al '08]



- Bound state must contribute as

$$\sigma(E) \simeq \frac{1}{m^4}\delta(E - 2m)\,|\Psi(0)|^2\,\alpha_S^{\,2}$$

- Using expression for wave-function:

$$\sigma(E) \simeq \frac{1}{m}\delta(E - 2m)\,\alpha_S^{\,2}\,a_s^{\,3}$$

N3LO correction

- As it stands, cannot arise in pure pQCD: it must not be there if repulsive coupling (a_S<0)

Binned distributions and bound-state contribution

- x-sec is measured in rather large Mtt bins (e.g. [340, 380] GeV, [300, 350] GeV).
  → Not enough resolution to see the bump.
- Enhanced α_S/v contributions are integrated: eventually sensitive to the velocity associated to the upper edge of the (1st) Mtt bin. Up to NNLO:

$$\int^{E_{cut}} dE\,\sigma(E) \sim \int^{v_{cut}} m\,dv^2\,\sigma(E) \approx \frac{\alpha_s^2 v_{\rm cut}^3}{m}\left(1,\ \frac{a_s}{v_{\rm cut}},\ \frac{a_s^2}{v_{\rm cut}^2}\right)$$

where $v_{cut} \simeq \sqrt{(E_{cut} - 2m)/m}$

- If far enough from threshold, **also at the order where bound states contribute**, such cross-section (i.e. the integral up to an energy cut) can be computed in pQCD, without explicitly separating bound states and continuum.

- If v_{cut} too small, resummation still needed.
  → with current Mtt bins, this doesn't seem to be very important.

- To understand better what happens at N3LO, ordinary QM helps.

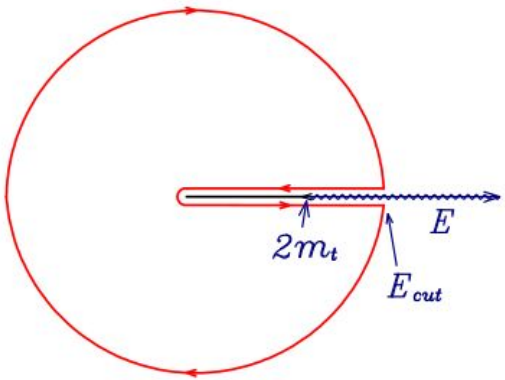
Bound-state contribution

- The cross section is related to the density of states ρ(E).
- Resolvent, i.e.time Fourier transform of Green's function

$$\frac{1}{E - H + i0} = \sum_n \frac{|n\rangle\langle n|}{E - E_n} + \int_{E_0}^{\infty} dE' \, \frac{|E'\rangle\langle E'|}{E - E'}$$

- $\frac{1}{x \pm i0} = \mathcal{P}\frac{1}{x} \mp i\pi\delta(x)$ → imaginary part of forward resolvent ~ spectral density.
- Integrating x-section up to a sufficiently large value of E_{cut} is equivalent to do a contour integral of the resolvent on a circle of radius E_{cut} .

  ⇒ away from threshold there should be no sensitivity to bound states, and the result should be convergent in perturbation theory (both bound states and continuum included).



- Intuitively: a "relatively large" Mtt bin defines a "relatively inclusive" cross section (think about e^+e^- → hadrons far from resonances).

Toy model (1d QM)

- Schroedinger's equation: single particle mass m in V(x) = - λ δ(x)

$$\left(-\frac{1}{2m}\frac{\mathrm{d}^2}{\mathrm{d}x^2} - \lambda\delta(x)\right)\psi = E\psi$$

- Eigenstates (even only):

$$\psi_b(x) = \theta(\lambda)\sqrt{k_b}\left[e^{k_b x}\theta(-x) + e^{-k_b x}\theta(x)\right] \quad k_b = m\lambda\,,\; E_b = -m\lambda^2/2\,,$$ *Bound states*

$$\psi_k(x) = \sqrt{\frac{2}{L(1+b_k^2)}}\left[\cos(kx) - \frac{x}{|x|}b_k\sin(kx)\right] \quad b_k = m\lambda/k \quad ,$$ *Free states*

- Density (imaginary part of forward resolvent):

$$\rho(E) \;=\; \theta(\lambda)\lambda m\,\delta\left(E + \frac{1}{2}m\lambda^2\right) + \frac{1}{\pi}\frac{m}{k_E}\frac{1}{1+\lambda^2/v_E^2} \qquad k_E = \sqrt{2mE}\,,\; v_E = k_E/m$$

- No power expansion in λ for ρ(E): first term contains a theta function; second term expanded in λ not integrable in dE.

Toy model (1d QM)

- However, full integral of density up to a given energy value can be expanded:

$$\int^{E'} \mathrm{d}E\,\rho(E) \;=\; \frac{1}{\pi}k' + m\underbrace{\left[\lambda\theta(\lambda) - \frac{|\lambda|}{2}\right]}_{=\lambda/2} + \frac{m\lambda^2}{\pi}\frac{m}{k'} + \dots$$

- a) Non-analytic term from continuum combined with bound states:
  → overall analytic term at order λ (contributing a half of the "bound state" only).
  b) Ordinary expansion in λ: $O(\lambda^2)$ term has given finite result:
  → $O(\lambda^2)$ term in ρ(E) to be interpreted as a distribution:

- $$\rho(E) \;=\; \frac{\lambda}{2}m\delta\left(E + \frac{1}{2}m\lambda^2\right) + \frac{1}{\pi}\frac{m}{k_E}\left(\frac{1}{1+\lambda^2/v_E^2}\right)_+$$

  ⇒ perturbative expression for ρ(E) possible, if coefficient interpreted as distributions.
  ⇒ Possible to verify this property explicitly: compute resolvent explicitly in pert theory, up to order λ, without "solving" the full QM problem; it agrees with the above eq.

- Such result can be generalized to the ttbar case.

pp→ ttbar

- $$\rho_l(\mathcal{E}) \to \frac{1}{2\pi r_l^3}\sum_{n=1}^{\infty}\frac{1}{n^3}\delta(\mathcal{E}-E_{l,n}) + \frac{m^{3/2}}{4\pi^2}\sqrt{\mathcal{E}}F^{+}(b_l v^{-1}) \qquad \mathcal{E} = M_{t\bar{t}} - 2m$$

$$r_l = \frac{2}{ma_l}, \quad E_{l,n} = -\frac{m}{4}\frac{a_l^2}{n^2}, \quad b_l = \pi a_l, \qquad F(z) = \frac{z}{1-\exp(-z)}$$

Sommerfeld factor

$$a_1 = C_F\alpha_s, \qquad a_8 = -\frac{\alpha_s}{2N_C}$$

- Density can be expanded up to order α_S^3

$$\frac{m^2}{4\pi^2}\left(v + \frac{b_l}{2} + \frac{b_l^2}{12v} + \frac{\zeta(3)}{4\pi^2}b_l^3 m\delta(\mathcal{E}) + \mathcal{O}(\alpha_s^4)\right)$$

- (N)NLO computations include, close to threshold, the 2nd and 3rd term.
  - At N3LO: bound states + open production, that cannot be distinguished without high resolution in Mtt.

[NB: m → m/2 (reduced mass)]

pp→ ttbar, in practice

- $$\frac{m^2}{4\pi^2}\left(v+\frac{b_l}{2}+\frac{b_l^2}{12v}+\frac{\zeta(3)}{4\pi^2}b_l^3 m\delta(\mathcal{E})+\mathcal{O}(\alpha_s^4)\right)$$

  Threshold corrections implemented, in practice, by replacing v with the above expression, starting from the known LO terms:

$$\sigma_{q\bar{q}}^{(8)} \approx \frac{\alpha_s^2}{m^2}\frac{\pi v}{9} \qquad \sigma_{gg} \approx \frac{\alpha_s^2}{m^2}\frac{\pi v}{192}\Big[\underbrace{2}_{\text{singlet}}+\underbrace{5}_{\text{octet}}\Big]$$

- Scale choice: appropriate scale to use for threshold corrections:
  → typical momentum of the top quark in ttbar rest frame (for a fixed value of Mtt=E_{cut}).

- Comment: in 2505.00096, we **did not have** a fully-differential MC generators implementing such effects; results were obtained by correcting MC results at the level of distributions.

pp→ ttbar, in practice

- (N)NLO (+PS) generators already include some of the above terms + different scale choices.

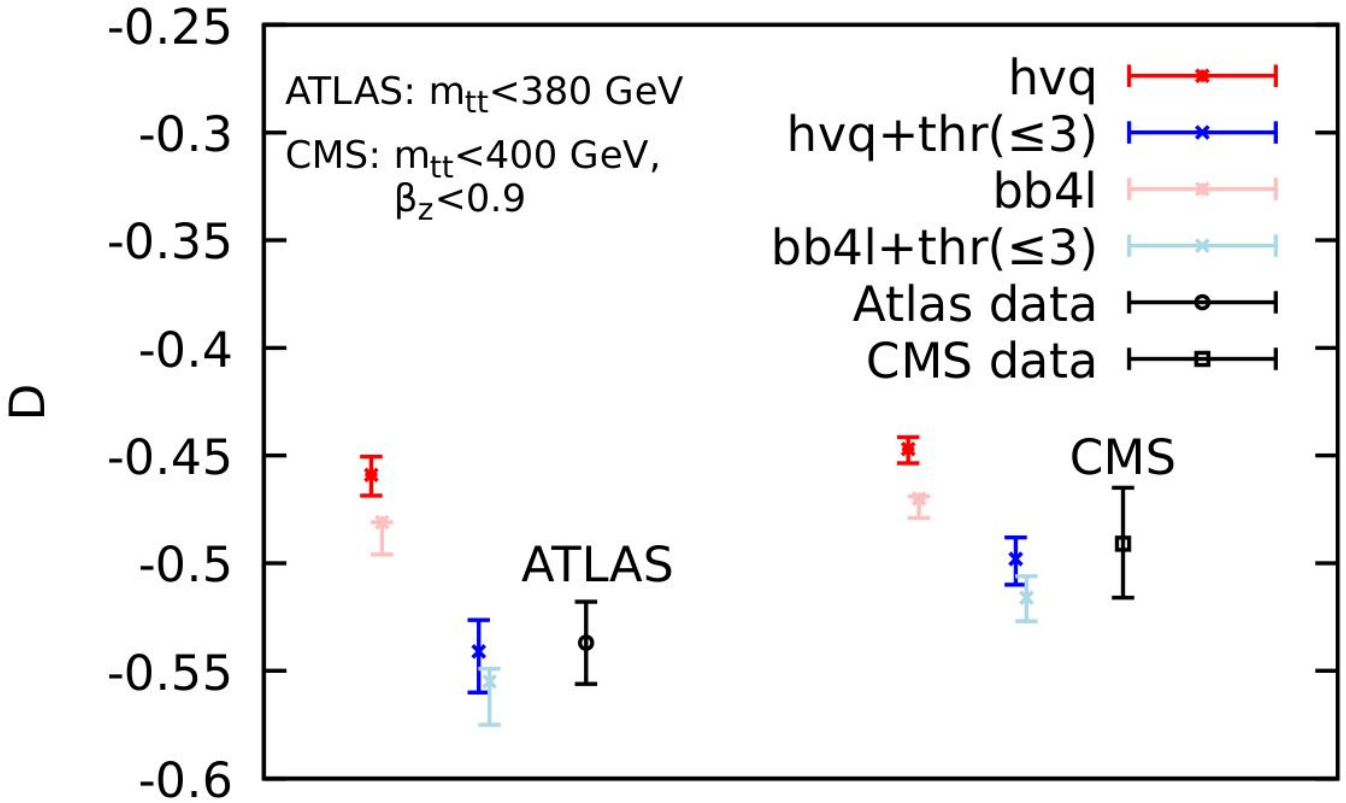
- Take care of overcounting correcting with the following factors:

$$F_{\mathrm{LO}}^{(\leq i)}(M) = F^{(\mathrm{LO})}(M) + \theta(i \geq 1)(F_0^{(\leq 1)}(M) - F^{(\mathrm{LO})}(M))\frac{\alpha_s(S(M))}{\alpha_0} + \theta(i \geq 2)(F_0^{(\leq 2)}(M) - F_0^{(\leq 1)}(M))\left(\frac{\alpha_s(S(M))}{\alpha_0}\right)^2 + \theta(i \geq 3)(F_0^{(\leq 3)}(M) - F_0^{(\leq 2)}(M))\left(\frac{\alpha_s(S(M))}{\alpha_0}\right)^3 \quad (5.8)$$

where $F_{\mathrm{LO}}^{(\leq i)}$ represent the LO cross section corrected with threshold enhanced contributions up to the order i. $S(M)$ is our choice of the renormalisation scale as a function of M, that we choose equal to one half of the top momentum in the $t\bar{t}$ rest frame:

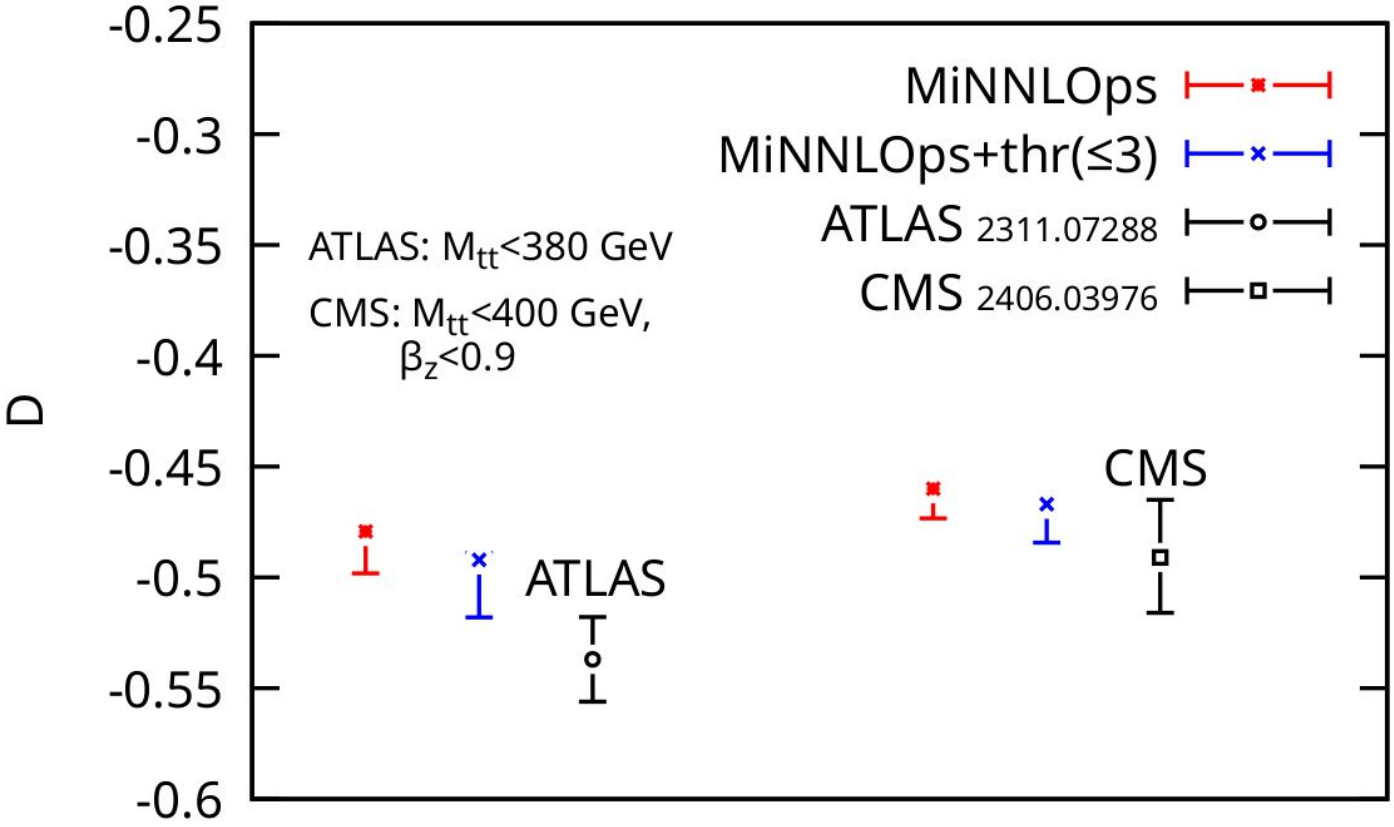
$$S(M) = \frac{1}{4}\sqrt{M^2 - 4m^2}. \quad (5.9)$$

TH vs data: NLO generators + threshold terms



⟶ tension with data seems to be gone; generator dependence: WIP.

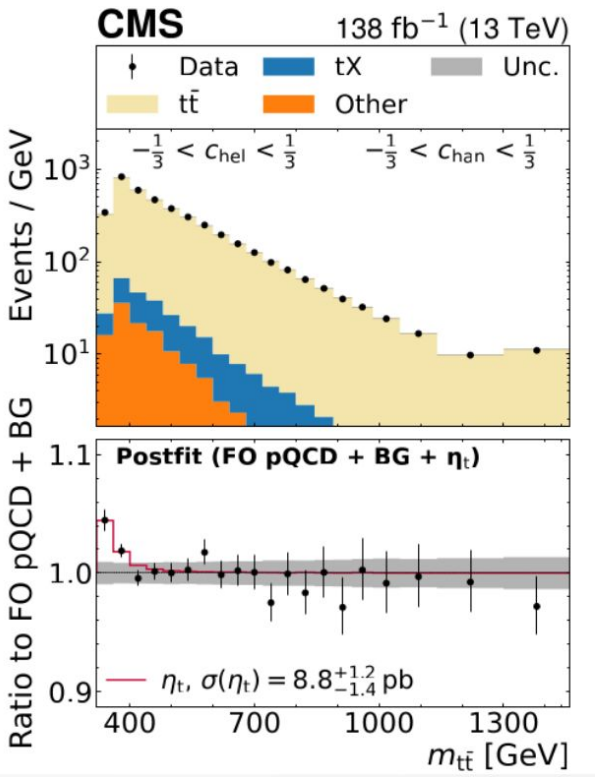
TH vs data: NNLO generators + threshold terms



a_S^3 correction:
→ small improvement

- NB: checked (after publication) that $(a_S/v)^n$ series converges, no need to resum.

TH vs data: CMS excess



- Excess (8.8 pb) on top of hvq generator, NNLO reweighted with MATRIX.

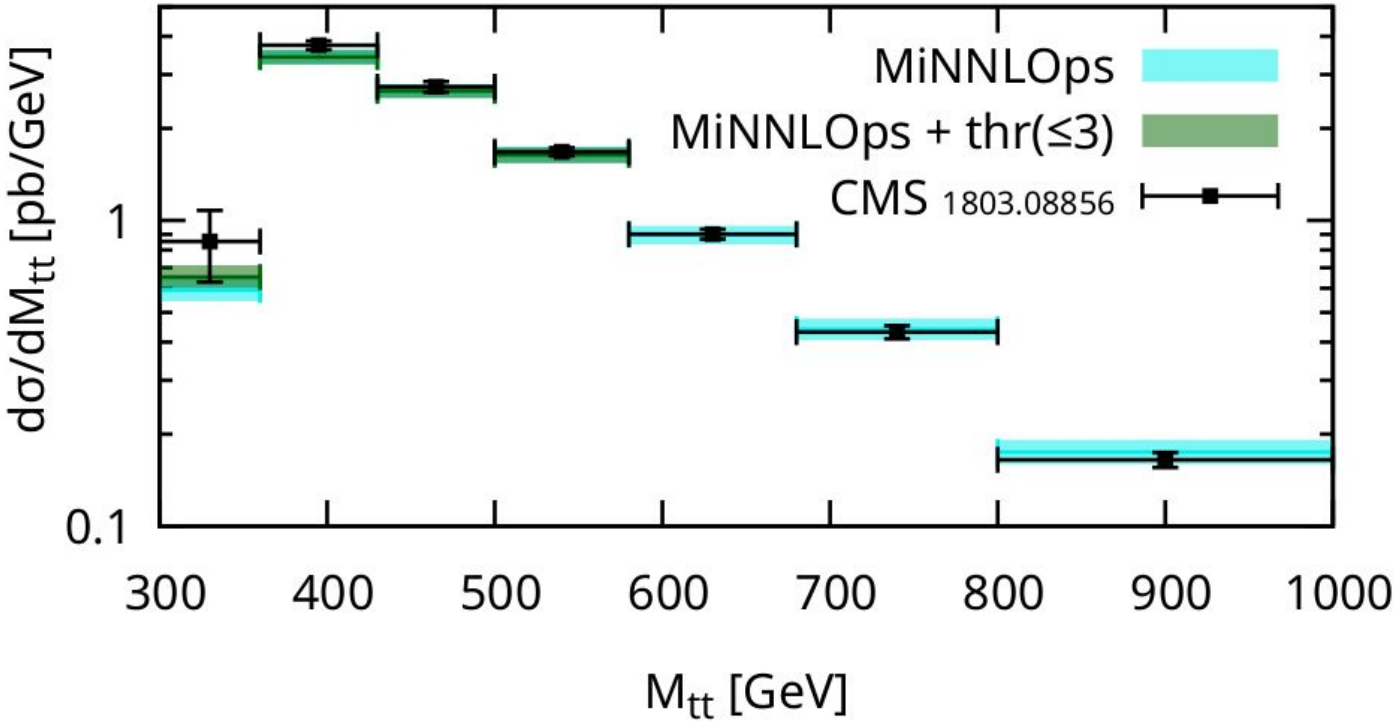
- Such excess argued to be consistent with Green's function method (that contains bound-state contribution).

- Our computation in first bin, Mtt<360 GeV:

$(a_S/v) \rightarrow 3.36$ pb
$(a_S/v)^2 \rightarrow 4.43$ pb
$(a_S/v)^3 \rightarrow 1.56$ pb

Compatible with 8.8 pb; however CMS baseline should already contain a good portion of the a_S/v and $(a_S/v)^2$ terms…

TH vs data: CMS Mtt distribution



Conclusions and prospects

- As long as Mtt resolution is not very high, we find that it's not necessary to fully include bound state effects to compare well with data (e.g. $O(\alpha_S^2\, a_S^3)$ term gives a minor effect).

- Desirable that event generators are able to provide reliable predictions also close to threshold. Achievable in practice, often with some approximations. Consistency not trivial:
  → reproducing the perturbative prediction for the *integrated cross section* over relatively large bins near threshold is challenging.

- Discrepancies with data to be understood; discussions are taking place in the LHCtopWG. Several groups are working on improving their predictions (e.g. Green-function reweighting in `MG5` [Fuks et al, 2411.18962], FO+NRQCD [Garzelli et al., 2604.09485]).

- We [Nason, Pelliccioli, ER, Rottoli] are currently working on including off-shell effects and threshold corrections, differentially, in hvq and in bb4l (possibly also in `MiNNLOps`), consistently with the results presented here. The idea is to use the resolvent with width dependence [Fadin,Khoze '87].

- Such effort might also allow to understand better the approximations used in `hvq` (and `MiNNLOps`) to include off-shell effects.