Top-antitop production and decay near threshold

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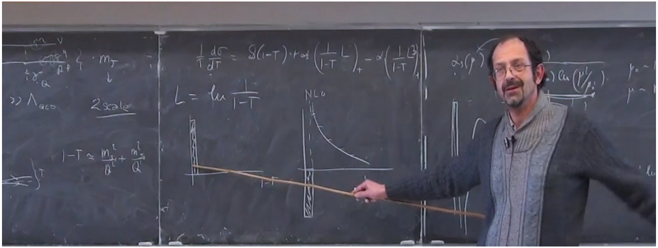

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In 1996 (Catani, Mangano, Trentadue, P.N.) I got involved, together with Stefano, in a research work where we examined the resummation of Sudakov logarithms in collider processes, in particular for applications to $t\bar{t}$ production in hadronic collisions.

The basic issue we dealt with: threshold resummation in x space for $t\bar{t}$ production leads naively to a form

$$\int_{\tau}^{1} \mathrm{d}x \exp[a \log^2(1-x)] \frac{\mathrm{d}}{\mathrm{d}x} \mathcal{L}\left(\frac{\tau}{x}\right), \tag{1}$$

that (although seemingly correct as far as the threshold logarithms that it generates) contains terms that are NOT enhanced by logs, but grow in value as the factorial of the order of the perturbative expansion, leading to divergent results.

These terms (later on dubbed "Sudakons" by Beneke) should be avoided to get physically reasonable results from resummation.

This was my first work with Stefano, and I enjoyed it a lot. It was a case where a simple observation made a difference in the progress of our field. This gave us that spark of enthusiasm that sometimes happens to enlighten our work ...

Much time has gone by since then. Some people did not take well our claims, and bitter arguments followed, mostly involving Michelangelo and myself. Now this is all forgotten, and our findings are seen as obvious.

Rather than reviewing these things, in choosing a topic for a talk in memory of Stefano, I have preferred to pick one that has recently given to me that same spark of enthusiasm and amusement that I felt for the '96 work. Incidentally, It still has to do to some extent with $t\bar{t}$ production near threshold, but it is something totally different, and is still work in progress.

Before starting with the discussion of this new topic, I would like to say one more thing regarding Stefan's work.

Since our 96 work I have collaborated with Stefano in several other occasions.
However, the paper that has most influenced my subsequent works was not one that I authored with him; it was the CKKW [Catani,Krauss,Kühn,Webber] paper.

Many ideas for conceiving the POWHEG method came from studying this paper, and subsequent progress in my work (the MiNLO development) took this paper as the starting point.

The top spin

It turns out that, in leptonic top decays, the direction of the anti-lepton in the top rest frame coincides with the top spin vector, i.e.

$$\hat{\vec{\ell}} \cdot \vec{\sigma}\, s_t = s_t$$

where s_t is the top non-relativistic spinor. (by CP, $\hat{\vec{\ell}} \cdot \vec{\sigma}\, s_{\bar{t}} = -s_{\bar{t}}$)

It is amusing that we can prove this fact in two lines of spinor algebra:

$$\begin{aligned}\mathcal{B}_D \sim & \bar{u}_b \gamma^\mu (1-\gamma_5) u_t \; \bar{u}_\ell \gamma_\mu (1-\gamma_5) v_\nu = -\bar{u}_b \gamma^\mu (1-\gamma_5) u_t \; \bar{u}_{\ell R} \gamma_\mu (1+\gamma_5) v_{\nu R} \\ = & -\left[\bar{u}_{\ell R}(1-\gamma_5) u_t\right] \left[\bar{u}_b (1+\gamma_5) v_{\nu R}\right],\end{aligned}$$

where the suffix R denotes the charge conjugate (right handed) spinor, and a Fierz identity has been used. Then one finds easily

$$\bar{u}_{\ell R} u_t = \bar{u}_{\ell R} \frac{1+\gamma_5 \hat{\not{\ell}}}{2} u_t$$

$t\bar{t}$ in singlet spin state

Production at threshold is dominated by s-wave $t\bar{t}$ states. In this limit 4 independent spin states for a $t\bar{t}$ pair can be constructed: a spin singlet (spin 0) and a spin triplet (spin 1) state.

Spin triplet production will yield a spin mixed state, since it will generally be the sum of three (spin 1) polarizations.

Spin singlet is instead a pure state

$$\frac{|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle}{\sqrt{2}}.$$

At threshold:

- $q\bar{q} \to t\bar{t}$ (at Born level) is dominated by the triplet state;
- $gg \to t\bar{t}$ (at Born level) is dominated by the singlet state, since a spin zero state cannot couple to two massless vectors (Landau-Yan theorem).

$t\bar{t}$ spin correlations at the LHC

In the dileptonic $t\bar{t}$ events one defines the observable

$$c_{\rm hel} = \vec{\ell}_+ \cdot \vec{\ell}_- \ .$$

For a (non-relativistic) $t\bar{t}$ pair in a spin singlet state, by simple Quantum Mechanics we find that $c_{\rm hel}$ is distributed as

$$\frac{1}{\sigma}\frac{{\rm d}\sigma}{{\rm d}c_{\rm hel}} = \frac{1+c_{\rm hel}}{2}$$

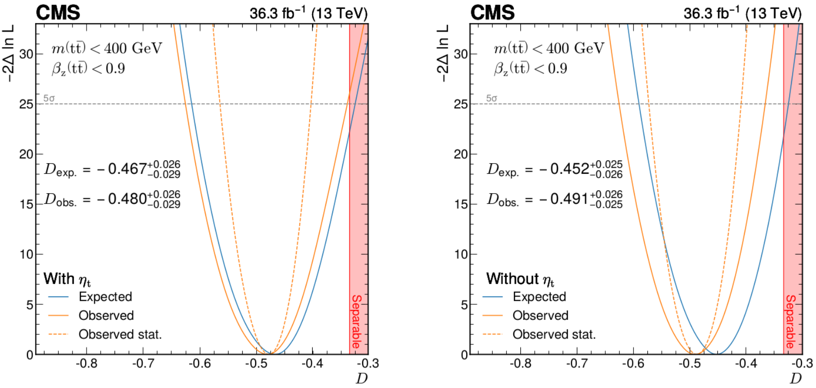
We also obtain immediately

$$\langle c_{\rm hel} \rangle = \frac{1}{3}$$

and also introduces the quantity $D = -3\langle c_{\rm hel}\rangle$, that equals -1 for a pure spin singlet state.

$t\bar{t}$ spin correlations at the LHC

ATLAS: "Observation of quantum entanglement with top quarks ..."
$D = -0.537 \pm 0.002(\text{stat.}) \pm 0.019(\text{syst.})$ for $340\text{GeV} < mtt < 380\text{GeV}$.



Expected value from various MC generators is about $D = -0.46$.
Tension with theoretical predictions: more singlet needed?

Searches for scalar and pseudo-scalar decaying into $t\bar{t}$

Interest in this topic is also fueled by experimental searches for BSM scalars and/or pseudoscalars coupled to the $t\bar{t}$ system. The pseudo-scalar decays into a $t\bar{t}$ paper in a spin singlet state, and correlation observables can help in enhancing the signal.

- The precision of these very delicate measurement is outstanding, and challenges our current production/decay models.
- Interest in this topic also for the search of scalar and pseudoscalar resonances in the $t\bar{t}$ channel.
- Notice the attempt to add a pseudoscalar $t\bar{t}$ bound state to the production model in order to ease the tension.

Current work

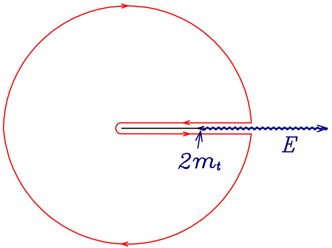
- Theoretical studies with models obtained by adding an η_t bound state to the SM production mechanism have been proposed by [Maltoni,Severy,Vryonidou,2024]
- Improving MC generator by including full treatment including all threshold-enhanced contributions to $t\bar{t}$ production in the non-relativistic approximation Fuks,Hagiwara,Ma,Zheng,2024.

These works emphasize the effect of toponium formation in enhancing the singlet signal in $t\bar{t}$ production.

THE ISSUE

Do we really need to include toponium effects for these observables?

- The experimental resolution Δ_{Mtt} for the measurement of $m_{t\bar{t}}$ is around 15 GeV (we will never really see a peak).
- The observables consider by the experiments involve an integration over $m_{t\bar{t}}$ up to 400 GeV, i.e. about 50 GeV above the threshold.
- Think in analogy to what happens for τ hadronic decays ... A cross section integral can be turned into a contour integral:



- When integrating along the contour we are far from the $v \to 0$ limit.

Resummation of $(\alpha_s/v)^k$ effects should not be needed ...

Toy model of bound state production

- Let us consider the Quantum mechanical system of a particle in a delta function potential, in one space dimension.
- It can be considered as the reduced problem of a two particle bound state.
- The finite width of the top plays no role for what I have to say ($\Gamma_t/2 \ll \Delta_{\mathrm{Mtt}}$).
- The system is exactly solvable.
- We can compare the exact solution to the one obtained in perturbation theory.

Toy model of bound state production

Schrödinger equation:

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

Eigenstates:

$$\begin{aligned}
\psi_0(x) &= \sqrt{k_0}\left[e^{k_0 x}\theta(-x) + e^{-k_0 x}\theta(x)\right], \qquad k_0 = m\lambda, \qquad E_0 = -\frac{m\lambda^2}{2}; \\
\psi_k(x) &= \sqrt{\frac{2}{L(1+\beta_k^2)}}\left[cos(kx) - \frac{x}{|x|}\beta_k \sin(kx)\right], \qquad \beta_k = \frac{m\lambda}{k}; \\
\hat{\psi}_k(x) &= \sqrt{2}L\sin(kx)
\end{aligned}$$

where L is the (large) size of the system.

We define the Green's function (or resolvent) in operator notation as

$$R(E) = \frac{1}{E - H},$$

that is defined for complex E. Since we know the spectrum, we can write

$$R(E, x_1, x_2) = \frac{\psi_0(x_1)\,\psi_0(x_2)}{E - E_0} + \left[\sum_k = \frac{L}{2\pi}\int \mathrm{d}k\right] \frac{\psi_k(x_1)\,\psi_k(x_2)}{E - E_k}.$$

in particular we need the forward Green's function (whose imaginary part is the cross section). We obtain

$$R(E, 0, 0) = \frac{k_0}{E - E_0} + \frac{1}{\pi}\int \mathrm{d}k \frac{1}{1 + \beta_k^2} \frac{1}{E - E_k},$$

We have $Im(R(E,0,0)) = 2\pi\rho(E)$, where ρ is the spectral density

$$\rho(E) = k_0\delta(E_0 - E) + \frac{1}{\pi}\int \mathrm{d}k \frac{1}{1+\beta_k^2}\delta(E_k - E) = k_0\delta(E - E_0) + \frac{1}{\pi}\frac{m}{k_E}\frac{1}{1+\beta_k^2}$$

that is proportional to the cross section for producing a final state of energy E_k.

Expanding in powers of λ for $E > 0$ we obtain

$$\rho(E) = \frac{1}{\pi}\frac{m}{k_E} - \frac{\lambda^2}{\pi}\left(\frac{m}{k_E}\right)^3 + \dots$$

showing the well-known λ/v singularities.

This naive perturbative expansion of ρ is invalid at threshold ...

We now consider the integral of the cross section the threshold up to a given energy E'. We get

$$\int^{E'} \mathrm{d}E\,\rho(E) = m\lambda + \frac{1}{\pi}\left[k' - m\lambda\, atan\,\frac{k'}{m\lambda}\right] = \frac{1}{\pi}k' + m\lambda\left[1 - \frac{1}{2}\right] + \frac{m\lambda^2}{\pi}\frac{m}{k'} + \ldots$$

where the 1 in the square bracket is from the bound state, and the $-1/2$ is from the continuum spectrum.

We conclude that the coefficients of the perturbative expansion of ρ should be interpreted as distributions:

$$\rho(E) = \frac{1}{\pi}\frac{m}{k_E} + \frac{m\lambda}{2}\delta(E) - \frac{\lambda^2}{\pi}\left(\frac{m^3}{k_E^3}\right)_+ + \ldots$$

using (as usual)

$$\int_0^{E'} \mathrm{d}E\left(\frac{m^3}{k_E^3}\right)_+ = -\int_{E'}^{\infty} \mathrm{d}E\,\frac{m^3}{k_E^3} = -\frac{m^2}{k'}.$$

We can use perturbation theory without passing through the exact solution:

$$\begin{aligned}
R(E) &= \frac{1}{H_0+V-E} = \frac{1}{H_0-E} - \frac{1}{H_0-E}V\frac{1}{H_0-E} + \dots \\
R(E,0,0) &= \frac{L}{2\pi}\int_0^\infty \mathrm{d}k \frac{|\psi_k(0)|^2}{E_k-E} - \lambda\left(\frac{L}{2\pi}\right)^2\int_0^\infty \mathrm{d}k\mathrm{d}k' \frac{|\psi_k(0)|^2|\psi'_k(0)|^2}{(E_k-E)(E_{k'}-E)} \\
&= \frac{1}{\pi}\int_0^\infty \mathrm{d}k \frac{1}{E_k-E} - \lambda\left[\frac{1}{\pi}\int_0^\infty \mathrm{d}k \frac{1}{E_k-E}\right]^2 \\
&= \sqrt{-\frac{m}{2E}} + \lambda\frac{m}{2E}
\end{aligned}$$

We now can turn the integral of $\rho(E)$ into a contour integral of $R(E)$

$$\int^{E'} \rho(E)\,\mathrm{d}E = \frac{1}{2\pi i}\oint \mathrm{d}E\, R(E) = \frac{k'}{\pi} + \lambda m \frac{1}{2}\left[= 1 - \frac{1}{2}\right] + \dots$$

Same as with the exact calculation, but no mention of the bound state!

What we have learned:

- If the cross section is integrated up to a velocity velocity Δ, we get a result with a well-defined perturbative expansion, containing terms of the form $(\lambda/\Delta)^k$.
- Full resummation is only needed if $(\lambda/\Delta) \lessapprox 1$.
- Care is needed in the computation of the perturbative expansion: the coefficients are distributions.

The $t\bar{t}$ case

We assume in the following that this works also for $yt\bar{t}$ production at threshold, or that at least NO ESSENTIAL COMPLICATIONS arise in this case.

In the perturbative expansion for $t\bar{t}$ production we have:

- Terms behaving like $(\alpha_s/v)^k$, where v is the velocity of the top in the $t\bar{t}$ rest frame, arise in perturbation theory.
- At NLO: α_s^3/v;
- At NNLO: α_s^4/v^2;
- At N^{3}LO: α_s^5/v^3; the $1/v^3$ singularity in not integrable in d^3k.

This is unlike the simple example shown earlier. The $1/v$ and $1/v^2$ terms at NLO and NNLO do not need any special attention, they are integrable

Examine now the contribution of a bound state:

- Peak cross section for an *s*-wave bound state:

$$\sigma_{\rm peak} \approx \frac{1}{m_t^2}\frac{|\psi(0)|^2}{\Gamma_T} \times \frac{\alpha_s^2}{m_t^2}$$

- The cross section near the peak is thus

$$\sigma(E) = \frac{\Gamma_t^2 \sigma_{\rm peak}}{(E-M)^2 + \Gamma_T^2}$$

($M \approx 2m_t$, $\Gamma_T \approx 2\Gamma_t$ are mass and width of the bound state.)

- The integral of the cross section around the peak yields

$$\frac{1}{m_t^2}|\psi(0)|^2 \times \frac{\alpha_s^2}{m_t^2} \approx \frac{\alpha_s^5}{m_t},$$

where I estimated $|\psi(0)|^2 \approx 1/r_b^3 \approx (\alpha_s m_t)^3$.

So: the bound state contribution to the cross section is of the same order of the terms that require "special" treatment in perturbation theory.

Phenomenology

Currently available NLO and NNLO generators for $t\bar{t}$ production already include enhanced effects of order $1/v$ and $1/v^2$

In the following we will examine to what extent the $1/v$ singularities are correctly treated be these generators, and whether, they can already explain the discrepancies found by the experiments for correlation observables.

Available calculations

- On shell top, no decay:
  - NLO: Dawson,Ellis,P.N.1987
  - NNLO: Barnreuther,Czakon,Mitov,2012
  - NNLO: q_T subtraction, public code Catani,Devoto,Grazzini,Kallweit,Mazzitelli,Sargsyan,2019
- Production and decay, narrow width limit:
  - NLO: Bernreuther,Brandenburg,Si,Uwer,2001
  - NNLO: Behring,Czakon,Mitov,Papanastasiou,Poncelet,2019, Czakon,Mitov,Poncelet,2021
- Full finite width effects in production and decay
  - NLO: Denner,Dittmaier,Kallweit,Pozzorini,2012
  - NLO + 1 jet: Bevilacqua,Hartanto,Kraus,Worek,2016

+ vast literature of additional implementations and added corrections.

The NLO+ps generators

There are several implementations of NLO+ps generators. Here I focus upon:

- NLO: hvq (POWHEG): Frixione,Ridolfi,P.N., 2007
- NLO: bb4l: Ježo,Lindert,Oleari,Pozzorini,P.N.,2016
- NNLO: MINNLOps
  Mazzitelli,Monni,Re,Wiesemann,Zanderighi,P.N.,2021

Another generator to consider is ttb_NLO_dec Campbell,Ellis,Re,P.N.2014 (not in this talk).

Treatment of correlations

- Both hvq and MiNNLOps generate undecayed, equal mass top quarks
- Correlation in decays are computed using a method introduced by Frixione,Laenen,Motylinski,Webber,2007 (also implemented as MADSPIN in MadGraph), that I will call the MadSpin method in the following
- bb4l fully accounts for correlations and off-shell effects from the start, as it implements the full process for the production of a $b\bar{b}$ pair accompanied by two lepton of opposite signs plus their two matching neutrinos.

hvq and MiNNLOps both include their own implementation of the MADSPIN method (that may differ from the MCatNLO one).
ttb_NLO_dec fully accounts for correlations, but in the narrow width limit.

Treatment of correlations: the MadSpin method

The hvq generator implements the MadSpin method as follows (and MiNNLOps is similar)

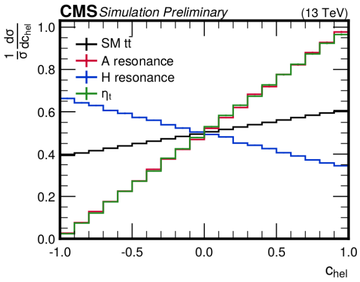
- Start from an hvq Les Houches event, typically made up of a $t\bar{t}$ pair plus a radiated parton, and more rarely by a $t\bar{t}$ pair with no accompanying partons.
- The event is transformed into an event that accounts for the top finite width, i.e. t and $\bar{t}$ are given virtualities distributed as Breit-Wigner resonances, and the momenta are reshuffled accordingly.
- The event is completed by generating a MadGraph event with the same kinematics of the transformed LH event, including the requested decay of the tops.

Thus, for example, a $gg \to t\bar{t}g$ Les Houches event is replaced by a $gg \to (t \to be^+\nu_e)(\bar{t} \to \bar{b}\mu\bar{\nu}_\mu)g$ event with off-shell tops.

At the LHC

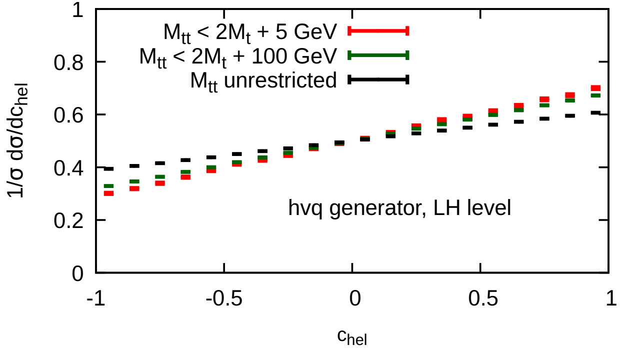
- $gg \to t\bar{t}$ prevails
- Near threshold: $t\bar{t}$ in s-wave: spin 0 (singlet) or 1 (triplet)
- Spin 1 forbidden by the Landau-Yang theorem (same that forbids $Z \to \gamma\gamma$): only singlet allowed (LY argument).

So: we expect a $(1 + c_{\mathrm{hel}})/2$ distribution, and $D \approx -1$ near threshold.
From CMS HIG-22-013-pas:



How do we reach the black line from the red-green one?

Our study: hvq at LH level (PRELIMINARY)

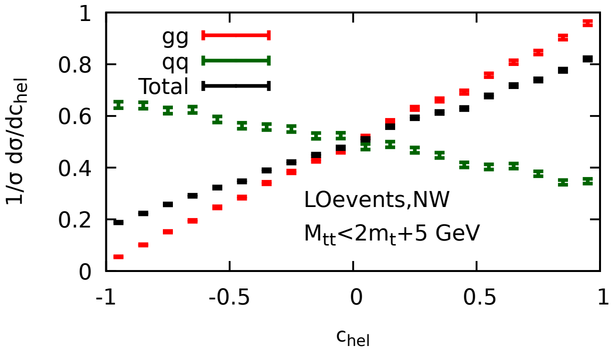


- Reproduces CMS for unrestricted M_{tt}.
- Correlations stronger in the low mass region. Still far from LY.

Deconstruct the result

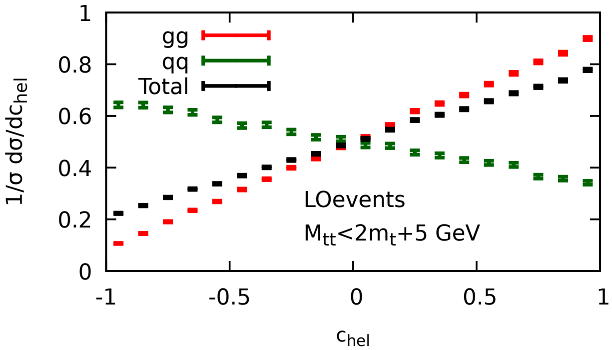
- - Run at Born level, with no radiation in LH file (`bornonly 1` and `LOevents 1` in powheg.input file).
  - Use very narrow width ($\Gamma_t = 0.1$)
  - Separate gg and qq
- Same for physical width ($\Gamma_t = 1.31$)
- Same for combined cross section ($gg + qq$).
- Combined cross section using only `bornonly 1`. In POWHEG, this is the analogue of MEC: underlying Born computed at LO, but radiation included in the event.

LOevents, NW



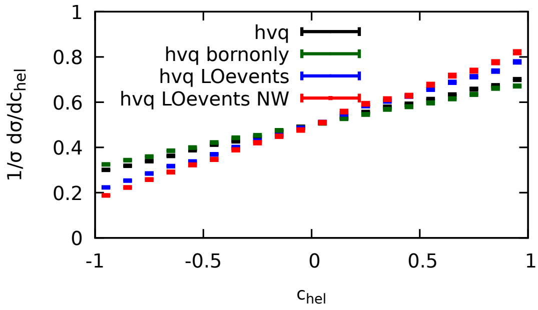
- *gg* contribution very consistent with LY argument
- Total closer to hvq full result.

LOevents



- *gg* contribution very consistent with LY argument
- Total closer to hvq full result.

Summary



- *qq* channel larger impact in deviation from LY.
- Radiation is next in importance (from LOevents to bornonly)
- Minor effect from finite width
- Adding full NLO corrections (from bornonly to hvq) increases slightly the correlation

NLO corrections and correlations

From NDE [Dawson,Ellis,P.N.,1988], near threshold:

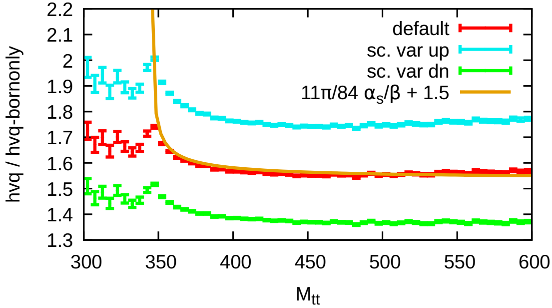
$$\sigma_{qq} \approx \frac{\alpha_s^2}{m_t^2}\left[\frac{\pi}{9}v\right]\left[1 - \frac{\pi}{12}\frac{\alpha_s}{v}\right],$$

$$\sigma_{gg} \approx \frac{\alpha_s^2}{m_t^2}\left[\frac{7\pi}{192}v\right]\left[1 + \frac{11\pi}{84}\frac{\alpha_s}{v}\right]$$

where v is the top velocity in the $t\bar{t}$ rest frame.

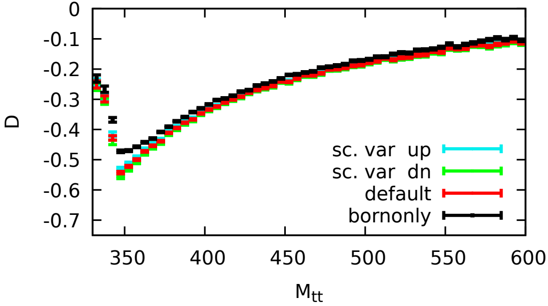
α_s/v enhancement in gg channel.

Threshold enhancement at NLO



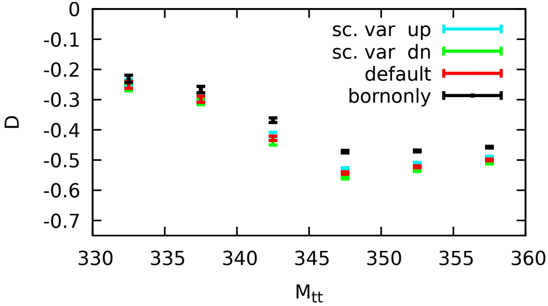
- the ratio of hvq to hvq-bornonly should better emphasize the $1/v$ singularity.
- the plot suggests that the effect is indeed visible
- Scale variations do not seem to affect the conclusion

Correlation enhancement at NLO

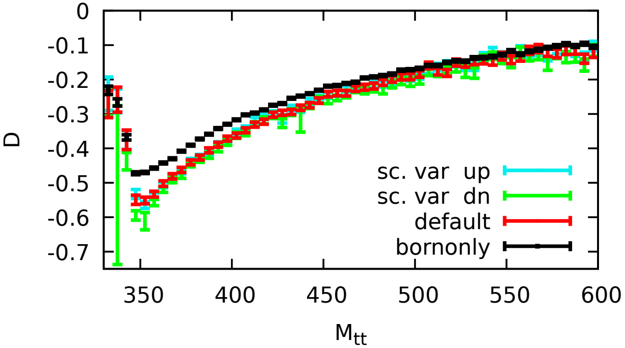


- Remember: $D = -3c_{\mathrm{hel}}$, and $D = -1$ is associated to pure singlet $t\bar{t}$ states.
- Correlations are enhanced near threshold at NLO.

Correlation enhancement at NLO

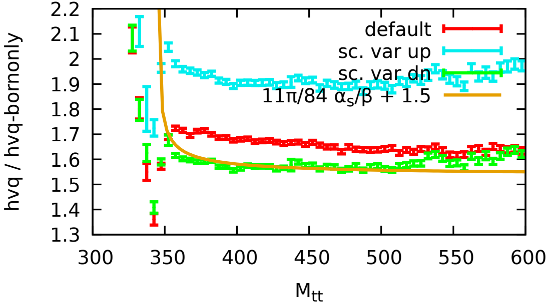


Correlation enhancement with bb4l



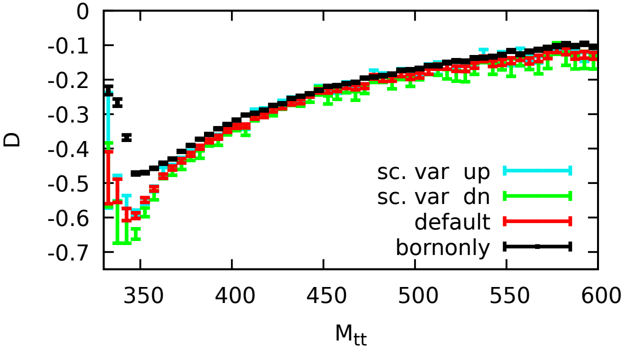
- Threshold enhancement even stronger with bb4l, especially for larger $M_{t\bar{t}}$ values.

Threshold enhancement with bb4l



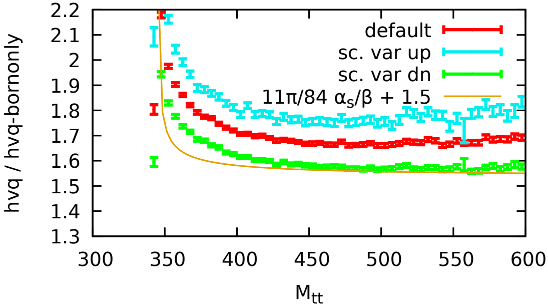
- Results are difficult to interpret.

Correlation enhancement with MiNNLOps



- Threshold enhancement also stronger with MiNNLOps, especially for $M_{t\bar{t}}$ very near threshold.

Threshold enhancement with MiNNLOps



- Enhancement stronger than in the NLO case (i.e. hvq).

Observations

Referring to hvq as the standard description of heavy quark pair production at the LHC, we find that:

- Better treatment of decay (i.e. bb4l) yields to an enhancement of correlations neat the threshold region.
- NNLO corrections also yields an enhancement near the threshold region

The two effects are likely to be independent, and lead us to speculate that together may bring about a stronger increase in the correlation near threshold.

Take Home Message

Can we explain the enhancements in bb4l and MiNNLOps?

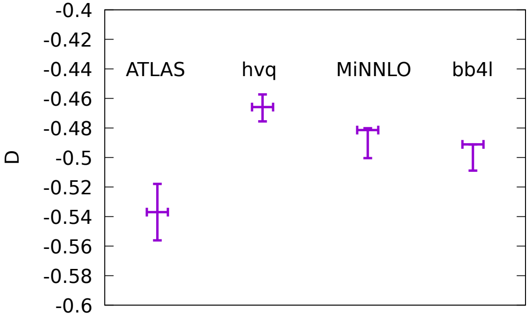
- In MiNNLOps there are further α_s^2/v^2 that increase the cross section near threshold, where it is more correlated.
- The bb4l enhancement is (likely) explained as follows. The enhancement near threshold strongly depends upon the $t\bar{t}$ spin state. But the MadSpin method is blind to these effects. bb4l is more likely to associate correctly the lepton correlation with the enhanced channels. (probably also ttb_NLO_dec).
- According to the above explanation, it makes sense to consider both effects as independent, i.e. they should add.

Do we need to include bound state effects?

- They can contribute at order NNNLO.
- Interplay with the FO may need clarifications.

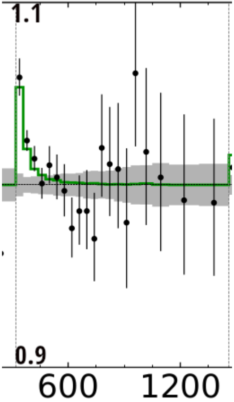
ATLAS result on correlations

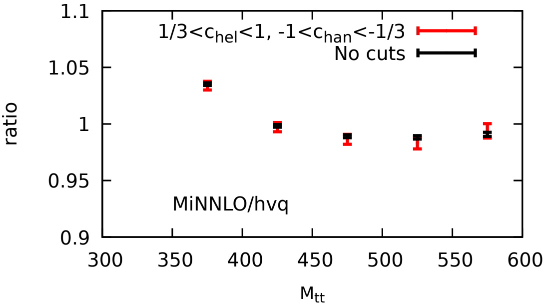
ATLAS finds: $D = -0.537 \pm 0.002(\mathrm{stat.}) \pm 0.019(\mathrm{syst.})$ for $340\mathrm{GeV} < mtt < 380\mathrm{GeV}$.



One can speculate that if the effect of MiNNLOps and bb4l could be added the discrepancy would be further reduced.

CMS,HIG-22-013-pas





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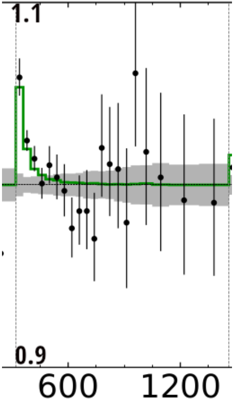

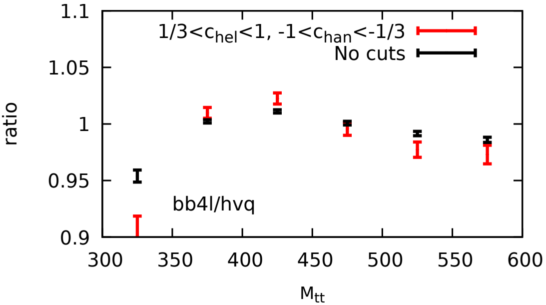

Conclusions

- Measurements of $t\bar{t}$ correlations near threshold by ATLAS and CMS are now challenging the precision of available generators.
- It is likely that inadequate treatment of correlations in decays may enhance current discrepancies between theoretical calculations and measurements. by including NNLO corrections
- Some generators at NLO, with very advanced treatment of decays, already ease the tension between data and simulations.
- There is room for improvements in generators, by adding systematically higher order leading $1/v$ effects.