aMC@NLO

Perturbative expansion

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

- The parton-level cross section can be computed as a series in perturbation theory, using the coupling constant as an expansion parameter, schematically:

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

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LO predictions

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LO predictions

NLO corrections

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LO predictions

NLO corrections

NNLO corrections

N3LO or NNNLO corrections

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LO predictions | NLO corrections | NNLO corrections | N3LO or NNNLO corrections

- Including higher corrections improves predictions and reduces theoretical uncertainties

Improved predictions

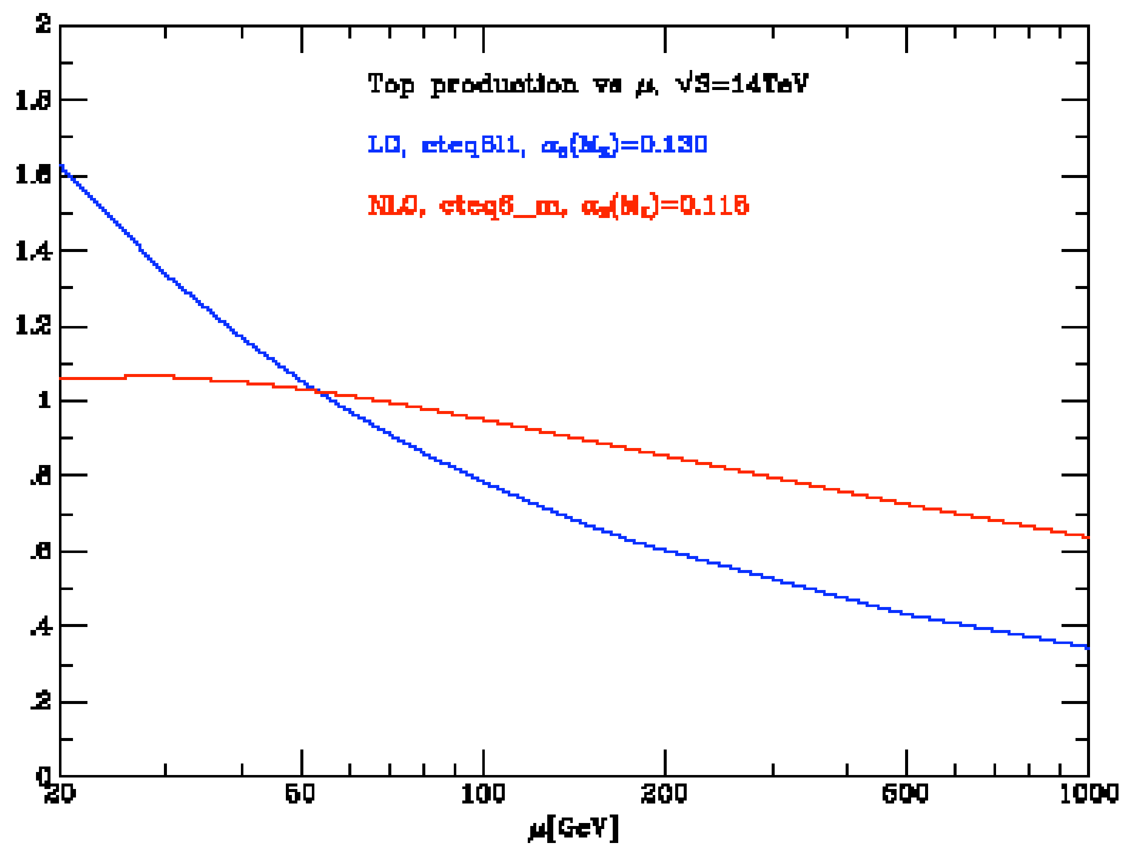
$$d\sigma = \sum_{a,b} \int dx_1 dx_2 \ f_a(x_1, \mu_F) f_b(x_2, \mu_F)\, d\hat{\sigma}_{ab\to X}(\hat{s}, \mu_F, \mu_R)$$

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

- Leading Order predictions can depend strongly on the renormalization and factorization scales
- Including higher order corrections reduces the dependence on these scales

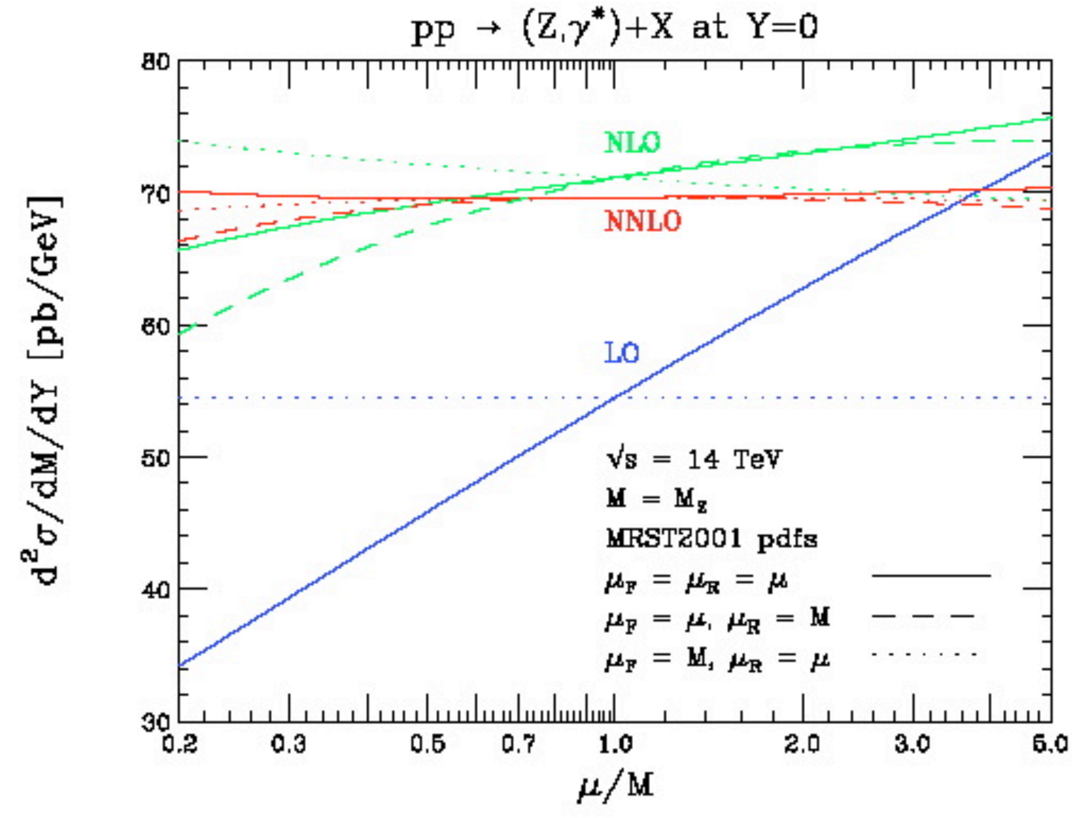
Going NLO

- 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

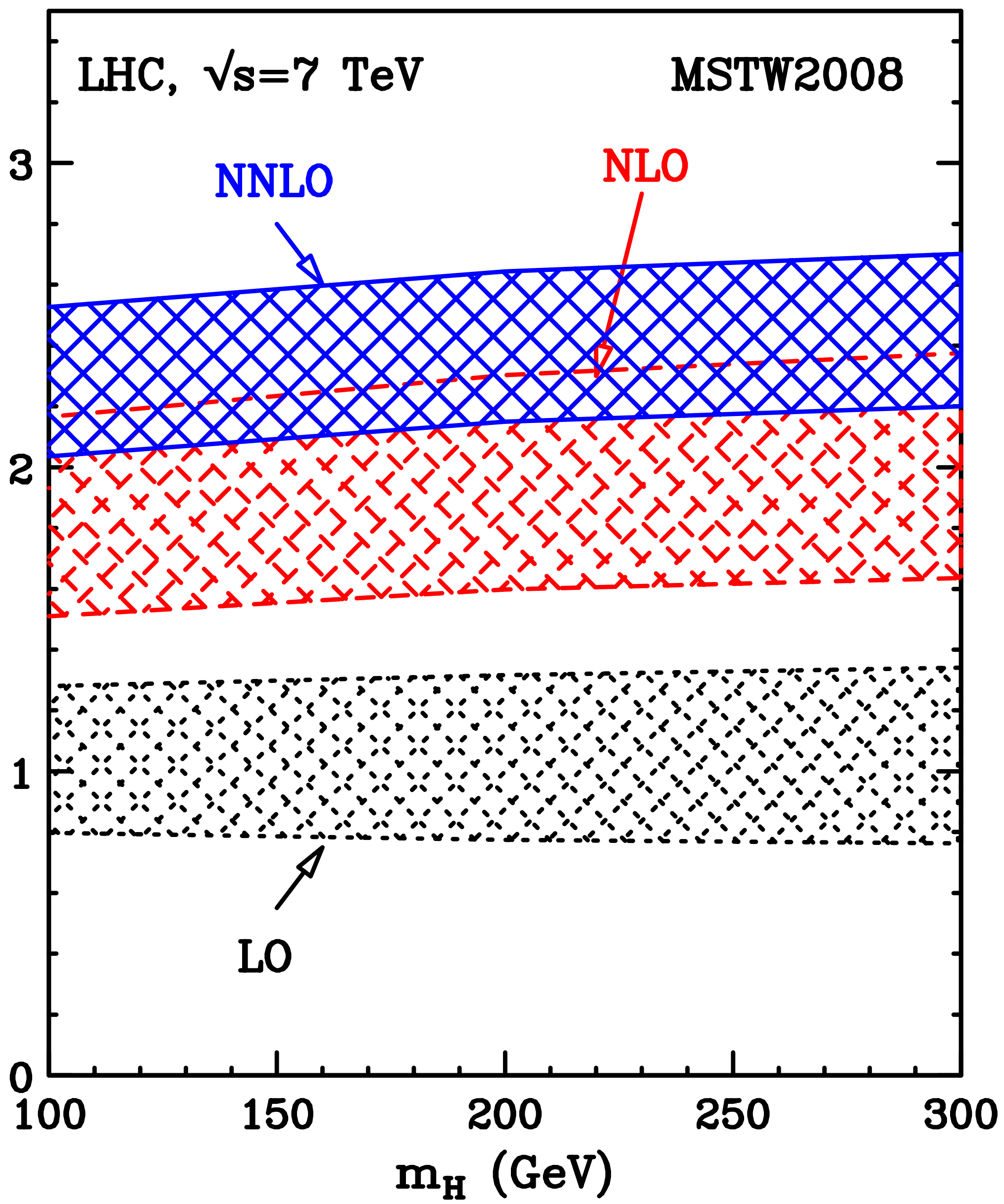


Going NNLO...?

- NNLO is the current state-of-the-art. There are only a few results available: Higgs, Drell-Yan, ttbar
- Why do we need it?
  - ➡ 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 needed for Standard Candles and very precise tests of perturbation theory, exploiting all the available information, e.g. for determining NNLO PDF sets



Higgs at NNLO



- LO calculation is not reliable,
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- NLO estimation of the uncertainties (by scale variation) works reasonably well

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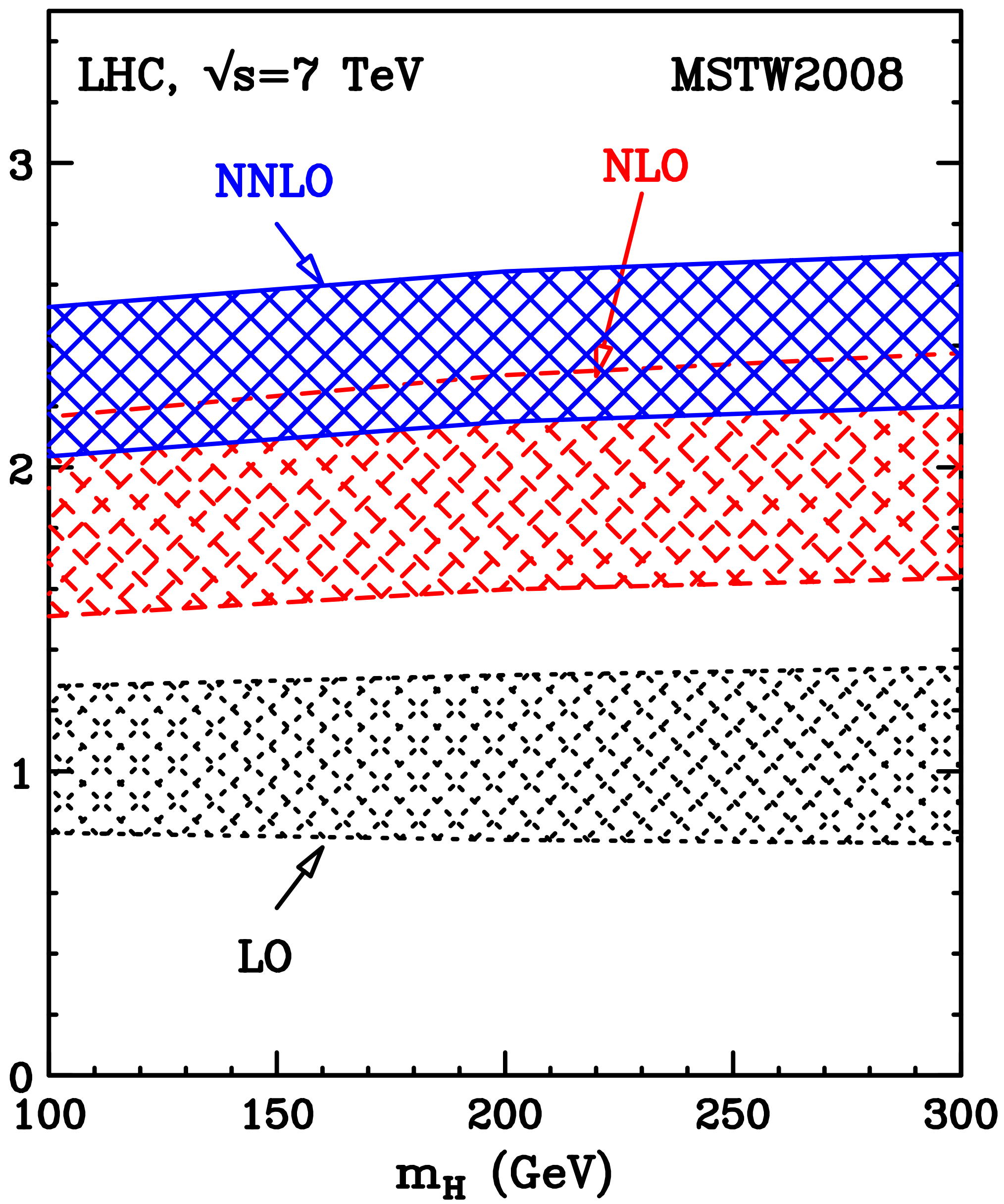

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Let's focus on NLO

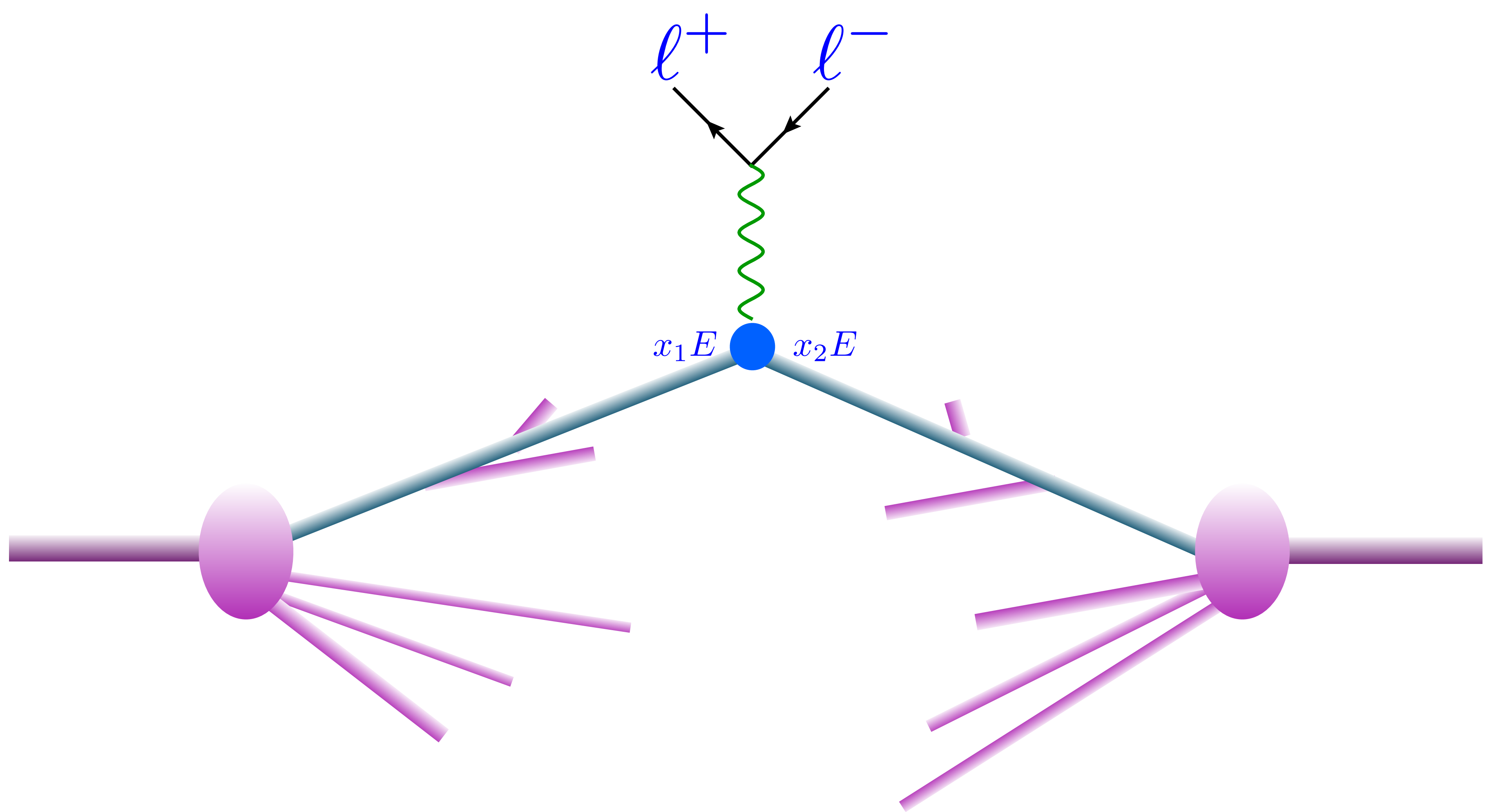
NLO corrections

- 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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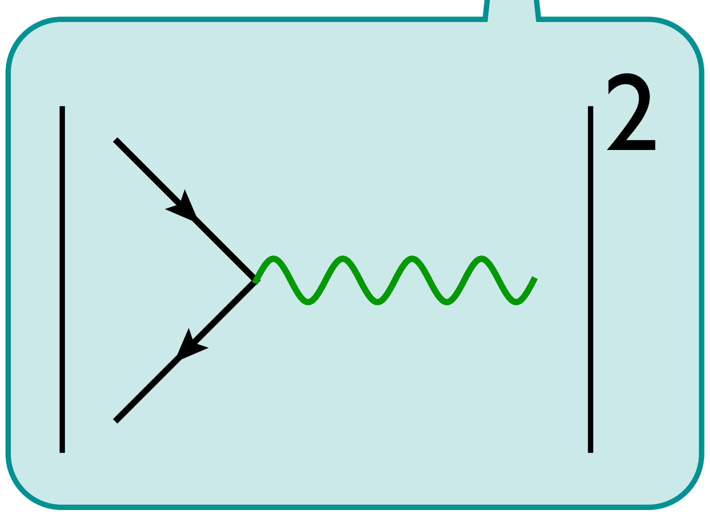

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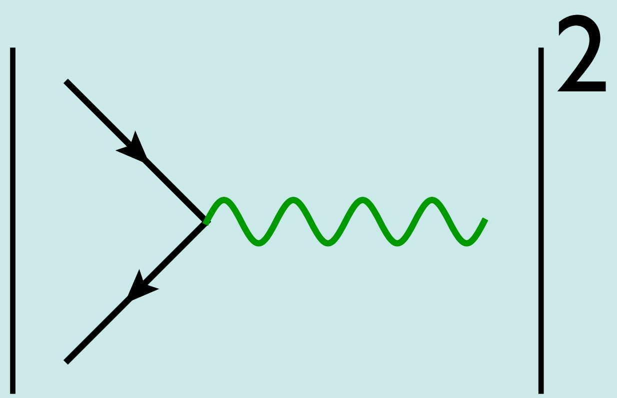

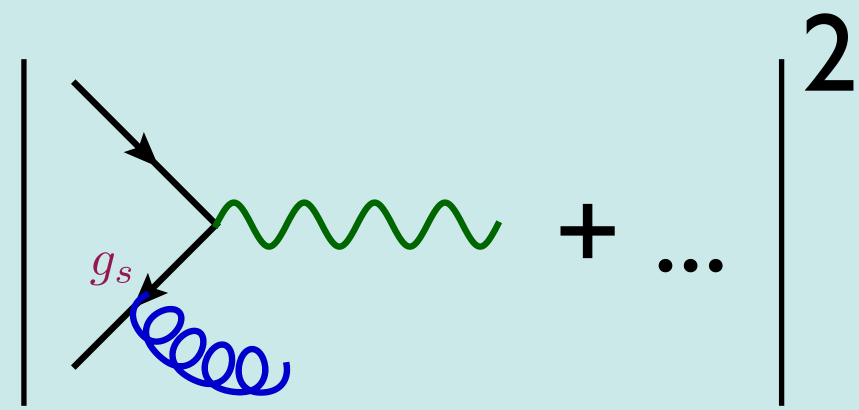

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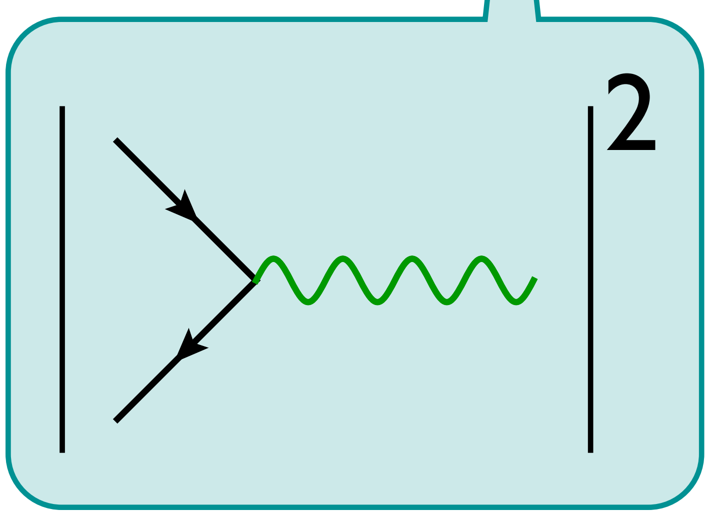

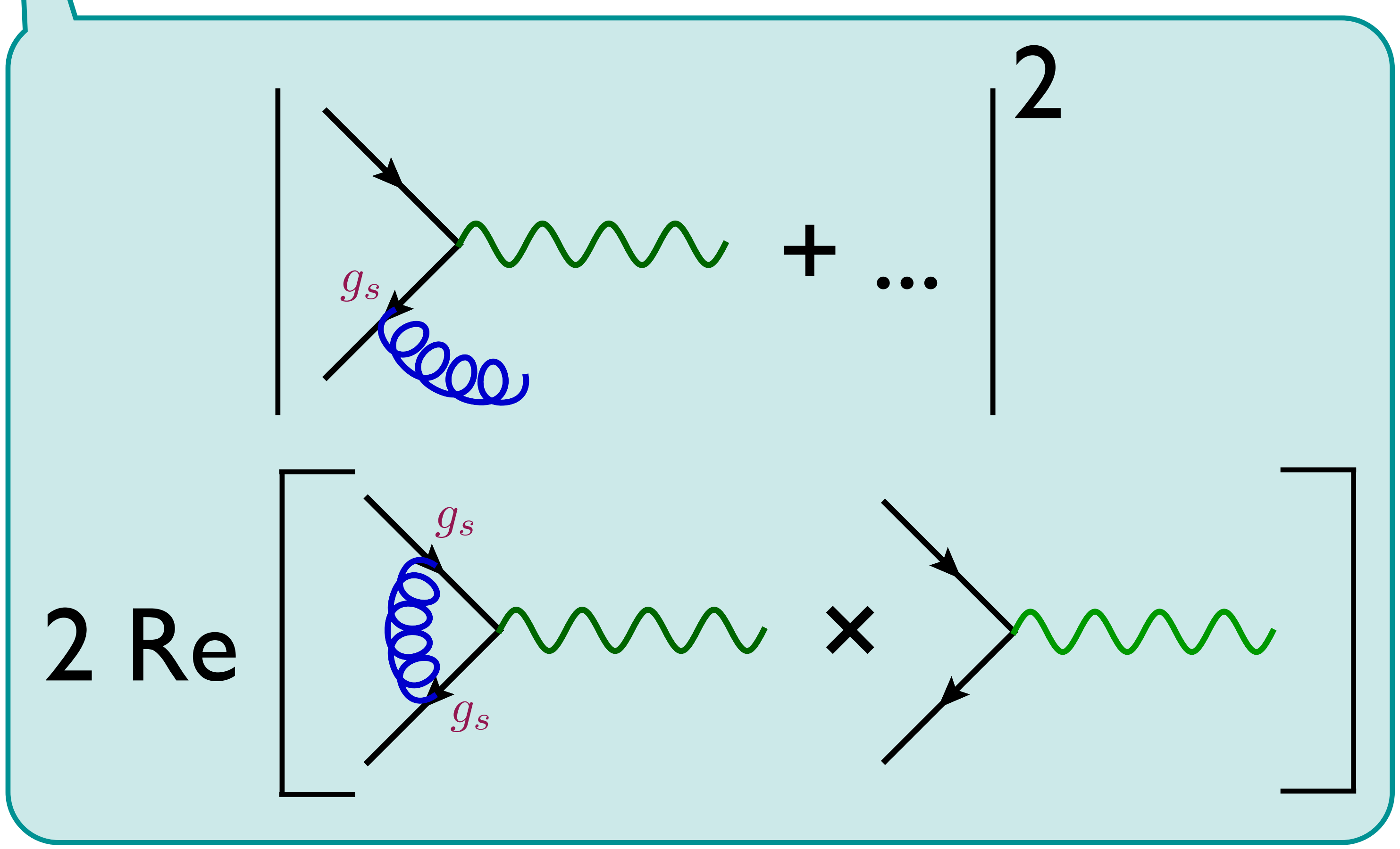

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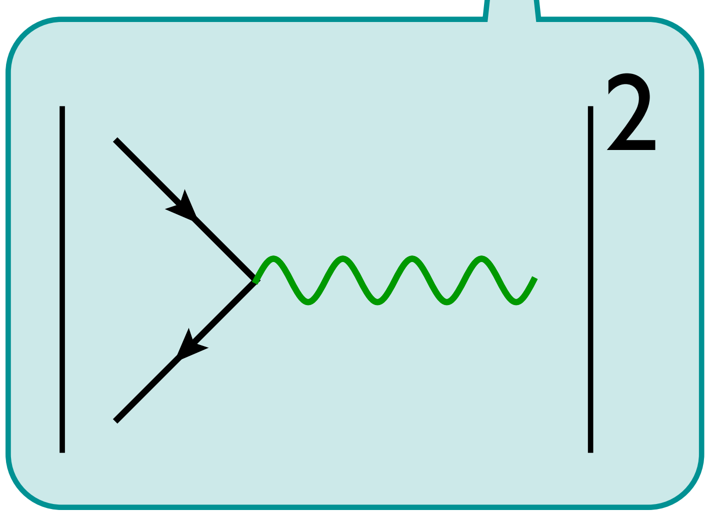
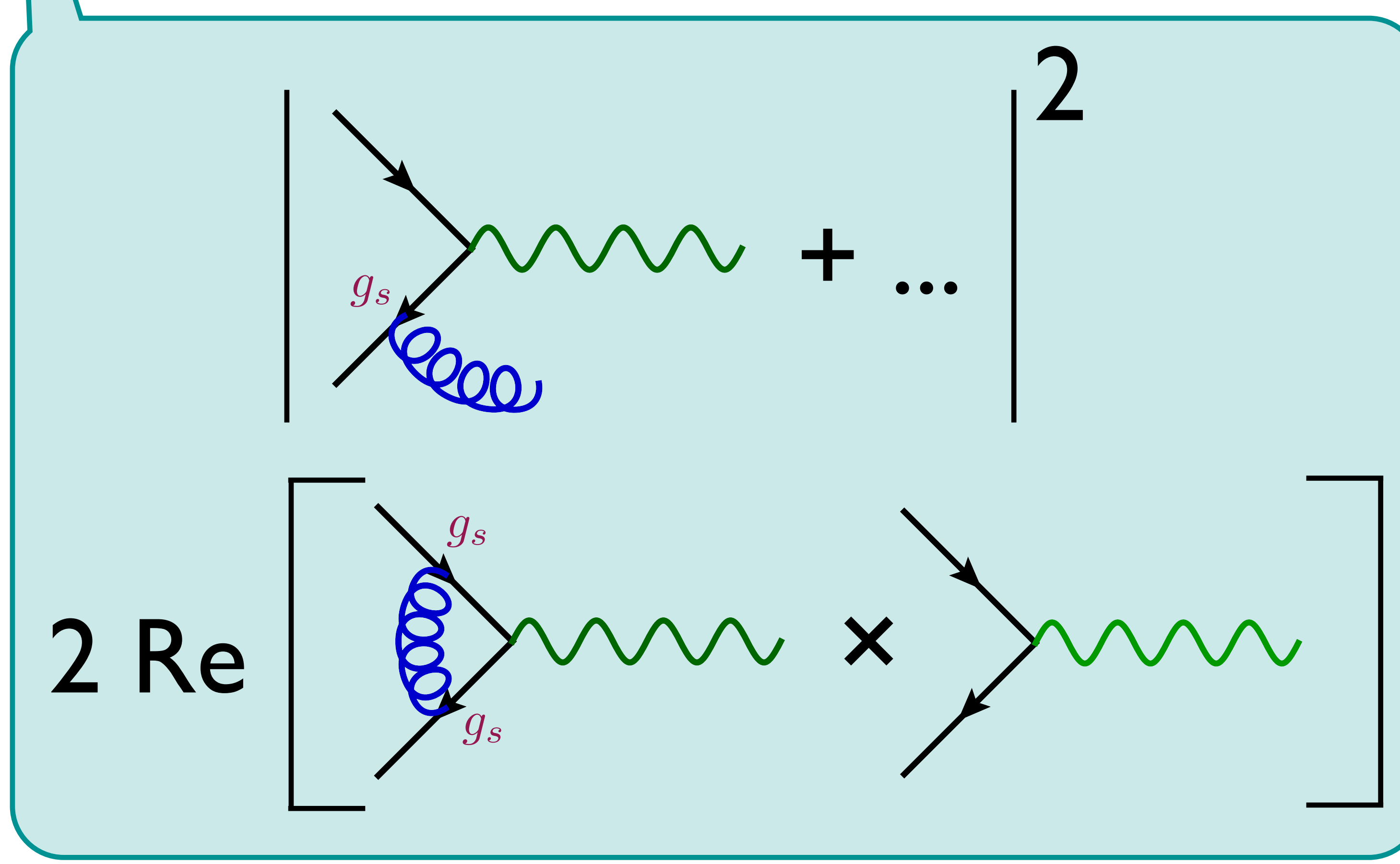
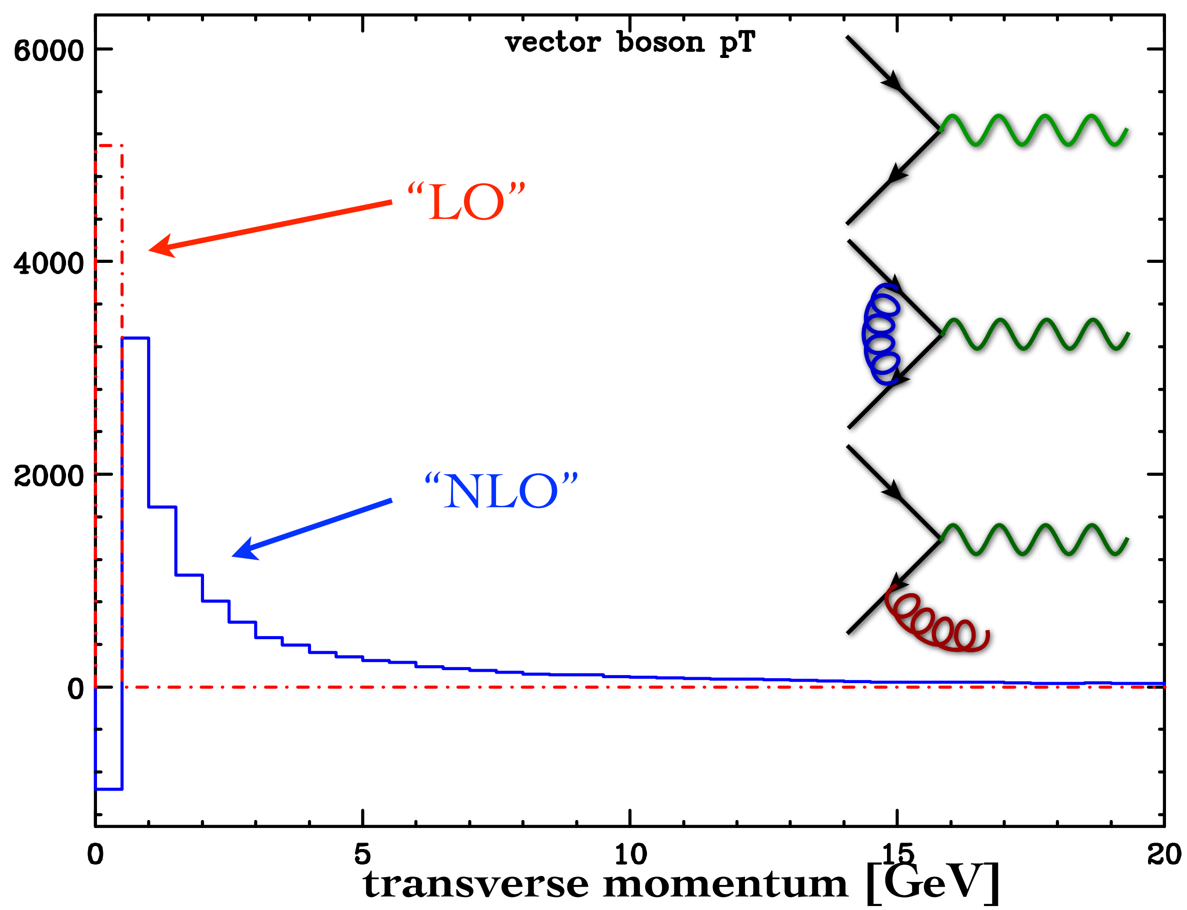
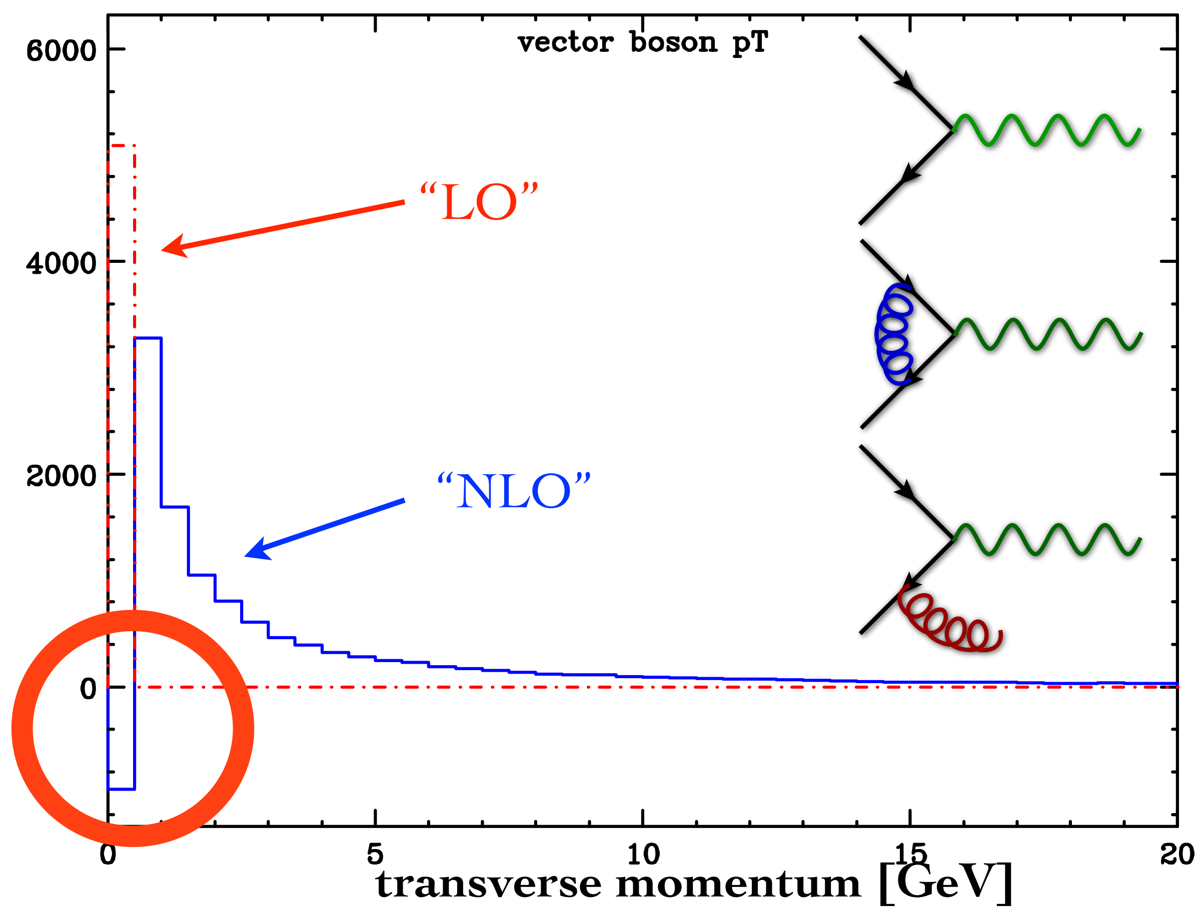




Not definite positive

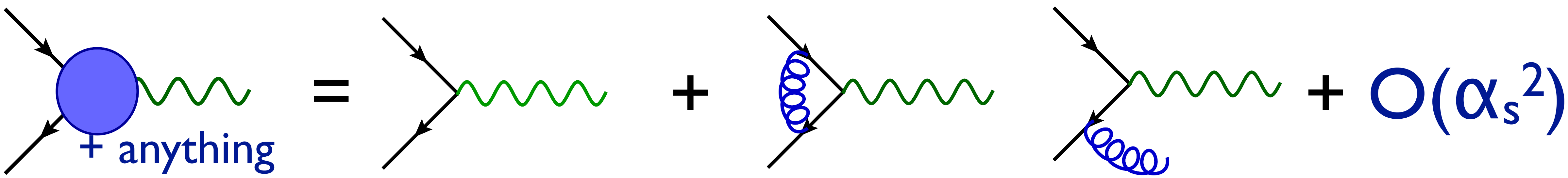
Fixed Order calculations





Negative contribution of the 0-bin

Difficulties



- Multiple steps
  - ➡ Fix divergencies
  - ➡ Virtual amplitudes: how to compute the loops automatically in a reasonable amount of time
  - ➡ How to deal with infra-red behavior for phase-space integration
  - ➡ How to match these processes to a parton shower without double counting

Infrared cancellation

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

- 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, $\epsilon \to 0$)

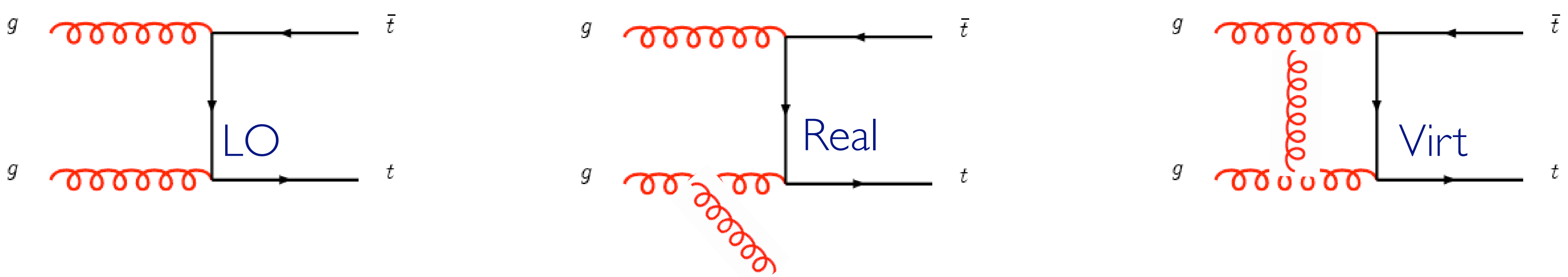
Infrared safe observables

- 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

- 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 $\longrightarrow$ ttbar



- ➡ Total cross section
- ➡ Transverse momentum of the top quark
- ➡ Transverse momentum of the top-antitop pair
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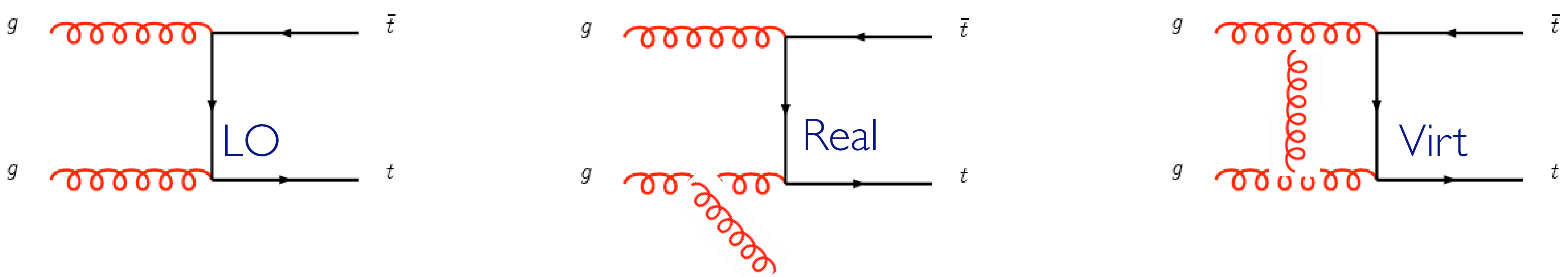

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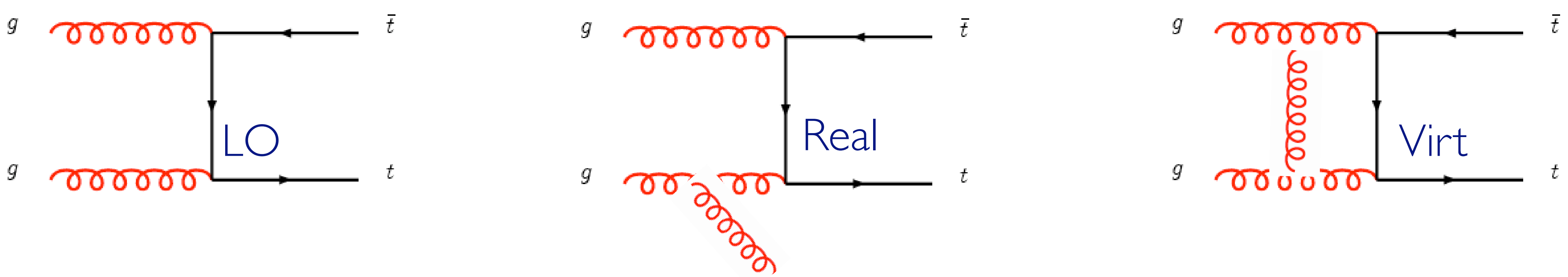

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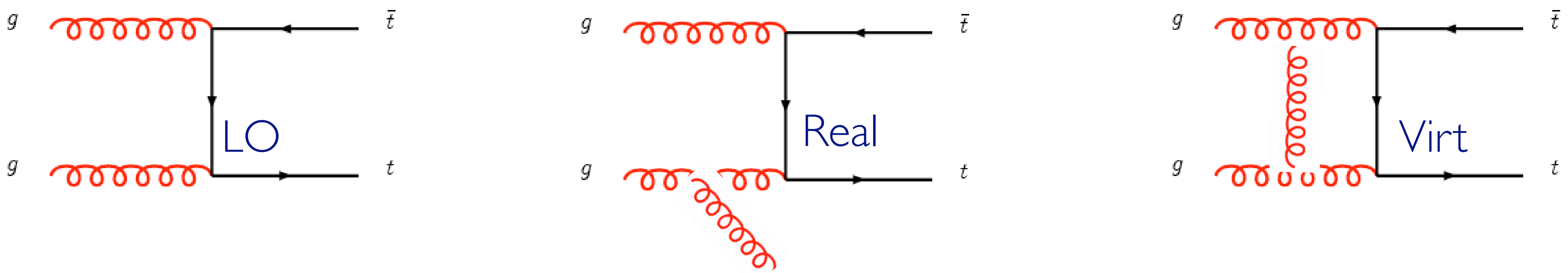

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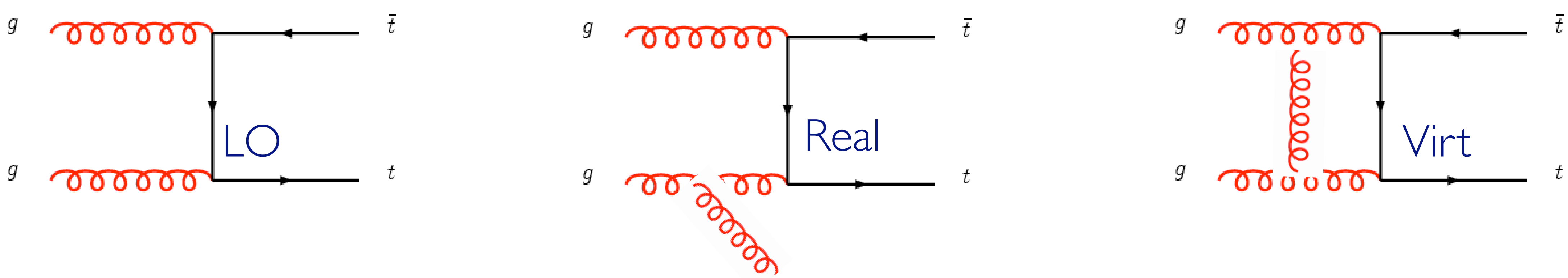

NLO?

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- ➡ Transverse momentum of the top-antitop pair ✘
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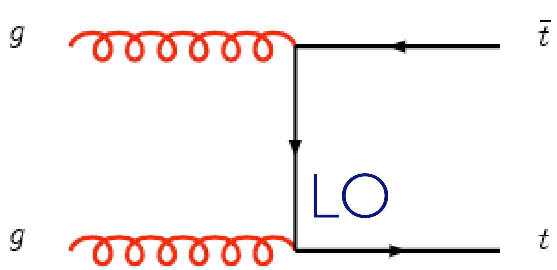

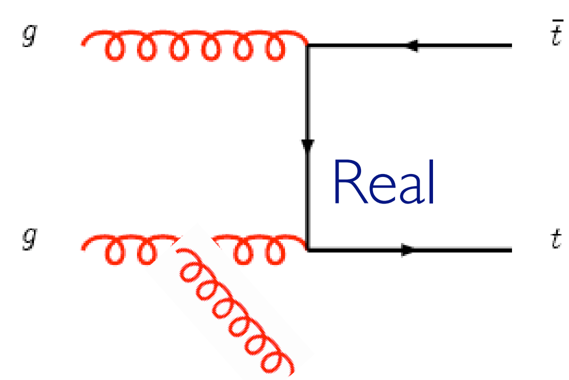

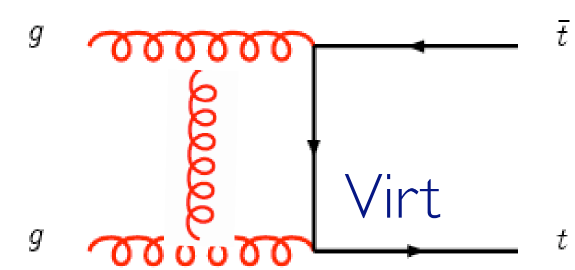

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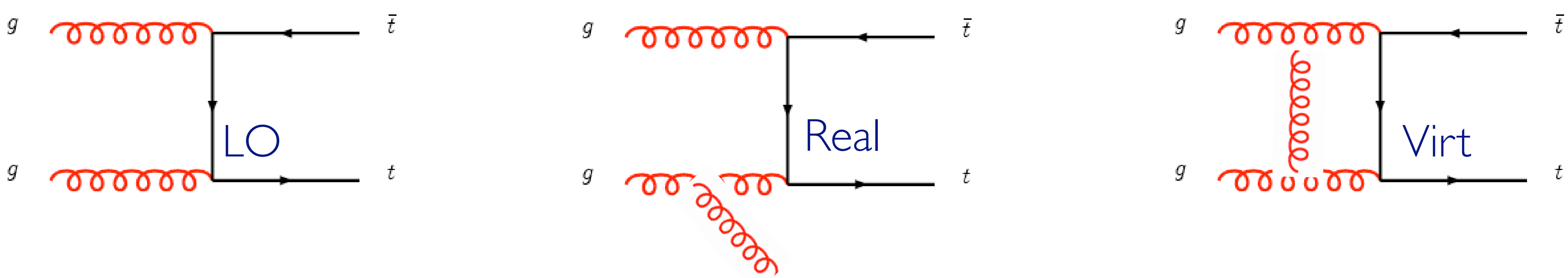

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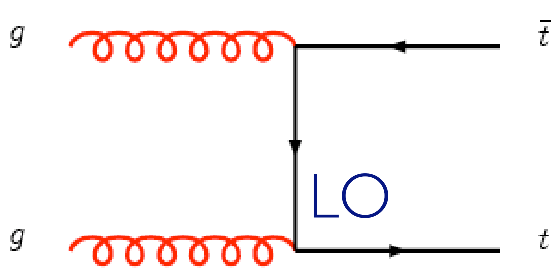

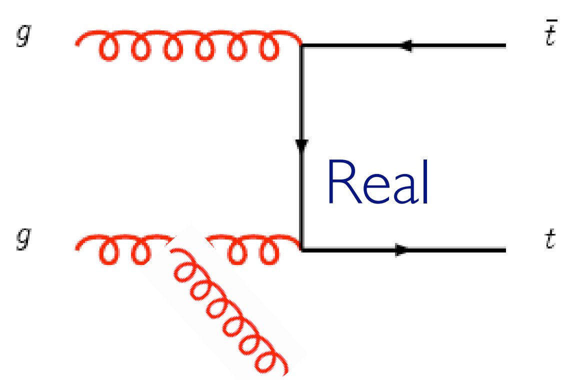

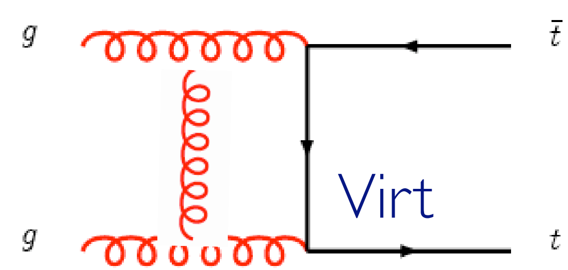

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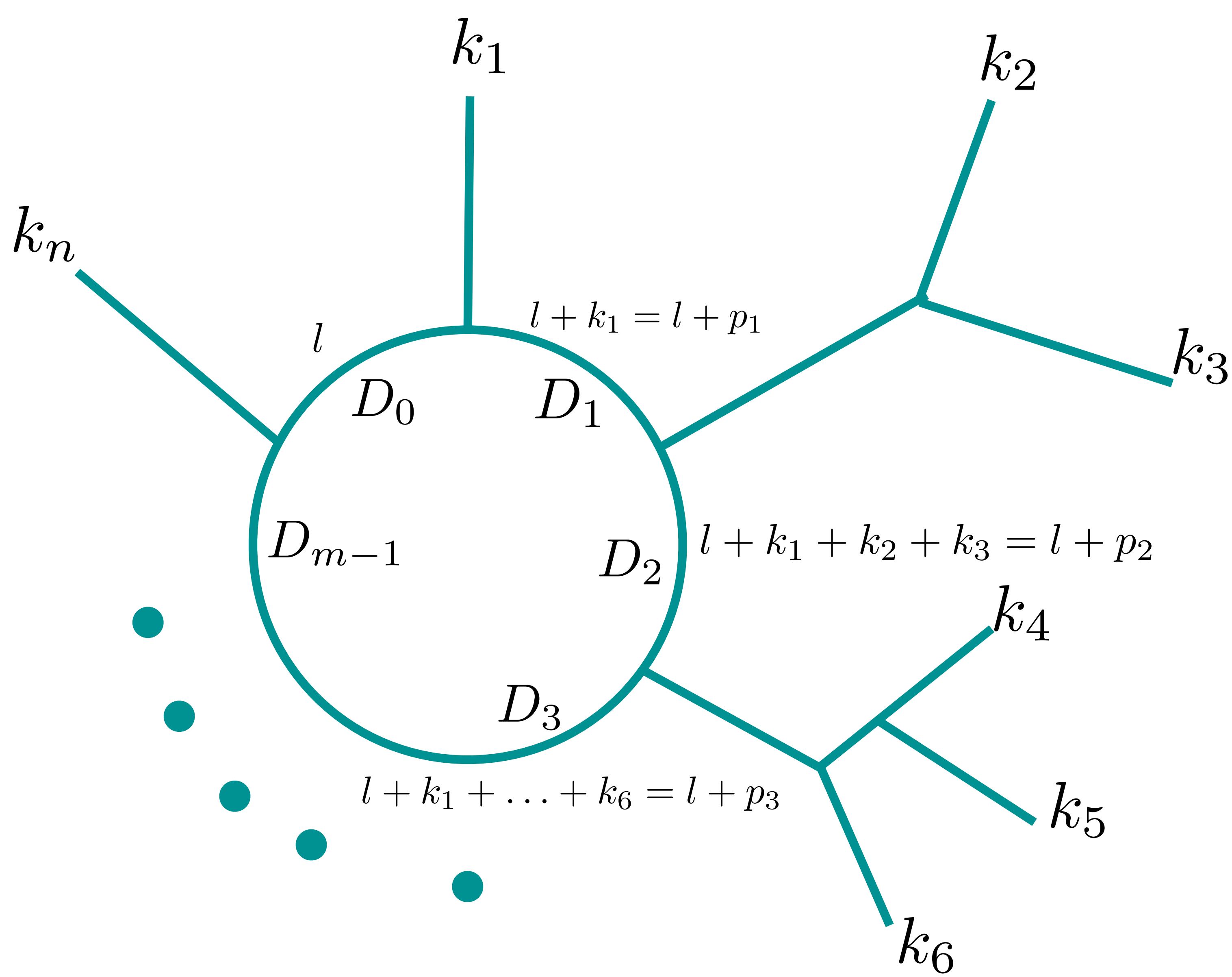
Loop Computation

one-loop integral



- Consider this *m*-point loop diagram with *n* external momenta

- The integral to compute is

$$\int d^d l \, \frac{N(l)}{D_0 D_1 D_2 \cdots D_{m-1}}$$

$$D_i = (l + p_i)^2 - m_i^2$$

Integrand reduction

- Any one-loop integral can be decomposed in scalar integrals
- The task is to find these coefficients efficiently (analytically or numerically)

Basis of scalar integrals

$$\mathcal{M}^{\text{1-loop}} = \sum_{i_0<i_1<i_2<i_3} d_{i_0 i_1 i_2 i_3} \text{Box}_{i_0 i_1 i_2 i_3} + \sum_{i_0<i_1<i_2} c_{i_0 i_1 i_2} \text{Triangle}_{i_0 i_1 i_2} + \sum_{i_0<i_1} b_{i_0 i_1} \text{Bubble}_{i_0 i_1} + \sum_{i_0} a_{i_0} \text{Tadpole}_{i_0} + R + \mathcal{O}(\epsilon)$$

- The a, b, c, d and R coefficients depend only on external parameters and momenta

$$D_i = (l + p_i)^2 - m_i^2$$

$$\text{Tadpole}_{i_0} = \int d^d l \frac{1}{D_{i_0}}$$

$$\text{Bubble}_{i_0 i_1} = \int d^d l \frac{1}{D_{i_0} D_{i_1}}$$

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$$\text{Box}_{i_0 i_1 i_2 i_3} = \int d^d l \frac{1}{D_{i_0} D_{i_1} D_{i_2} D_{i_3}}$$

- All these scalar integrals are known and available in computer libraries (FF [v. Oldenborgh], QCDLoop [Ellis, Zanderighi], OneLOop [v. Hameren])

Divergences

$$\mathcal{M}^{\text{1-loop}} = \sum_{i_0<i_1<i_2<i_3} d_{i_0i_1i_2i_3}\text{Box}_{i_0i_1i_2i_3} + \sum_{i_0<i_1<i_2} c_{i_0i_1i_2}\text{Triangle}_{i_0i_1i_2} + \sum_{i_0<i_1} b_{i_0i_1}\text{Bubble}_{i_0i_1} + \sum_{i_0} a_{i_0}\text{Tadpole}_{i_0} + R + \mathcal{O}(\epsilon)$$

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$$\text{Box}_{i_0i_1i_2i_3} = \int d^dl \frac{1}{D_{i_0}D_{i_1}D_{i_2}D_{i_3}}$$

- ➡The coefficients d, c, b and a are finite and do not contain poles in $1/\epsilon$
- ➡The $1/\epsilon$ dependence is in the scalar integrals (and the UV renormalization)
- ➡When we have solved this system (and included the UV renormalization) we have the full dependence on the soft/collinear divergences in terms of coefficients in front of the poles. These divergences should cancel against divergences in the real emission corrections (according to KLN theorem)

$$\text{Virtual} \sim v_0 + \frac{v_1}{\epsilon} + \frac{v_2}{\epsilon^2}$$

OPP Reduction

- The decomposition to scalar integrals presented before works at the level of the integrals

$$
\begin{aligned}
\mathcal{M}^{\text{1-loop}} = & \sum_{i_0<i_1<i_2<i_3} d_{i_0 i_1 i_2 i_3} \mathrm{Box}_{i_0 i_1 i_2 i_3} \\
& + \sum_{i_0<i_1<i_2} c_{i_0 i_1 i_2} \mathrm{Triangle}_{i_0 i_1 i_2} \\
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& + R + \mathcal{O}(\epsilon)
\end{aligned}
$$

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- If we would know a similar relation at the integrand level, we would be able to manipulate the integrands and extract the coefficients without doing the integrals

OPP Reduction

- The decomposition to scalar integrals presented before works at the level of the integrals

$$\mathcal{M}^{\text{1-loop}} = \sum_{i_0<i_1<i_2<i_3} d_{i_0 i_1 i_2 i_3} \text{Box}_{i_0 i_1 i_2 i_3} + \sum_{i_0<i_1<i_2} c_{i_0 i_1 i_2} \text{Triangle}_{i_0 i_1 i_2} + \sum_{i_0<i_1} b_{i_0 i_1} \text{Bubble}_{i_0 i_1} + \sum_{i_0} a_{i_0} \text{Tadpole}_{i_0} + R + \mathcal{O}(\epsilon)$$

- If we would know a similar relation at the integrand level, we would be able to manipulate the integrands and extract the coefficients without doing the integrals

$$\begin{aligned} N(l) = & \sum_{i_0<i_1<i_2<i_3}^{m-1} \left[d_{i_0 i_1 i_2 i_3} + \tilde{d}_{i_0 i_1 i_2 i_3}(l) \right] \prod_{i \neq i_0,i_1,i_2,i_3}^{m-1} D_i \\ & + \sum_{i_0<i_1<i_2}^{m-1} \left[c_{i_0 i_1 i_2} + \tilde{c}_{i_0 i_1 i_2}(l) \right] \prod_{i \neq i_0,i_1,i_2}^{m-1} D_i \\ & + \sum_{i_0<i_1}^{m-1} \left[b_{i_0 i_1} + \tilde{b}_{i_0 i_1}(l) \right] \prod_{i \neq i_0,i_1}^{m-1} D_i \\ & + \sum_{i_0}^{m-1} \left[a_{i_0} + \tilde{a}_{i_0}(l) \right] \prod_{i \neq i_0}^{m-1} D_i \\ & + \tilde{P}(l) \prod_{i}^{m-1} D_i \end{aligned}$$

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Spurious term

How it works...

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To solve the OPP reduction, choosing special values for the loop momenta helps a lot

For example, choosing *l* such that

$$D_0(l^\pm) = D_1(l^\pm) = D_2(l^\pm) = D_3(l^\pm) = 0$$

sets all the terms in this equation to zero except the first line

There are two (complex) solutions to this equation due to the quadratic nature of the propagators

How it works...

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How it works...

- For each phase-space point we have to solve the system of equations
- Due to the fact that the system reduces when picking special values for the loop momentum, the system greatly reduces
- We can decompose the system at the level of the squared matrix element, amplitude, diagram or anywhere in between. As long as we provide the corresponding numerator function. Since each reduction with CutTools is computationally heavy, we directly reduce the squared element with MadGraph.
- For a given phase-space point, we have to compute the numerator function several times (~50 or so for a box loop)

Complications in d dimensions

- In the previous consideration I was very sloppy in considering if we are working in 4 or d dimensions
- In general, external momenta and polarization vectors are in 4 dimensions; only the loop momentum is in d dimensions
- To be more correct, we compute the integral

$$\int d^d l \, \frac{N(l,\tilde{l})}{\bar{D}_0 \bar{D}_1 \bar{D}_2 \cdots \bar{D}_{m-1}}$$

$$\bar{l} = l + \tilde{l}$$

d dim, 4 dim, epsilon dim

$$\bar{D}_i = (\bar{l} + p_i)^2 - m_i^2 = (l + p_i)^2 - m_i^2 + \tilde{l}^2 = D_i + \tilde{l}^2$$

$$l \cdot \tilde{l} = 0 \qquad \bar{l} \cdot p_i = l \cdot p_i \qquad \bar{l} \cdot \bar{l} = l \cdot l + \tilde{l} \cdot \tilde{l}$$

Implications

$$\sum_{0\le i_0<i_1<i_2<i_3}^{m-1} d(i_0 i_1 i_2 i_3) \int d^d\bar{\ell}\, \frac{1}{\bar{D}_{i_0}\bar{D}_{i_1}\bar{D}_{i_2}\bar{D}_{i_3}}$$
$$+ \sum_{0\le i_0<i_1<i_2}^{m-1} c(i_0 i_1 i_2) \int d^d\bar{\ell}\, \frac{1}{\bar{D}_{i_0}\bar{D}_{i_1}\bar{D}_{i_2}}$$
$$+ \sum_{0\le i_0<i_1}^{m-1} b(i_0 i_1) \int d^d\bar{\ell}\, \frac{1}{\bar{D}_{i_0}\bar{D}_{i_1}}$$
$$+ \sum_{i_0=0}^{m-1} a(i_0) \int d^d\bar{\ell}\, \frac{1}{\bar{D}_{i_0}}$$
$$+ R\,.$$

- The decomposition in terms of scalar integrals has to be done in d dimensions
- This is why the rational part *R* is needed

Rational terms

$$R = R_1 + R_2$$

Rational terms

- In the OPP method, they are split into two contributions, generally called $$R = R_1 + R_2$$
- Both have their origin in the UV part of the model, but only R_1 can be directly computed in the OPP reduction and is given by the CutTools program

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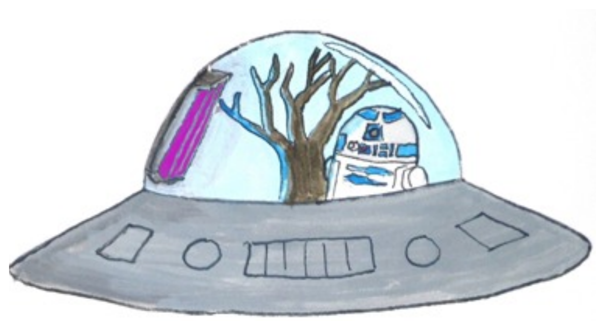
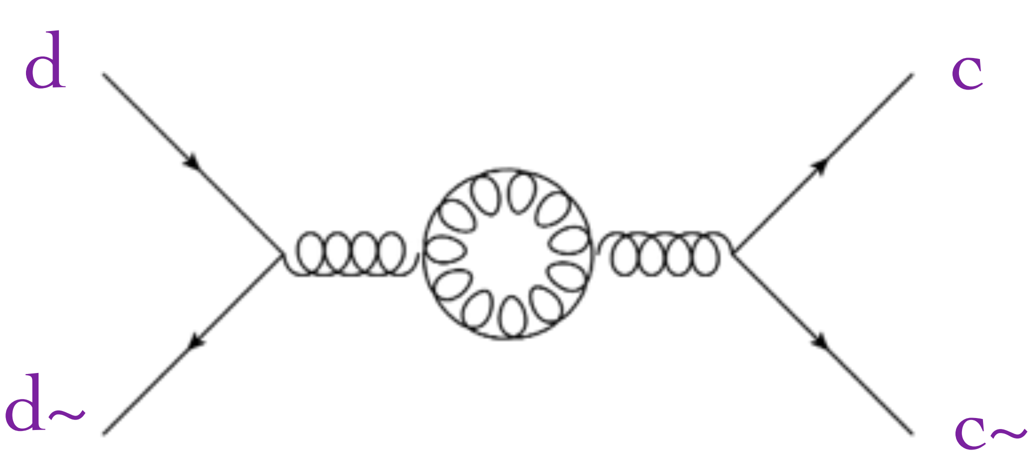


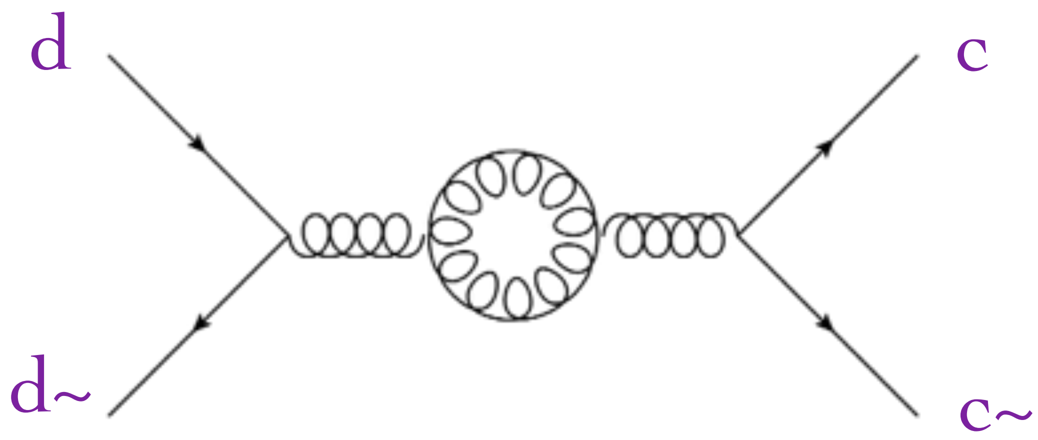
Remember:



$$\mathcal{N}(l^{\mu})$$

Remember:

➡ For a given phase-space point, we have to compute the numerator function several times (~50 or so for a box loop) per external phase-space point.



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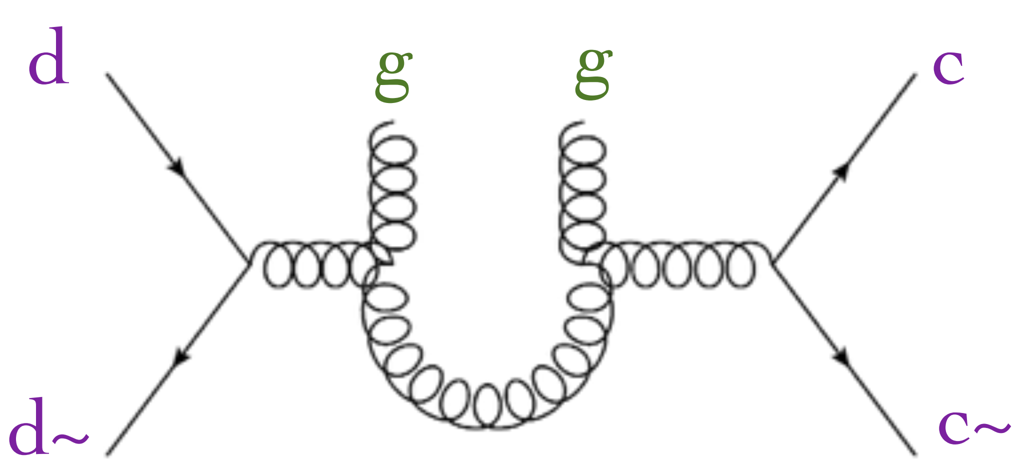
- ➡ For a given phase-space point, we have to compute the numerator function several times (~50 or so for a box loop) per external phase-space point.
  - ➡ Cut the Loop and use HELAS (with no denominator)
    - ➡ Generic
    - ➡ recycling



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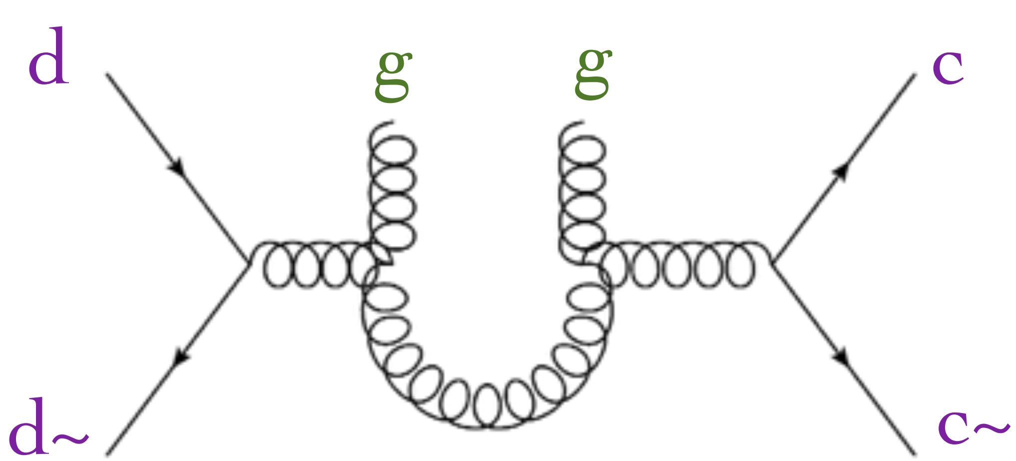
- Need to upgrade MadGraph so to generate loop diagrams and numerical code for the integrand N(q)



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MadLoop

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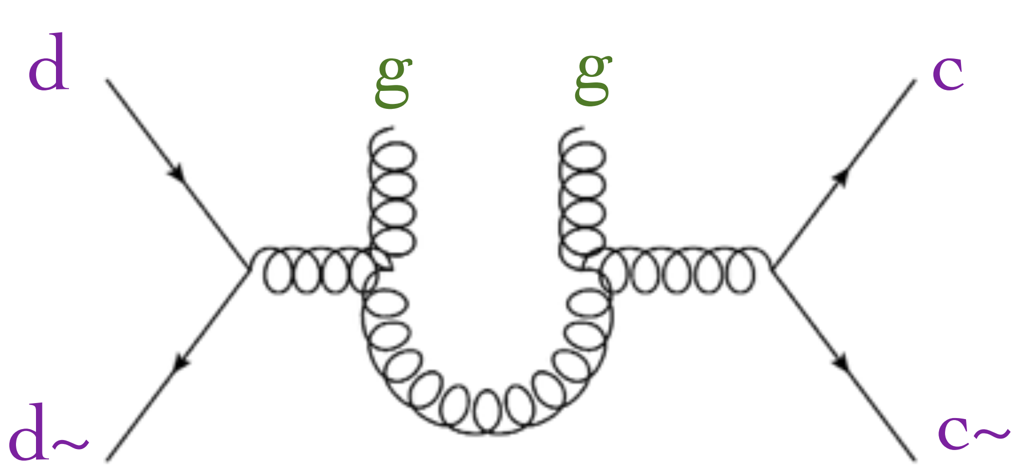
OpenLoop: [S. Pozzorini & al.(2011)]



$$\mathcal{N}(l^\mu) = \sum_{r=0}^{r_{max}} C^{(r)}_{\mu_0\mu_1\cdots\mu_r} l^{\mu_0} l^{\mu_1} \ldots l^{\mu_r}$$

coefficient computed iteratively by ALOHA

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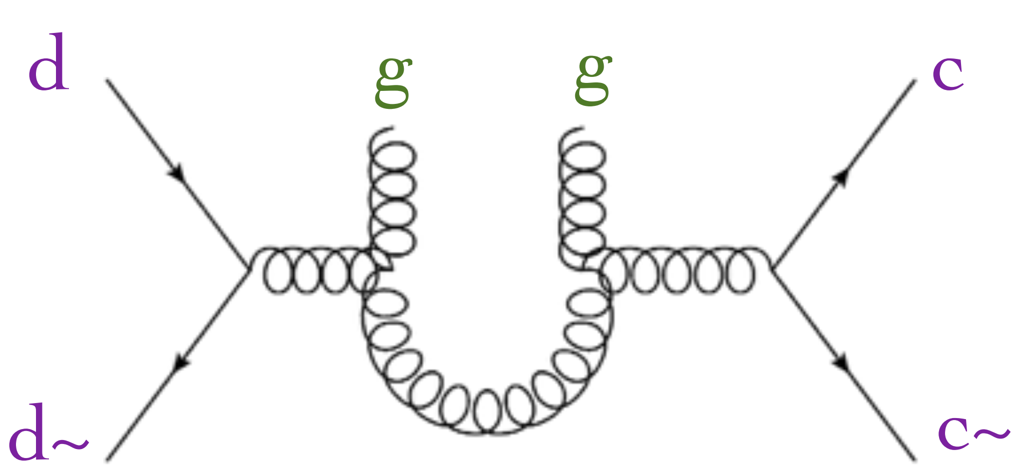

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5-10 times faster

coefficient computed iteratively by ALOHA

FKS

phase-space integration

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

- 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

I skipped this interesting topic here!

NLO+PS MATCHING

ME

1. Fixed order calculation
2. Computationally expensive
3. Limited number of particles
4. Valid when partons are hard and well separated
5. Quantum interference correct
6. Needed for multi-jet description

Shower MC

1. Resums logs to all orders
2. Computationally cheap
3. No limit on particle multiplicity
4. Valid when partons are collinear and/or soft
5. Partial interference through angular ordering
6. Needed for hadronization

Approaches are complementary: merge them!

Difficulty: avoid double counting, ensure smooth distributions

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No longer true at NLO!

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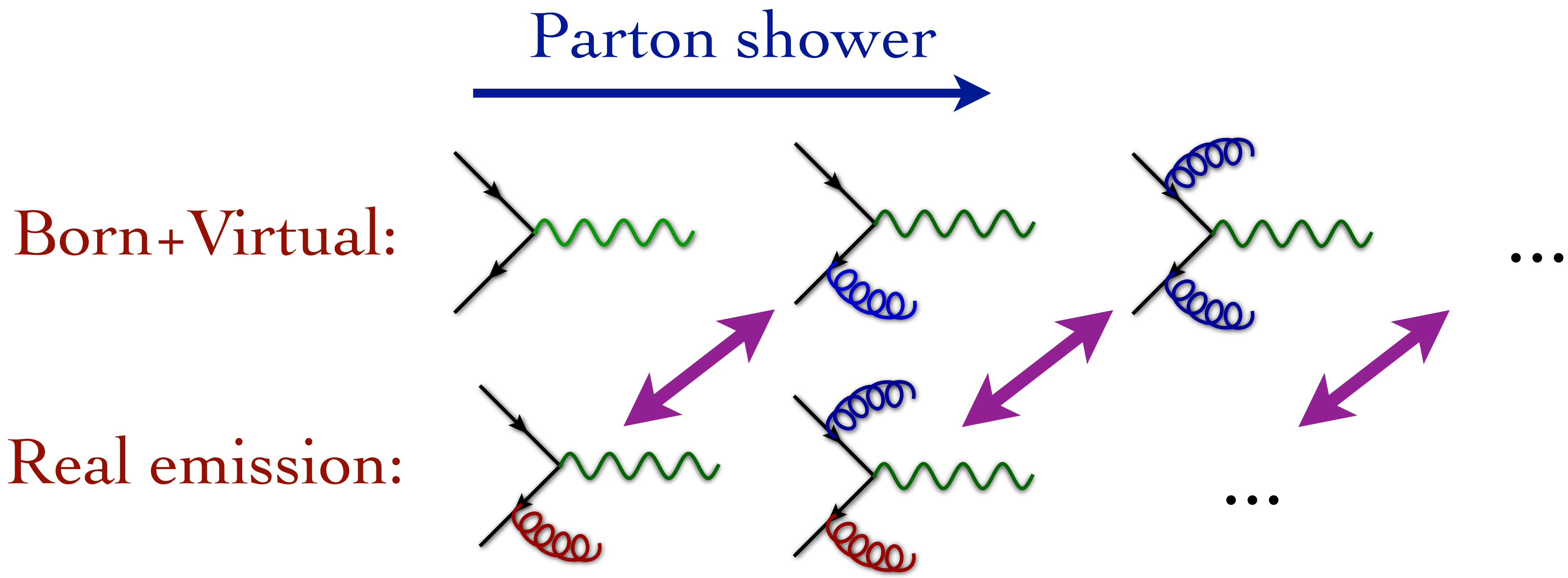
Difficulty: avoid double counting, ensure smooth distributions

Matching NLO

- At NLO one faces even more severe double-counting issues:



- And also part of the virtual contribution is double counted through the definition of the Sudakov factor Δ

MC@NLO

1. PSMC dependent
2. Some negative weighted events
3. Quantum interference exact
4. Used by both MG5_aMC and Sherpa.

POWHEG

1. PSMC independent
2. Only positive unit weight
3. Can use existing NLO results via the POWHEG-Box
4. Used by HELAC

Double counting

- The Sudakov factor Δ (which is responsible for the resummation of all the radiation in the shower) is the no-emission probability
- It's defined to be Δ = 1 - *P*, where P is the probability for a branching to occur
- By using this conservation of probability in this way, Δ contains contributions from the virtual corrections implicitly
- Because at NLO the virtual corrections are already included via explicit matrix elements, Δ is double counting with the virtual corrections
- In fact, because the shower is unitary, what we are double counting in the real emission corrections is exactly equal to what we are double counting in the virtual corrections (but with opposite sign)!

MC@NLO procedure

[Frixione & Webber (2002)]

- To remove the double counting, we can add and subtract the same term to the m and m+1 body configurations

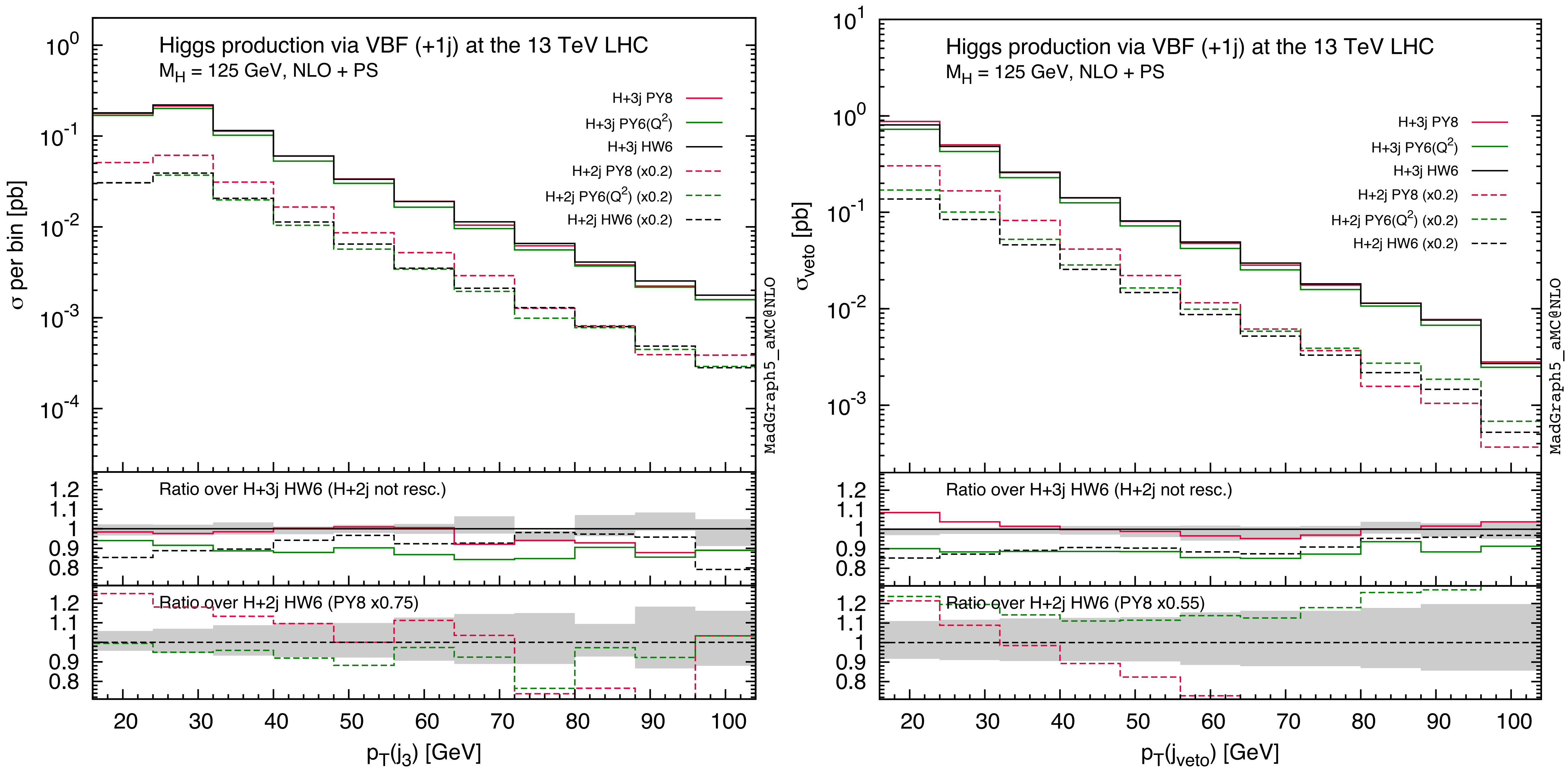
$$\frac{d\sigma_{\mathrm{NLOwPS}}}{dO} = \left[d\Phi_m \left(B + \int_{\mathrm{loop}} V + \int d\Phi_1 MC \right) \right] I_{\mathrm{MC}}^{(m)}(O) + \left[d\Phi_{m+1} (R - MC) \right] I_{\mathrm{MC}}^{(m+1)}(O)$$

- Where the MC are defined to be the contribution of the parton shower to get from the m body Born final state to the m+1 body real emission final state

Negative weights

$$\frac{d\sigma_{\mathrm{NLOwPS}}}{dO} = \left[d\Phi_m \left(B + \int_{\mathrm{loop}} V + \int d\Phi_1 MC \right) \right] I_{\mathrm{MC}}^{(m)}(O)$$
$$+ \left[d\Phi_{m+1} (R - MC) \right] I_{\mathrm{MC}}^{(m+1)}(O)$$

- We generate events for the two terms between the square brackets (S- and H-events) separately
- There is no guarantee that these contributions are separately positive (even though predictions for infra-red safe observables should always be positive!)
- Therefore, when we do event unweighting we can only unweight the events **up to a sign**. These signs should be taken into account when doing a physics analysis (i.e. making plots etc.)
- The events are only physical when they are showered.


Higgs production via VBF (+1j) at the 13 TeV LHC
M_H = 125 GeV, NLO + PS
H+3j PY8
H+3j PY6(Q^2)
H+3j HW6
H+2j PY8 (x0.2)
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σ per bin [pb]
MadGraph5_aMC@NLO
Ratio over H+3j HW6 (H+2j not resc.)
Ratio over H+2j HW6 (PY8 x0.75)
$p_T(j_3)$ [GeV]
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σ_{veto} [pb]
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$p_T(j_{veto})$ [GeV]

Conclusion

- Shower Monte Carlo
  - ➡ QCD in colinear approximation
  - ➡ key object is the Sudakov factor
- Matching/Merging at LO
  - ➡ How to use it/check it
- NLO
  - ➡ Automated for the SM
  - ➡ All observable are not NLO accurate
  - ➡ Fixed Order computation are not definite positive
  - ➡ NLO+PS events are not physical before the shower

Remark

- Never trust a code (even mine)
  - ➡ Always check!
- Never use those as full black box.