

Theory aspects of top-pair production near threshold

M. Beneke (TU München)

Precision calculations for future e^+e^- colliders: targets and tools
CERN, June 7 - 17, 2022

MB, Kiyo, Schuller, Part I 1312.4791 [hep-ph] and Part II in preparation

MB, Kiyo, Marquard, Penin, Piclum, Steinhauser, 1506.06864 [hep-ph]

MB, Maier, Piclum, Rauh, 1506.06865 [hep-ph]

MB, Maier, Rauh, Ruiz-Femenia, 1711.10429

including earlier results from

MB, Schuller, Kiyo, hep-ph/0501289

MB, Kiyo, 0804.4004 [hep-ph]

MB, Jantzen, Ruiz-Femenia, 1004.2188 [hep-ph]

Jantzen, Ruiz-Femenia, 1307.4337 [hep-ph]

Marquard, Piclum, Seidel, Steinhauser, 1401.3004 [hep-ph]

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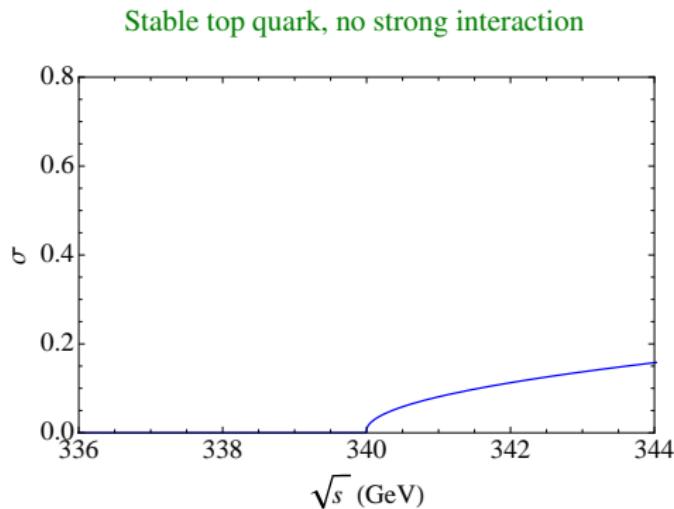
QQbar_threshold code MB, Kiyo, Maier, Piclum, 1605.03010 [hep-ph]

<https://www.hepforge.org/downloads/qqbartthreshold/>



Pair production threshold – Strong Coulomb force and Weak Decay

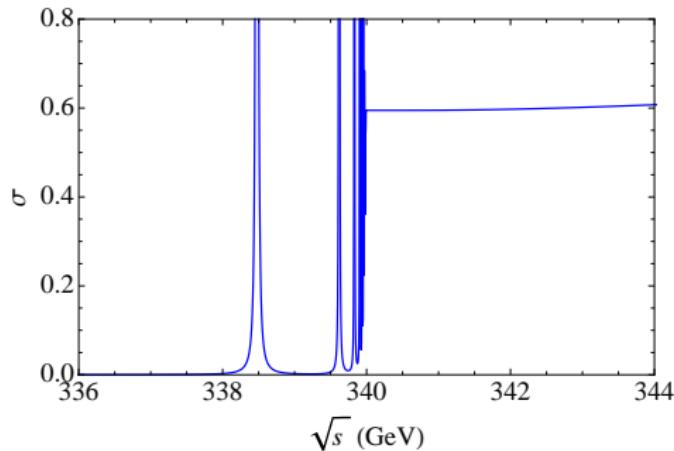
- Ultra-precise mass measurement, order of magnitude relative to pp
- “Spectroscopic” measurement utilizing unique QCD dynamics
- Free from uncertainties of interpretation of mass definition
- Sensitivity to Higgs Yukawa force, too?



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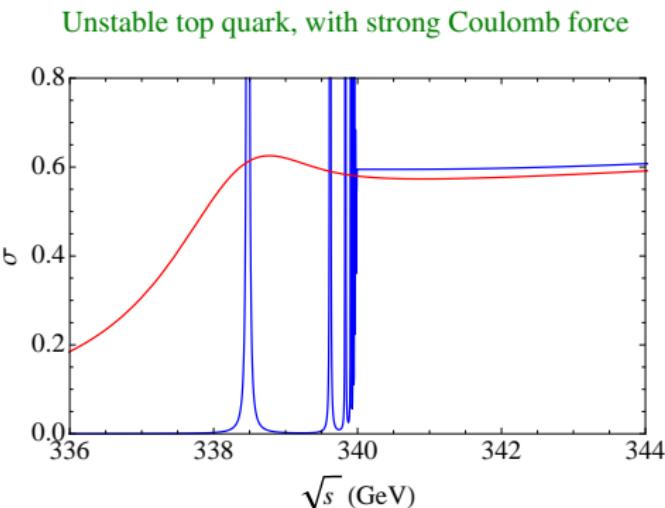
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Stable top quark, with strong Coulomb force



Pair production threshold – Strong Coulomb force and Weak Decay

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Challenges for theory

Scales

$$\underbrace{m_t, m_t v, m_t v^2}_{\text{QCD dynamics}}, \quad \underbrace{m_{W,H}, \Gamma_t}_{\text{EW}}, \quad \underbrace{\ln m_e}_{\text{QED ISR}}$$

- Weak coupling but non-perturbative QCD (strong Coulomb force)
 - ▶ NNNLO MB, Kiyo, Marquard, Penin, Piclum, Steinhauser, 1506.06864 [hep-ph]
 - ▶ NNLL (almost) Hoang, Stahlhofen, 1309.6323 [hep-ph]
- The rest of the SM: Electroweak, Higgs and QED
- Non-resonant production $e^+ e^- \rightarrow W^+ W^- b\bar{b}$ and cuts
- QED initial state radiation / parton distribution effects

QCD Theory

Non-perturbative but weak coupling. Expansion in α_s and $v = \sqrt{\frac{E}{m}} = \sqrt{\frac{\sqrt{q^2} - 2m_t}{m_t}}$, while $\alpha_s/v = O(1)$

$$R \sim v \sum_k \left(\frac{\alpha_s}{v} \right)^k \cdot \left\{ \underbrace{1 \text{ (LO)}}_{\text{Fadin, Khoze}} ; \underbrace{\alpha_s, v \text{ (NLO)}}_{\text{Peskin, Strassler}} ; \underbrace{\alpha_s^2, \alpha_s v, v^2}_{\text{1998}} \text{ (NNLO)} ; \underbrace{\alpha_s^3, \alpha_s^2 v, \alpha_s v^2, v^3}_{\text{2005-2015}} \text{ (N3LO)} ; \dots \right\}$$

$$(q_\mu q_\nu - q^2 g_{\mu\nu}) \Pi(q^2) = i \int d^4x e^{iq \cdot x} \langle 0 | T(j_\mu(x) j_\nu(0)) | 0 \rangle, \quad j^\mu(x) = [\bar{Q} \gamma^\mu (\gamma_5) Q](x)$$

Summation through Schrödinger equation

$$\text{Im } \Pi(E) = \frac{N_c}{2m^2} \underbrace{\sum_{n=1}^{\infty} Z_n \times \pi \delta(E_n - E) + \Theta(E)}_{\text{bound states}} \underbrace{\text{Im } \Pi(E)_{\text{cont}}}_{\text{continuum}}$$

$$R \equiv \frac{\sigma_{e^+ e^- \rightarrow WWb\bar{b}X}}{\sigma_0} = 12\pi e_t^2 K \text{ Im } \Pi(E + i\Gamma_t) + [\text{EWC} + \text{non-resonant}]$$

Tools

Multiple scales m_t , $m_t v$ integrated out in steps through a sequence of non-relativistic effective theories and the threshold expansion. See [MB, Kiyo, Schuller, arXiv:1312.4791 [hep-ph]]

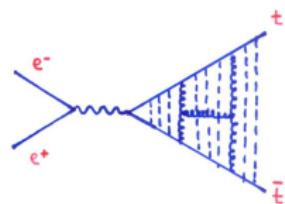
$$\mathcal{L}_{\text{QCD}} [Q(h, s, p), g(h, s, p, us)] \quad \mu > m$$



$$\mathcal{L}_{\text{NRQCD}} [Q(s, p), g(s, p, us)] \quad mv < \mu < m$$



$$\mathcal{L}_{\text{PNRQCD}} [Q(p), g(us)] \quad \mu < mv$$



$$\sigma_{e+e- \rightarrow \bar{t}t} = \frac{16\pi^2 \alpha_{\text{em}}^2 e_t^2}{s} \text{Im} \left[\frac{N_c}{2m^2} \left(\textcolor{red}{c}_v \left[\textcolor{red}{c}_v - \frac{E}{m} \left(c_v + \frac{d_v}{3} \right) \right] G_{\text{PNRQCD}}(E) + \dots \right) \right],$$

$$\begin{aligned} \delta_3 G_{\text{PNRQCD}}(E) &= \langle \mathbf{0} | \hat{G}_0(E) i \delta V_1 i \hat{G}_0(E) i \delta V_1 i \hat{G}_0(E) i \delta V_1 i \hat{G}_0(E) | \mathbf{0} \rangle \\ &\quad + 2 \langle \mathbf{0} | \hat{G}_0(E) i \delta V_1 i \hat{G}_0(E) i \delta V_2 i \hat{G}_0(E) | \mathbf{0} \rangle + \langle \mathbf{0} | \hat{G}_0(E) i \delta V_3 i \hat{G}_0(E) | \mathbf{0} \rangle + \delta^{us} G(E) \end{aligned}$$

The effective Lagrangian

Integrating out soft fluctuations results in a spatially non-local effective Lagrangian since $[k^i]_{\text{soft}} \sim [k^i]_{\text{pot.}}$

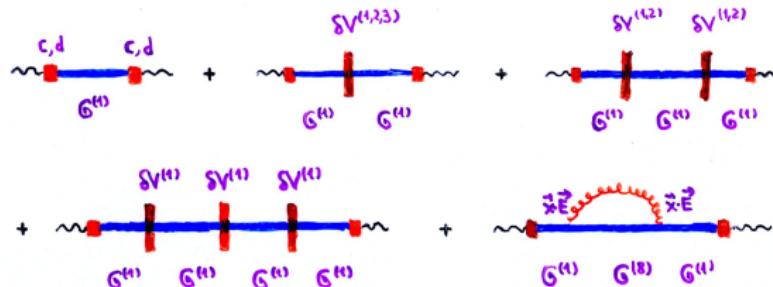
$$\begin{aligned}\mathcal{L}_{\text{PNRQCD}} = & \psi^\dagger \left(iD_0 + i\frac{\Gamma_t}{2} + \frac{\partial^2}{2m} + \frac{\partial^4}{8m^3} \right) \psi + \chi^\dagger \left(iD_0 - i\frac{\Gamma_t}{2} - \frac{\partial^2}{2m} - \frac{\partial^4}{8m^3} \right) \chi \\ & + \int d^{d-1} \mathbf{r} [\psi^\dagger \psi](x + \mathbf{r}) \left(-\frac{\alpha_s C_F}{r} + \delta V(r, \boldsymbol{\theta}) \right) [\chi^\dagger \chi](x) \\ & - g_s \psi^\dagger(x) \mathbf{x} \mathbf{E}(t, \mathbf{0}) \psi(x) - g_s \chi^\dagger(x) \mathbf{x} \mathbf{E}(t, \mathbf{0}) \chi(x)\end{aligned}$$

- The leading-order Coulomb potential is part of the unperturbed Lagrangian. The asymptotic states correspond to the composite field $[\psi^\dagger \chi](\mathbf{R}, \mathbf{r})$ with free propagation in the cms coordinate. **The propagation in the relative coordinate is determined by the Coulomb Green function $G_c^{(1)}(\mathbf{r}, \mathbf{r}'; E)$**
- Perturbations consist of **kinetic energy corrections, perturbation potentials, and ultrasoft gluon interactions.**

NNNLO calculation

The NNNLO contribution to the PNRQCD correlation function is

$$G^{(3)} = -G_c^{(1)} \delta V_1 G_c^{(1)} \delta V_1 G_c^{(1)} \delta V_1 G_c^{(1)} + 2G_c^{(1)} \delta V_1 G_c^{(1)} \delta V_2 G_c^{(1)} - G_c^{(1)} \delta V_3 G_c^{(1)} + \delta G_{\text{us}}$$



where

$$G_c^{(1,8)}(\mathbf{r}, \mathbf{r}', E) = \frac{m\gamma}{2\pi} e^{-y(r+r')} \sum_{l=0}^{\infty} (2l+1)(2\gamma r)^l (2\gamma r')^l P_l \left(\frac{\mathbf{r} \cdot \mathbf{r}'}{rr'} \right) \sum_{s=0}^{\infty} \frac{s! L_s^{(2l+1)} (2\gamma r) L_s^{(2l+1)} (2\gamma r')}{(s+2l+1)! (s+l+1-\lambda)}$$

$$y = \sqrt{-m(E + i\epsilon)}, \lambda = \frac{m\alpha_s}{2\gamma} \times \{C_F \text{ (singlet)}; C_F - C_A/2 \text{ (octet)}\}$$

For singlet need only $l = 0$, for octet only $l = 1$.

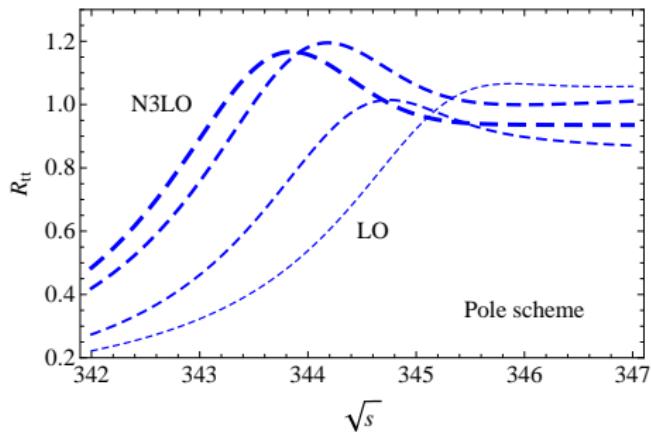
3rd order ingredients

- Bound state quantities (S-wave)
 - E_n – Kniehl, Penin, Smirnov, Steinhauser (2002); MB, Kiyo, Schuller (2005); Penin, Smirnov, Steinhauser (2005)
 - $|\psi_n(0)|^2$ – MB, Kiyo, Schuller (2007); MB, Kiyo, Penin (2007)
- Matching coefficients
 - a_3 – Anzai, Kiyo, Sumino (2009); Smirnov, Smirnov, Steinhauser (2009)
 - c_3 – Marquard, Piclum, Seidel, Steinhauser (2014) [2009]
- Continuum (PNRQCD correlation function)
 - ultrasoft – MB, Kiyo (2008)
 - potential – MB, Kiyo, [Schuller], in preparation [2007]
 - P-wave – MB, Piclum, Rauh (2013)

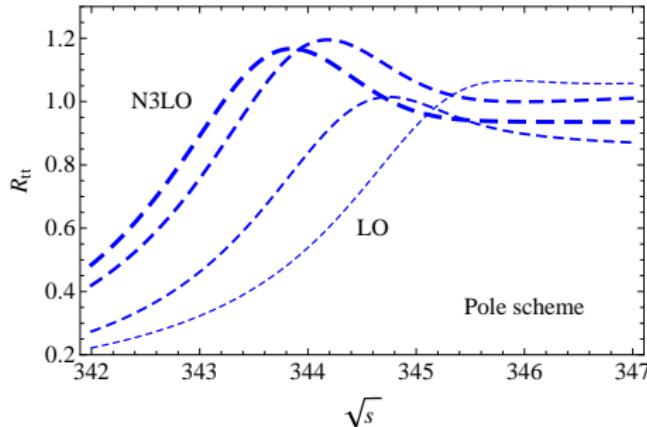
Note: logarithmically enhanced 3rd order terms known before or resummed [Hoang et al. 2001-2013; Pineda et al. 2002-2007]. But non-log terms are as large in individual terms.

2nd order available since end of 1990s.

Mass scheme issues



Mass scheme issues



- Pole mass cannot be determined with an accuracy better than $\mathcal{O}(\Lambda_{\text{QCD}})$ [MB, Braun, 1994; Bigi et al., 1994].
Pole mass renormalon seeds to spurious shifts in the peak position of the $t\bar{t}$ cross section [MB, 1998]
- Solution (“Kill two birds with one stone”): intermediate mass definition m_{PS} , which can be related precisely to the $\overline{\text{MS}}$ mass (\rightarrow top Yukawa coupling) AND avoids large, spurious corrections to the cross section.

Mass scheme issues

- Potential-subtracted mass [MB, 1998]

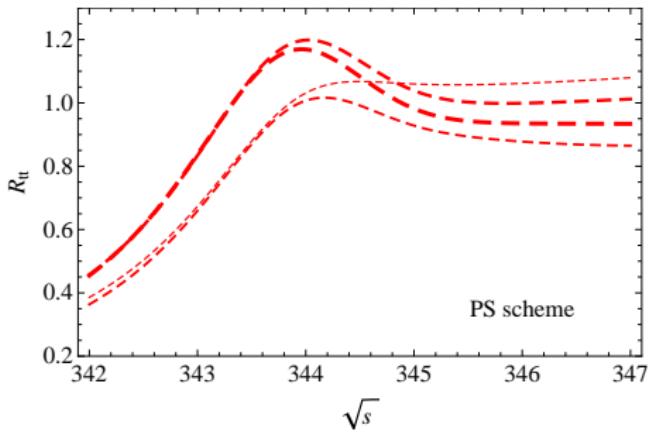
$$m_{\text{PS}}(\mu_f) \equiv m_{\text{pole}} + \frac{1}{2} \int_{|\vec{q}| < \mu_f} \frac{d^3 \vec{q}}{(2\pi)^3} \tilde{V}_{\text{Coulomb}}(\vec{q})$$

$$m_{\text{PS}}(\mu_f) - \bar{m}(\bar{m}) = \underbrace{[m_{\text{PS}}(\mu_f) - m_{\text{pole}}]}_{\text{known to } \mathcal{O}(\mu_f \alpha_s^4) \text{ [hep-ph/0501289]}} + \underbrace{[m_{\text{pole}} - \bar{m}(\bar{m})]}_{\text{known to } \mathcal{O}(m_t \alpha_s^4) \text{ [1502.01030]}}$$

Conversion precision ≈ 20 MeV.

Cancellation of large perturbative contributions from the IR.

In the following use
 $m_{t,\text{PS}}(20 \text{ GeV}) = 171.5 \text{ GeV}$.

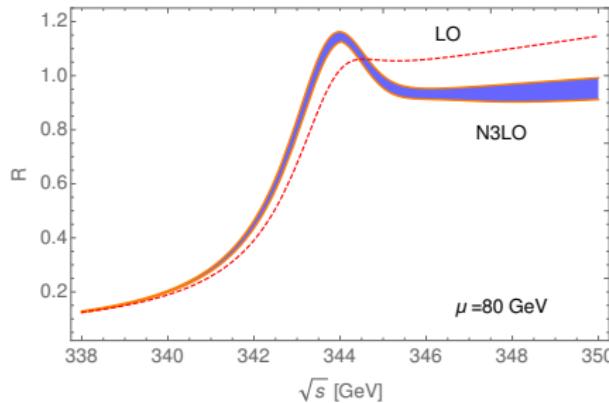


NNNLO QCD result

[MB, Kiyo, Marquard, Penin, Piclum, Steinhauser, 1506.06864]

Photon exchange and Z-vector coupling only.

$m_{t,\text{PS}}(20 \text{ GeV}) = 171.5 \text{ GeV}$, $\Gamma_t = 1.33 \text{ GeV}$, $\alpha_s(m_Z) = 0.1185 \pm 0.006$, $\sin^2 \theta_W = 0.23$,
 $\mu = (50 \dots 80 \dots 350) \text{ GeV}$, $\mu_w = 350 \text{ GeV}$.

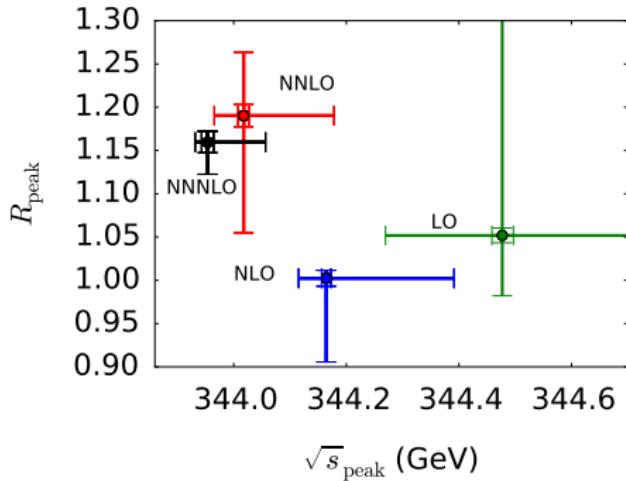
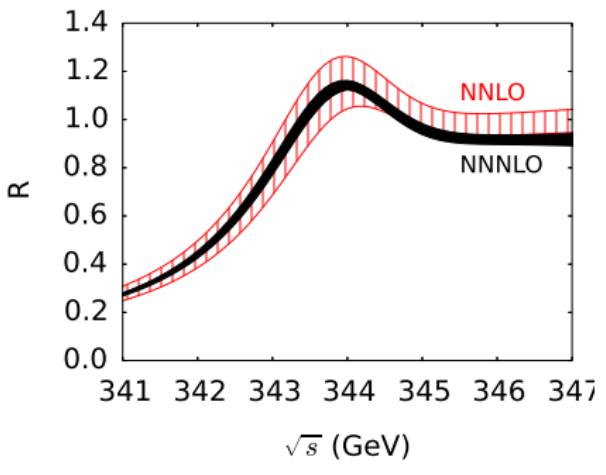


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Position shift: 310 MeV (LO to NLO) 150 MeV (to NNLO) 64 MeV (to NNNLO)
Improvement of factor 3 in uncertainty in peak height.

From QCD $t\bar{t}$ threshold to a realistic prediction

- Axial-vector Z-coupling (not a non-QCD effect), P-wave production
N3LO [MB, Piclum, Rauh, 2013] [starts at **NNLO**]
- QED effects
N3LO [MB, Maier, Rauh, Ruiz-Femenia, 2017] [starts at **NLO**, Pineda, Signer, 2006; MB, Jantzen, Ruiz-Femenia, 2010]
- Electroweak matching coefficients absorptive parts [Hoang, Reisser, 2004] and electroweak corrections in general [Guth, Kühn, 1992]
NNLO [MB, Maier, Rauh, Ruiz-Femenia, 2017] [starts at **NNLO**] [$\alpha_{EW} \sim \alpha_s^2$]
- Higgs contributions [Eiras, Steinhauser, 2006; MB, Maier, Piclum, Rauh, 2015]
N3LO [starts at **NNLO**]
- Non-resonant contributions: $\sigma_{e^+ e^- \rightarrow W^+ W^- b\bar{b}_{\text{nonres}}} (\mu_w)$
Mostly inclusive, possibly invariant mass cuts.
NNLO [MB, Maier, Rauh, Ruiz-Femenia, 2017] [starts at **NLO**, MB, Jantzen, Ruiz-Femenia, 2010; Penin, Piclum, 2011, Jantzen, Ruiz-Femenia, 2013; Ruiz-Femenia, 2014]]
- QED initial state radiation
Formally **NNLO**, but large logs of m_e . Effectively **LO**. [MB, Maier, Rauh, Ruiz-Femenia, 2017]

Systematics of Yukawa coupling effects

Power counting of new parameters m_H, λ_t :

- $m_H \sim m_t$ or $m_H \sim m_t v$ [Strassler, Peskin, 1991]
- $\lambda_t \sim \alpha_s$ or $\lambda_t \sim \alpha_{\text{EW}} \sim \alpha_s^2$

Adopt $m_H \sim m_t$ and $\lambda_t = y_t^2/(4\pi)$ as electroweak coupling.

Higgs-exchange Yukawa potential is effectively local

$$\frac{y_t^2}{\vec{q}^2 + m_H^2} \rightarrow \frac{y_t^2}{m_H^2} \quad \Rightarrow \quad \delta\sigma \propto -\frac{y_t^2}{m_H^2} \text{Im}[G_0(E)^2]_{\overline{\text{MS}}}$$

N3LO effect relative to $-g_s^2/\vec{q}^2$.

Need only single insertion of Higgs-exchange tree-level potential into Coulomb Green function.
Formally not the dominant Yukawa coupling effect.

Short-distance Yukawa coupling effects

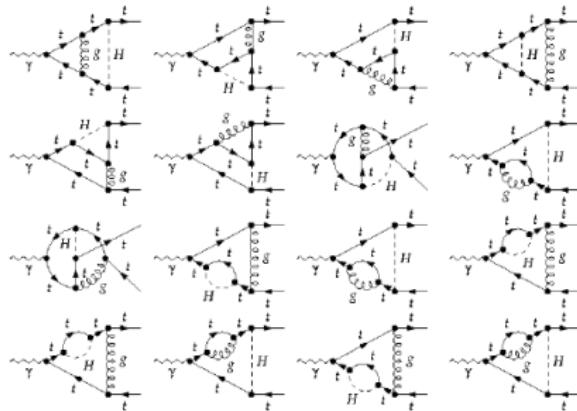
Modification of the $t\bar{t}$ production vertex

NNLO – 1-loop correction to vector-current matching [Guth, Kühn, 1991]

N3LO – Mixed 2-loop Higgs-QCD correction to vector-current matching [Eiras, Steinhauser, 2006]

$$c_v = 1 - \underbrace{0.103|_{\alpha_s} - 0.022|_{\alpha_s^2} + 0.031|_{y_t^2}}_{\text{NNLO}} - \underbrace{0.070|_{\alpha_s^3} - 0.019|_{y_t^2 \alpha_s}}_{\text{NNNLO}} + \dots,$$

Local approximation of the Higgs potential required for consistent cancellation of factorization scale dependence.



Finite-width divergence and scale-dependence

The pure-QCD calculation in the (P)NRQCD framework is technically inconsistent from NNLO.
Uncancelled $1/\epsilon$ poles.

- Finite-width divergences (overall log divergence, already at NNLO):

$$[\delta G(E)]_{\text{overall}} \propto \frac{\alpha_s}{\epsilon} \cdot E$$



Since $E = \sqrt{s} - 2m_t + i\Gamma$, the divergence survives in the imaginary part:

$$\text{Im} [\delta G(E)]_{\text{overall}} \propto m_t \times \frac{\alpha_s \alpha_{ew}}{\epsilon} \quad \Rightarrow \quad \ln(\mu_w / (m_t E))$$

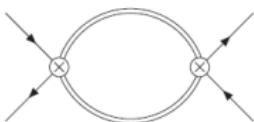
- Electroweak effect. Must consider $e^+ e^- \rightarrow W^+ W^- b\bar{b}$.

$$\sigma_{e^+ e^- \rightarrow W^+ W^- b\bar{b}} = \underbrace{\sigma_{e^+ e^- \rightarrow [t\bar{t}]_{\text{res}}} (\mu_w)}_{\text{pure (PNR)QCD}} + \sigma_{e^+ e^- \rightarrow W^+ W^- b\bar{b}_{\text{nonres}}} (\mu_w)$$

Non-resonant starts at NLO (overall linear divergence) [MB, Jantzen, Ruiz-Femenia, 2010; Penin, Piclum, 2011]. Finite-width scale dep must cancel. Need consistent dim reg calculation.

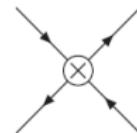
Unstable particle effective theory

Unstable particle EFT provides a systematic expansion of the amplitude in powers of Γ/m . [MB, Chapovsky, Signer, Zanderighi, 2003]



Resonant contributions

Production of an on-shell, non-relativistic $t\bar{t}$ pair and subsequent decay $t \rightarrow W^+ b$. Effective non-relativistic propagator contains on-shell width.



Non-resonant contributions

All-hard region. Off-shell lines. Full theory diagrams expanded around $s = 4m_t^2$. No width in propagators.

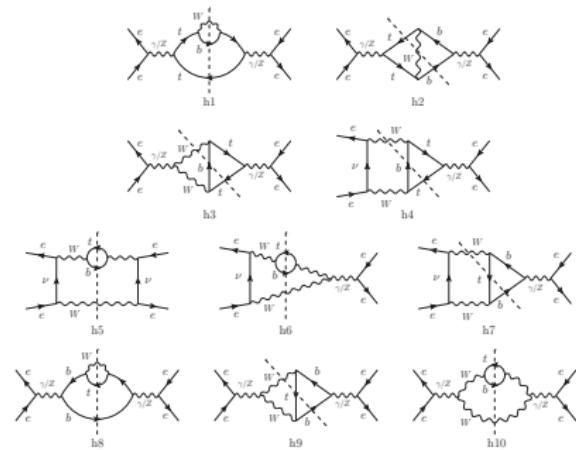
$$i\mathcal{A} = \sum_{k,l} C_p^{(k)} C_p^{(l)} \int d^4x \langle e^- e^+ | T[i\mathcal{O}_p^{(k)\dagger}(0) i\mathcal{O}_p^{(l)}(x)] | e^- e^+ \rangle + \sum_k C_{4e}^{(k)} \langle e^- e^+ | i\mathcal{O}_{4e}^{(k)}(0) | e^- e^+ \rangle$$

$$\mathcal{O}_p^{(v,a)} = \bar{e}_{c_2} \gamma_i(\gamma_5) e_{c_1} \psi_t^\dagger \sigma^i \chi_t$$
$$\mathcal{O}_{4e}^{(k)} = \bar{e}_{c_1} \Gamma_1 e_{c_2} \bar{e}_{c_2} \Gamma_2 e_{c_1},$$

$$\sigma_{\text{non-res}} = \frac{1}{s} \sum_k \text{Im} \left[C_{4e}^{(k)} \right] \langle e^- e^+ | i\mathcal{O}_{4e}^{(k)}(0) | e^- e^+ \rangle$$

Separately divergent and factorization (“finite-width”) scale-dependent.

Non-resonant corrections at NLO & NNLO

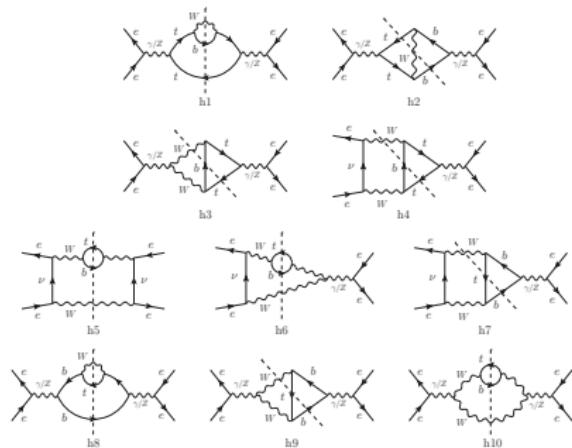


Equivalent to the dimensionally regulated $e^+e^- \rightarrow bW^+\bar{t}$ process with $\Gamma_t = 0$, expanded in the hard region around $s = 4m_t^2$.

NNLO: $\mathcal{O}(\alpha_s)$ corrections to this process

[MB, Maier, Rauh, Ruiz-Femenia, 2017]

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NNLO: $\mathcal{O}(\alpha_s)$ corrections to this process

[MB, Maier, Rauh, Ruiz-Femenia, 2017]

$$\int_{\Delta^2}^{m_t^2} dp_t^2 (m_t^2 - p_t^2)^{\frac{d-3}{2}} H_i \left(\frac{p_t^2}{m_t^2}, \frac{M_W^2}{m_t^2} \right)$$

$$p_t^2 \equiv (p_b + p_{W+})^2$$

$$H_1 \left(\frac{p_t^2}{m_t^2}, \frac{M_W^2}{m_t^2} \right) \xrightarrow{p_t^2 \rightarrow m_t^2} \text{const} \times \frac{1}{(m_t^2 - p_t^2)^2}$$

Linearly IR divergent at NLO. Finite in dim reg.

Log divergent at NNLO

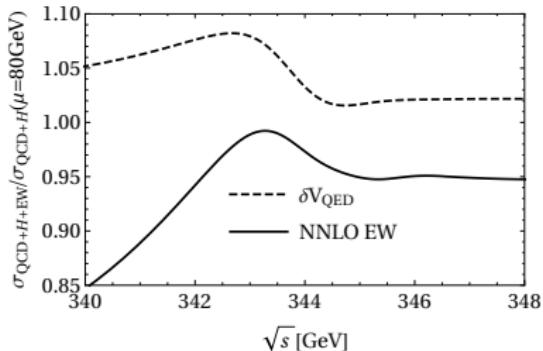
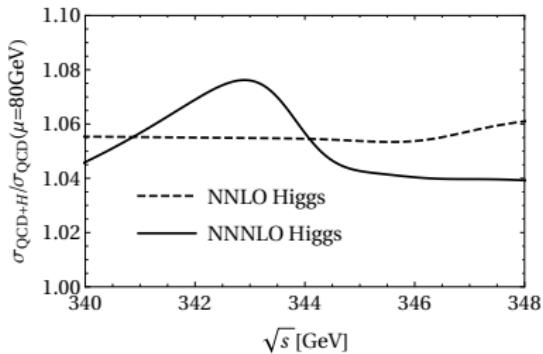
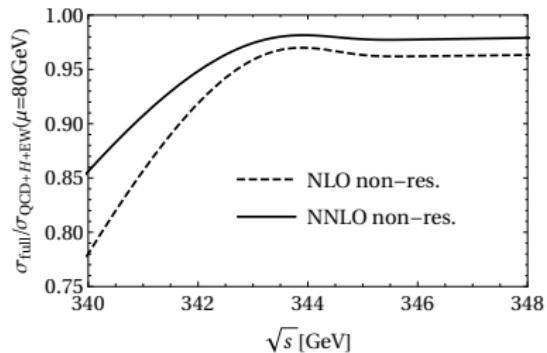
Can impose invariant mass cuts on top decay products. $\Delta^2 = M_W^2$ for inclusive cross section.

EFT works differently for loose and wide cuts [Actis, MB, Falgari, Schwinn, 2008]

Here: wide cuts

Size of non-QCD effects

- QCD = NNNLO QCD including P-wave
- NNNLO Higgs (top-Yukawa)
- NNLO electroweak+QED
- NNLO non-resonant

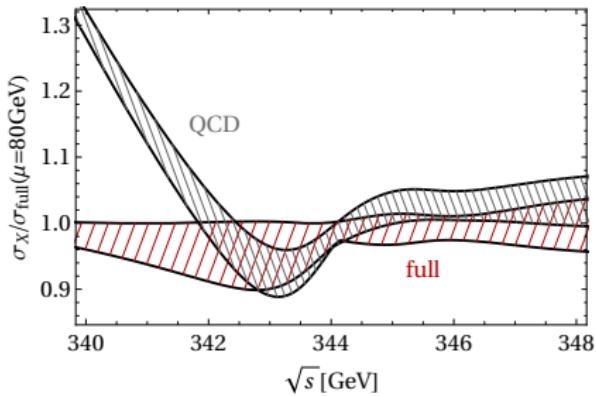
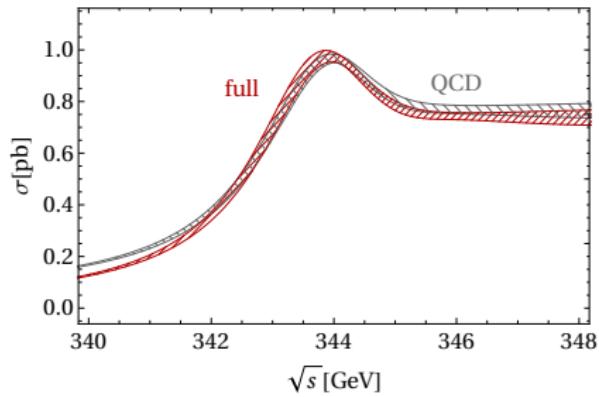


NNNLO (QCD+Higgs) + NNLO (EW+QED+non-resonant)

[MB, Maier, Piclum, Rauh, 2015; MB, Maier, Rauh, Ruiz-Femenia, 1710.10429]

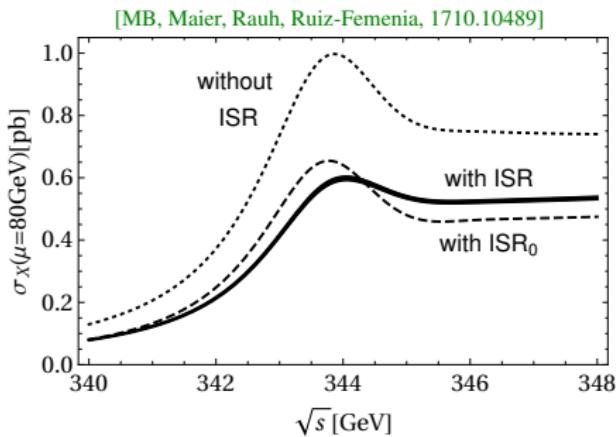
Inclusive $e^+ e^- \rightarrow W^+ W^- b\bar{b}$ cross section

$m_{t,\text{PS}}(20 \text{ GeV}) = 171.5 \text{ GeV}$, $\Gamma_t = 1.33 \text{ GeV}$, $\alpha_s(m_Z) = 0.1185 \pm 0.006$, $\sin^2 \theta_W = 0.2229$,
 $\mu = (50 \dots 80 \dots 350) \text{ GeV}$, $\mu_w = 350 \text{ GeV}$.



QED ISR

Should be part of the theoretical prediction, because separation from the “partonic cross section” depends on a factorization scheme.



QED parton distributions at large- x in LL approximation (as detailed in the LEP-1 Yellow report)

→ major theoretical uncertainty
can be improved (see Frixione's talk)

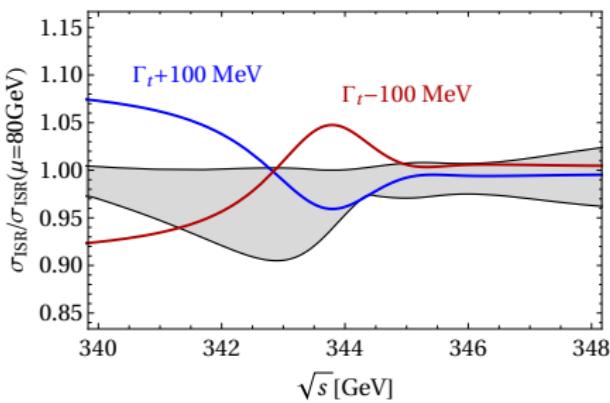
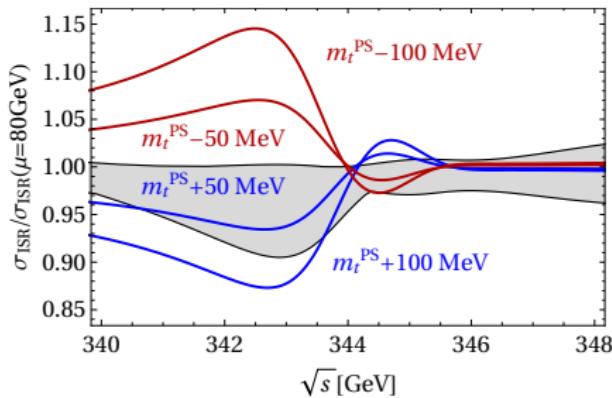
Sensitivity to (m_t, Γ_t) vs. theoretical uncertainty

Shaded band: Relative scale uncertainty

$$\frac{\delta\sigma}{\sigma} = \pm(2 \dots 3.5)\%$$

Superimposed: Variation with shifted top mass or width input normalized to reference.

[MB, Maier, Piclum, Rauh, 2015; MB, Maier, Rauh, Ruiz-Femenia, 2017]



Sensitivity to y_t and α_s

- Add

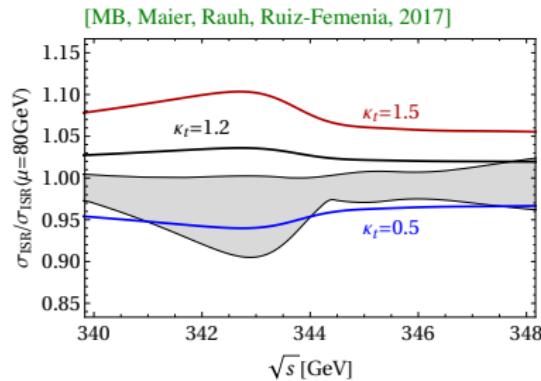
$$\Delta \mathcal{L} = -\frac{c_{\text{NP}}}{\Lambda^2} (\phi^\dagger \phi) (\bar{Q}_3 \tilde{\phi} t_R) + \text{h.c.}$$

to the SM Lagrangian

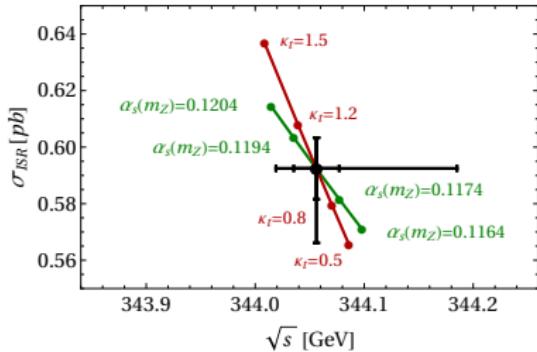
$$\kappa_t \equiv \frac{y_t}{\sqrt{2}m_t/v} = 1 + \frac{c_{\text{NP}}}{\Lambda^2} \frac{v^3}{\sqrt{2}m_t}$$

Treat top mass and Yukawa coupling as independent parameters.

- Caveat: In the framework of SMEFT there are many more and possibly more important anomalous coupling effects.



Peak position of (κ_t, α_s) vs. th. uncertainty



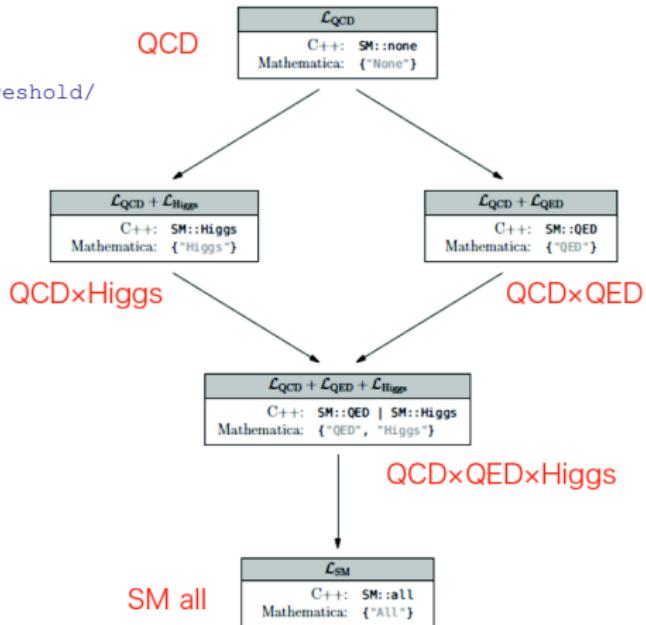
QQbar_threshold code

All results implemented in the code
QQbar_threshold available from

<https://www.hepforge.org/downloads/qqbarthreshold/>

[MB, Kiyo, Maier, Piclum, 1605.03010]

- C++ code
Mathematica interface via Mathlink
- Possibility to choose different models (QCD, SM,)
- Also for bottom, bound state energy and decay, mass scheme conversion.



QQbar_threshold code

examples/Mathematica/xsection_1.m

```
Needs["QQbarThreshold`"];

LoadGrid[GridDirectory -> "ttbar_grid.tsv"];
With[
{
  mu = 50.,
  mtPS = 168.,
  width = 1.4,
  muWidth = 350.,
  order = "N3LO"
},
Do[
  Print[
    sqrts, "\t",
    TTbarXSection[sqrts, {mu, muWidth}, {mtPS, width}, order]
  ],
  {sqrts, 330., 345., 1.}
];
];
```

Evaluation time per cross section point approx 5ms

Summary

I $e^+e^- \rightarrow t\bar{t}X$ cross section near threshold now computed at NNNLO in (PNR)QCD
+ top-Yukawa effects

- Sizeable 3rd order corrections and reduction of theoretical uncertainty to about $\pm 3\%$.

II Realistic predictions for $e^+e^- \rightarrow W^+W^- b\bar{b}$ near top-pair threshold

- NNLO available, including cuts invariant mass cuts.

III Parameter dependences ($m_t, \Gamma_t, y_t, \alpha_s$) can be studied.

- (m_t, Γ_t) with unrivaled accuracy.
- y_t with 20% accuracy from threshold already challenging.

IV Further requirements:

- ISR / QED PDF's for $x \rightarrow 1$ with NLL evolution
- N4LO QCD would be reassuring, but appears prohibitive.

<https://www.hepforge.org/downloads/qqbarthreshold/>