

Heavy quarks and new scales: Understanding subtleties of QCD

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CTEQ Collaboration

CTEQ

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1 Heavy quarks

- Charm, beauty and truth
- What is a heavy quark?

2 Using heavy quarks to understand QCD

- Going beyond DIS and Drell Yan
- Interpreting the initial state
- Matrix elements
- Interpreting the final state
- Tying it together: scales and consequences

3 Summary

1 Heavy quarks

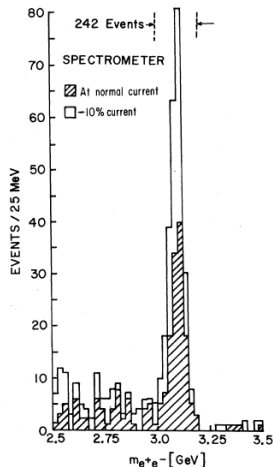
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A charming discovery



The first heavy quark, **charm** was discovered in 1974 in $p\bar{p}$ collisions at BNL and e^+e^- at SLAC

The observations were published together:

PRL 33, 1404 (1974); PRL 33, 1406 (1974)

The J/ψ was recognized as a $c\bar{c}$ bound state

$\Rightarrow m_c \sim 1.5$ GeV

The existence of a 4th quark confirmed the Glashow-Iliopoulos-Maiani explanation for why FCNC decays ($s \rightarrow d\nu\bar{\nu}$) did not occur.

— And it loosened the shackles of $SU(3)_{\text{flavor}}$, **Gell-Mann's "Eightfold way"**

A charming crisis

While the J/ψ was clearly a quark bound state, it had an extremely narrow width of 88 keV.

This caused a minor crisis in the fledgling QCD...

After all how could a strongly interacting state be narrow?

$\Gamma_\rho \sim 150$ MeV, $\Gamma_\omega \sim 8.5$ MeV, $\Gamma_\phi \sim 4.3$ MeV, $\Gamma_{J/\psi} \sim 88$ keV

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An explanation was found by Appelquist and Politzer, PRL 34, 43 (75).

Write the width as

$$\Gamma(^3S_1 \rightarrow 3 \text{ gluons}) = |R(0)|^2 |M(q\bar{q} \rightarrow ggg)|^2$$

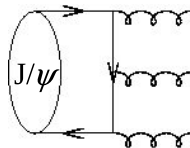
Following the model of positronium, solve the Schroedinger Eqn. for $R(r) = \frac{2}{a_0^{3/2}} e^{-r/a_0}$,

where $a_0 = \frac{1}{\alpha_s m_c/2}$.

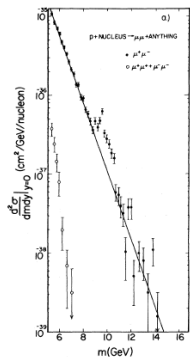
$|M(q\bar{q} \rightarrow ggg)|^2 \sim \alpha_s^3$ — one power for each gluon

$\Rightarrow \Gamma(^3S_1 \rightarrow 3 \text{ gluons}) \sim 0.2 \alpha_s^6 m_c \sim 90$ keV; $\alpha_s \approx 0.26$

Homework: Why do we not see $J/\psi \rightarrow gg$?



A beautiful discovery

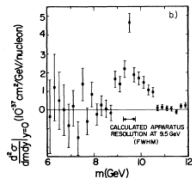


In 1975 the τ was discovered and led to the search for other 3rd-generation particles.

In 1977 the Upsilon (a $b\bar{b}$ bound state) was observed at the Fermilab Tevatron. PRL 39, 252 (1977)

(The Upsilon is also very narrow.)

Once the bottom quark was found it was clear that a sixth quark was needed to complete the family structure.



matter: fermions

quarks	u	c	t	+2/3
	d	s	b	-1/3
leptons	e	μ	τ	-1
	ν_e	ν_μ	ν_τ	0

“The top quark was discovered several times!”

ABSTRACT

A clear signal is observed for the production of an isolated large-transverse-momentum lepton in association with two or three centrally produced jets. The two-jet events cluster around the W^2 mass, indicating a novel decay of the Intermediate Vector Boson. The rate and features of these events are not consistent with expectations of known quark decays (charm, bottom). They are, however, in agreement with the process $W \rightarrow l\bar{\nu}$ followed by $t \rightarrow b\bar{q}$, where t is the sixth quark (top) of the weak Cabibbo current. If this is indeed so, the bounds on the mass of the top quark are $30 \text{ GeV}/c^2 < m_t < 50 \text{ GeV}/c^2$.

UA1, Phys. Lett. B 147, 493 (1984)

IT IS LIKELY THAT $m_t < m_W$

F. Halzen ^{*})

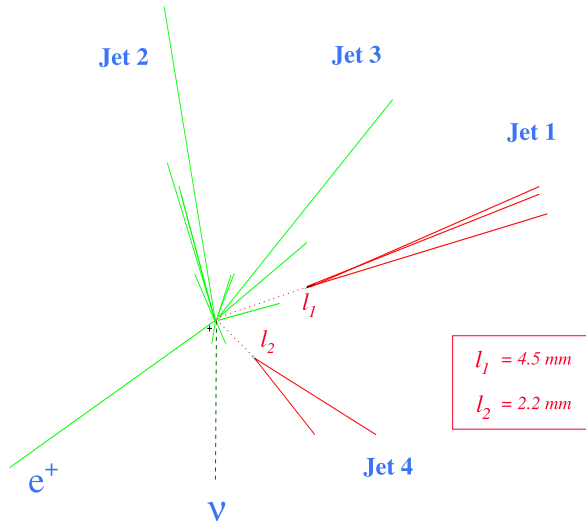
CERN - Geneva

Phys. Lett. B 182, 388 (1986)

A B S T R A C T

Within the standard model with three generations, the experimental data on the rate of W versus Z events in $p\bar{p}$ collisions favour $m_t < m_W$. The bound is sharpened for $N_\nu > 3$. We discuss the virtues as well as the shortcomings in the procedure to determine the t-quark mass from such data. Neutrino experiments sensitive to $u(x)/d(x)$ structure function ratios can help.

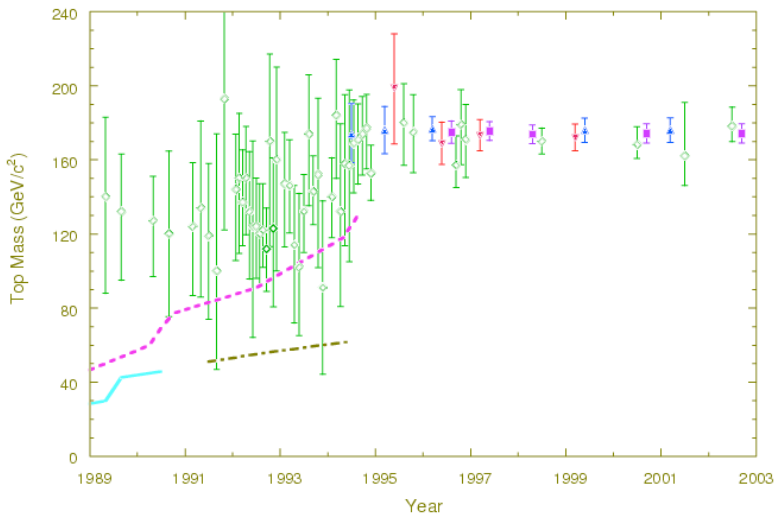
“This is the top quark!”



$$M_{\text{top}}^{\text{Fit}} = 170 \pm 10 \text{ GeV}/c^2$$

24 September, 1992
run #40758, event #44414

“Was the top quark mass predicted?”



Did LEP predict the mass? Look at Sept. 1992 . . .

Quigg

What is a “heavy quark?”

Usual definition: A heavy quark is a quark with $m_q \gg \Lambda_{\text{QCD}}$.

	Pole mass M	$\overline{\text{MS}}$ mass $\overline{m}(\overline{m})$
Charm	$\sim 1.3\text{--}1.7$ GeV	1.275 ± 0.025 GeV
Bottom	$\sim 4.5\text{--}5$ GeV	4.18 ± 0.03 GeV
Top	173.1 ± 0.6 GeV (?)	$160^{+4.8}_{-4.3}$ GeV

PDG (5/30/17)

Top: TEVEWWG: $174.30 \pm 0.35 \pm 0.54$ GeV, LHC: $172.64 \pm 0.25 \pm 0.55$ GeV

Pole Mass: $\sim \frac{1}{\not{p} - M}$

TeV vs. LHC $\sim 3\sigma$

$\overline{\text{MS}}$ Mass: Related to pole mass by

$$\frac{M}{\overline{m}(\overline{m})} = 1 + \frac{4}{3} \left(\frac{\alpha_s}{\pi} \right) + \left(\frac{\alpha_s}{\pi} \right)^2 (-1.0414 \ln(M^2/\overline{m}^2) + 13.4434) + \dots$$

It seems kind of funny to list 2 different masses...

c and b masses are best written in $\overline{\text{MS}}$ scheme.

t mass is given in pole-mass scheme.

What is a heavy quark mass?

Answer 1: A parameter of the Lagrangian $\mathcal{L} \sim m_t \bar{t}t$

A weak answer, but if the number is big enough we can expand in inverse powers of the mass to create a convergent series. (E.g., HQET)

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Answer 2: An effective (Yukawa) coupling between t - t - h

$m_t = Y_t / (2\sqrt{2}G_F)^{1/2}$, $Y_t \approx 1.00$ in the SM

This is better, as the Standard Model predicts that quark masses are not fundamental, but rather an artifact of dynamical interactions.

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Answer 3: The kinematic mass seen by the experiments

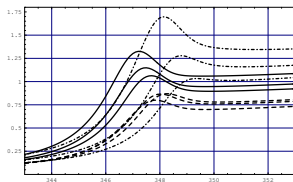
Right after the discovery of the top quark, Martin Smith and Scott Willenbrock asked this question about the “pole mass” of the top quark. They showed that a renormalon (the closest pole of the Borrel transform) induced an ambiguity of $\mathcal{O}(\Lambda_{QCD})$ in the definition of the pole mass.

Top mass from $t\bar{t}$ threshold at a e^-e^+ collider

There is a subtle question when you try to make a precision measurement of QCD:
What mass do you use?

The pole mass is not defined beyond Λ_{QCD} .

In fact it is not well-defined at all, since there are no free quarks.



Yakovlev, Grootte PRD63, 074012(01)

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Solution: Use the 1S mass (pseudo bound state)

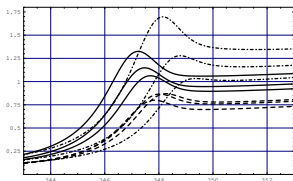
There are large non-relativistic corrections

$$\sigma_{t\bar{t}} \propto v \sum \left(\frac{\alpha_s}{v} \right) \times \left\{ \frac{1}{\sum (\alpha_s \ln v)} \right\} \\ \times \left\{ \begin{array}{l} \text{LO}(1) + \text{NLO}(\alpha_s, v) + \text{NNLO}(\alpha_s^2, \alpha_s v, v^2) \\ \text{LL} + \text{NLL} + \text{NNLL} \end{array} \right\}$$

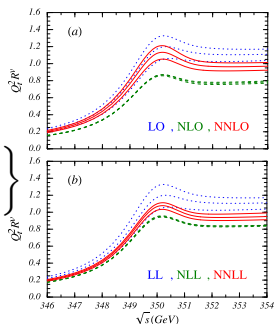
Normalization changes, but peak stable.

$\delta\sigma_{t\bar{t}}$ is $\pm 6\%$ before ISR/beamstrahlung

$\delta m_t \sim 100$ MeV is attainable



Yakovlev, Groote PRD63, 074012(01)



Hoang, et al. PRD69, 034009(04)

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Right after the discovery of the top quark, Martin Smith and Scott Willenbrock asked this question about the “pole mass” of the top quark. They showed that a renormalon (the closest pole of the Borrel transform) induced an ambiguity of $\mathcal{O}(\Lambda_{QCD})$ in the definition of the pole mass.

This led to the recommended use of the $\overline{\text{MS}}$ mass for top quarks.

We theorists are good at setting standards that make our life easier ... most perturbative calculations use the $\overline{\text{MS}}$ mass for simplicity.

Of course mass is NOT measured directly. Instead, it affects the distribution of events that are measured, and that distribution is used to INFER the mass by matching to a calculation. ...

What is a heavy quark mass?

Answer 4: A new scale in the problem.

This will both complicate our calculations and lead to new insights into the meaning of QCD structures that are hidden when we ignore quark masses.

The key is context.

Depending on the other scales in the problem, a heavy quark mass may teach us something deep about the physics, or be completely irrelevant.

E.g., most mass corrections go like $\mathcal{O}(m^2/\mu^2)$

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Homework: Show in the top quark width $\Gamma(t \rightarrow bW)$, dropping m_b loses terms of $\mathcal{O}(m_b^2/m_t^2) \sim 1\%$.

In the rest of this lecture we will concentrate on what we learn from physics with corrections that go like $\mathcal{O}[\ln(m_t^2/m_b^2)]$.

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Structure of an observable cross section

$$\sigma_{\text{obs.}} = \int f_1(x_1, \mu_1) f_2(x_2, \mu_2) \otimes \overline{|M|^2} \otimes d\text{P.S.} \otimes D_i(p_i) \dots D_n(p_n)$$

Theorists factorize (break) the cross section into:

- Initial-state IR singularities swept into parton distribution “functions”.

These are not physical, but include scheme dependent finite terms:

$\overline{\text{MS}}$ — the current standard

DIS — ambiguous in modern PDF sets, could be fixed, but why?

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⇒ Exclusive cross sections (jet counting), angular correlations

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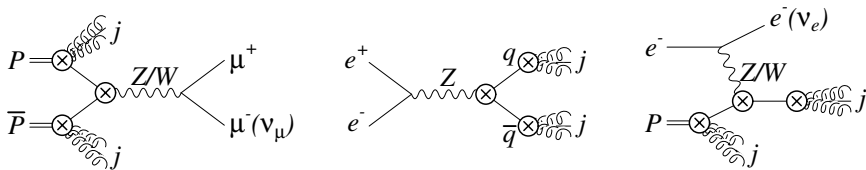
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- A squared matrix element, which represents the bulk of the perturbative calculation effort.
- Phase space which you may not want to completely integrate out.
⇒ Exclusive cross sections (jet counting), angular correlations
- Fragmentation functions or jet definitions.
These provide the coarse graining to hide final-state IR singularities.

Drell-Yan and DIS

The traditional testbed of perturbative QCD have been restricted to Drell-Yan production, e^+e^- to jets, or deeply inelastic scattering (DIS).

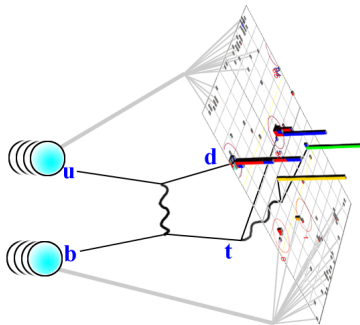


A key property that all three processes share is a complete factorization of QCD radiation between different parts of the diagrams.

- Drell-Yan \rightarrow Initial-state (IS) QCD radiation only.
- $e^+e^- \rightarrow$ jets \rightarrow Final-state (FS) QCD radiation only.
- DIS \rightarrow Proton structure and fragmentation functions probed. Simple color flow.

A heavy quark testbed for QCD: single top

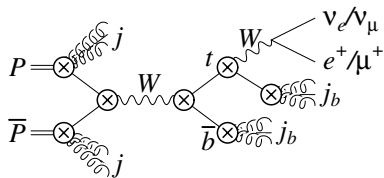
Experimentalist: Single top quark production is the observation of $b \ell^\pm \cancel{E}_T$ that reconstruct to a top quark mass, plus an extra jet (or two).



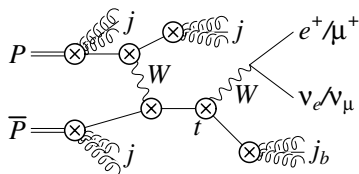
Theorist: Single top quark production is a playground in which we refine our understanding of perturbative QCD in the presence of heavy quarks.

s-/t-channel single-top-quark production (A generalized Drell-Yan and DIS)

A perfect factorization through next-to-leading order (NLO) makes single-top-quark production mathematically *identical*[†] to DY and DIS!



Generalized Drell-Yan.
IS/FS radiation are independent.

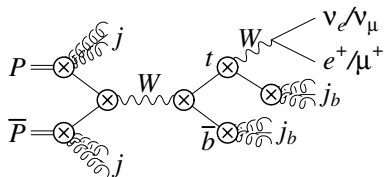


Double-DIS (DDIS) w/ 2 scales:
 $\mu_l = Q^2$, $\mu_h = Q^2 + m_t^2$

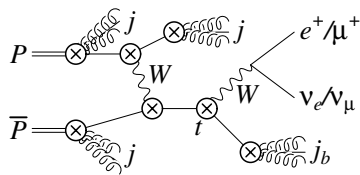
[†] Massive forms: m_t , m_b , and m_t/m_b are relevant.

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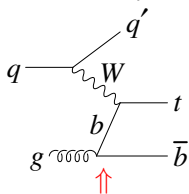
Double-DIS (DDIS) w/ 2 scales:
 $\mu_l = Q^2$, $\mu_h = Q^2 + m_t^2$

Color conservation forbids the exchange of just 1 gluon between the independent fermion lines.

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Rethinking the initial state: W -gluon fusion \rightarrow t -channel single-top

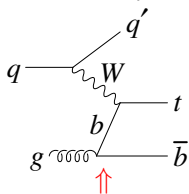
W -gluon fusion (circa 1996)



$$\sim \alpha_s \ln \left(\frac{Q^2 + m_t^2}{m_b^2} \right) + \mathcal{O}(\alpha_s)$$

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$$\sim \alpha_s \ln \left(\frac{Q^2 + m_t^2}{m_b^2} \right) + \mathcal{O}(\alpha_s)$$

Look at the internal b .

The propagator is

$$\frac{1}{(P_g - P_{\bar{b}})^2 - m_b^2} = \frac{1}{-2P_g \cdot P_{\bar{b}}}$$

$$P_g = E_g(1, 0, 0, 1), P_{\bar{b}} = (E_b, \vec{p}_T, p_z)$$

$$P_g \cdot P_{\bar{b}} = E_g(p_z \sqrt{1 + \frac{p_T^2 + m_b^2}{p_z^2}} - p_z)$$

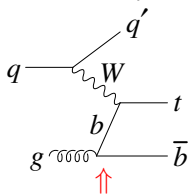
$$\approx E_g p_z \left(\frac{p_T^2 + m_b^2}{2p_z^2} \right) \sim (p_T^2 + m_b^2)$$

$$\int_{p_T \text{ cut}} \frac{dp_T^2}{p_T^2 + m_b^2} \rightarrow \ln \left(\frac{1}{p_{T \text{ cut}}^2 + m_b^2} \right)$$

Rethinking the initial state:

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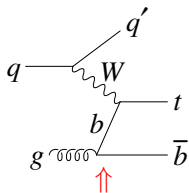
The same procedure for the W leads to the **massive** formula for DIS.

$$\sigma \sim \alpha_s \ln \left(\frac{Q^2 + m_t^2}{p_{T \text{ cut}}^2 + m_b^2} \right)$$

We now have multiple scales entering the problem: $Q, m_t, m_b, p_{T \text{ cut}}$

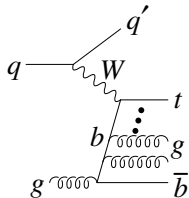
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W-gluon fusion (circa 1996)



$$\sim \alpha_s \ln \left(\frac{Q^2 + m_t^2}{m_b^2} \right) + \mathcal{O}(\alpha_s)$$

$$m_t \approx 35 m_b! \quad \alpha_s \ln \sim .7-.8$$



Each order adds

$$\frac{1}{n!} \left[\alpha_s \ln \left(\frac{Q^2 + m_t^2}{m_b^2} \right) \right]^n$$

Looks bad for
perturbative
expansion...

Look at the internal b .

The propagator is

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Resummation of large logs and b PDF

The Dokshitzer-Gribov-Lipatov-Altarelli-Parisi (DGLAP) equation sums large logs in (almost) collinear singularities in gluon splitting.

$$\frac{db(\mu^2)}{d \ln(\mu^2)} \approx \frac{\alpha_s}{2\pi} P_{bg} \otimes g + \frac{\alpha_s}{2\pi} \cancel{P_{bb}} \otimes b; \quad b \ll g$$

$$P_{bg}(z) = \frac{1}{2} [z^2 + (1-z)^2]$$

$$b(x, \mu^2) = \frac{\alpha_s(\mu^2)}{2\pi} \ln \left(\frac{\mu^2}{m_b^2} \right) \int_x^1 \frac{dz}{z} P_{bg}(z) g \left(\frac{x}{z}, \mu^2 \right)$$



Barnett, Haber, Soper, NPB 306, 697 (88)

Olness, Tung, NPB 308, 813 (88)

Aivazis, Collins, Olness, Tung, PRD 50, 3102 (94)

The procedure is the same for c or t .

Resummation of large logs and b PDF

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$$\frac{db(\mu^2)}{d \ln(\mu^2)} \approx \frac{\alpha_s}{2\pi} P_{bg} \otimes g + \frac{\alpha_s}{2\pi} \cancel{P_{bb}} \otimes b; \quad b \ll g$$

$$P_{bg}(z) = \frac{1}{2} [z^2 + (1-z)^2]$$

$$b(x, \mu^2) = \frac{\alpha_s(\mu^2)}{2\pi} \ln\left(\frac{\mu^2}{m_b^2}\right) \int_x^1 \frac{dz}{z} P_{bg}(z) g\left(\frac{x}{z}, \mu^2\right)$$



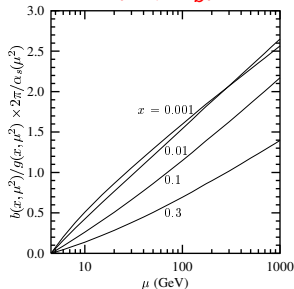
Barnett, Haber, Soper, NPB 306, 697 (88)

Olness, Tung, NPB 308, 813 (88)

Aivazis, Collins, Olness, Tung, PRD 50, 3102 (94)

The procedure is the same for c or t .

$$b \propto \alpha_s \ln(\mu^2/m_b^2) \times g$$



Stelzer, ZS, Willenbrock, PRD 56, 5919 (1997)

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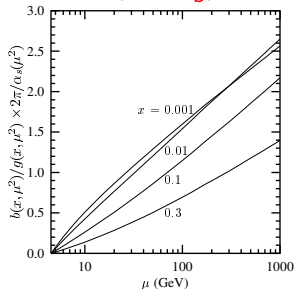
Aside: In the $\overline{\text{MS}}$ scheme, $b(\mu \leq m_b) \equiv 0$.

DIS scheme is not uniquely defined for heavy quarks.

Do you choose $F_2 \equiv 0$ (traditional) or define w.r.t. $\overline{\text{MS}}$?

The first attempt to calculate single-top failed because the DIS scheme was used.

$$b \propto \alpha_s \ln(\mu^2/m_b^2) \times g$$

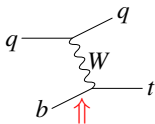


Stelzer, ZS, Willenbrock, PRD 56, 5919 (1997)

Bordes, van Eijk, NPB435, 23 (95)

Remove 1 scale (m_b) w/improved perturbation theory

New Leading Order

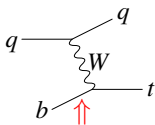


$$b \sim \alpha_s \ln \left(\frac{\mu^2}{m_b^2} \right) \times g$$

The t -channel W exchange naturally lead to the nomenclature of t -channel production

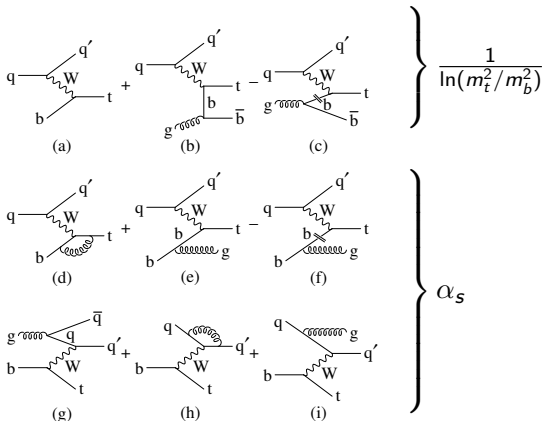
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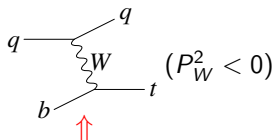
NLO: Terms that generated large logs are already resummed.

⇒ Must subtract overlap to avoid double-counting (general issue)

⇒ Reorders PT into 2 types of corrections: α_s and $\frac{1}{\ln(m_t^2/m_b^2)}$ w.r.t. LO

New nomenclature and classification

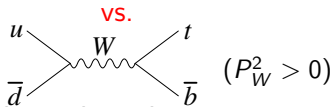
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t -channel production

Named for the “ t -channel”
exchange of a W boson.

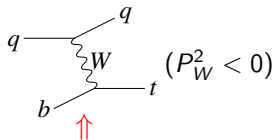


s -channel production

Named for the “ s -channel”
exchange of a W boson.

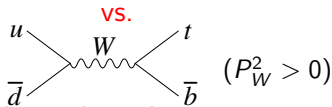
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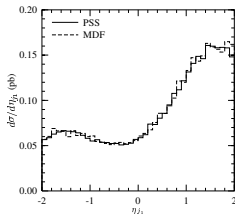
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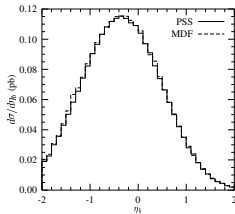
s-channel production
Named for the “*s*-channel”
exchange of a *W* boson.

Classifying processes by analytical structure
leads directly to kinematic insight:

Jets from *t*-channel processes are more
forward than those from *s*-channel.

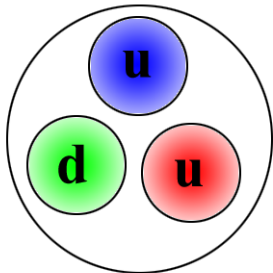


jet from *t*-channel



b jet from *s*-channel

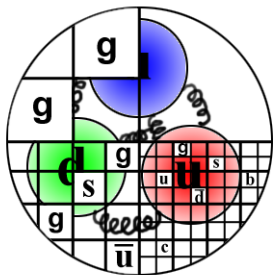
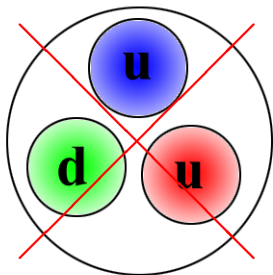
Rethinking the proton



Using DGLAP was NOT just a math trick!

This “valence” picture of the proton is not complete.

Rethinking the proton

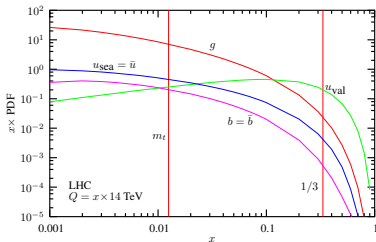


Using DGLAP was NOT just a math trick!

This “valence” picture of the proton is not complete.

Larger energies resolve smaller structures.

The probability of finding a particle inside the proton is given by PDFs (Parton Distribution Functions)



b (and c) quarks are full-fledged members of the proton structure.

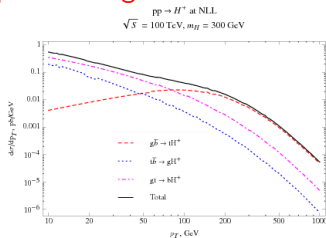
The top quark as a parton

In general, we do not consider the top quark when discussing proton structure.

The reason is simple: We do not tend to measure at scales far enough above m_t to ignore its mass.

Dawson, Ismail, and Low (PRD90, 014005(14)) revisited this issue and demonstrated it was indeed not sensible for inclusive cross sections at 100 TeV.

However, the p_T distributions for some processes, such as $H^+ + X$ production need a top PDF to get the correct result.



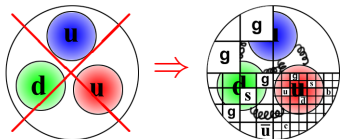
Summary Day 1

“Heavy quarks” (c , b , and t) are interesting because their mass adds a new scale to any problem.

$$\sigma \sim \alpha_s \ln \left(\frac{\mu^2}{p_{T \text{ cut}}^2 + m_Q^2} \right)$$

Single-top-quark production is the new DIS and Drell-Yan

$$\sigma_{\text{obs.}} = \int f_1(x_1, \mu_1) f_2(x_2, \mu_2) \otimes |\overline{M}|^2 \otimes dP.S. \otimes D_i(p_i) \dots D_n(p_n)$$



- b/c PDFs are inside the proton
- For construction and uncertainties cf. Dr. Nadolsky's talks
- Analytic structure gives direct kinematical insight

Homework: Why do we not see $J/\psi \rightarrow gg$?

Homework: Show in the top quark width $\Gamma(t \rightarrow bW)$, dropping m_b loses terms of $\mathcal{O}(m_b^2/m_t^2) \sim 1\%$.

Intermission

1 Heavy quarks

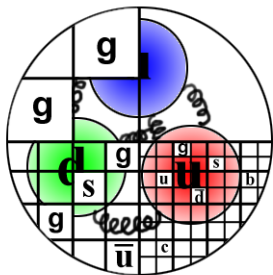
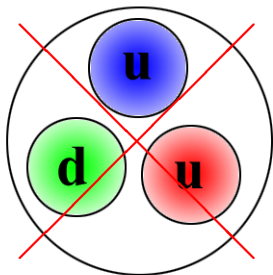
- Charm, beauty and truth
- What is a heavy quark?

2 Using heavy quarks to understand QCD

- Going beyond DIS and Drell Yan
- Interpreting the initial state
- Matrix elements
- Interpreting the final state
- Tying it together: scales and consequences

3 Summary

Rethinking the proton

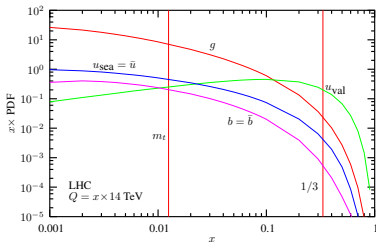


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Larger energies resolve smaller structures.

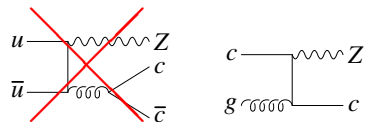
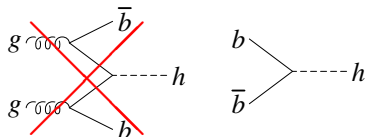
The probability of finding a particle inside the proton is given by PDFs (Parton Distribution Functions)



b (and c) quarks are full-fledged members of the proton structure.

Rethinking several physical processes

Why is this important?



Starting with a c/b gives us:

$b\bar{b} \rightarrow h$ **Largest** SUSY Higgs cross section

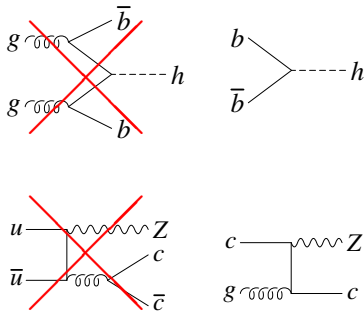
Zb/Zc Affects LHC luminosity monitor

Zbj/Zcj Higgs background

Wbj Largest single-top background

etc.

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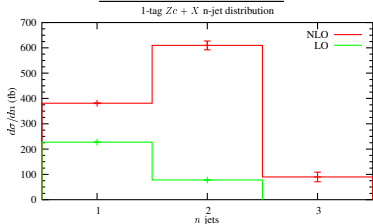
Zbj/Zcj Higgs background

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etc.

Why is this important?

Zc at Tevatron



Parton luminosity and large logs can be more important than counting powers of α_s !

This can be exaggerated at LHC

$Z \approx Z + 1 \text{ jet} \approx Z + 2 \text{ jets!}$

(w/ reasonable cuts)

What is LO when 0/1/2 jets are all the same?

1 Heavy quarks

- Charm, beauty and truth
- What is a heavy quark?

2 Using heavy quarks to understand QCD

- Going beyond DIS and Drell Yan
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- Matrix elements
- Interpreting the final state
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3 Summary

Rethinking the matrix element: A practical problem for experiments

The same large logs that lead to a reordered perturbation for t -channel single-top, implied a potentially large uncertainty in measurable cross sections when cuts were applied.

Recall: t -channel and s -channel are distinguished by the number of b -jets.

Rethinking the matrix element: A practical problem for experiments

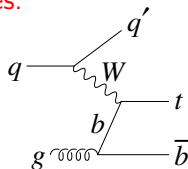
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A problem: About 20% of the time, the extra \bar{b} -jet from the t -channel process is hard and central — mixing s -/ t -channel samples.

Real problem: Is the b contamination 20%, 30%, 10%?

Large $\ln\left(\frac{Q^2+m_t^2}{p_{T\text{ cut}}^2+m_b^2}\right)$ terms return



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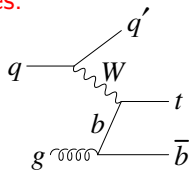
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Another problem: To distinguish from $t\bar{t}$, the cross section in the $W + 2$ jet bin has to be known.

Counting jets is IDENTICAL to performing a jet veto.

Inclusive cross sections are not enough, we need to calculate **exclusive cross sections**

Fully Differential NLO Techniques

- In 2001, there were few matrix-element techniques or calculations that could deal IR singularities in processes with massive particles.
- Experiments were mostly stuck using LO matrix elements to predict semi-inclusive or exclusive final states.
- We needed methods to provide the 4-vectors, spins, and corresponding weights of exclusives final-state configurations.

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- We needed methods to provide the 4-vectors, spins, and corresponding weights of exclusives final-state configurations.

These needs led to work on 3 techniques:

- Phase space slicing method with 2 cutoffs.
 - L.J. Bergmann, Ph.D. Thesis, FSU (89)
 - cf. H. Baer, J. Ohnemus, J.F. Owens, PRD 40, 2844 (89)
 - B.W. Harris, J.F. Owens, PRD 65, 094032 (02)
- Phase space slicing method with 1 cutoff.
 - W.T. Giele, E.W.N. Glover, PRD 46, 1980 (92)
 - cf. W.T. Giele, E.W.N. Glover, D.A. Kosower, NPB 403, 633 (93)
 - E. Laenen, S. Keller, PRD 59, 114004 (99)
- Massive dipole formalism (a subtraction method) coupled with a helicity-spinor calculation. **Invented to solve single-top production.**
 - cf. L. Phaf, S. Weinzierl, JHEP 0104, 006 (01)
 - S. Catani, S. Dittmaier, M. Seymour, Z. Trocsanyi, NPB 627,189 (02)

Phase Space Slicing Method (2 cutoffs)

B.W. Harris, J.F. Owens, PRD 65, 094032 (02)

The essential challenge of NLO differential calculations is dealing with initial- and final-state soft or collinear IR divergences.

$$\sigma_{\text{obs.}} \sim \int \frac{1}{s_{ij}} \sim \int \frac{dE_i dE_j d\cos\theta_{ij}}{E_i E_j (1 - \cos\theta_{ij})}$$

If $E_{i,j} \rightarrow 0$ “soft” singularity

If $\theta_{ij} \rightarrow 0$ “collinear” singularity

IDEA: Introduce arbitrary cutoffs
(δ_s, δ_c) to remove the singular
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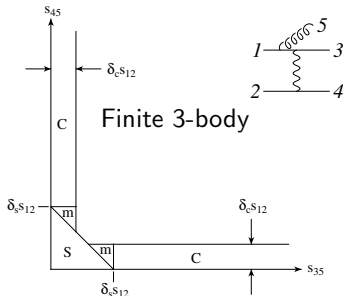
Divide phase space into 3 regions:

① **soft:** $E_g \leq \delta_s \sqrt{\hat{s}}/2$ gluons only

② **collinear:** $\hat{s}_{35}, \hat{s}_{45}, \dots < \delta_c \hat{s}$;

③ **hard non-collinear:** (finite, particles well separated, $E > 0$)

Phase space plane (s_{35}, s_{45})



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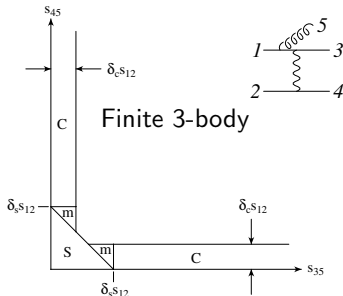
We traded dependence on physical observables (energy, angles) for logarithmic dependence on arbitrary parameters ($\ln \delta_s$, $\ln \delta_c$)

When a massive quark radiates, $(1 - \beta \cos\theta_{ij})$ has no collinear singularity

Divide phase space into 3 regions:

- 1 soft: $E_g \leq \delta_s \sqrt{\hat{s}}/2$ gluons only
- 2 collinear: $\hat{s}_{35}, \hat{s}_{45}, \dots < \delta_c \hat{s}$;
- 3 hard non-collinear: (finite, particles well separated, $E > 0$)

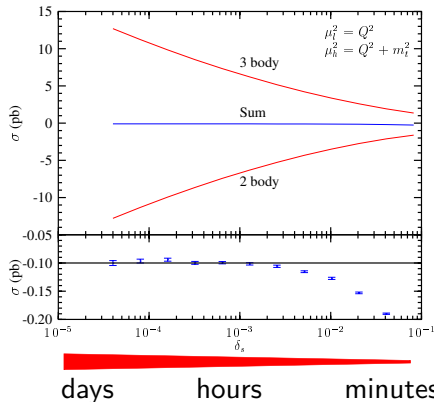
Phase space plane (s_{35} , s_{45})



Cut-off dependence of NLO correction

Each term is logarithmically divergent for small δ_s, δ_c

Logarithmic dependence on the cutoffs cancels in any IR-safe observable at the histogramming stage.



At the end we take δ_s and δ_c to zero via numerical computation. This can take a long time...

Massive Dipole Formalism (subtraction)

$$\begin{aligned}\sigma_{NLO} &= \int_{n+1} d\sigma^{\text{Real}} + \int_n d\sigma^{\text{Virtual}} \\ &= \int_{n+1} \left(d\sigma^R - d\sigma^A \right) + \int_n \left(d\sigma^V + \int_1 d\sigma^A \right)\end{aligned}$$

- $d\sigma^A$ is a sum of color-ordered dipole terms.
 - $d\sigma^A$ must have the same point-wise singular behavior in D dimensions as $d\sigma^R$.
 $\Rightarrow d\sigma^A$ is a local counterterm for $d\sigma^R$.
 - $\int_1 d\sigma^A$ is analytic in D dimensions, and reproduces the soft and collinear divergences of $d\sigma^R$.
- Some advantages over Phase Space Slicing are:
 - You can easily project out spin eigenstates.
 \Rightarrow Explicitly test different spin bases at NLO after cuts.
 - Event generators use color-ordered matrix elements.
- Both methods have some contribution to n -body final states from $n + 1$ phase-space. Hence, you must do 2 separate integrations.

Subtraction vs. phase space slicing

In practical terms, the difference in methods is in how to integrate in the presence of infrared singularities.

$$I = \lim_{\epsilon \rightarrow 0^+} \left\{ \int_0^1 \frac{dx}{x} x^\epsilon F(x) - \frac{1}{\epsilon} F(0) \right\}$$

Subtraction: Add and subtract $F(0)$ under the integral

$$\begin{aligned} I &= \lim_{\epsilon \rightarrow 0^+} \left\{ \int_0^1 \frac{dx}{x} x^\epsilon [F(x) - F(0) + F(0)] - \frac{1}{\epsilon} F(0) \right\} \\ &= \int_0^1 \frac{dx}{x} [F(x) - F(0)], \text{ finite up to machine precision} \end{aligned}$$

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PSS: Integration region divided into two parts $0 < x < \delta$ and $\delta < x < 1$, with $\delta \ll 1$. A Maclaurin expansion of $F(x)$ yields

$$\begin{aligned} I &= \lim_{\epsilon \rightarrow 0^+} \left\{ \int_0^\delta \frac{dx}{x} x^\epsilon F(x) + \int_\delta^1 \frac{dx}{x} x^\epsilon F(x) - \frac{1}{\epsilon} F(0) \right\} \\ &= \int_\delta^1 \frac{dx}{x} F(x) + F(0) \ln \delta + \mathcal{O}(\delta), \text{ take } \lim_{\delta \rightarrow 0} \text{ numerically} \end{aligned}$$

Remaining $\ln \delta$ singularities removed by summing all integrals I_i .

Rethinking jet definitions and phase space: Experiments need exclusive $t + 1$ jet at NLO

ZTOP, Z.S., PRD 70, 114012 (2004)

Tevatron # b -jets	t_j (Wbj)	t_{jj} ($Wbjj$)
s-channel = 2	0.620 pb $^{+13\%}_{-11\%}$	0.168 pb $^{+24\%}_{-19\%}$
= 1	0.022 pb $^{+24\%}_{-19\%}$	(NNLO)
t-channel = 1	0.950 pb $^{+16\%}_{-15\%}$	0.152 pb $^{+17\%}_{-14\%}$
= 2	0.146 pb $^{+21\%}_{-16\%}$	0.278 pb $^{+21\%}_{-16\%}$

Cuts: $p_{Tj} > 15$ GeV, $|\eta_j| < 2.5$, no cuts on t

Jet definition: $\Delta R_{k_T} < 1.0$ ($\approx \Delta R_{\text{cone}} < 0.74$)

Breakdown of *shape-independent* uncertainties

Process	$\times \delta m_t$ (GeV)	$\mu/2-2\mu$	PDF	b mass	$\alpha_s(\delta_{\text{NLO}})$
s-channel $p\bar{p}$	$^{-2.33\%}_{+2.71\%}$	$^{+5.7\%}_{-5.0\%}$	$^{+4.7\%}_{-3.9\%}$	$< 0.5\%$	$\pm 1.4\%$
pp	$^{-1.97\%}_{+2.26\%}$	$\pm 2\%$	$^{+3.3\%}_{-3.9\%}$	$< 0.4\%$	$\pm 1.2\%$
t-channel $p\bar{p}$	$^{-1.6\%}_{+1.75\%}$	$\pm 4\%$	$^{+11.3\%}_{-8.1\%}$	$< 1\%$	$\pm 0.01\%$
pp	$^{-0.73\%}_{+0.78\%}$	$\pm 3\%$	$^{+1.3\%}_{-2.2\%}$	$< 1\%$	$\pm 0.1\%$

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ZTOP, Z.S., PRD 70, 114012 (2004)

Tevatron # b -jets	t_j (Wb_j)	t_{jj} ($Wbjj$)
s-channel = 2	0.620 pb $^{+13\%}_{-11\%}$	0.168 pb $^{+24\%}_{-19\%}$
= 1	0.022 pb $^{+24\%}_{-19\%}$	(NNLO)
t-channel = 1	0.950 pb $^{+16\%}_{-15\%}$	0.152 pb $^{+17\%}_{-14\%}$
= 2	0.146 pb $^{+21\%}_{-16\%}$	0.278 pb $^{+21\%}_{-16\%}$

Cuts: $p_{Tj} > 15$ GeV, $|\eta_j| < 2.5$, no cuts on t
 Jet definition: $\Delta R_{k_T} < 1.0$ ($\approx \Delta R_{\text{cone}} < 0.74$)

Breakdown of *shape-independent* uncertainties

Process	$\times \delta m_t$ (GeV)	$\mu/2-2\mu$	PDF	b mass	$\alpha_s(\delta_{\text{NLO}})$
s-channel $p\bar{p}$	-2.33%	+5.7%	+4.7%	< 0.5%	$\pm 1.4\%$
	+2.71%	-5.0%	-3.9%		
	-1.97%		+3.3%	< 0.4%	$\pm 1.2\%$
pp	+2.26%	$\pm 2\%$	-3.9%		
t-channel $p\bar{p}$	-1.6%	$\pm 4\%$	+11.3%	< 1%	$\pm 0.01\%$
	+1.75%		-8.1%		
	-0.73%	$\pm 3\%$	+1.3%	< 1%	$\pm 0.1\%$
pp	+0.78%		-2.2%		

Every number here, even the concept of t -channel single-top, required a new or revised understanding of QCD.

- b PDFs \rightarrow t -channel
- PDF uncertainties
- multiple scales: m_t/m_b
- 2 expansions: α_s , $1/\ln$
- Fully differential NLO jet calculations
- . . .

1 Heavy quarks

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2 Using heavy quarks to understand QCD

- Going beyond DIS and Drell Yan
- Interpreting the initial state
- Matrix elements
- Interpreting the final state
- Tying it together: scales and consequences

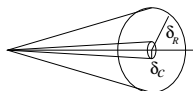
3 Summary

Thinking about the final state: How do we interpret exclusive NLO calculations?

Z.S., PRD 70, 114012 (2004)

“Paradigm of jet calculations”

- We are calculating extensive objects, i.e., **jets** not “improved quarks.”
- Unlike **inclusive** NLO calculations, **exclusive** NLO calculations are only well-defined in the presence of a jet definition or hadronization function. ($D_i(p_i)$)
⇒ The mathematics of quantum field theory tells us we **cannot** resolve the quarks inside of these jets!



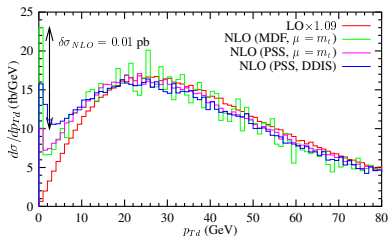
- “Bad things” happen if you treat jets as NLO partons. . .

Transverse momenta distributions at NLO

At LO, a d -quark recoils against the top quark in t -channel.



NLO “ d -jet” (no cuts)



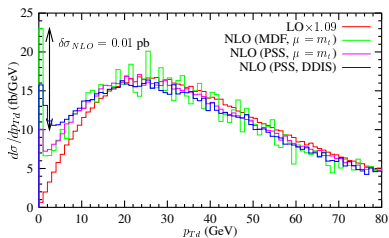
- Perturbation theory is not terribly stable at low p_{T_d} (or even high p_{T_d}).
- This is not what we want.
Be careful what you ask for!

Transverse momenta distributions at NLO

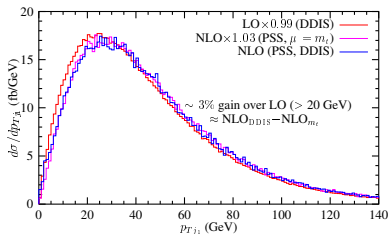
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We measure the highest E_T jet



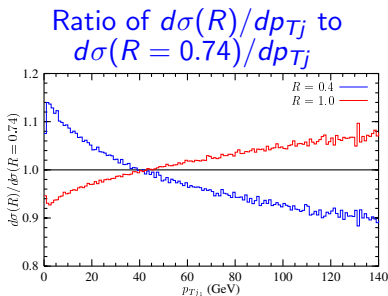
- Perturbation theory is not terribly stable at low $p_{T,D}$ (or even high $p_{T,D}$).
- This is not what we want.

Be careful what you ask for!

The highest E_T jet recoils against the top. The measurable change in shape is comparable to the scale uncertainty.

Jet distributions depend on jet definition

Just like the experimentalists, theorists must study the effect jet algorithms with different cone sizes R will have on measurable properties.



For “reasonable” values of R the variation is $< 10\%$, but this must be checked for all observables. (Note: theoretical uncertainty $< 5\%$)

Upshot: NLO exclusive calculations give jets not partons.

Without some thought, mismatches between theory and experiment can be larger than the theory error alone would indicate.

THEORY

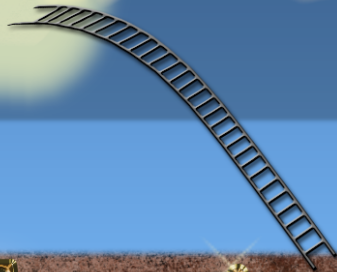
Experiment

THEORY

Event Generators

Experiment

THEORY



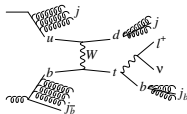
Experiment

Event generators vs. NLO t -channel $t\bar{b}$ ($Wb\bar{b}$)

Z.S., PRD 70, 114012 (2004)

Initial-state radiation (ISR) is generated by backward evolution of angular-ordered showers.

⇒ The jet containing the extra \bar{b} comes from **soft** ISR.

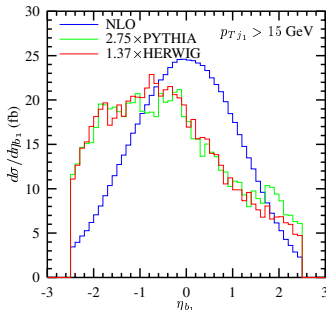
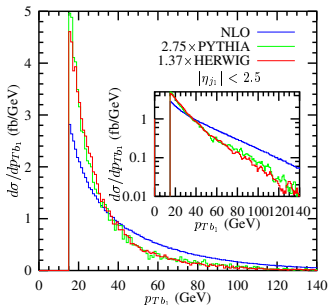
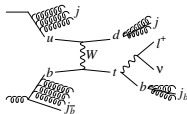


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- **Lesson:** n -jets+showers $\neq n + 1$ jets. ⇒ **Need NLO matching.** (Schemes have since proliferated: MLM, CKKW, SCET, ...)
- **Showing can be improved:** Including b mass effects in splitting kernels for shower helps (Nagy, Soper JHEP 06(14)179)
NLO Implementation for ttj is promising (Czakon et al. JHEP 06(15)033)

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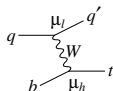
Scale (μ) dependence of the t -channel jets and top

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s-channel $p\bar{p}$	-2.33%	+5.7%	+4.7%	< 0.5%	$\pm 1.4\%$
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Why do we vary scales to estimate higher order corrections?

The large logs that we resummed appear at every order with similar coefficients, and we expect them to dominate the variation.

- The shapes of the p_T and η distributions do not change if you vary the scales. Only the normalization changes.
- If you vary the 4 independent scales[†] at the same time you underestimate the uncertainty.



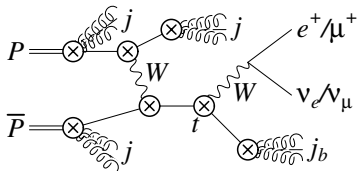
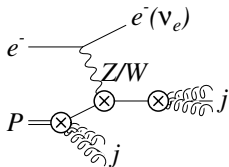
$\mu/2 - 2\mu$	$\text{LO}_t(m_t)$	$\text{NLO}_t(m_t)$	$\text{LO}_t(\text{DDIS})$	$\text{NLO}_t(\text{DDIS})$
fixed	0.95 pb	1.03 pb	1.07 pb	1.06 pb
μ_l & μ_h	$\pm 1\%$	$\pm 2.5\%$	+0.1%	$\pm 3.5\%$
μ_h	-7.5%	-3.5%	-2%	-3%
μ_l	+5.5%	+4%	+5.2%	+4%
	+6.7%	$\pm 1\%$	+8%	$\pm 0.6\%$
	-5.8%		-6.8%	

[†] (2 factorization, 2 renormalization)

PDFs and scales — a subtlety

Standard lore says that the choice of scale in a perturbative calculation is arbitrary. . . **Standard lore is not quite correct.**

$$\sigma_{\text{obs.}} = \int f_1(x_1, \mu_1) f_2(x_2, \mu_2) \otimes \overline{|M|^2} \otimes dP.S. \otimes D_i(p_i) \dots D_n(p_n)$$



DIS is measured at 1 scale:

$$\mu^2 = Q^2$$

Double-DIS (DDIS) probes 2 scales:

$$\mu_l^2 = Q^2, \mu_h^2 = Q^2 + m_t^2$$

Fits can be done at LO or NLO to extract PDFs, but. . . the most important *mathematical* constraint is that a *calculation* must give the the same answer for these *inclusive* observables at LO or NLO.

$$\sigma^{LO} = \sigma^{NLO}$$

Data is data. You are just undoing the original PDF fits.

How well does this work? Well, it used to...

Z.S. arXiv:1711.04018 [hep-ph]

Important: D-DIS scales used ($\mu_l = Q^2$, $\mu_h = Q^2 + m_t^2$); $m_t = 172.5$ GeV

LO means (LO ME, $\alpha_s(M_Z) = 0.130$, LO PDFs)

NLO means (NLO ME, $\alpha_s(M_Z) = 0.118$, NLO PDFs)

Tevatron (1.96 TeV) $t + \bar{t}$ inclusive cross section

PDF	LO (pb)	NLO (pb)	
CTEQ4L/4M	2.26	2.41	(6% not great, known α_s bug)
CTEQ5L/5M1	2.08	2.07	< 0.5% (bug fixed)
CTEQ6L1/6M	2.07	2.086	< 0.5%
CTEQ6L1/6M	1.83	2.086	Scales set to m_t , 12% as expected

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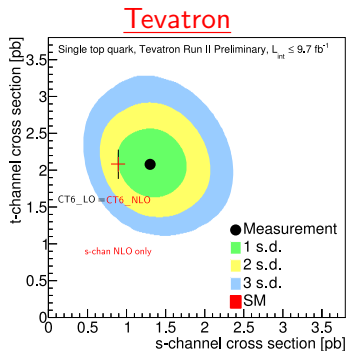
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CTEQ14llo/nlo	2.39	2.00	(20% deviation!)
HERAPDF1.5lo/nlo	1.965	1.798	(9.3% deviation!)
HERAPDF2lo/nlo	1.910	1.762	(8.4% deviation)
NNPDF30lo/nlo	2.33	2.21	(5.4% deviation)

Total PDF uncertainty expected to be $+8.8 - 7.3\%$ at 90% C.L.

1. LO is not equal to NLO any more! We do *not* get back to data!
2. NLO calculations w/ different PDFs disagree by $\sim 5\sigma$!

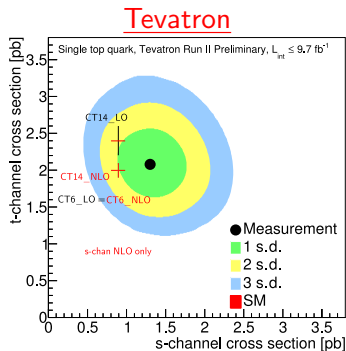
LO at Tevatron shifted, LHC not much help



I modified 1503.05027

t -channel scale uncertainties shown (LO and NLO)
 1σ PDF uncertainties similar to NLO scale uncertainty
(NLO s -channel: CTEQ 6 \equiv CTEQ 14 to $< 0.1\%$)

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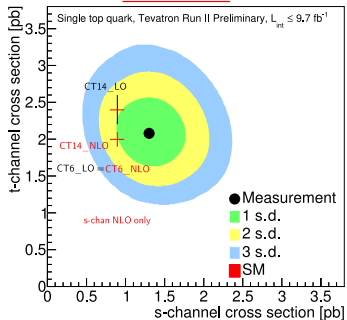


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Tevatron



I modified 1503.05027

LHC 13 TeV

CMS has measured:

$$t \quad 141.5 \pm 12.2 \text{ pb}$$

$$\bar{t} \quad 81.0 \pm 10.4 \text{ pb}$$

	LO (pb)	NLO (pb)
t	141	140
t	134	137
t	147	145
\bar{t}	79.2	80.8
\bar{t}	76.4	79.5
\bar{t}	85.4	85.6

LHC LO/NLO agree to 2% or better

t -channel scale uncertainties shown (LO and NLO)

1σ PDF uncertainties similar to NLO scale uncertainty

(NLO s -channel: CTEQ 6 \equiv CTEQ 14 to $< 0.1\%$)

What happened? We aren't certain yet...

- Perhaps like CTEQ 4, α_s in LHAPDF is off.
 - In fact it was off in LHAPDF 5 with multisets on, this same t -channel calculation found it ... it is now fixed in LHAPDF 6.
- Maybe LHAPDF is not a good reproduction of the fits.
 - There are small differences, but they are $\leq 0.1\%$
Still be warned, it can take millions of events at NLO or NNLO to reproduce cross sections if there are large cancellations.
- Maybe the LO fits are just poor.
 - This is a distinct possibility. Mostly NLO (or higher) distributions are fit, then LO formally extracted, but not always with as much data.

What has changed since the days of CTEQ 6?

LHC data has been added, HERA has been updated.

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LHC data has been added, HERA has been updated.

- HERA fits DIS directly.

PDF	LO (pb)	NLO (pb)	
HERAPDF2lo/nlo	1.910	1.762	(8% deviation)
HERA20 ("JETS")	(1.910)	1.830	4% — +c, dijets, α_s

HERA "JETS" uses charm and multijets (technically differential DIS).

Recall $\sigma \sim \ln\left(\frac{Q^2}{p_T^2}\right)$ in the massless case.

Summary

“Heavy quarks” (c , b , and t) are interesting because their mass adds a new scale to any problem.

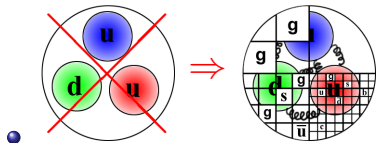
$$\sigma \sim \alpha_s \ln \left(\frac{\mu^2}{p_{T \text{ cut}}^2 + m_Q^2} \right)$$

These terms can appear in the initial or final state, and need to be resummed.

When you see logs of this type, it is often a hint there is something deeper to be learned.

Single-top-quark production is the new DIS and Drell-Yan

$$\sigma_{\text{obs.}} = \int f_1(x_1, \mu_1) f_2(x_2, \mu_2) \otimes |\overline{M}|^2 \otimes dP.S. \otimes D_i(p_i) \dots D_n(p_n)$$



- b/c PDFs are inside the proton
- For construction and uncertainties cf. Dr. Nadolsky's talks
- Analytic structure gives direct kinematical insight
- ⇒ New processes & new questions

Summary

- Many techniques exist to calculate perturbative matrix elements to higher orders
 - They only agree at the level of well-defined observables, which means that experimentalists and theorists must take care to ask the same questions.
- Exclusive jet observables require careful mathematical techniques
 - Requires an understanding of jet definitions, cf. Dr. Larkowski.
 - Experiments need to use NLO matched Monte Carlo programs, cf. Dr. Kuttimalai and the tutorials.
- Scale choices are not always free
 - DIS and DY-like processes have had (until now) a hidden correlation with choices made in PDF fits.
 - **Clear and large discrepancies** exist in single-top quark production due to large logarithms and delicate analytic cancelations in **all modern PDF sets**.
Resolving this issue will require a much deeper understanding of proton structure that will almost certainly require new data from an Electron Ion Collider.

THANK YOU