Quantum Chromodynamics

Lecture 4: Higher orders and all that

Hadron Collider Physics Summer School 2010

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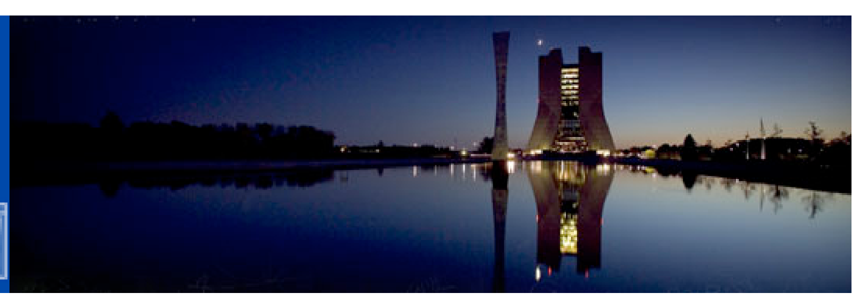


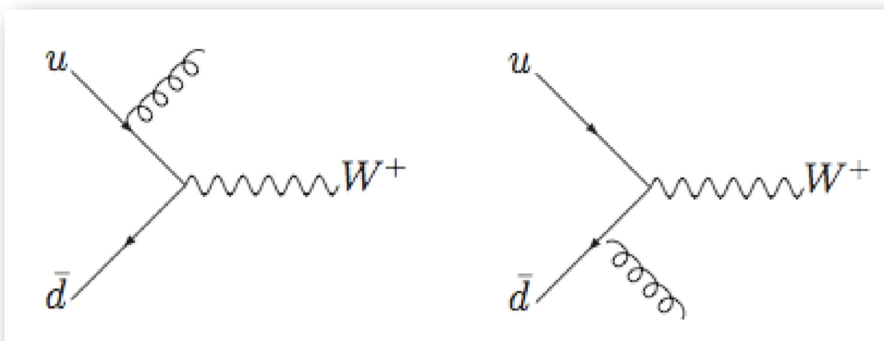
Tasks for today

- Understand general features of higher order calculations.
  - infrared singularities and calculational framework.
- Investigate improvements to parton shower predictions.
  - matching/merging and including higher orders.
- Discuss other pertinent breakthroughs.
  - jets at hadron colliders.

General structure: NLO

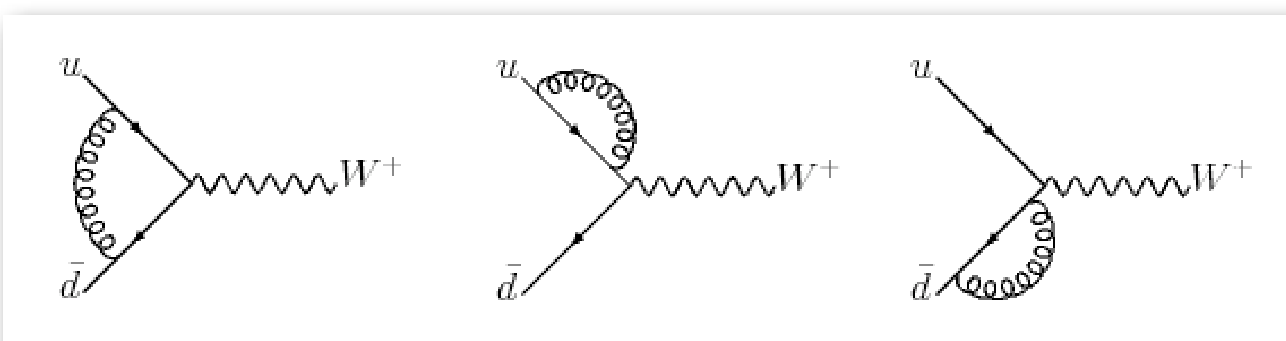
- We have seen some of the motivation for computing cross sections beyond leading order. We'll now look at some of the details.

- In the DGLAP evolution we already saw that radiating a gluon contributes in two ways. Example: W production (Drell-Yan process).



additional radiation present in the final state

"real radiation"



additional radiation emitted and reabsorbed internally

"virtual" or "1-loop" diagrams

- Contribute at the same order in the strong coupling:

$$|\mathcal{M}_{W+g}|^2 \sim (g_s)^2 \;, \quad (\mathcal{M}_{W,1-\mathrm{loop}} \times \mathcal{M}_{W,\mathrm{tree}}) \sim g_s^2 \times 1$$

Real radiation

- We already know that the real radiation contribution suffers from infrared singularities. This time we will regularize them with dimensional regularization.

- In our discussion of factorization in the small angle approximation we had:

$$d\sigma_{(\ldots)ac} \sim \int |\mathcal{M}_{(\ldots)ac}|^2 E_a^2 dE_a \, \theta_a d\theta_a \sim d\sigma_{(\ldots)b} \left(\frac{\alpha_s}{2\pi}\right) \frac{dt}{t} P_{ab}(z) \, dz$$

- Moving from 4 to 4-2ε dimensions we pick up some extra factors that we can again write in terms of *t* and *z*:

$$E_a^2 dE_a \, \theta_a d\theta_a \to E_a^{2-2\epsilon} dE_a \, \theta_a^{1-2\epsilon} d\theta_a = E_a^2 dE_a \, \theta_a d\theta_a \, z^{-2\epsilon} \left[\frac{t(1-z)}{z\theta_a^2}\right]^{-\epsilon} \theta_a^{-2\epsilon}$$

$$= E_a^2 dE_a \, \theta_a d\theta_a \, z^{-\epsilon} (1-z)^{-\epsilon} \, t^{-\epsilon}$$

- Hence our new factorization is:

$$d\sigma_{(\ldots)ac}^{4-2\epsilon} = d\sigma_{(\ldots)b} \left(\frac{\alpha_s}{2\pi}\right) \frac{dt}{t^{1+\epsilon}} P_{ab}(z) z^{-\epsilon} (1-z)^{-\epsilon} \, dz$$

- NB: in contrast to regularization of UV-divergent loop integrals, need ε<0 here.

Pole structure

- Schematically, we can see the structure that will emerge.

$$\int \frac{dt}{t^{1+\epsilon}} \to \frac{1}{\epsilon}$$

collinear pole

$$\int dz (1-z)^{-\epsilon} \left(\frac{1}{1-z} \right) \to \frac{1}{\epsilon}$$

additional pole from soft behavior

factor present in, for example, Pqq and Pgg

- Unlike the case of parton branching, we cannot simply treat the radiation from the quark and the antiquark separately. In our case:

universal pole structure

$$d\sigma_{W+g} = \left(\frac{2}{\epsilon^2} + \frac{3}{\epsilon} - \frac{2}{\epsilon} P_{qq} + \mathcal{O}(\epsilon^0) \right) d\sigma_{W,\text{tree}}$$

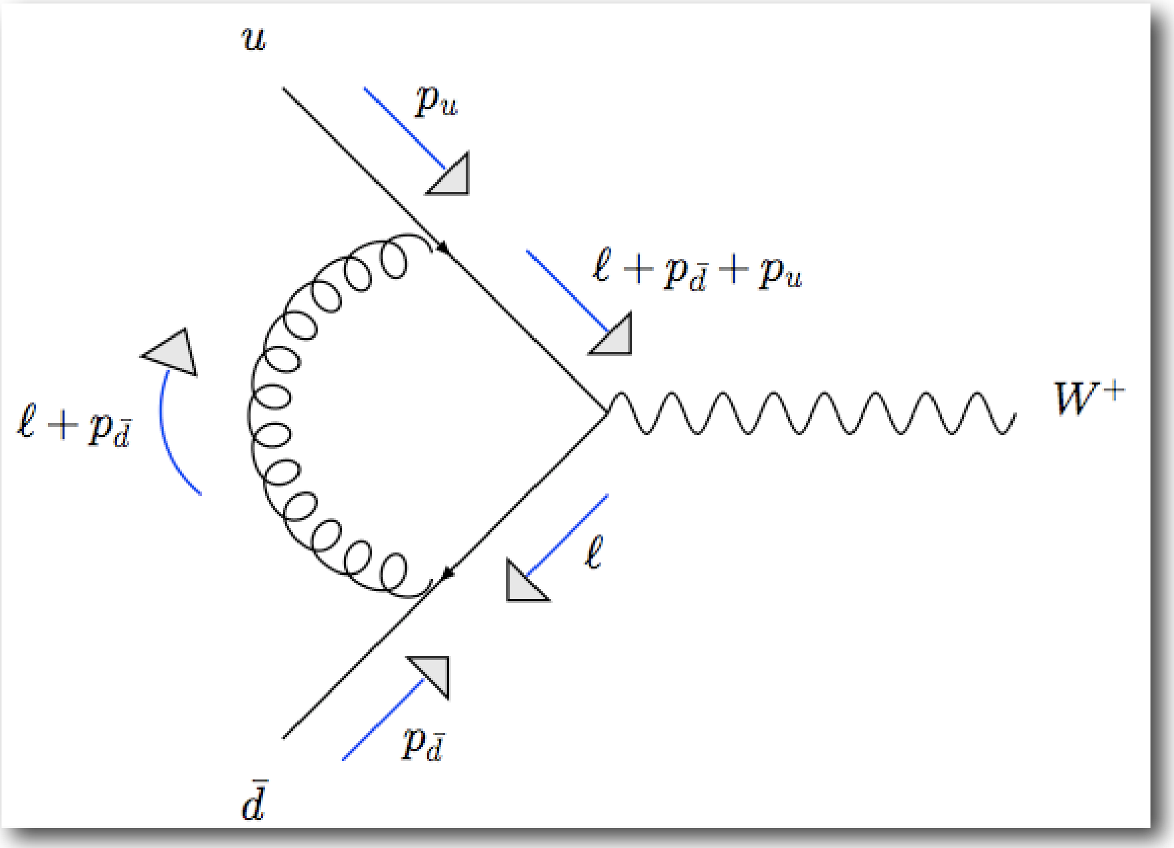
soft

collinear

initial state: absorbed into pdf

Virtual corrections

- We know that the remaining poles must cancel in the end (KLN theorem) so now turn to the virtual (loop) corrections.
- Only one diagram to calculate in the end (self-energy corrections on massless lines are zero in dim. reg.).
- General structure of amplitude is:



$$\int \frac{d^{4-2\epsilon}\ell \quad \mathcal{N}}{\ell^2(\ell + p_{\bar{d}})^2(\ell + p_{\bar{d}} + p_u)^2}$$

with Dirac structure in numerator:

$$\mathcal{N} = \left[\bar{u}(p_{\bar{d}})\gamma^\alpha \not{\ell} \gamma^\mu (\not{\ell} + \not{p}_{\bar{d}} + \not{p}_u)\gamma_\alpha u(p_u)\right] V_\mu(p_W) \ .$$

- Difficult part is performing the integral over the loop momentum. First we'll inspect the integrand.

Infrared singularities

- Inspection of the denominators reveals the now-familiar problems. They are best seen by shifting the loop momentum:

$$\ell^2(\ell+p_{\bar{d}})^2(\ell+p_{\bar{d}}+p_u)^2 \longrightarrow \ell^2(\ell-p_{\bar{d}})^2(\ell+p_u)^2 \qquad [\ell \to \ell - p_{\bar{d}}]$$

- There is a soft singularity as $\ell \to 0$ and two collinear singularities, when ℓ is proportional to either of the external momenta.
- These will again be handled by dim. reg., which is already being used anyway to handle the UV singularity (two powers of ℓ) - not to mention on the real side.
- Just as in the real radiation case, these singularities will be proportional to tree-level matrix elements.
- In our case (and in general) the procedure is greatly complicated by the Dirac structure in the numerator.
  - as a simple case, consider the case with no numerator ("scalar integral").

Quick calculation

- The normal method is to combine the denominators with Feynman parameters (x_1, x_2, x_3 here) and shift the loop momentum:

$$\frac{1}{\ell^2(\ell+p_{\bar{d}})^2(\ell+p_{\bar{d}}+p_u)^2} = 2\int_0^1 dx_1 \int_0^1 dx_2 \int_0^1 dx_3 \, \frac{\delta(x_1+x_2+x_3-1)}{\left[x_1\ell^2 + x_2(\ell+p_{\bar{d}})^2 + x_3(\ell+p_{\bar{d}}+p_u)^2\right]^3}$$

$$= 2\int_0^1 dx_1 \int_0^{1-x_1} dx_3 \, \frac{1}{(L^2-\Delta)^3}$$

$$L = \ell + (1-x_1)\,p_{\bar{d}} + x_3\,p_u$$

$$\Delta = -2x_1x_3\,p_u\cdot p_{\bar{d}}$$

- Evaluate this using the identity:

$$\int \frac{d^dL}{(2\pi)^d}\frac{1}{(L^2-\Delta)^n} = i\frac{(-1)^n}{(4\pi)^{d/2}}\frac{\Gamma\left(n-\frac{d}{2}\right)}{\Gamma(n)}\Delta^{d/2-n}$$

- Obtain:

$$\int_0^1 dx_1 \int_0^{1-x_1} dx_3 \,(-2x_1x_3\,p_u\cdot p_{\bar{d}})^{-1-\epsilon} = (-2p_u\cdot p_{\bar{d}})^{-1-\epsilon}\int_0^1 dx_1\, x_1^{-1-\epsilon}\left(-\frac{1}{\epsilon}\right)x_1^{-\epsilon}$$

$$= (-2p_u\cdot p_{\bar{d}})^{-1-\epsilon}\left(-\frac{1}{\epsilon}\right)\frac{\Gamma(-\epsilon)\Gamma(1-\epsilon)}{\Gamma(1-2\epsilon)} \quad = (-2p_u\cdot p_{\bar{d}})^{-1-\epsilon}\left(\frac{1}{\epsilon^2}\right)\frac{\Gamma^2(1-\epsilon)}{\Gamma(1-2\epsilon)}$$

soft singularity exposed

W production: final result

- Since this is a simple calculation, this method can actually used to perform the entire calculation;
  - loop shift in numerator gives different Feynman parameter integrals.
  - in general, we need to do more work.
- A detailed account of the full calculation can be found online:

See notes by Keith Ellis on Indico web-page

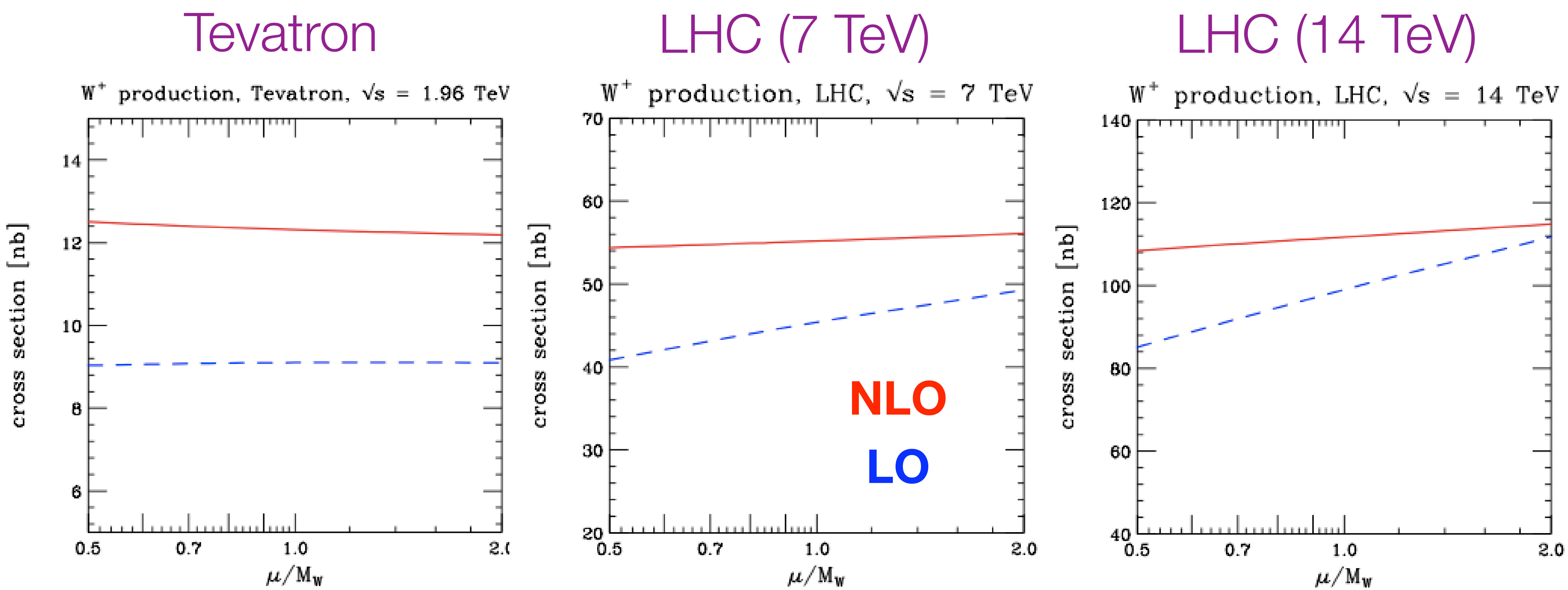
- Here, I'll just draw attention to the pertinent features:

$$d\sigma_{W,1-\mathrm{loop}} = \left(-\frac{2}{\epsilon^2} - \frac{3}{\epsilon} + \mathrm{finite}\right) d\sigma_{W,\mathrm{tree}}$$

- The poles are proportional to the tree level contribution and are equal and opposite to those from the real contribution. Their sum is therefore finite.
- In this case the finite term is also proportional to the tree-level result.
  - this is not true in general: it is process-specific and hard to calculate.

W^+ cross sections at LO and NLO

- Numerical results at LO and NLO, Tevatron and two LHC energies, setting $\mu_R=\mu_F$ and varying about M_W (pdf set: MSTW08).



- LO: cross section depends only on μ_F (but on both at NLO).
  - mostly independent of scale at Tevatron; this is because typical *x* ~ 0.05, in the region of no scaling violations (c.f. earlier HERA data).
- Behavior of the theoretical predictions quite different at the two machines.

More complicated NLO calculations

- In general the method outlined here does not scale to complex final states. Briefly mention two of the issues here.
- Computing the relevant loop integrals with more particles in the final state generates very complicated and length expressions.
  - this has led to a revolution in the way that virtual amplitudes are computed. Nowadays, most new calculations rely on either a numerical or analytical implementation of unitarity techniques.
  - these rely on sewing together tree level diagrams and replacing integrals with algebraic manipulations.
  - analytic methods yield compact results; numerical methods allow calculations of unprecedented difficulty (e.g. W+4 jets from earlier)
- Although the infrared pole structure of the real radiation contribution is known, the phase space integrals cannot actually be performed analytically.
  - we need a way to extract the poles to cancel with the 1-loop diagrams, so that the remainder of the integrals can be performed numerically.

Real radiation: toy model

- There are two methods that are widely used in existing NLO calculations. They both rely on the fact that, in the singular regions, both the phase-space and the matrix elements factorize against universal functions.
  - these are called phase space slicing and subtraction methods.
- Briefly demonstrate the features of each with reference to a toy model:

$$\mathcal{I} = \int_0^1 \frac{dx}{x}\, x^{-\epsilon} \mathcal{M}(x)$$

- *M(x)* represents the real matrix elements, with *M(0)* the lowest order.
- We know that this toy model exhibits the correct features of the soft and collinear limits in dimensional regularization.

Phase space slicing

Giele, Glover and Kosower, 1980;
Keller and Laenen, 1999;
Harris and Owens, 2002.

- In the slicing approach, an additional theoretical parameter (δ) is introduced which is used to define the singular region. Close to the singular region, the matrix elements are approximated by the leading order ones.
  - In our toy model, this means choosing $\delta \ll 1$ and approximating *M(x)* by *M(0)* when $x<\delta$.
- In that case we can split the integral into two regions thus:

$$\begin{aligned}
\mathcal{I} &= \mathcal{M}(0) \int_0^\delta \frac{dx}{x} x^{-\epsilon} + \int_\delta^1 \frac{dx}{x} x^{-\epsilon} \mathcal{M}(x) \\
&= -\frac{1}{\epsilon}\delta^{-\epsilon}\mathcal{M}(0) + \int_\delta^1 \frac{dx}{x}\mathcal{M}(x) \\
&= \left(-\frac{1}{\epsilon} + \underbrace{\log\delta\right)\mathcal{M}(0) + \int_\delta^1 \frac{dx}{x}\mathcal{M}(x)}_{\text{finite, ready to be integrated numerically}}
\end{aligned}$$

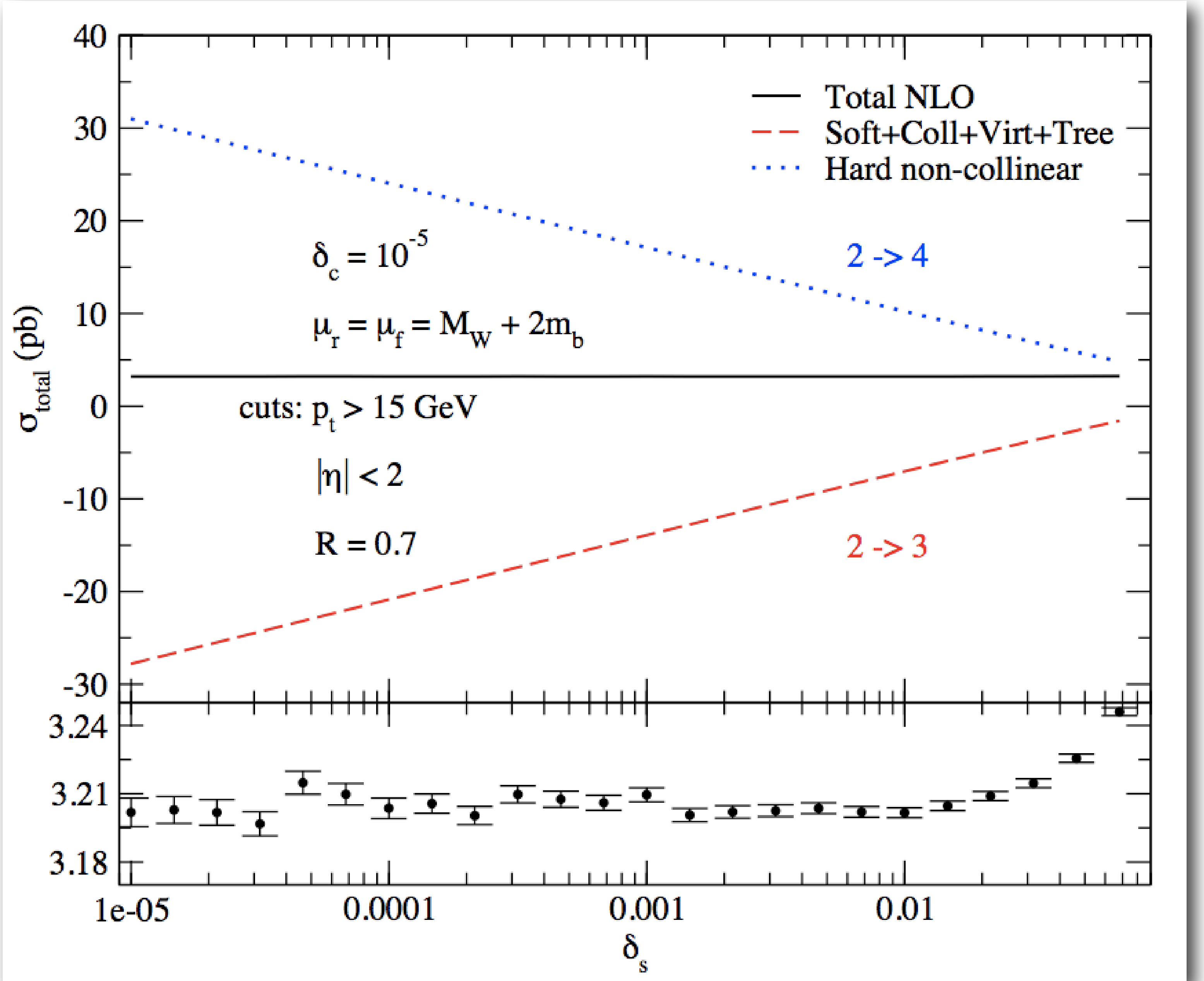
isolated singularity

- The final result should be independent of δ, via an implicit cancellation of logarithms between the exposed log and the lower limit of the integral.

Slicing: example

- Tension between retaining a good soft/collinear approximation (wanting small δ) and reducing numerical-log cancellations (large δ).

- Example: *Wbb* production (with massive b-quarks).
- Actually uses two cutoffs, one for soft (δ_s) and one for collinear (δ_c) singularities.



Febres Cordero, Reina, Wackeroth (2006)

Subtraction

Ellis, Ross and Terrano, 1981
Catani and Seymour, 2002

- Subtract from the integrand, in each singular region, a local counterterm with exactly the same singular behaviour.
- In the toy model the counterterm is obvious:

$$\mathcal{I} = \int_0^1 \frac{dx}{x} x^{-\epsilon} \left[\mathcal{M}(x) - \mathcal{M}(0)\right] + \mathcal{M}(0) \int_0^1 \frac{dx}{x} x^{-\epsilon}$$

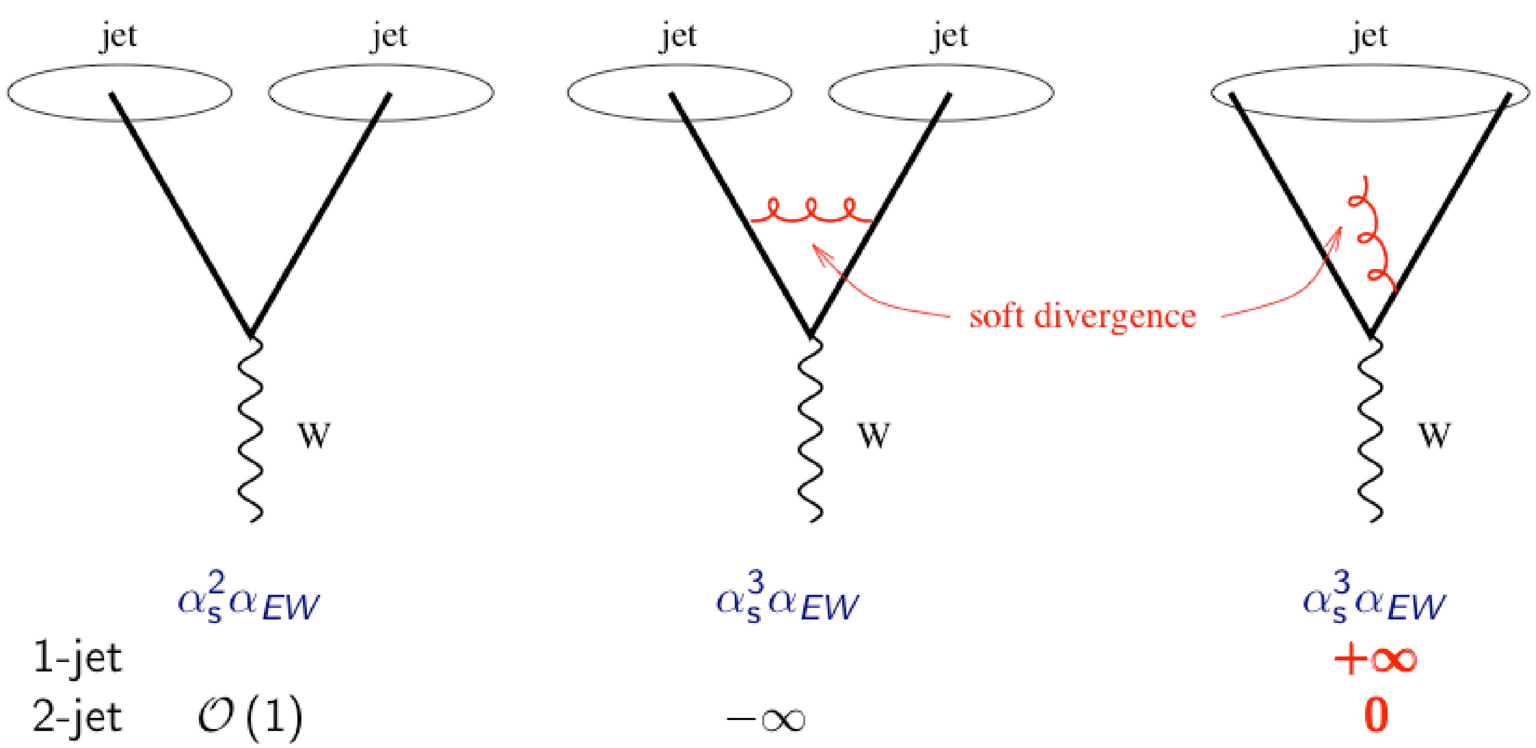
$$= \underbrace{\int_0^1 \frac{dx}{x} \left[\mathcal{M}(x) - \mathcal{M}(0)\right]}_{\text{suitable for numerical integration}} - \frac{1}{\epsilon}\mathcal{M}(0)$$

isolated singularity

- Although apparently straightforward, there are still shortcomings.
- For numerical stability still need a cutoff in practise, since it is impractical to integrate the subtracted singularity completely (to zero, in our toy example).
- In addition, the trick here is to construct the singular terms in such a manner that they are both universal and readily integrated analytically.
- Such a formulation is provided by the dipole subtraction procedure.

Infrared safety

- After isolating the divergent terms from the real contribution, the cancellation of them against the virtual contributions is very delicate.
- It relies on the fact that both types of event should have the same number of jets in the final state.
- This can be a problem in some jet algorithms, which are the means by which calorimeter towers (partons) are combined into jets.
  - an algorithm is called infrared unsafe when the addition of a soft particle changes the configuration of jets found by the algorithm.



Infrared unsafety

- On the theory side, higher order calculations cannot be used in situations (a combination of algorithm and observable) which are infrared unsafe.
- In the interpretation of experimental data (or in a parton shower) such singularities of course do not occur
    - however, they are replaced by large logarithms in an (almost certainly) unpredictable way - due to details of the detector (or parton shower).
- As a result, comparisons between different experiments and with higher order theoretical predictions can become difficult.
- Typical jet algorithms used at the Tevatron (e.g. cone, midpoint cone, JetClu) do indeed suffer from infrared unsafety.
    - but often only for large numbers of jets (not so common at the Tevatron).
- Solution for the LHC: use infrared and collinear safe algorithms from the start.
    - now possible thanks to a new generation of jet algorithms.

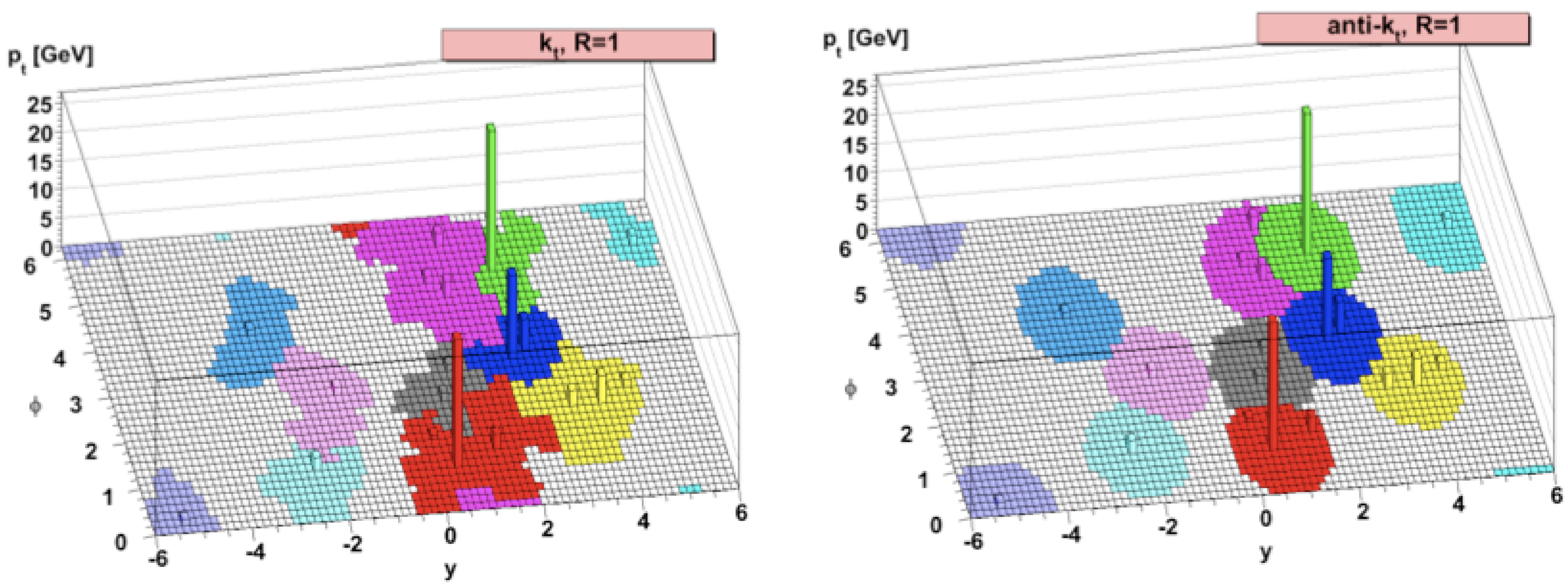
Excellent, comprehensive review: Salam, arXiv:0906.1833

Jet algorithms for the LHC

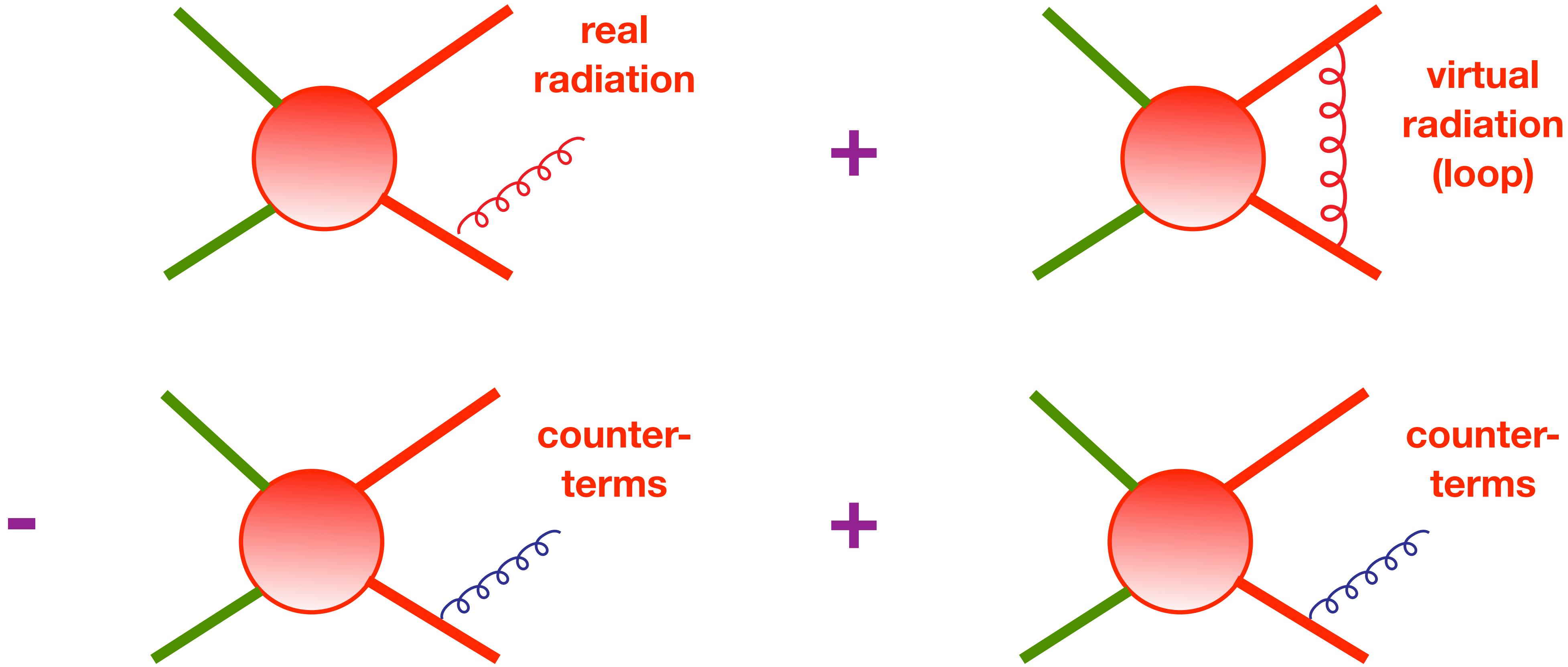
- Two algorithms of most importance:

SISCone	Salam and Soyez (2007)
anti-k_T	Cacciari, Salam and Soyez (2008); Delsart

- Traditionally, cone algorithms have advantages when analyzing data while the k_T algorithm (to which anti-k_T is closely related) has better theoretical properties.
  - with advent of SISCone and anti-k_T, they are now on a more even footing.



General structure of NLO



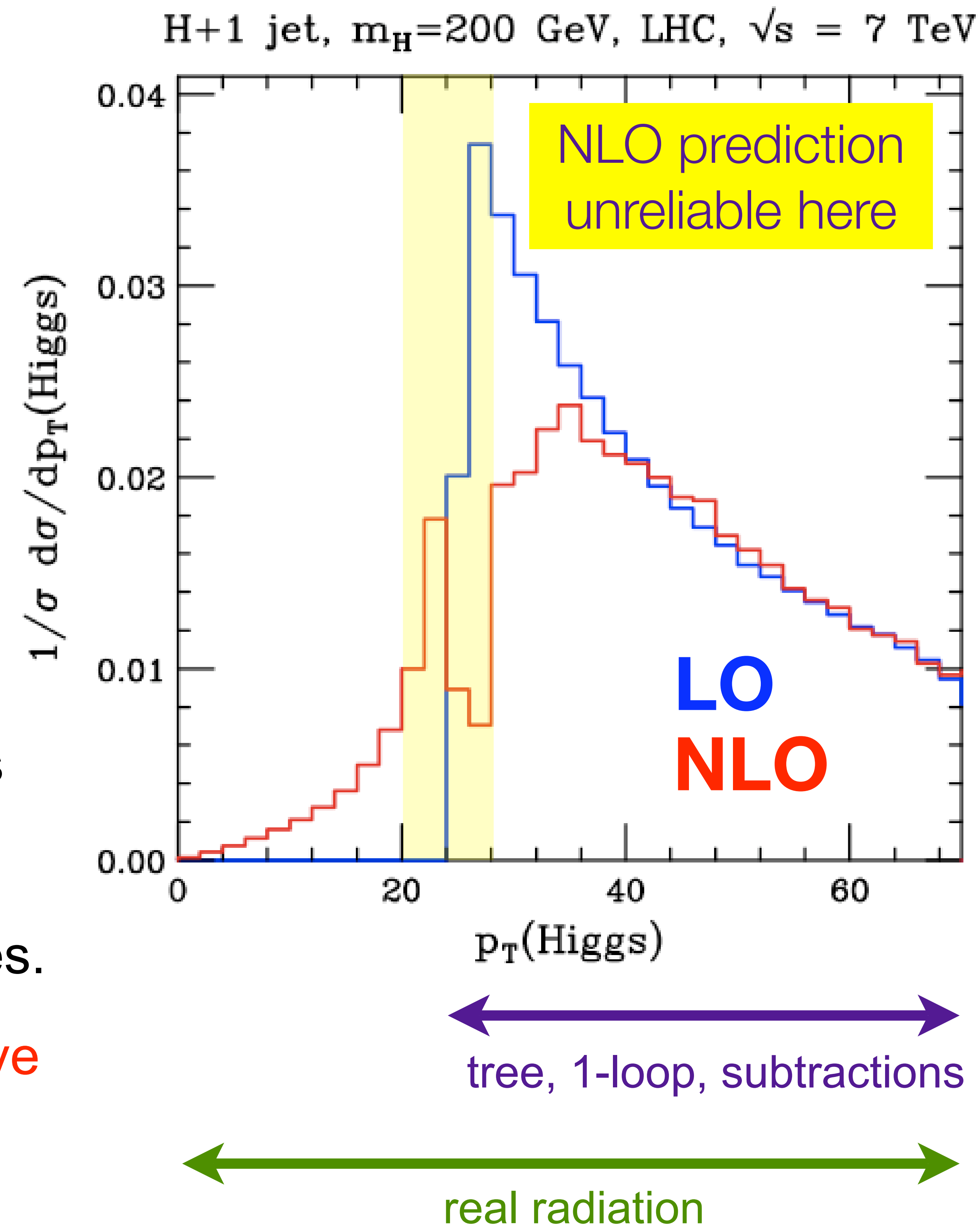
soft/collinear singularities cancelled numerically

singularities cancelled analytically

- In general: many subtractions (“counter-events”) for each real radiation event.
- Common parton level NLO programs:
MCFM, NLOJET++, Blackhat, Rocket, HELAC-1loop.

Other features of NLO

- Compared to LO (without a shower) additional benefits include:
    - exposure to wider range of initial states;
    - sensitivity to final state features such as details of jet algorithm;
    - extended kinematic range.
- Major disadvantages:
    - while calculating LO cross sections is a solved problem, only very recently have we had NLO calculations beyond 2→3 processes.
    - without using a shower, no exclusive hadron-level predictions (just partons).



Beyond NLO: next-to-next-to-leading order

- We've already seen how the scale dependence is expected to be reduced even further at the next order of perturbation theory.
  - can expect real precision from the theoretical prediction ("few percent").
- The normalization of a cross section begins to be trustworthy at NLO, but the theoretical uncertainty associated with it is only reasonably estimated at NNLO.
- In addition, many of the arguments for NLO apply again at NNLO - e.g. even more sensitivity to jet algorithms, still larger phase space, etc.
- The ingredients for a NNLO calculation are similar to, but more complicated than, those that enter at NLO.
  - as a result, relatively few predictions at this order yet:

Drell-Yan, Higgs (gluon fusion and WBF)	hadron colliders
2- and 3-jet production	lepton colliders

NNLO complexity

- One way to envision the different NNLO contributions is to consider all possible cuts of a 3-loop diagram.

- Example: 3-jet production in e^+e^- annihilation.

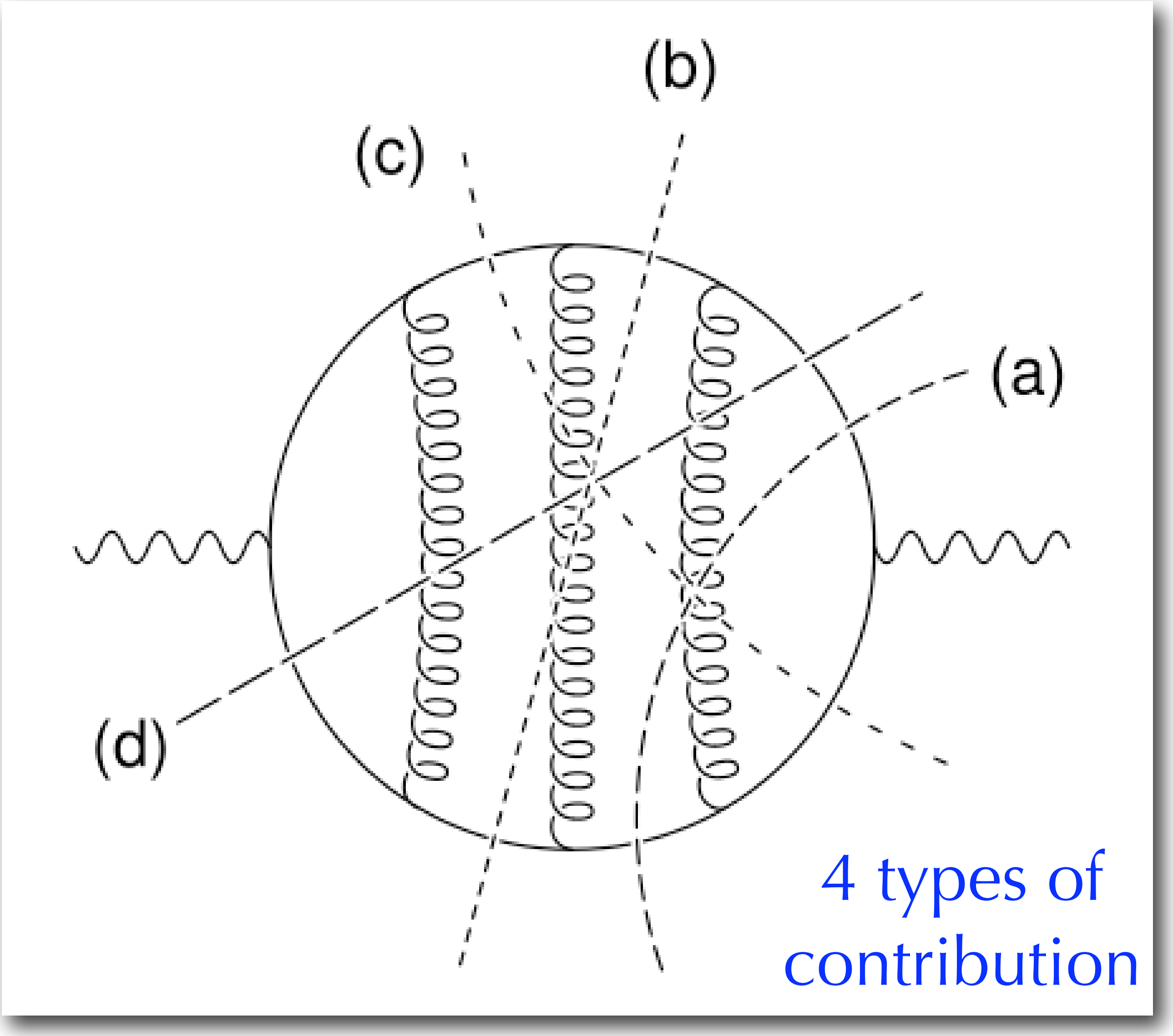
  (a) 2-loop virtual diagrams.

  (b) 1-loop squared.

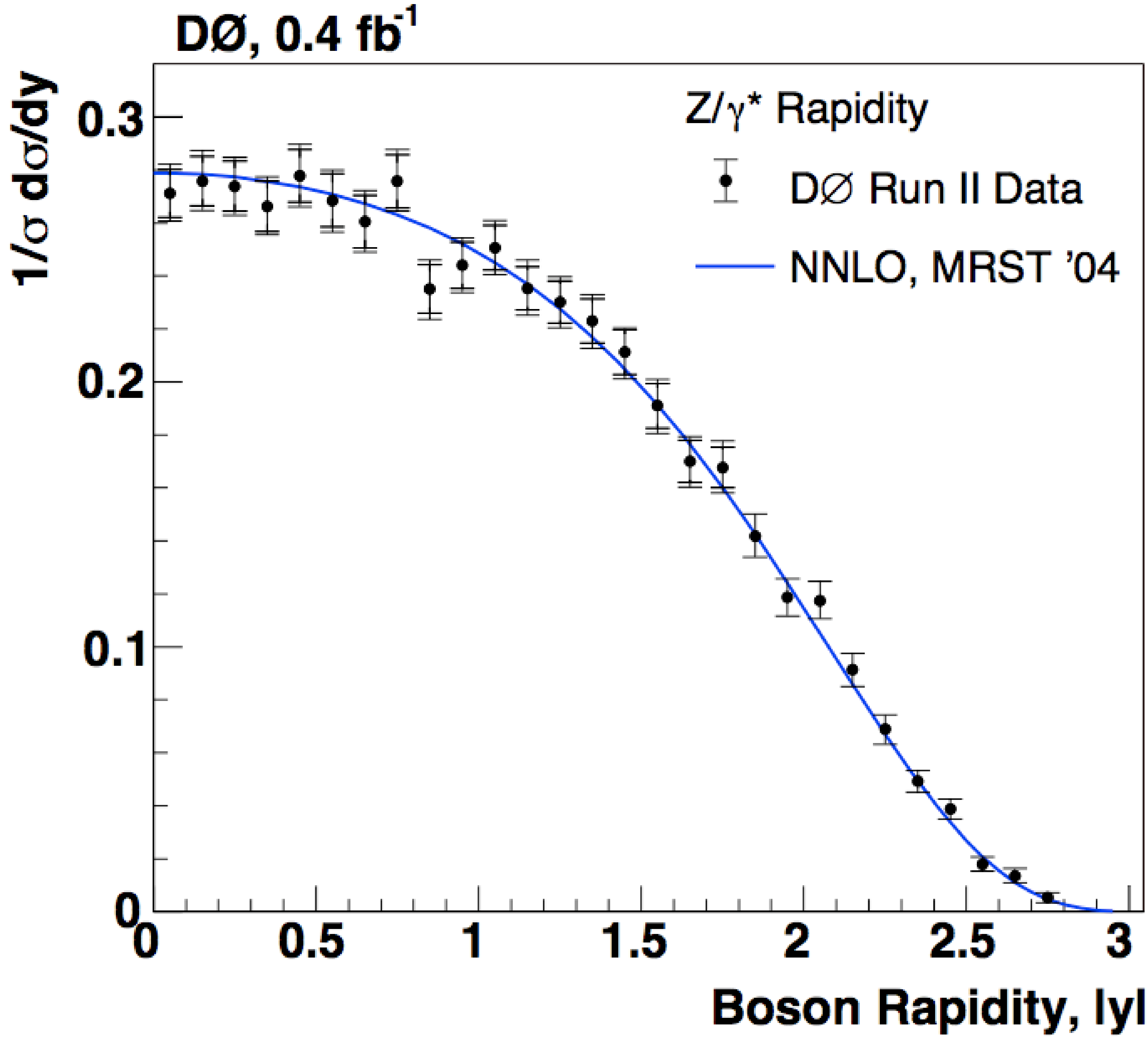
  (c) interference of 1-loop and tree, both with extra parton → infrared singularities (easy)

  (d) tree with two extra partons → [infrared singularities]^2

- At present, no universal procedure (like dipole subtraction) formulated.



Example: NNLO vs. data



NNLO calculation:

Anastasiou, Dixon, Melnikov, Petriello (2003).

Higher orders: practical advice

- Orders of calculation populate different jet bins at differing orders of accuracy.

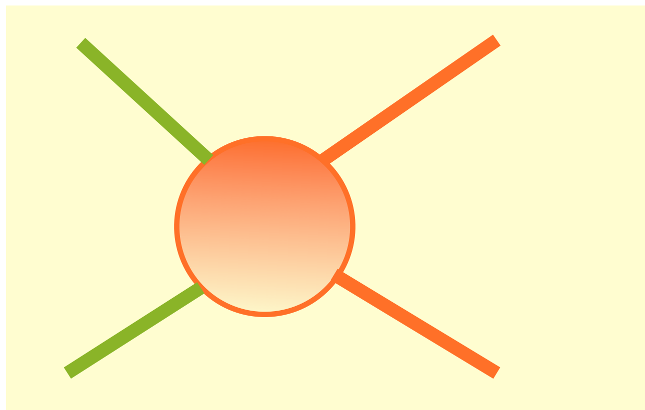
- When moving beyond normalizing a total cross section, better to think of order of observable rather than calculation.

LO ballpark

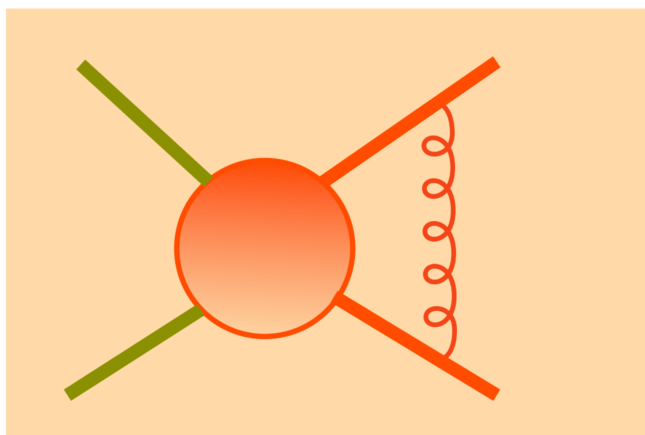
NLO trustworthy

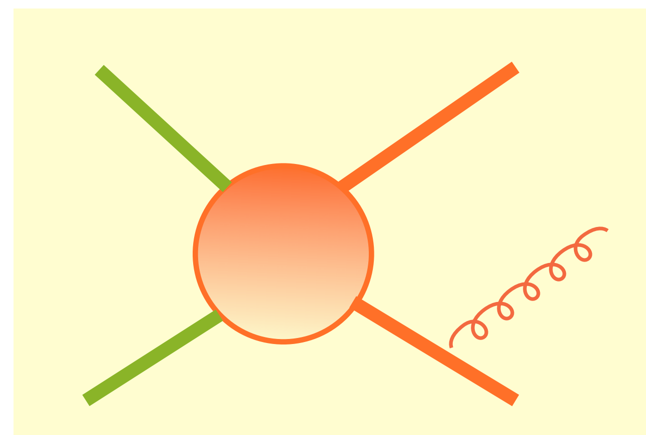
NNLO precision

LO N-jet calculation

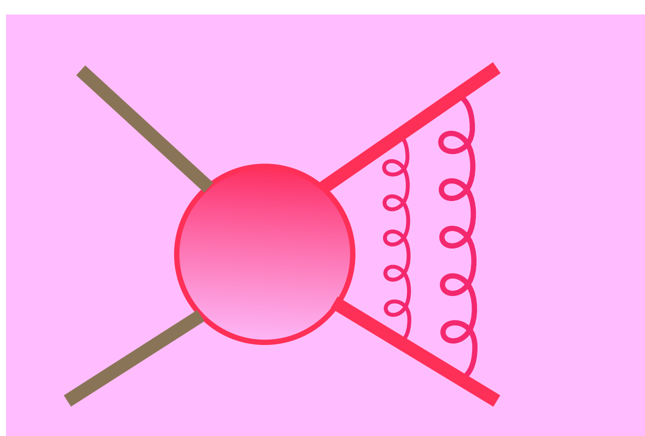


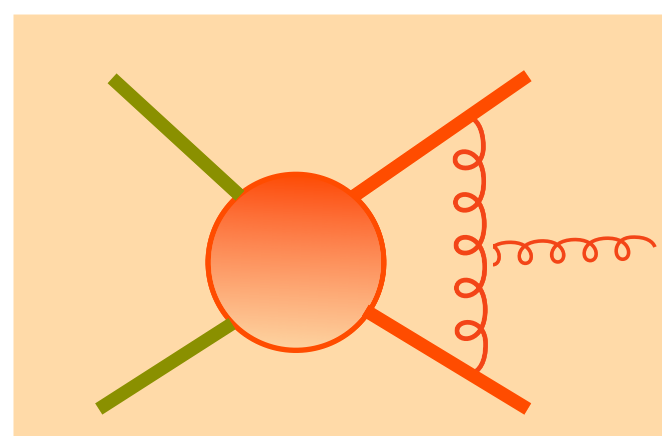
NLO N-jet

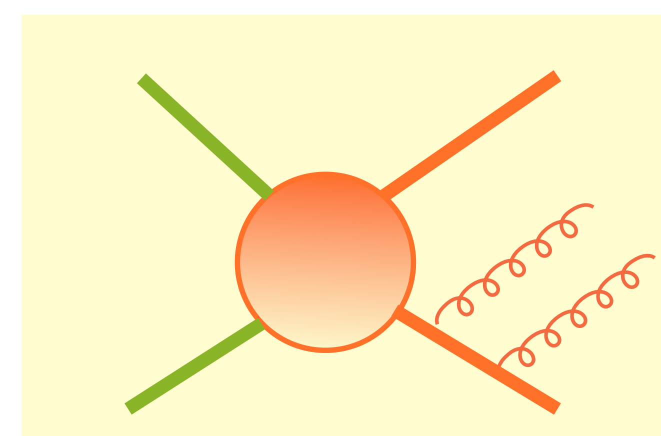




NNLO N-jet



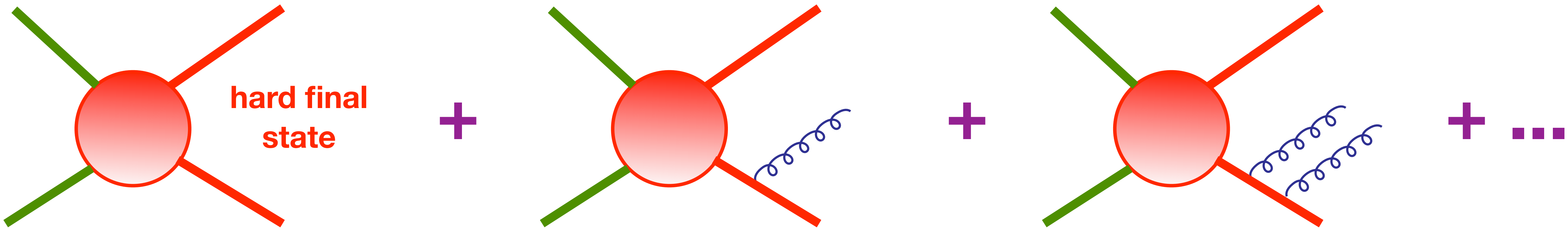




N-jet kinematics | **(N+1)-jet** | **(N+2)-jet**

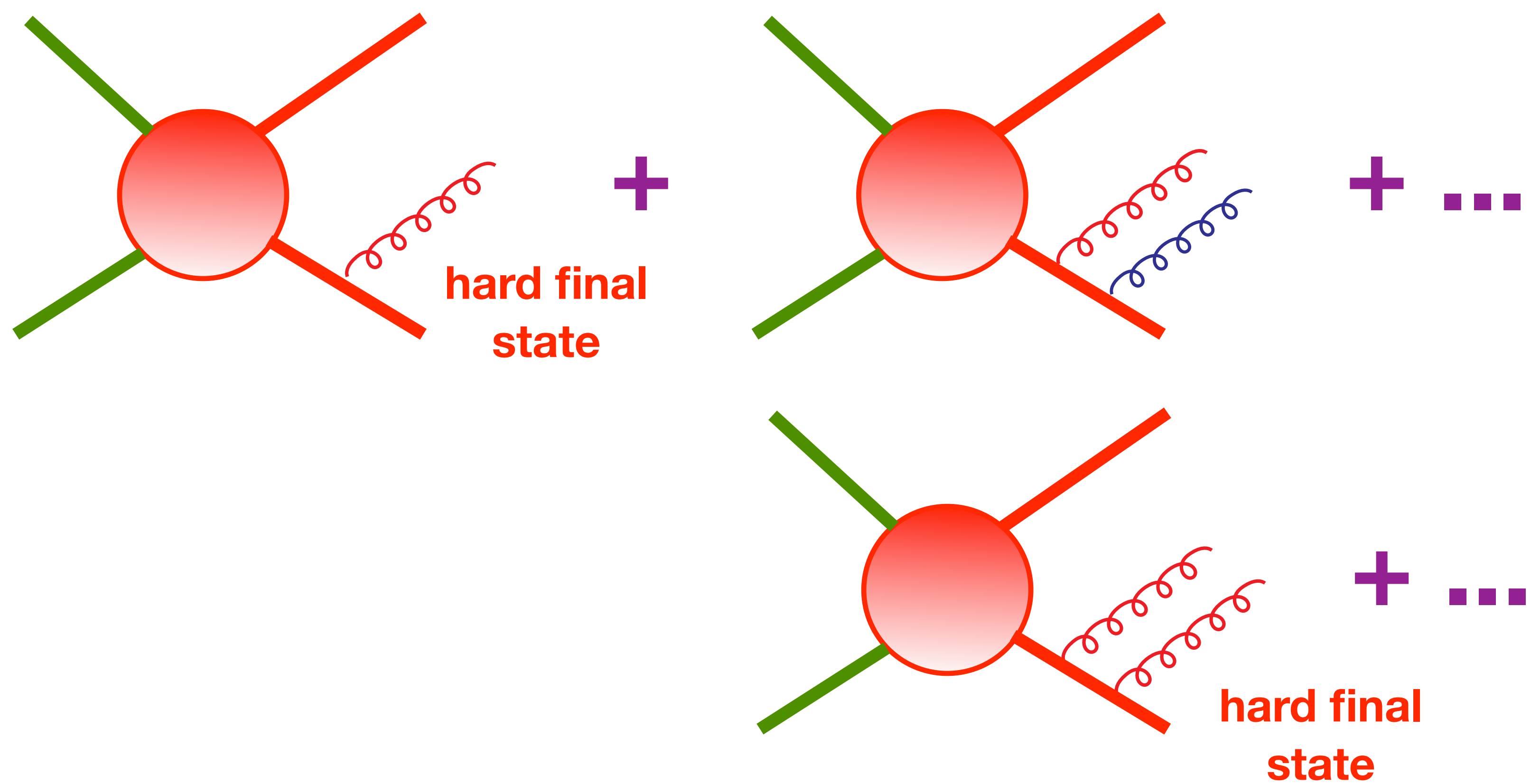
Improving parton showers

- We know that the parton shower approach we developed earlier suffers from the approximation that all additional radiation is soft or collinear.
- Solution: include more exact matrix elements as initial hard scatters.



- Avoid double counting
  → ME matching/merging.
- Many different universal schemes for doing this, e.g. MLM, CKKW, ME&TS (“matrix element +truncated shower”)

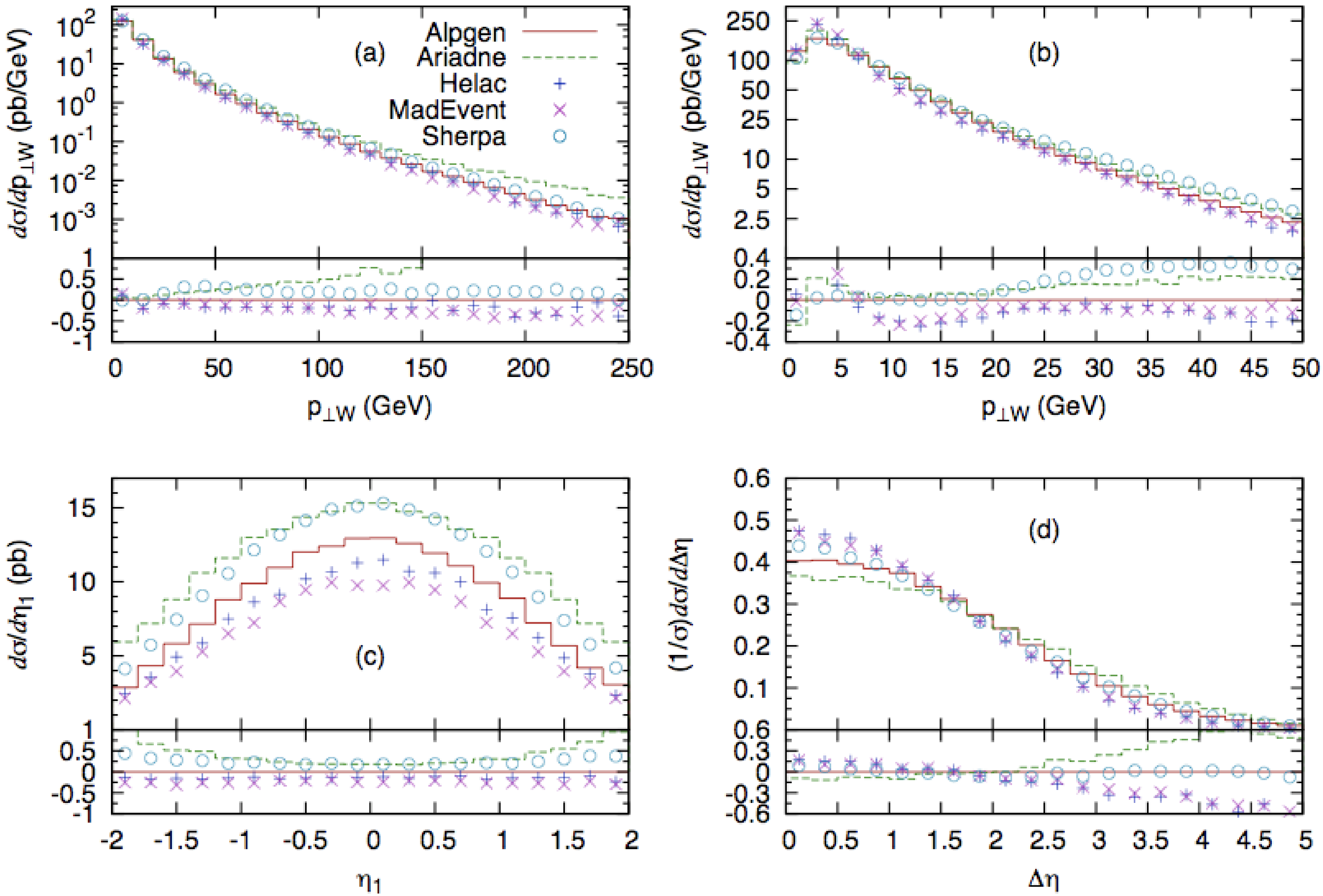
Built in to Alpgen, Sherpa



Comparison of merging techniques

Alwall et al. (2007)

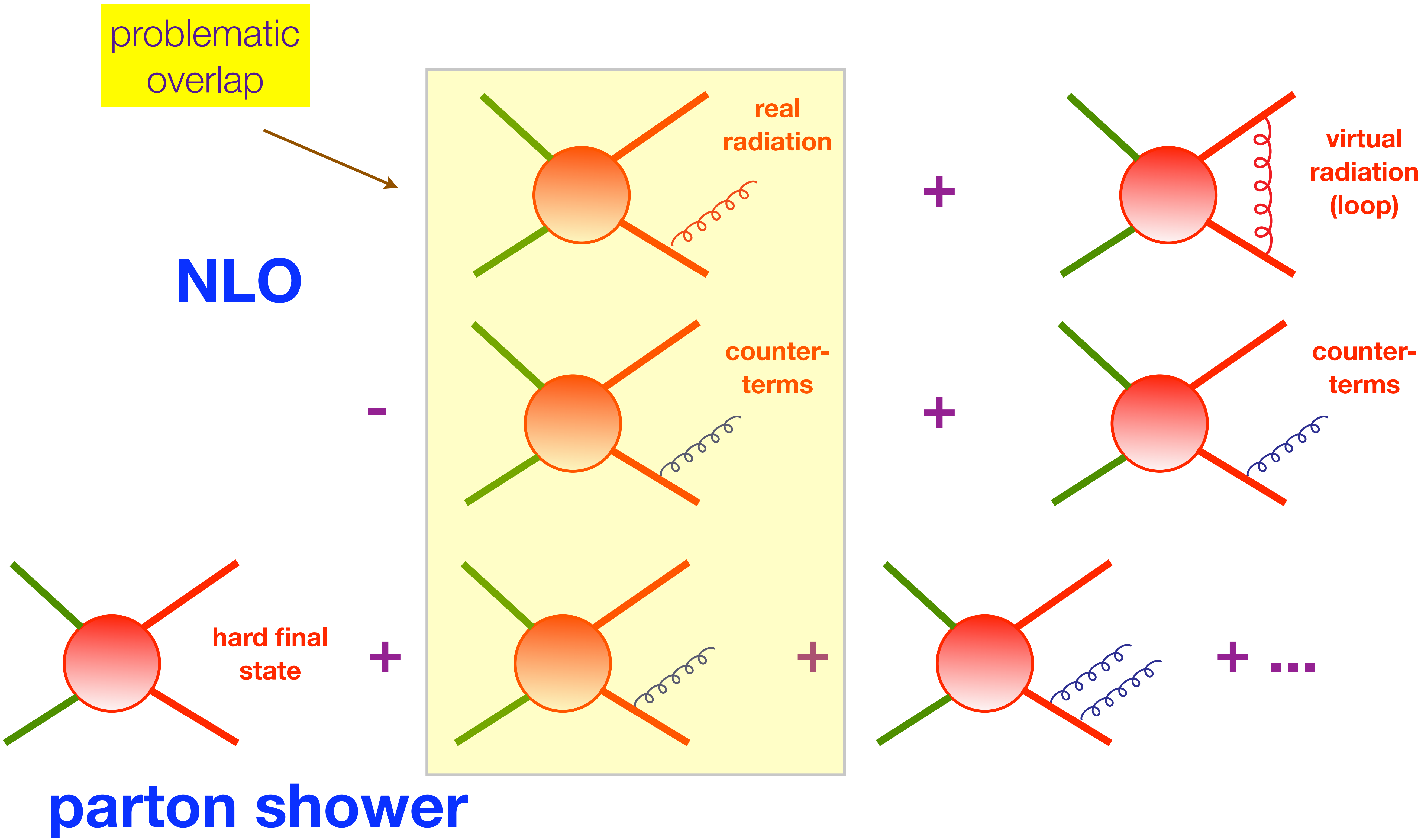
Tevatron



Limits of LO+parton shower

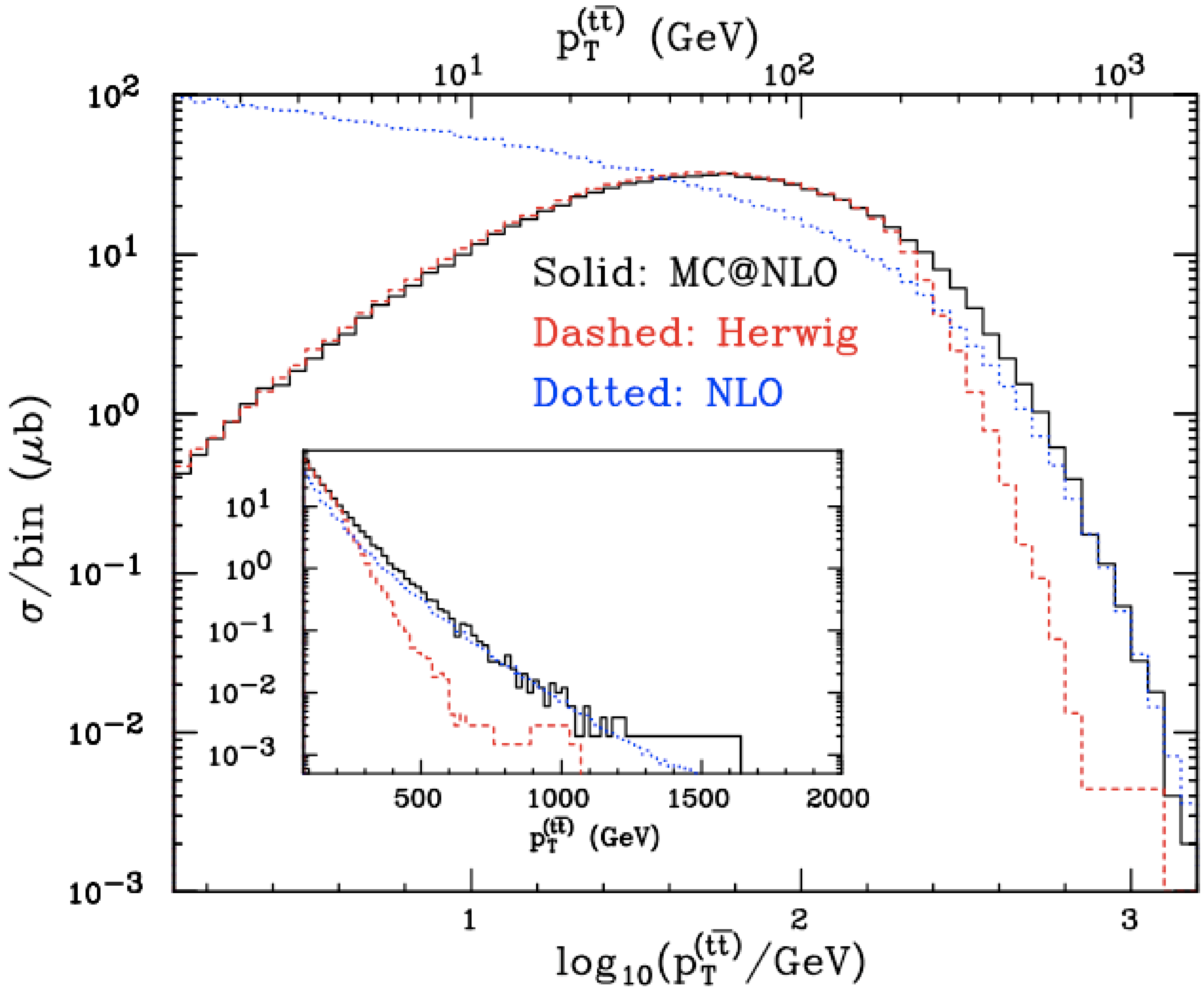
- Even after adding additional hard radiation onto a parton shower, overall normalization of cross section remains a leading order estimate
  - usual disadvantages, such as sensitivity to scale choices.
- Natural question: can one add a parton shower on top of NLO?
  - obtain NLO accuracy, but exclusive hadron-level predictions.
- Obvious problem:
  - NLO already includes one extra parton emission.
  - the hard part of this can be matched as before.
  - the soft/collinear part contains singularities that must be extracted in a particular way (e.g. subtraction). How can that be combined with a shower?
- Solution: generate the subtraction terms from the shower.
  - simplest implementation is process-dependent and still complicated.

Schematic: NLO+parton shower



NLO + PS: MC@NLO

- First real matching of a parton shower (HERWIG) onto a NLO calculation.

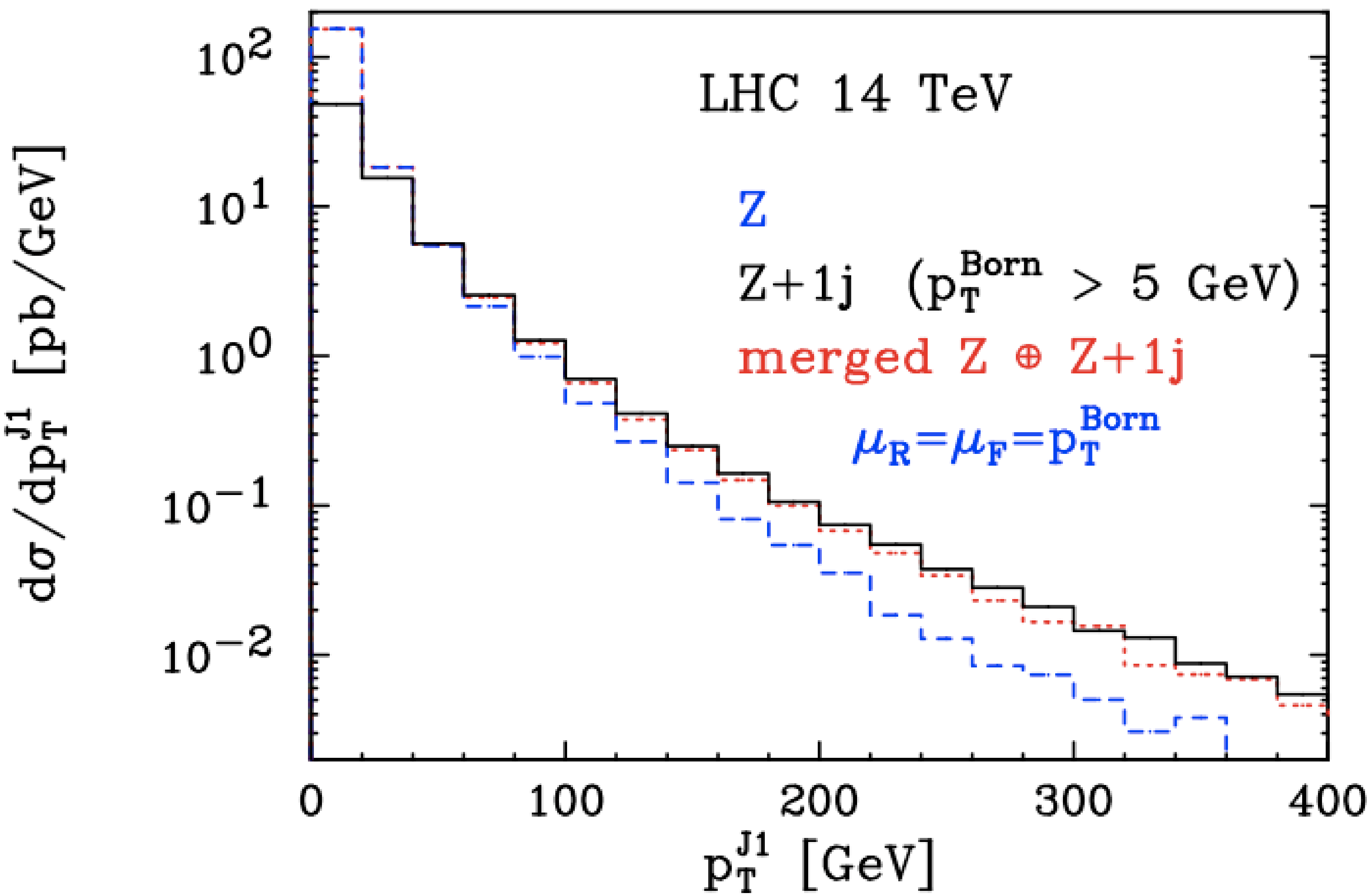


transverse momentum of top pairs, from MC@NLO

Frixione and Webber (2003)

NLO + PS: POWHEG

- More recent implementation, promising simpler procedure through which to incorporate parton-level NLO calculations.
- Shower not fixed by the implementation, so any can be used.



transverse momentum of leading jet in Z+X, from POWHEG

Merging between Z and Z+jet samples

Oleari et al. (2010)

Parton shower vs. higher order: quandaries

- At present there is no implementation of a NLO parton shower that considers hadron collider processes with two or more jets in the final state, nor a NNLO+parton shower tool at all.
  - how do we best use N(NLO) information when no NLO+PS is available?
- Some possible options:
  - ☆ Use higher orders for overall inclusive normalization only
    - ✔ simple to implement, defensible theoretically
    - ✘ misses potentially important shape and/or kinematic information
  - ☆ Split events into jet bins and normalize by best prediction in each bin
    - ✔ simple, uses best information, defensible
    - ✘ as above + sum of bin cross sections is not a well-defined quantity
  - ☆ Pick an important distribution and reweight shower to reproduce NLO
    - ✔ relatively simple
    - ✘ throws away some PS shower information; other distributions okay?

Recap

- Next-to-leading order calculations include virtual and real radiation diagrams
  - each set contains infrared singularities that cancel in the sum
  - in order to realise this cancellation, the singularities are usually isolated by a subtraction or slicing procedure (→ additional types of “event”)
  - predictions are available for many processes through a number of different codes; current limit of complexity is 5 particles in the final state.
- NNLO has more contributions, but similar features
  - no universal scheme for handling IR issues, single particle final states only
- Two (mostly) orthogonal directions for improving parton showers
  - include more hard matrix elements to seed the shower, need to worry about matching event samples properly
  - improve accuracy from LO to NLO; a much more difficult problem (no universal solution) but solutions available for a select no. of processes.