NLO QCD Calculations I

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Contents

- Today:
  - Ingredients to a NLO calculations
    - Dealing with divergent integrals
- Tomorrow:
  - Computing loops efficiently

Master equation for hadron colliders

$$d\sigma = \sum_{a,b} \int dx_1 dx_2 \;\; f_a(x_1,\mu_F) f_b(x_2,\mu_F) \; d\hat{\sigma}_{ab\to X}(\hat{s},\mu_F,\mu_R)$$

Parton density functions

Parton-level (differential) cross section

- Parton-level cross section from matrix elements: model and process dependent
- Parton density (or distribution) functions: process independent
- Differences between colliders given by parton luminosities

Perturbative expansion

$d\hat{\sigma}_{ab\to X}(\hat{s}, \mu_F, \mu_R)$ Parton-level cross section

$$\hat{\sigma} = \sigma^{\mathrm{Born}}\left(1 + \frac{\alpha_s}{2\pi}\sigma^{(1)} + \left(\frac{\alpha_s}{2\pi}\right)^2\sigma^{(2)} + \left(\frac{\alpha_s}{2\pi}\right)^3\sigma^{(3)} + \ldots\right)$$

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LO predictions | NLO corrections | NNLO corrections | NNNLO corrections

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Improved predictions

$$d\sigma = \sum_{a,b} \int dx_1 dx_2 \;\; f_a(x_1, \mu_F) f_b(x_2, \mu_F) \, d\hat{\sigma}_{ab\to X}(\hat{s}, \mu_F, \mu_R)$$

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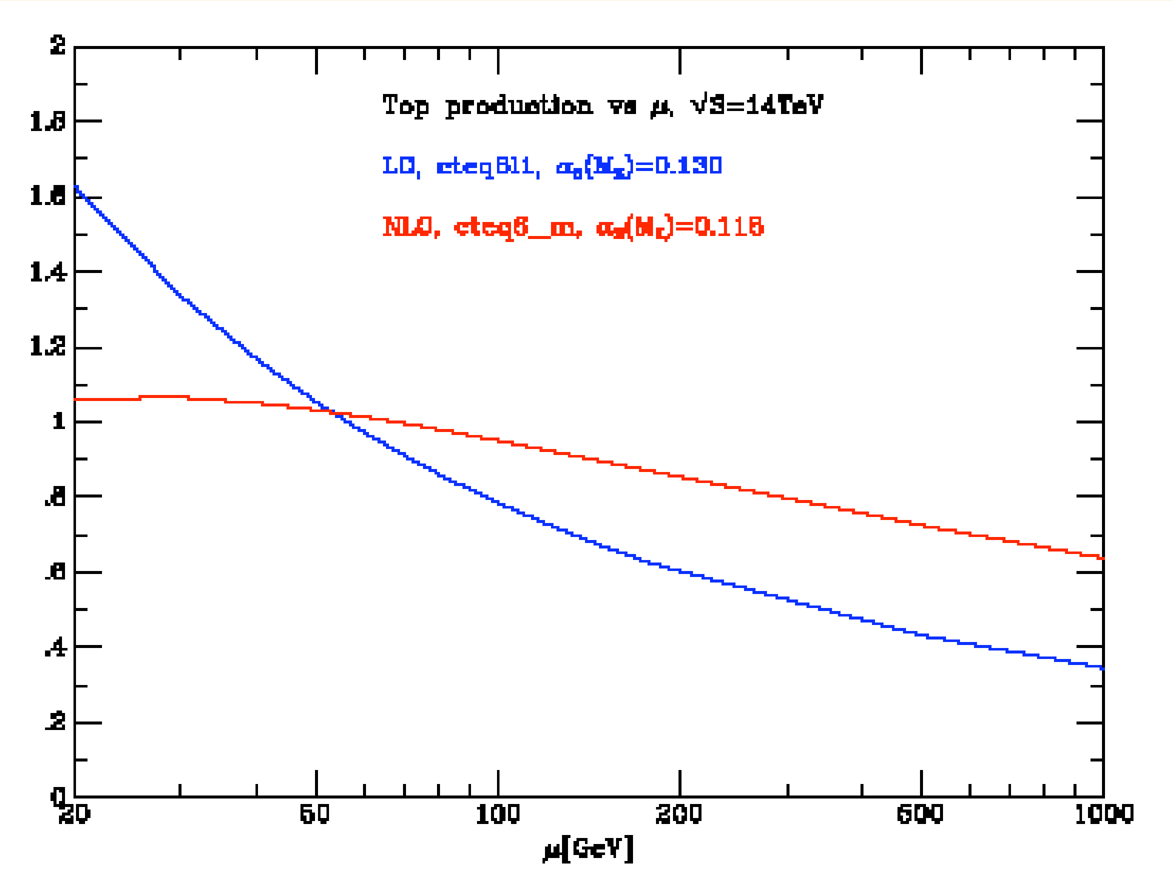
- Remember, **predictions are inclusive**: also at LO initial state radiation is included via the PDF; final state radiation by the definition of the parton, which represents all final state evolutions
  - Can be made explicit by using a parton shower (which is unitary)
- Due to these approximations, Leading Order predictions can depend strongly on the renormalization and factorization scales
- Including higher order corrections reduces the dependence on these scales

Going NLO

- At NLO the dependence on the renormalization and factorization scales is reduced
  - First order where scale dependence in the running coupling and the PDFs is compensated for via the loop corrections: **first reliable estimate of the total cross section**
  - Better description of final state: impact of extra radiation included (e.g. jets can have substructure)
  - Opening of additional initial state partonic channels



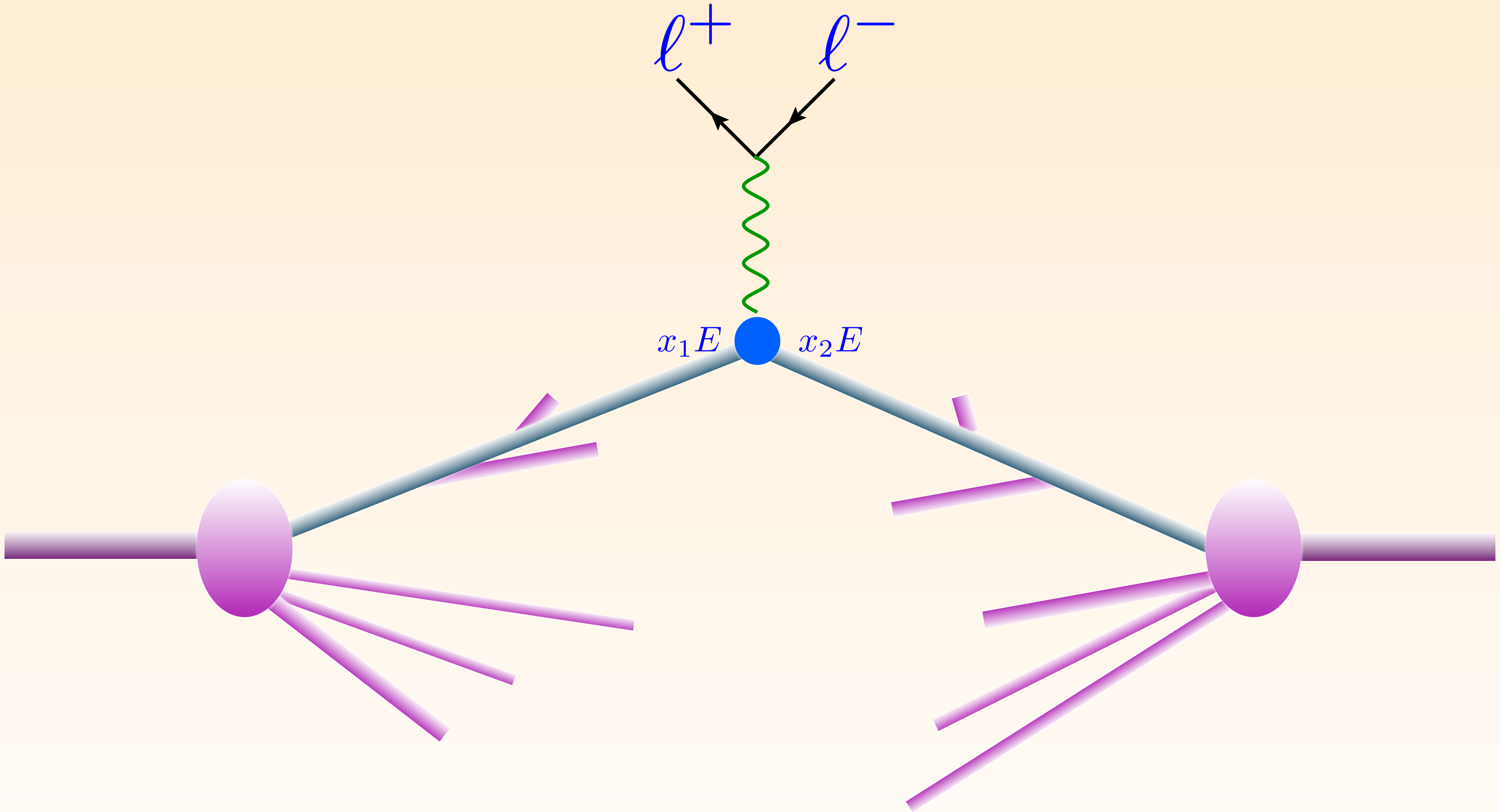
NLO corrections

- NLO corrections have three parts:
  - The Born contribution, i.e. the Leading order.
  - Virtual (or Loop) corrections: formed by an amplitude with a closed loop of particles interfered with the Born amplitudes
  - Real emission corrections: formed by amplitudes with one extra parton compared to the Born process
- Both Virtual and Real emission have one power of α_s extra compared to the Born process

$$\sigma^{\mathrm{NLO}} = \int_m d\sigma^B + \int_m d\sigma^V + \int_{m+1} d\sigma^R$$

NLO predictions

- As an example, consider Drell-Yan Z/γ* production



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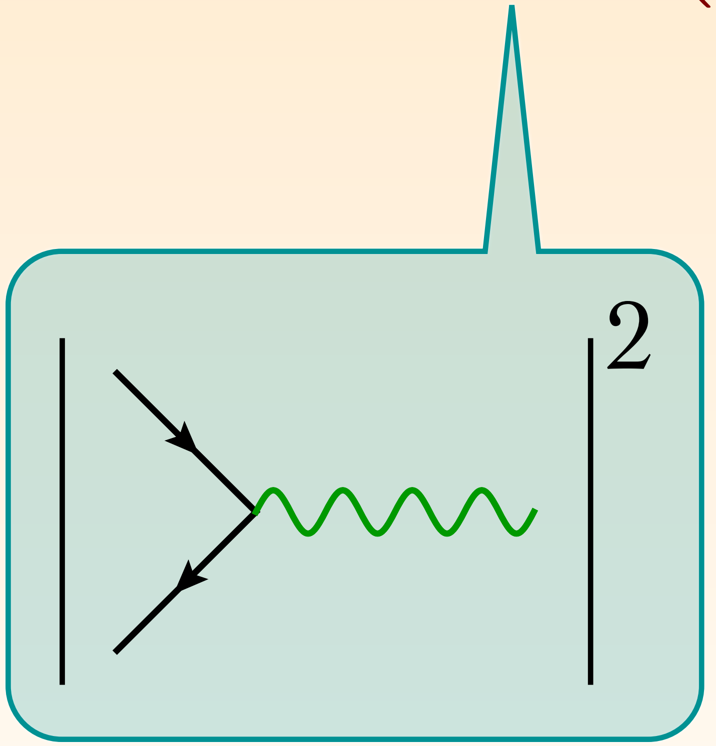

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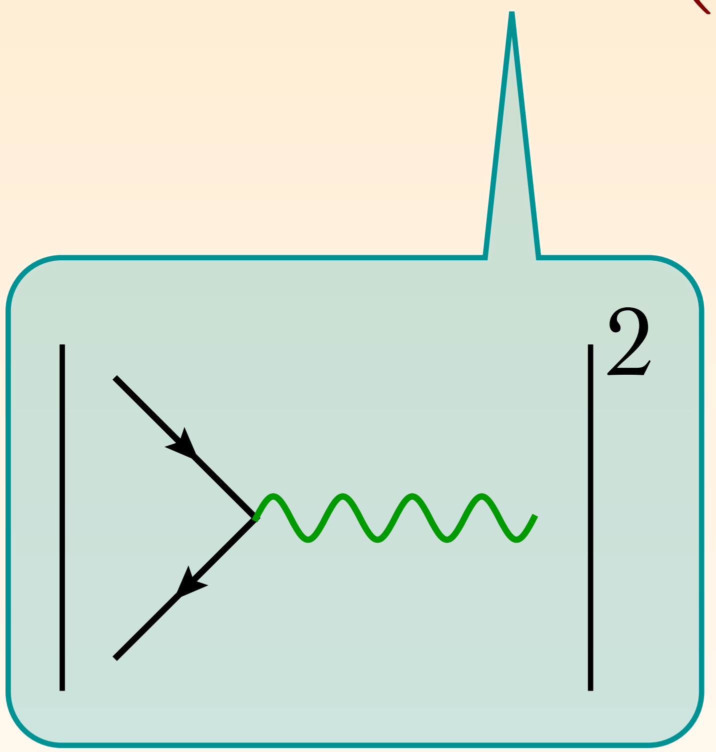

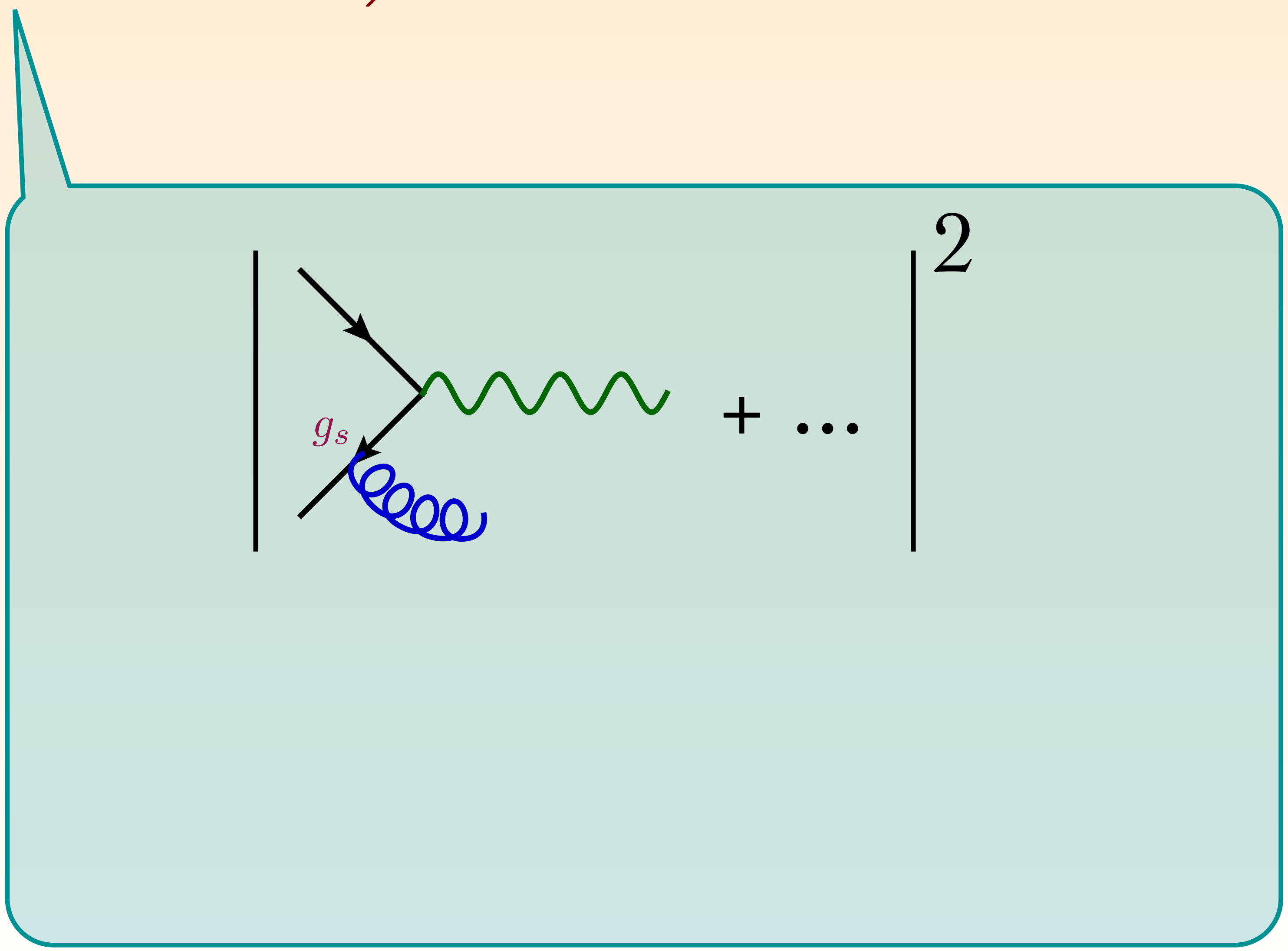

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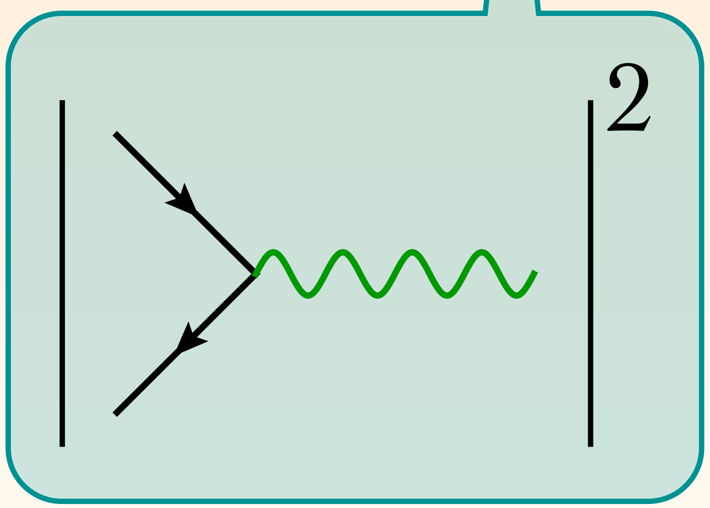
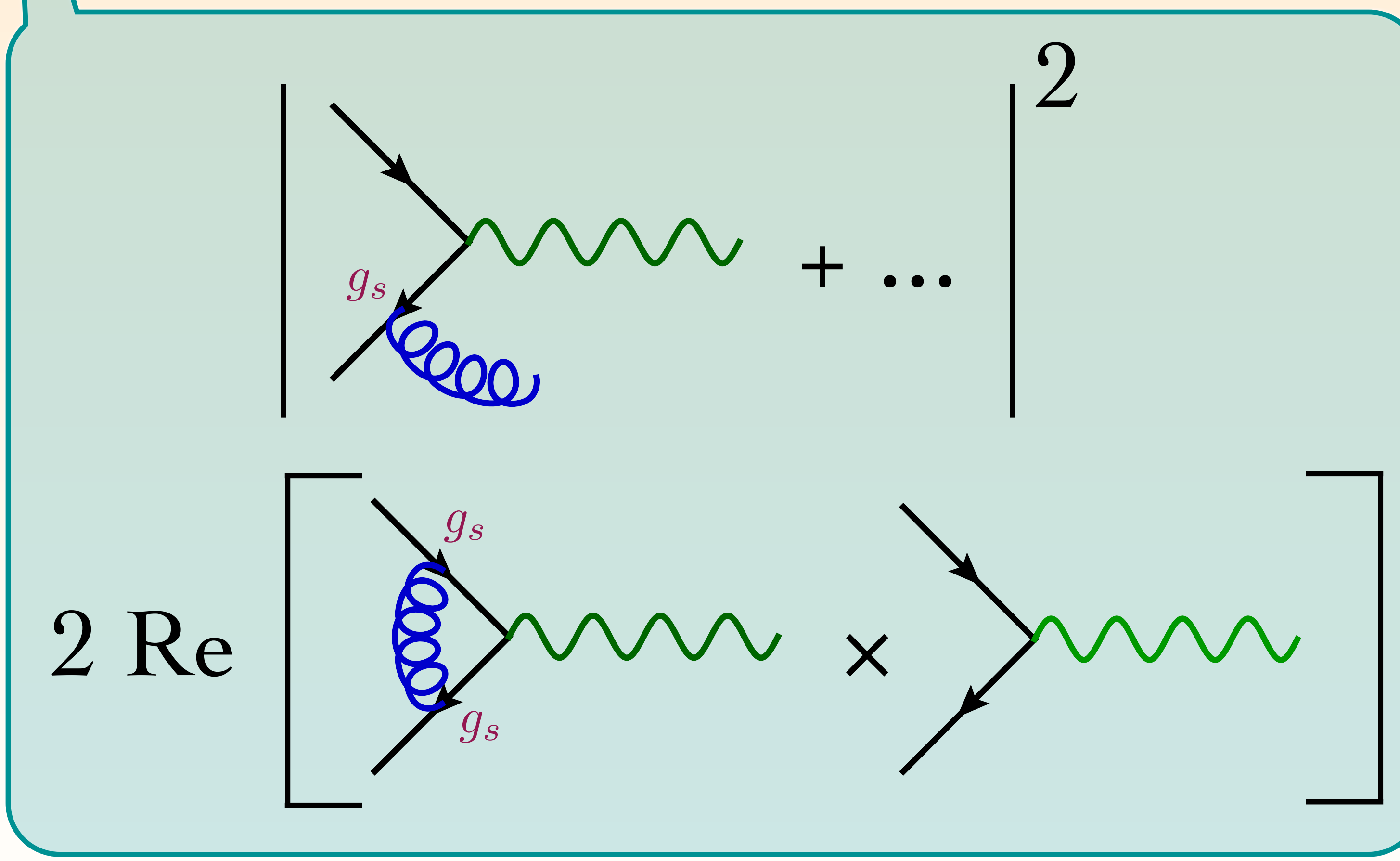
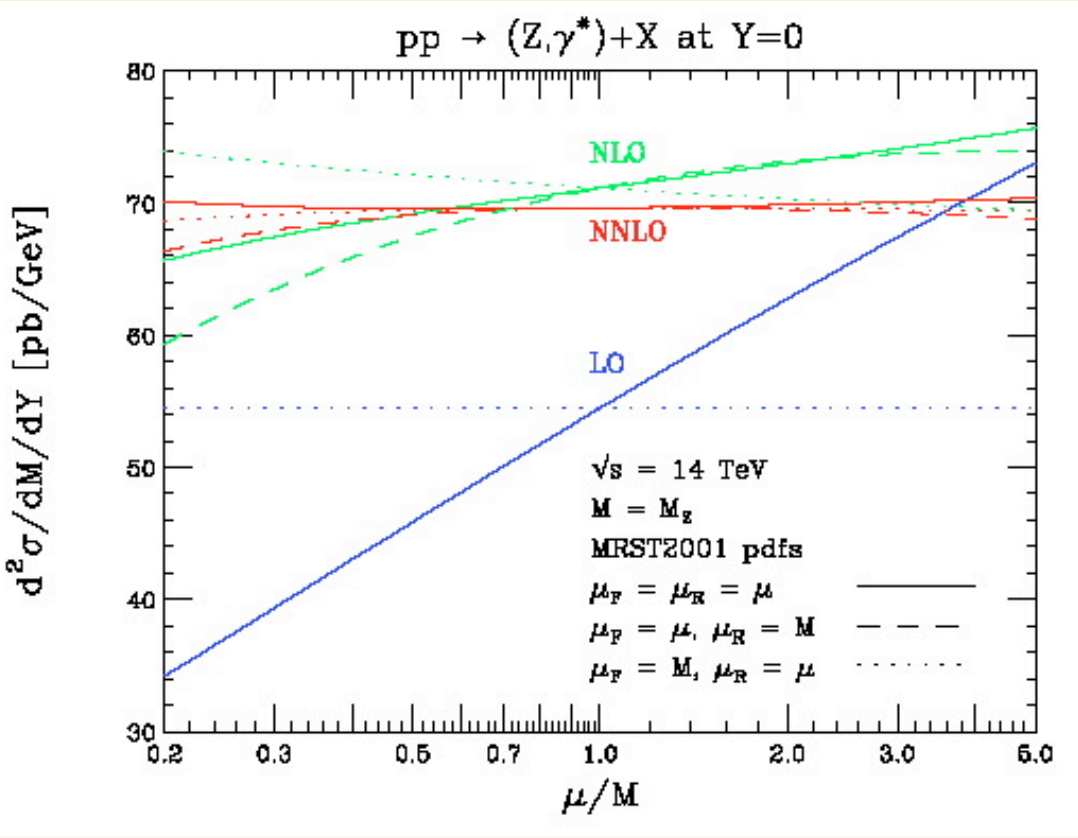


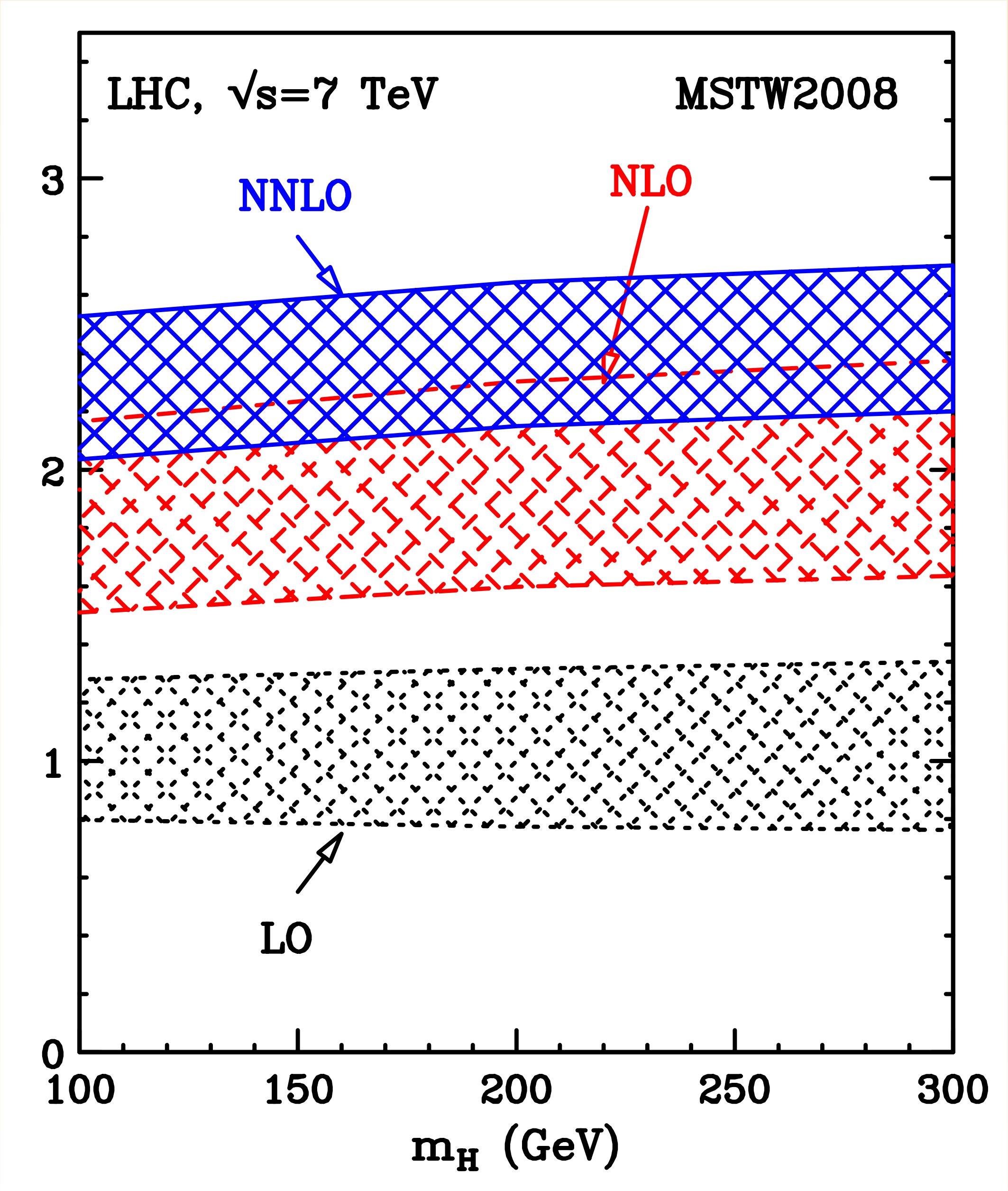


Going NNLO...?

- NNLO is the current state-of-the-art. There are only a few complete results available, but this year great progress has been made and NNLO results for ttbar, H+1j, dijet appeared
- Why do we need it?
  - An NNLO calculation gives control of the uncertainties in a calculation
  - It is "mandatory" if NLO corrections are very large to check the behavior of the perturbative series
  - It is the best we have! It is needed for Standard Candles and very precise tests of perturbation theory, exploiting all the available information, e.g. for determining NNLO PDF sets

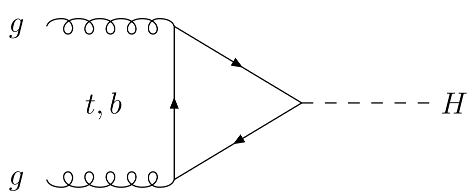


Higgs predictions at NNLO

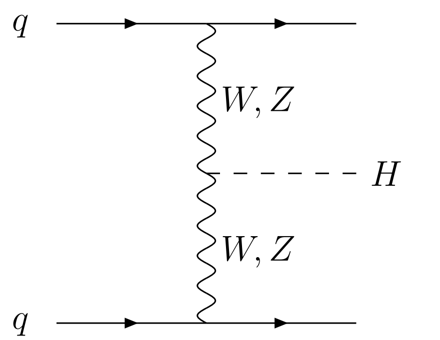


- LO calculation is not reliable,
- but the perturbative series stabilizes at NNLO
- NLO estimation of the uncertainties (by scale variation) works reasonably well

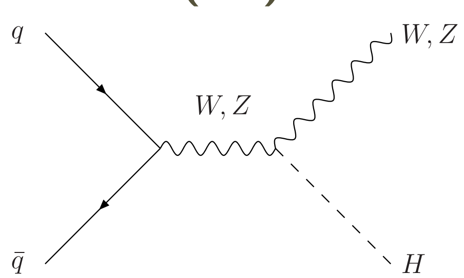
Higgs predictions at LHC



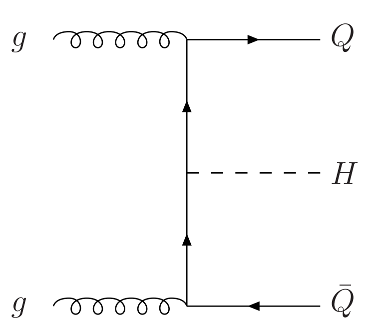
GluonFusion



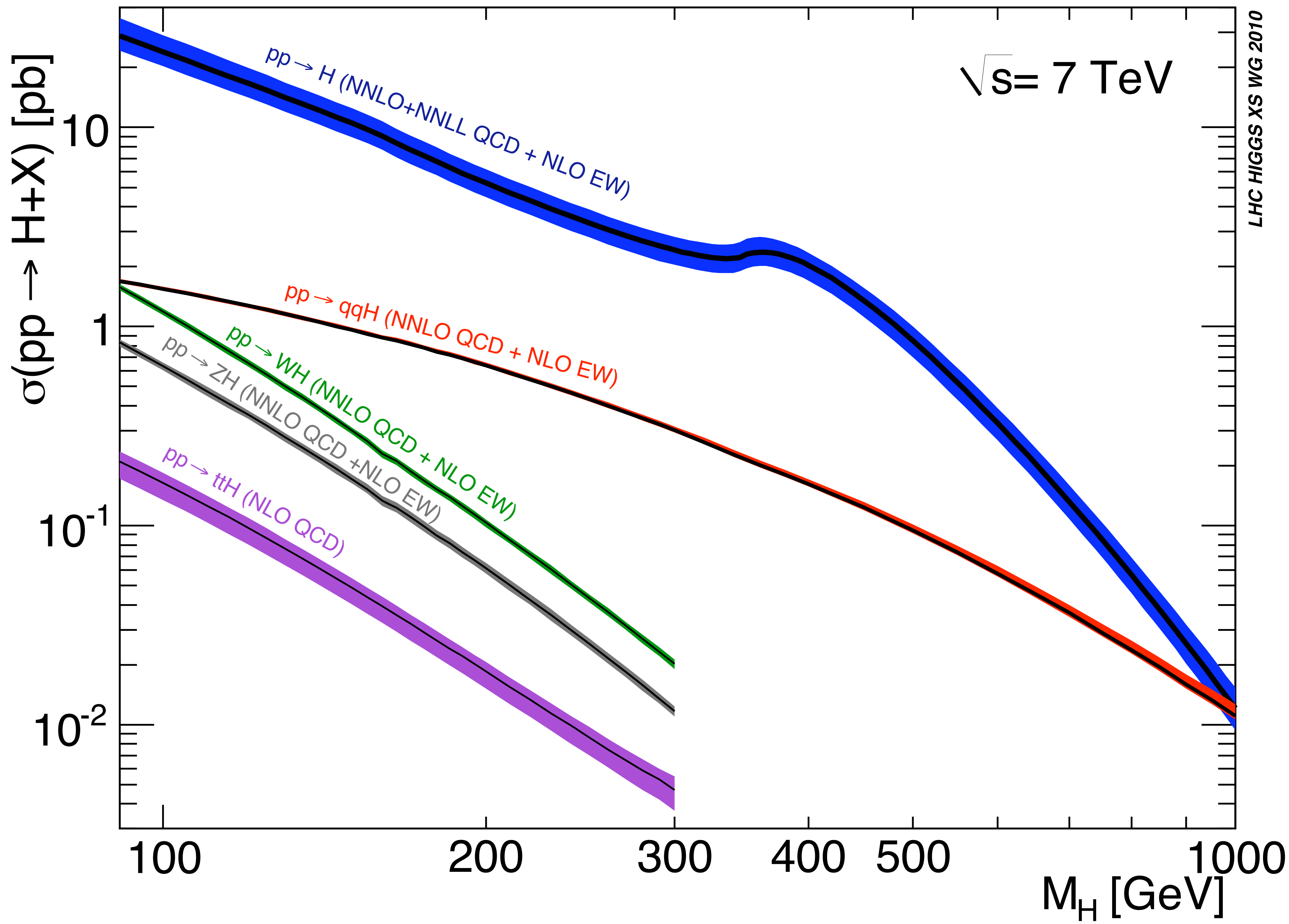
vector boson fusion (VBF)



associated production with vector bosons

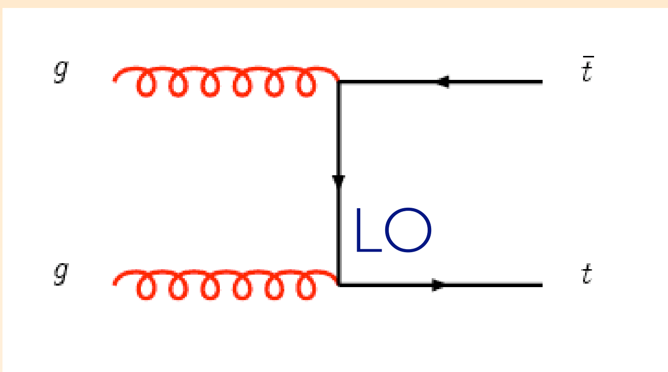


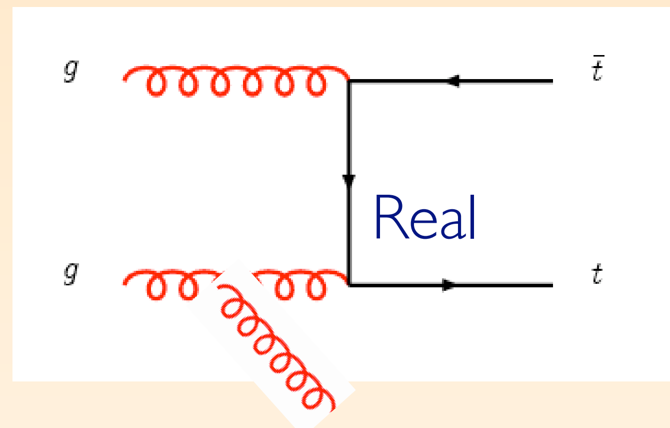
associated production with heavy quarks

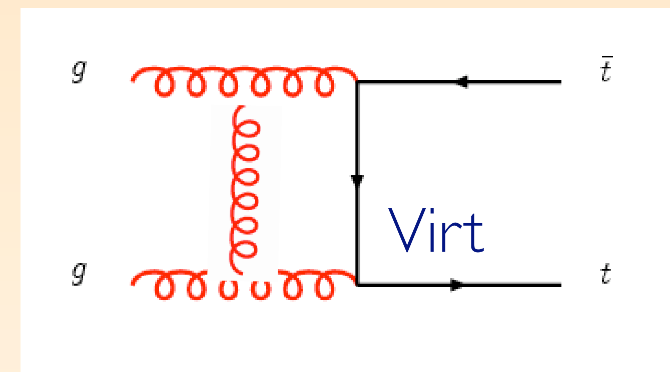


NLO...?

- Are all (IR-safe) observables that we can compute using a NLO code correctly described at NLO? Suppose we have a NLO code for pp ⟶ ttbar







  - Total cross section
  - Transverse momentum of the top quark
  - Transverse momentum of the top-antitop pair
  - Transverse momentum of the jet
  - Top-antitop invariant mass
  - Azimuthal distance between the top and anti-top

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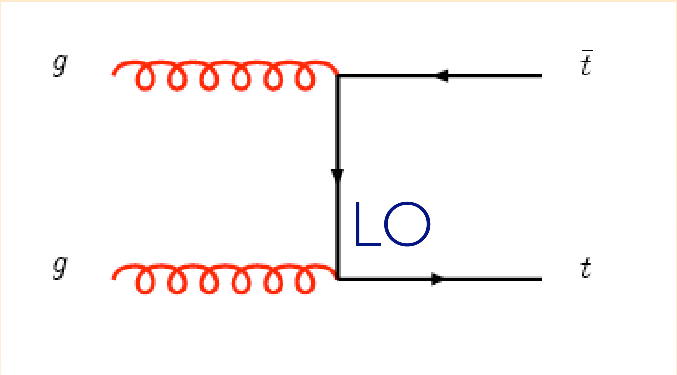

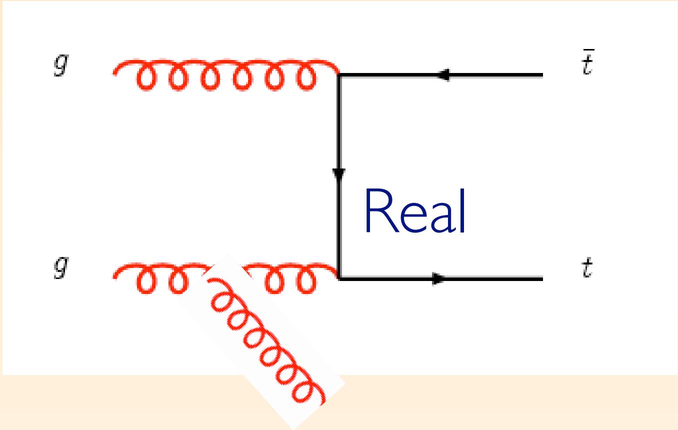

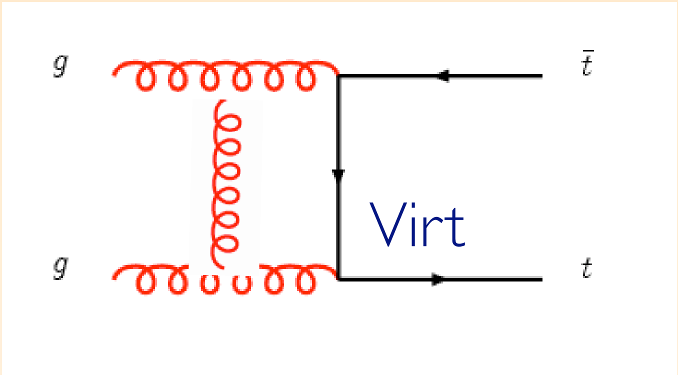

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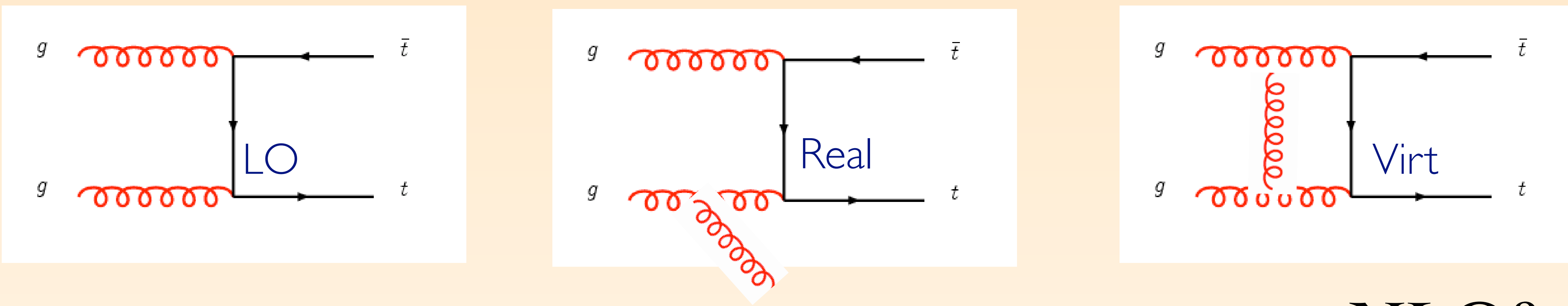

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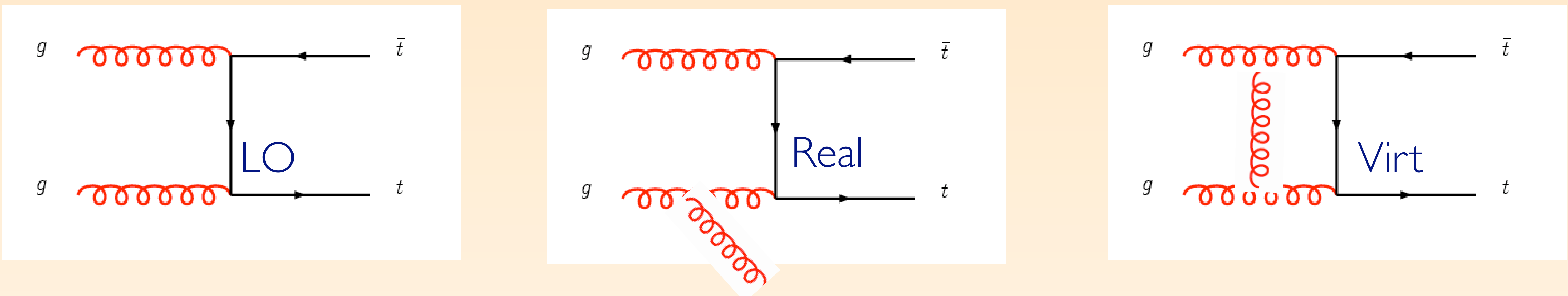

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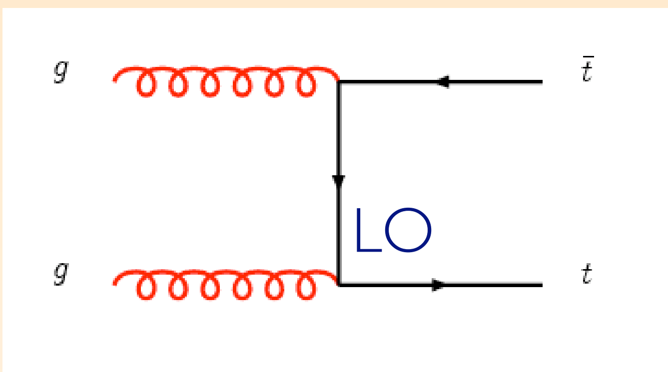

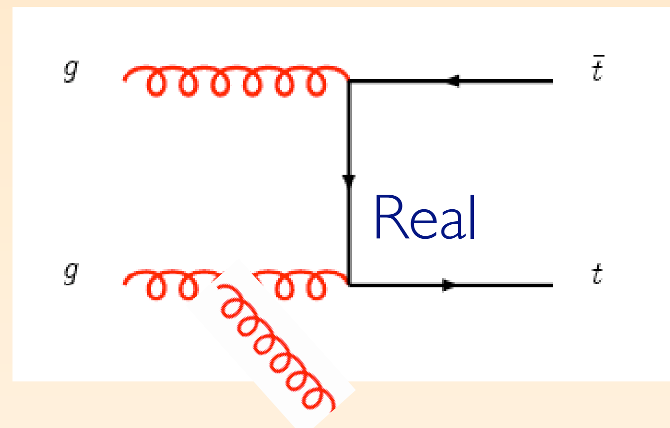

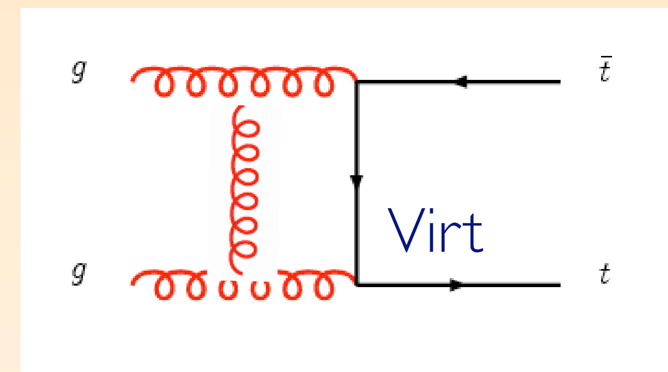

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Total cross section	✔
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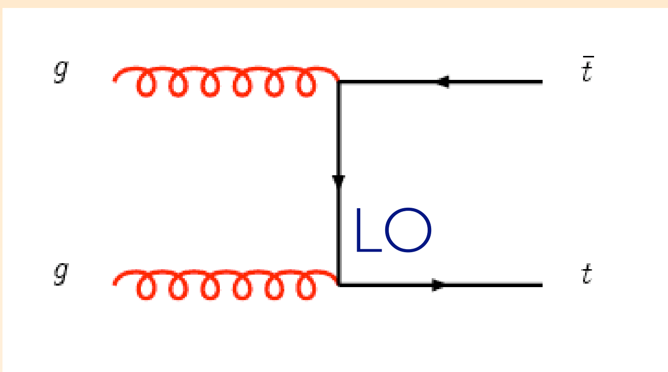

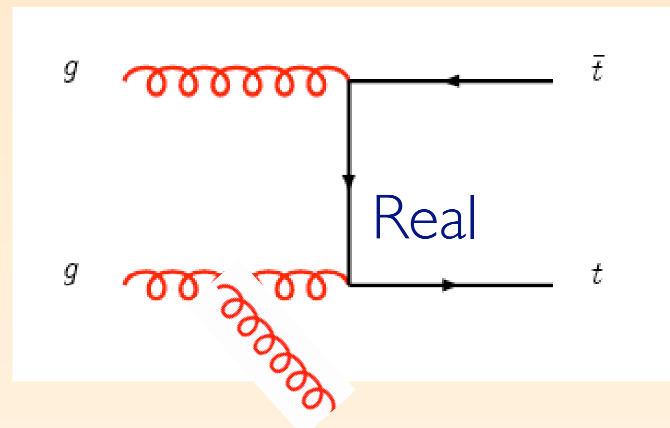

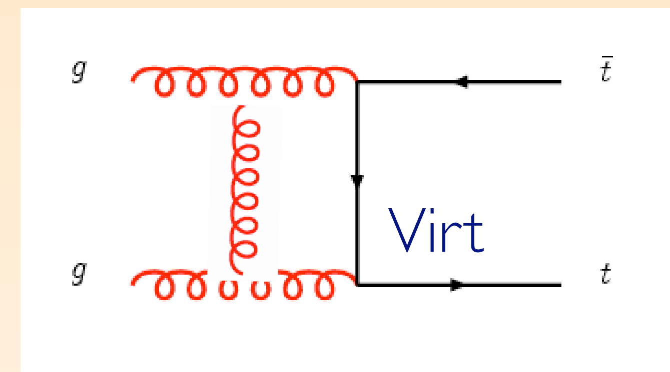

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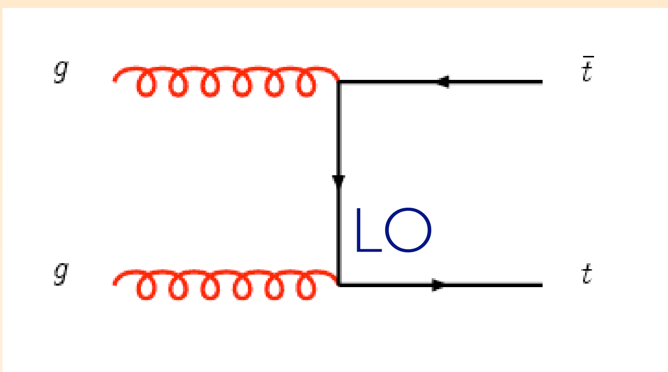

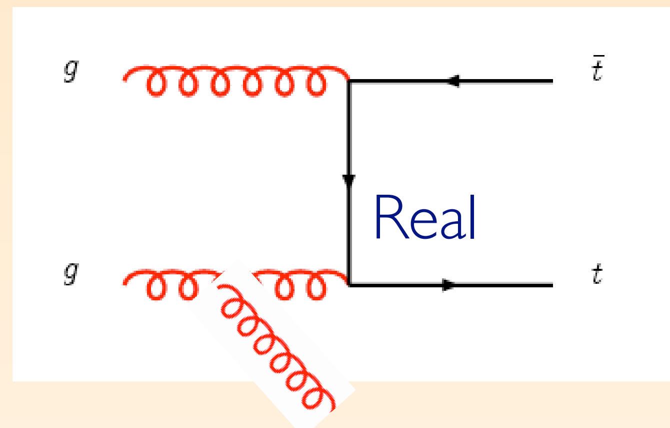

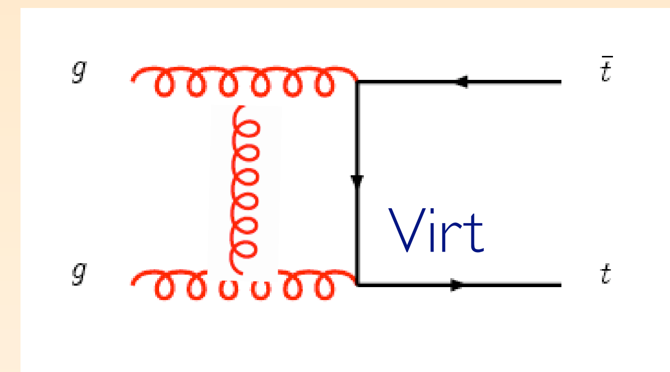

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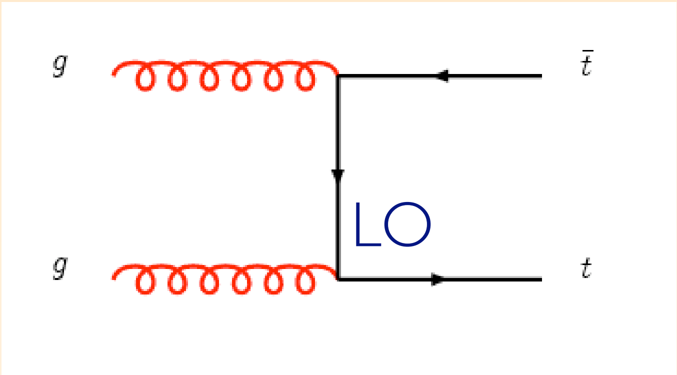

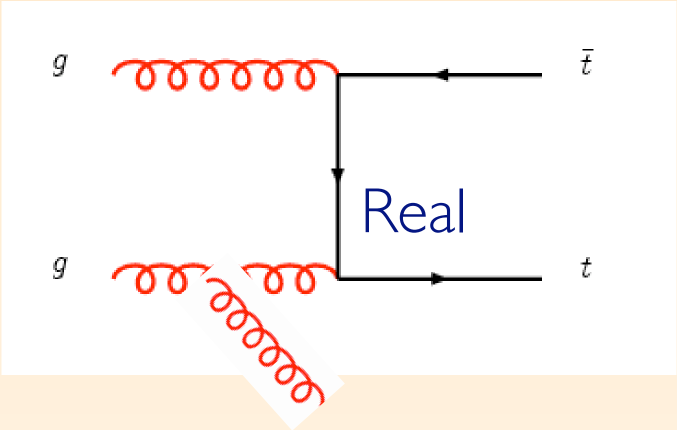

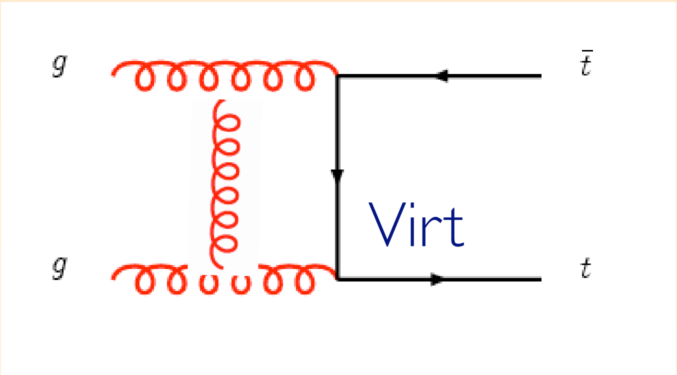

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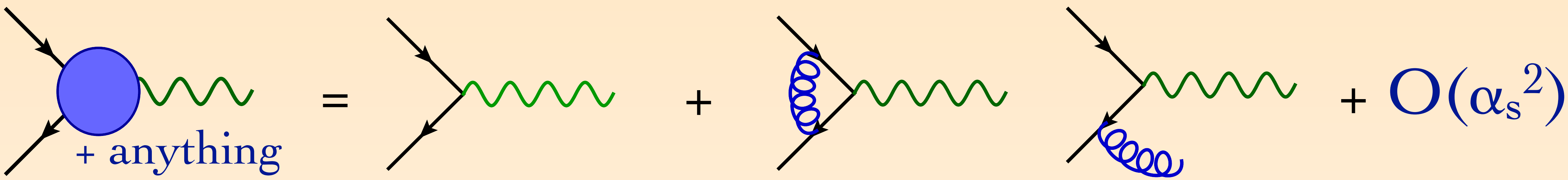
Obstacles



- Let us focus on NLO… there are already enough steps to be taken:
  - Virtual amplitudes: how to compute the loops automatically in a reasonable amount of time
  - How to deal with infra-red divergences: virtual corrections and real-emission corrections are separately divergent and only their sum is finite (for IR-safe observables) according to the KLN theorem
  - How to match these processes to a parton shower without double counting

Canceling infrared divergences

NLO predictions

- As an example, consider Drell-Yan production

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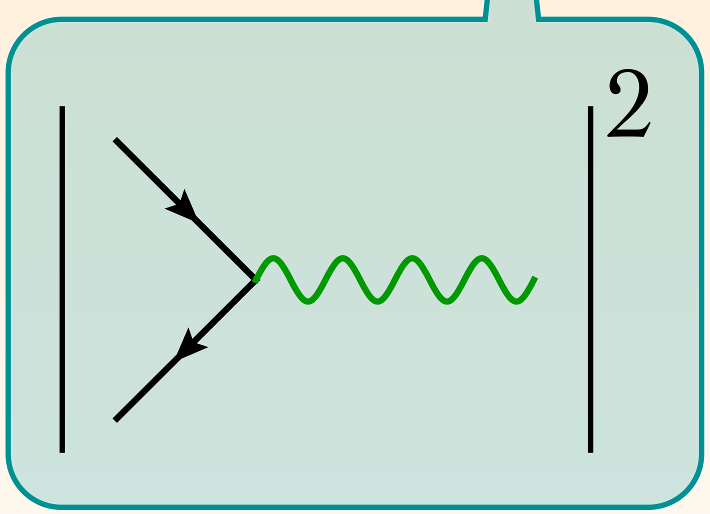
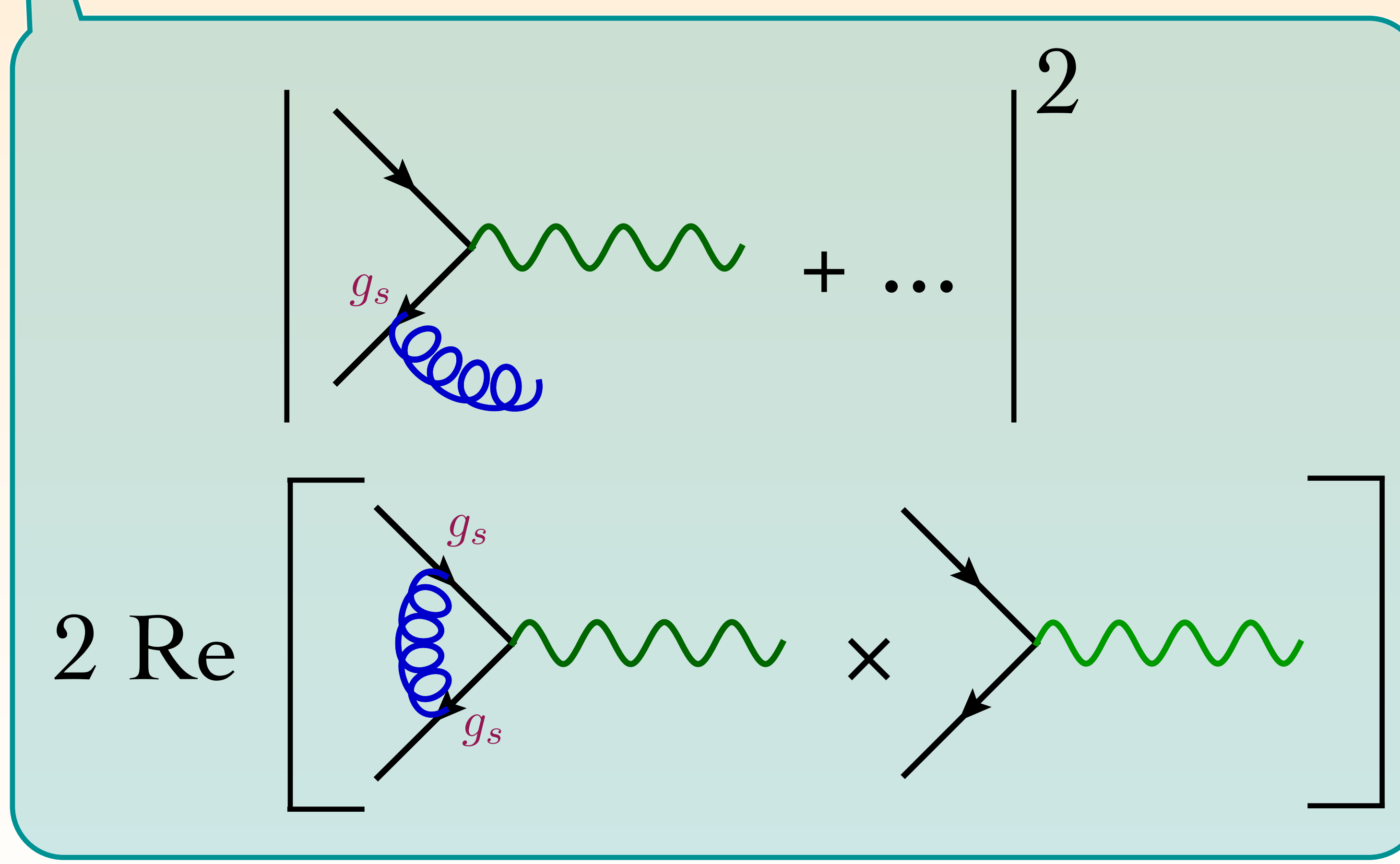
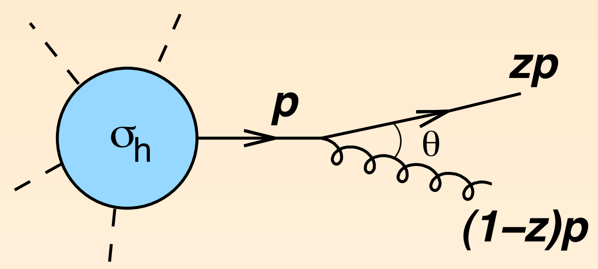




Branching

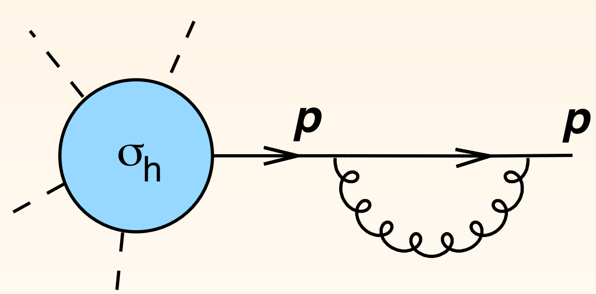
- In the soft and collinear region, the branching of a gluon from a quark can be written as



$$\sigma_{h+g} \simeq \sigma_h \frac{\alpha_s C_F}{\pi} \frac{dz}{1-z} \frac{dk_t^2}{k_t^2}$$

where k_t is the transverse momentum of the gluon, $k_t = E \sin\theta$.

- The singularities cancel against the singularities in the virtual corrections, which result from the integral over the loop momentum of the function



$$\sigma_{h+V} \simeq -\sigma_h \frac{\alpha_s C_F}{\pi} \frac{dz}{1-z} \frac{dk_t^2}{k_t^2}$$

- The sum is finite for observables that cannot distinguish between two collinear partons ($k_t \longrightarrow 0$); a hard and a soft parton ($z \longrightarrow 1$); and a single parton (in the virtual contributions)

Infrared cancellation

$$\sigma^{\rm NLO} \sim \int d^4\Phi_m\, B(\Phi_m) + \int d^4\Phi_m \int_{\rm loop} d^d l\, V(\Phi_m) + \int d^d\Phi_{m+1}\, R(\Phi_{m+1})$$

- The KLN theorem tells us that divergences from virtual and real-emission corrections cancel in the sum for observables insensitive to soft and collinear radiation ("IR-safe observables")
- When doing an analytic calculation in dimensional regularization this can be explicitly seen in the cancellation of the $1/\epsilon$ and $1/\epsilon^2$ terms (with ϵ the regulator, $\epsilon \rightarrow 0$)
- In the real emission corrections, the explicit poles enter after the phase-space integration (in d dimensions)

Infrared safe observables

- For an observable to be calculable in fixed-order perturbation theory, the observable should be infrared safe, i.e., it should be insensitive to the emission of soft or collinear partons.
- In particular, if p_i is a momentum occurring in the definition of an observable, it most be invariant under the branching

$$p_i \longrightarrow p_j + p_k,$$

whenever p_j and p_k are collinear or one of them is soft.
- Examples
  - "The number of gluons" produced in a collision is not an infrared safe observable
  - "The number of hard jets defined using the k_T algorithm with a transverse momentum above 40 GeV," produced in a collision is an infrared safe observable

PHASE-SPACE INTEGRATION

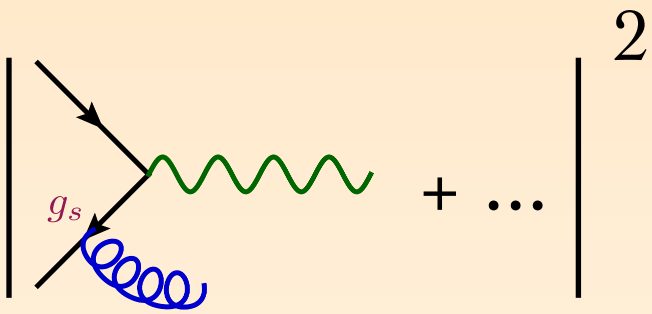
$$\sigma^{\rm NLO} \sim \int d^4\Phi_m\, B(\Phi_m) + \int d^4\Phi_m \int_{\rm loop} d^d l\, V(\Phi_m) + \int d^d\Phi_{m+1}\, R(\Phi_{m+1})$$

- For complicated processes we have to result to numerical phase-space integration techniques ("Monte Carlo integration"), which can only be performed in an integer number of dimensions
  - Cannot use a finite value for the dimensional regulator and take the limit to zero in a numerical code
- But we still have to cancel the divergences explicitly
- Use a subtraction method to explicitly factor out the divergences from the phase-space integrals

Example

- Suppose we want to compute the integral ("real emission radiation", where the 1-particle phase-space is referred to as the 1-dimensional x)

$$\int_0^1 dx\, f(x)$$



where $f(x) = \dfrac{g(x)}{x}$ and $g(x)$ is finite everywhere

- Let's introduce a regulator

$$\lim_{\epsilon \to 0} \int_0^1 dx\, \frac{g(x)}{x^{1+\epsilon}} = \lim_{\epsilon \to 0} \int_0^1 dx\, x^{-\epsilon} f(x)$$

for any non-integer non-zero value for ϵ this integral is finite

- We would like to factor out the explicit poles in ϵ so that they can be canceled explicitly against the virtual corrections

Subtraction method

$$\lim_{\epsilon\to 0}\int_0^1 dx\, x^{-\epsilon} f(x) \qquad\qquad f(x) = \frac{g(x)}{x}$$

- Add and subtract the same term

$$\begin{aligned}
\lim_{\epsilon\to 0}\int_0^1 dx\, x^{-\epsilon} f(x) &= \lim_{\epsilon\to 0}\int_0^1 dx\, x^{-\epsilon}\left[\frac{g(0)}{x} + f(x) - \frac{g(0)}{x}\right] \\
&= \lim_{\epsilon\to 0}\int_0^1 dx\left[g(0)\frac{x^{-\epsilon}}{x} + \frac{g(x)-g(0)}{x^{1+\epsilon}}\right] \\
&= \lim_{\epsilon\to 0}\frac{-1}{\epsilon}g(0) + \int_0^1 dx\,\frac{g(x)-g(0)}{x}
\end{aligned}$$

- We have factored out the $1/\epsilon$ divergence and are left with a finite integral
- According to the KLN theorem the divergence cancels against the virtual corrections

Limitations

"Plus distribution"

Subtraction: $\int_0^1 dx \, \frac{g(x) - g(0)}{x}$

- Even though the divergence is factored, there are cancellations between large numbers: if for an observable O, if $\lim_{x \to 0} O(x) \neq O(0)$ or we choose the bin-size too small, instabilities render the computation useless
  - We already knew that! KLN is sufficient; one must have infra-red safe observables and cannot ask for infinite resolution (need a finite bin-size)

NLO with Subtraction

$$\sigma^{\rm NLO} \sim \int d^4\Phi_m\, B(\Phi_m) + \int d^4\Phi_m \int_{\rm loop} d^d l\, V(\Phi_m) + \int d^d\Phi_{m+1}\, R(\Phi_{m+1})$$

- With the subtraction method this is replace by

$$\begin{aligned}\sigma^{\rm NLO} \sim & \int d^4\Phi_m\, B(\Phi_m) \\ & + \int d^4\Phi_m \left[\int_{\rm loop} d^d l\, V(\Phi_m) + \int d^d\Phi_1 G(\overline{\Phi}_{m+1})\right]_{\epsilon\to 0} \\ & + \int d^4\Phi_{m+1}\left[R(\Phi_{m+1}) - G(\overline{\Phi}_{m+1})\right]\end{aligned}$$

- Terms between the brackets are finite. Can integrate them numerically and independent from one another in 4 dimensions

Subtraction methods

- $G(\overline{\Phi}_{m+1})$ should be defined such that

  1) it exactly matches the singular behavior of $R(\Phi_{m+1})$

  2) its form is convenient for numerical integration techniques

  3) it is exactly integrable in d dimensions over the one-particle subspace $\int d^d\Phi_1 G(\overline{\Phi}_{m+1})$, leading to soft and/or collinear divergences as explicit poles in the dimensional regulator

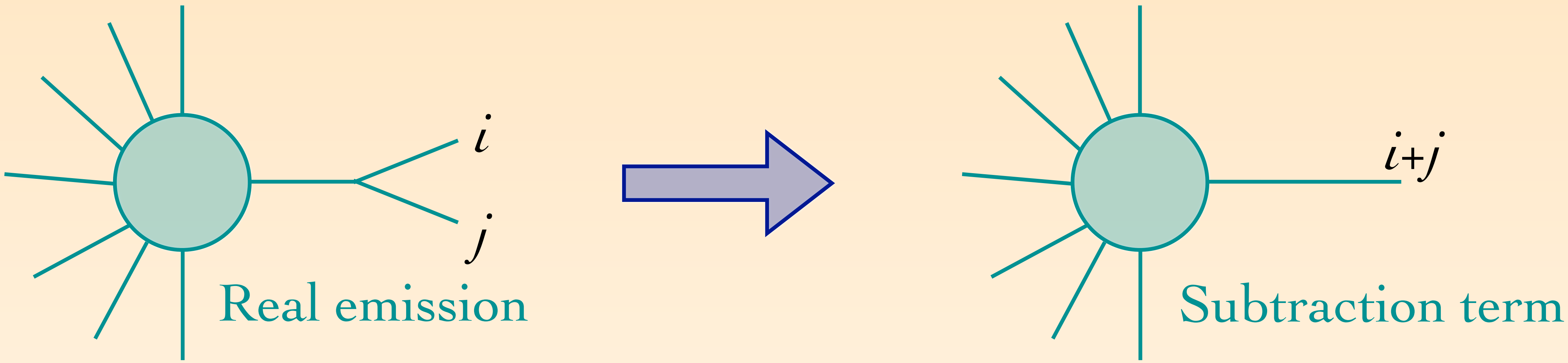
  4) it is universal, i.e. process independent
  → overall factor times the Born process

Two methods

- **Catani-Seymour (CS) dipole subtraction**
  - Most used method
  - Clear written paper on how to use this method in practice
  - Recoil taken by one (color-connected) parton: N^3 scaling
  - Method evolved from cancellation of the soft divergence
  - Proven to work for simple as well as complicated processes
  - Automation in publicly available packages: MadDipole, AutoDipole, Helac-Dipoles, Sherpa

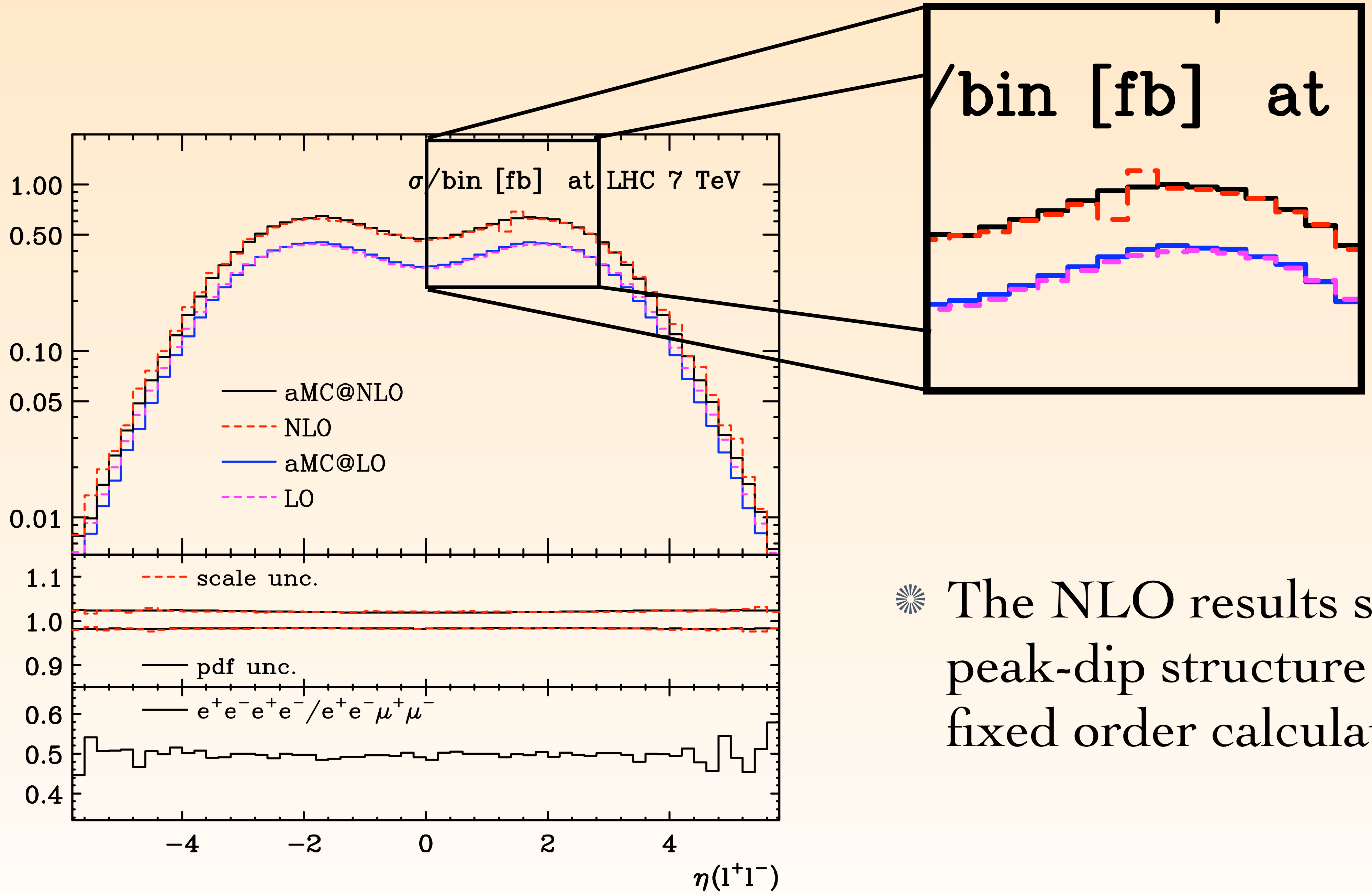
- **Frixione-Kunszt-Signer (FKS) subtraction**
  - Not so well-known
  - (Probably) more efficient, because less subtraction terms are needed
  - Recoil evenly distributed by all particles: N^2 scaling
  - Collinear divergences as a starting point
  - Proven to work for simple as well as complicated processes
  - Automated in aMC@NLO & POWHEG BOX

Kinematics of counter events



- If *i* and *j* are two on-shell particles that are present in a splitting that leads to an singularity, for the counter events we need to combine their momenta to a new on-shell parton that's the sum of *i+j*
- This is not possible without changing any of the other momenta in the process
- When applying cuts or making plots, events and counter events might end-up in different bins
  - Use IR-safe observables and don't ask for infinite resolution! (KLN theorem)

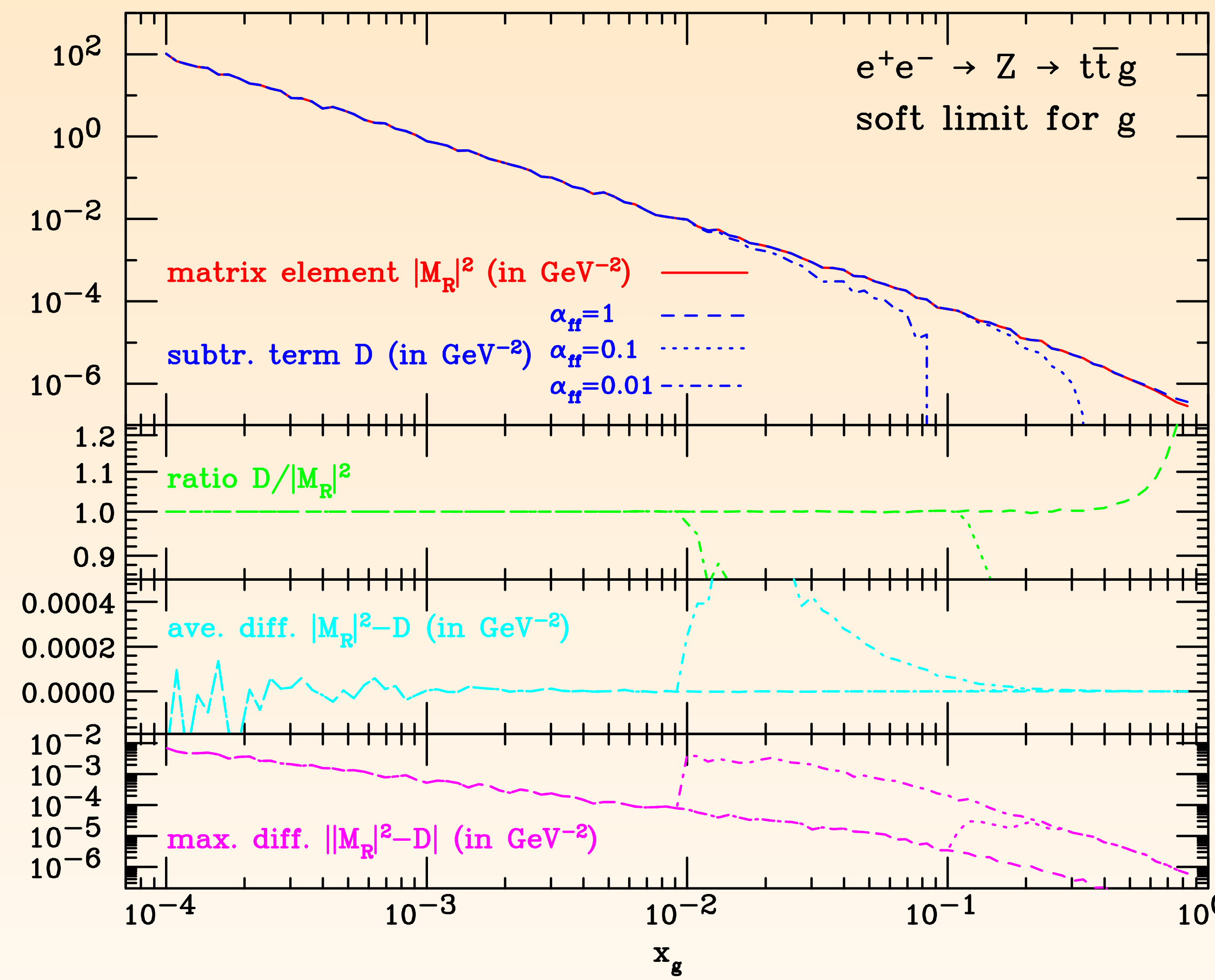
Example in 4 charged lepton production

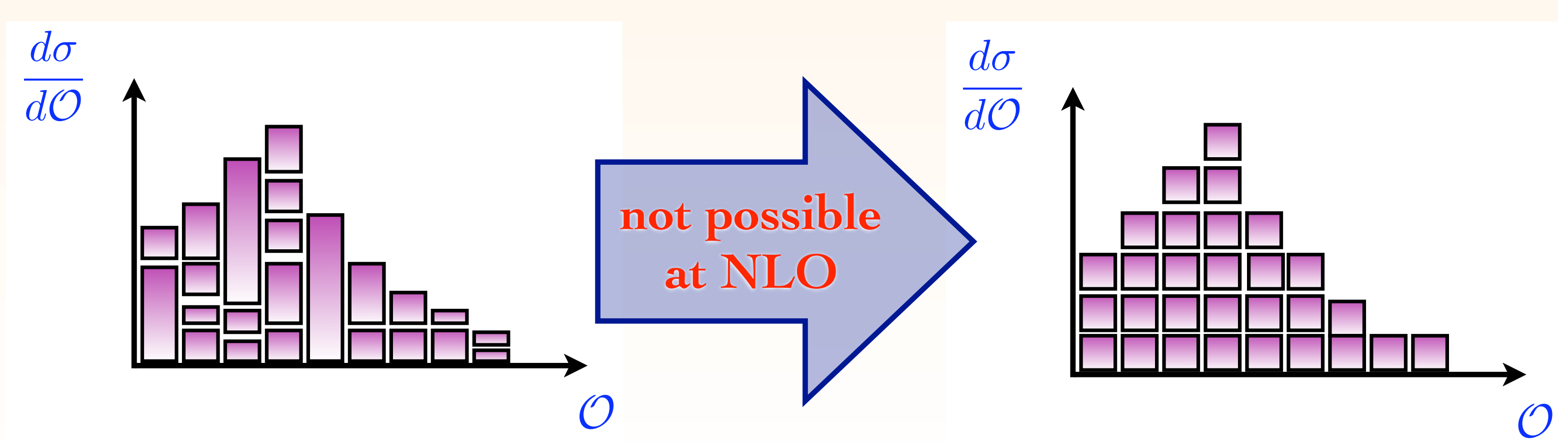


- The NLO results shows a typical peak-dip structure that hampers fixed order calculations

Event unweighting?

- Another consequence of this kinematic mismatch is that we cannot generate events at fixed order NLO
  - Even though the integrals are finite, they are not bounded (compare with $\int_0^1 dx \, \frac{1}{\sqrt{x}}$), so there is no maximum to unweight against: a single event can have an arbitrarily large weight!
  - Furthermore, event and counter event have different kinematics: which one to use for the unweighted event?





Filling histograms on-the-fly

$$\sigma^{\text{NLO}} \sim \int d^4\Phi_m\, B(\Phi_m) + \int d^4\Phi_m \left[\int_{\text{loop}} d^d l\, V(\Phi_m) + \int d^d\Phi_1 G(\overline{\Phi}_{m+1}) \right]_{\epsilon\to 0} + \int d^4\Phi_{m+1} \left[R(\Phi_{m+1}) - G(\overline{\Phi}_{m+1}) \right]$$

- In practice, when we do the MC integration we generate 2 sets of momenta

  1. An *m*-body set (for the Born, virtual and integrated counter terms)
  2. An *m*+1-body (for the NLO) which we map to the counter term momenta (for the counter terms)

- We compute the above formula; and apply cuts and fill histograms using the momenta corresponding to each term with the weight of that corresponding term

SUMMARY

- Both the virtual and real-emission corrections are IR divergent, but their sum is finite: We can use a subtraction methods to factor the divergences in the real-emission phase-space integration and cancel them explicitly against the terms in the virtual corrections
- This generates events and counter events with slightly different kinematics. This means we cannot generate unweighed events (integrals are not bounded), but we can fill plots with weighted events: MC integrator (not an MC event generator)
- When making plots or applying cuts, use only IR safe observables with finite resolution
- Phase-space integrals are finite, but not bounded: cannot unweight the events