

Stefano Frixione

# QCD and advanced Monte Carlo tools

*CERN-FNAL HCP summer school – Lecture 3*

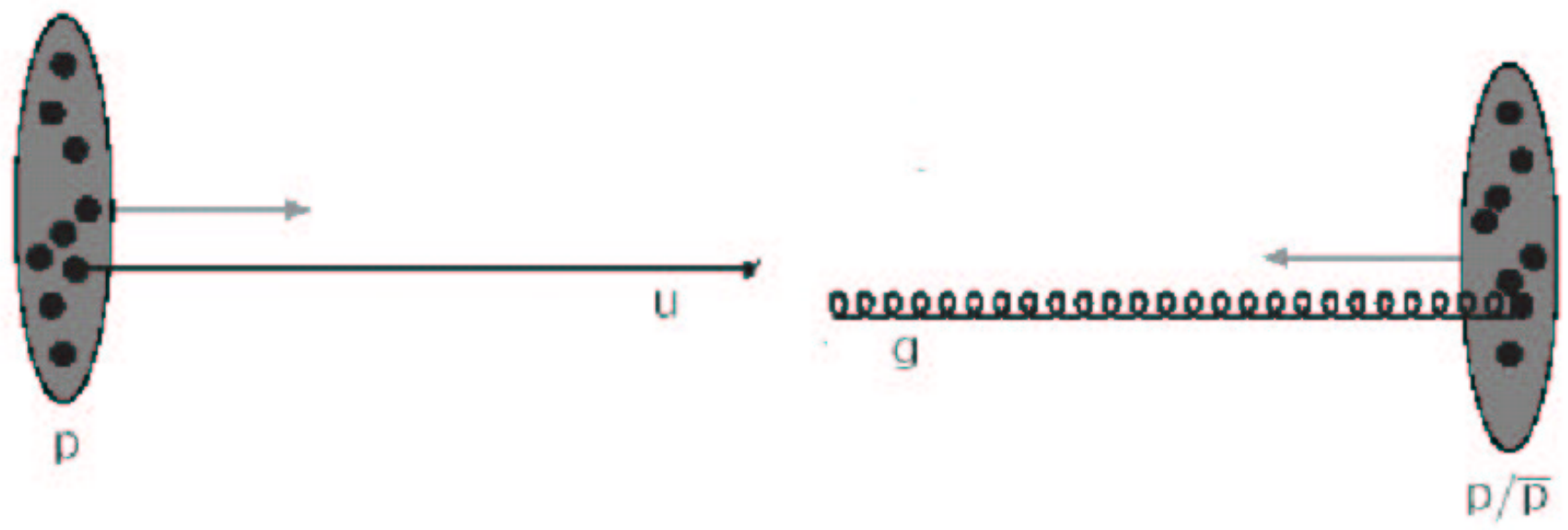
CERN, 10/6/2011

## Summary of lecture 2

- ◆ With the help of hadron-parton duality, infrared safety, and factorization theorems we can use perturbation theory for collider physics
- ◆ The leading kinematical behaviour of the matrix elements is due to soft and collinear configurations
- ◆ In these configurations, the matrix elements factorize universal kernels
- ◆ The simulation of an event typically requires the separation between large- and small- $p_T$  phenomena. The former are computed exactly, the latter are approximated or modelled

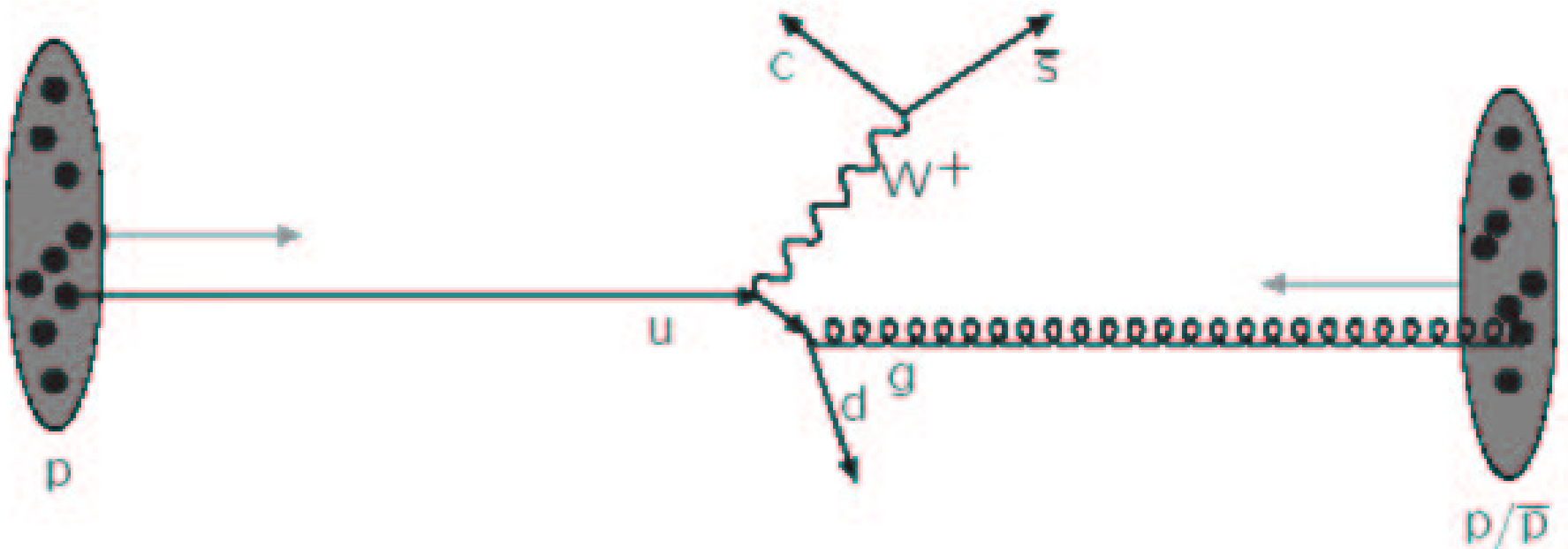
# THE PHYSICS OF EVENT GENERATORS

Plot: T. Sjöstrand

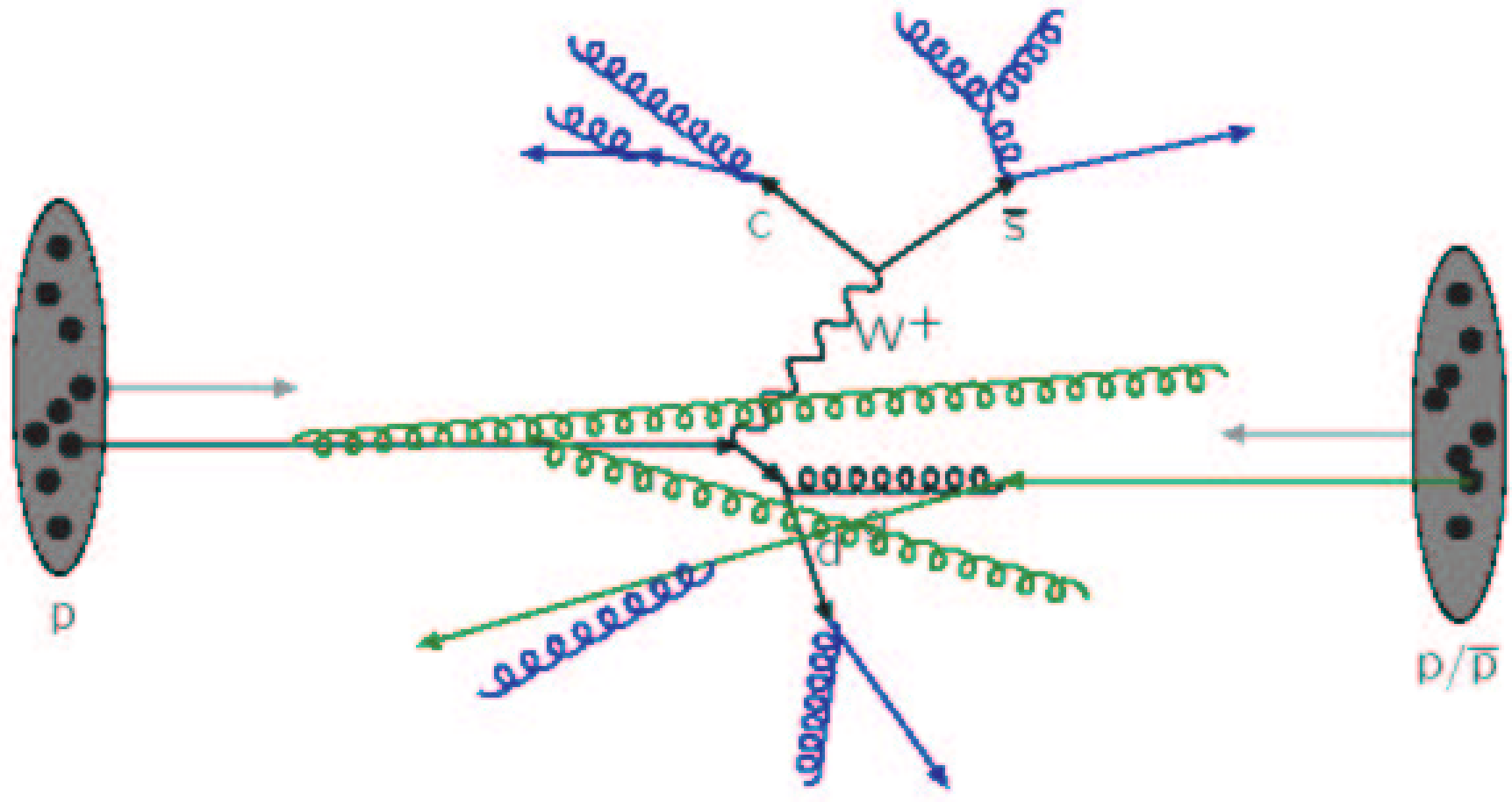


0. Pull out one parton from each of the incoming hadrons  
(use PDFs to choose flavour and  $x$ )

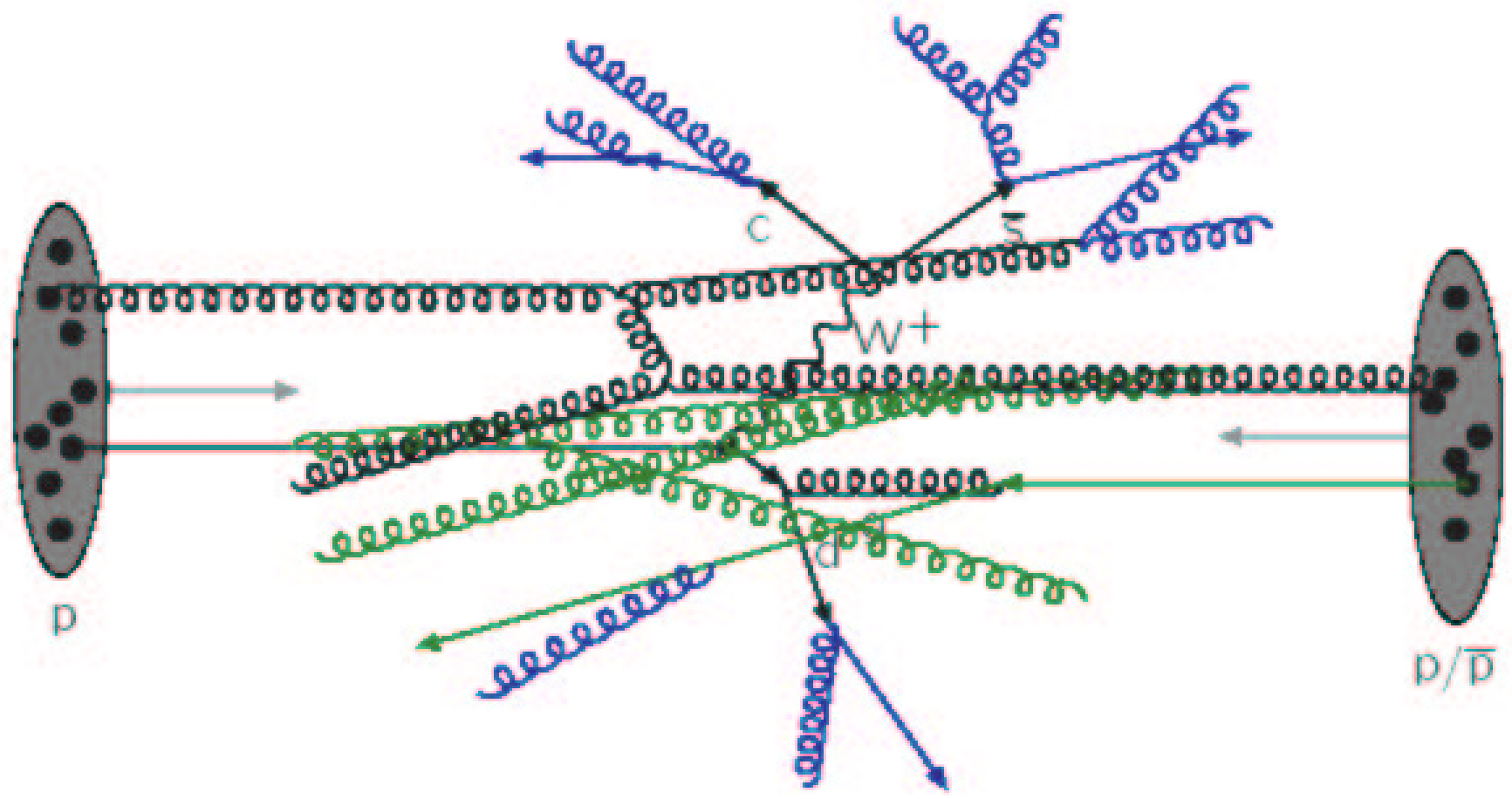
Plot: T. Sjöstrand



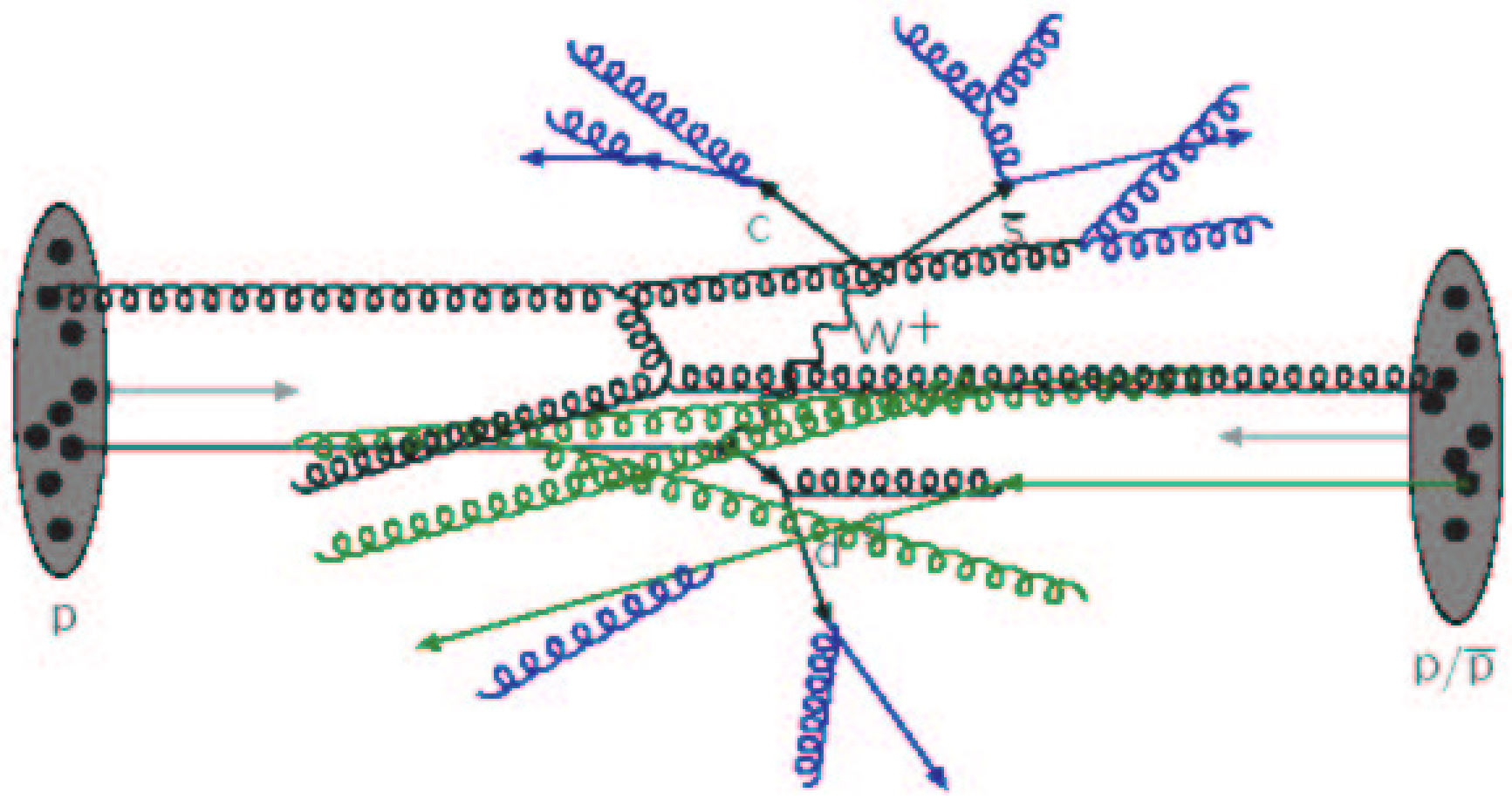
1. Make them collide and produce *large- $p_T$  stuff* (Hard Subprocess)



2. Let quarks and gluons emit other quarks and gluons (Parton Shower) – small *relative*  $p_T$



3. Other partons may undergo the same fate *at smaller  $p_T$ 's*  
(MPI + beam remnants  $\equiv$  Underlying Event)



4. Convert quarks and gluons into physical hadrons (Hadronization)



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4. Hadronization. Not so well understood. Based on models, with pretty good fits to data. Largely energy-independent, so extrapolations (e.g. Tevatron  $\longrightarrow$  LHC) are considered to be reliable
3. Underlying Event. Poorly understood. Models are not well constrained by data, and extrapolations are affected by very large uncertainties

Traditionally, activity in EvG's was limited to 2 (shower), 3 (UE), and 4 (hadronization). Step 1 (hard subprocess) was performed at the lowest order in pQCD.

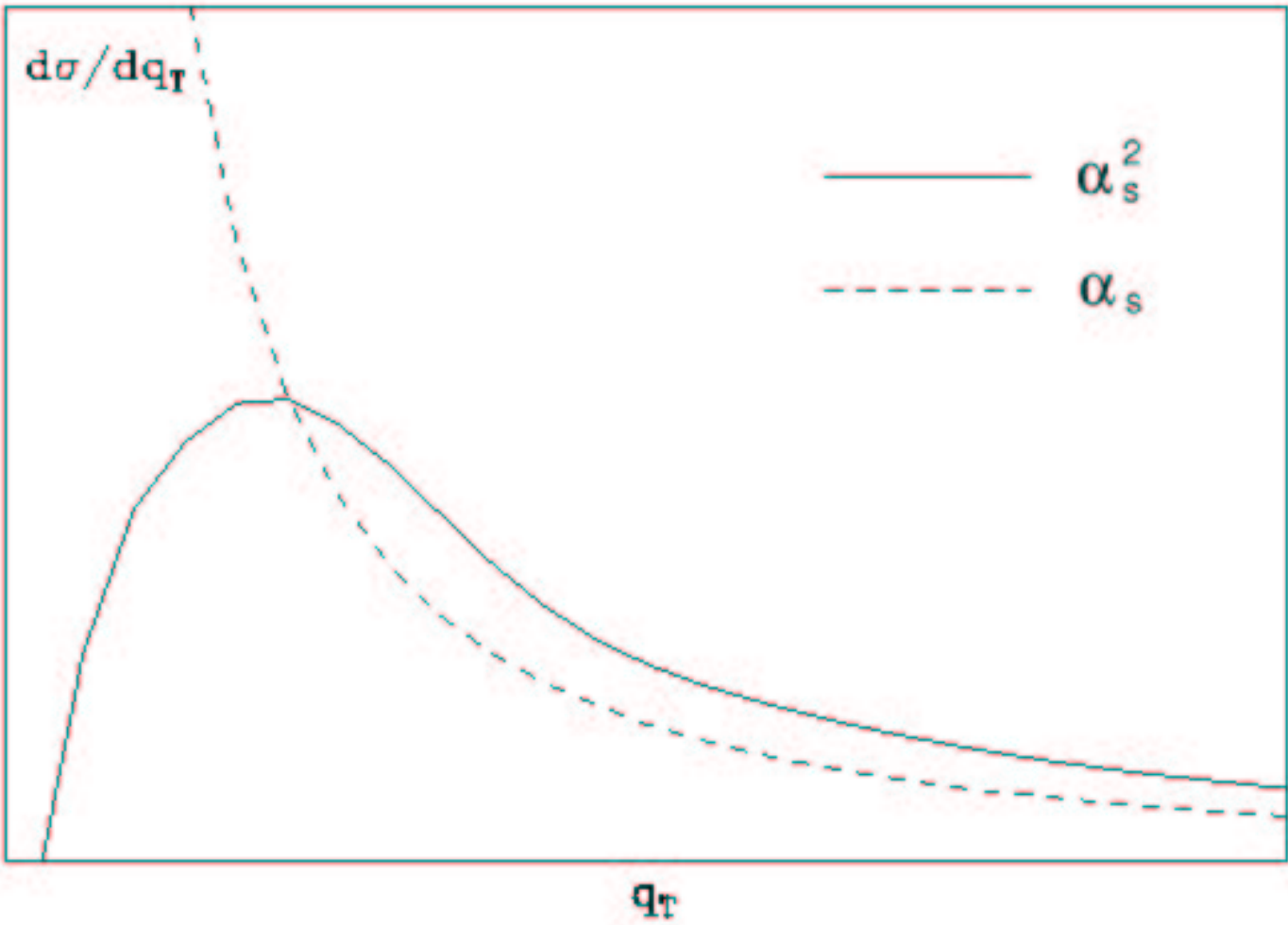
This has now changed, and I'll talk about that later.

For the moment, I'll concentrate on parton showers. Keep in mind that:

A Parton Shower is a way to compute Feynman diagrams to all order in pQCD, by retaining their dominant contributions

We already know that dominant contributions are associated with soft and collinear singularities. So now we set out to study them to all orders

Note that, even if one were able to compute exactly quite a lot of Feynman diagrams (e.g., NLO, NNLO, ...), the results wouldn't always be meaningful



$$p_T(W) \equiv q_T(W)$$

This quantity diverges order-by-order in pQCD at  $p_T(W) = 0$  — it's IR sensitive, in spite of being IR safe

Before tackling parton showers, let me stress that the problem of the sensible generation of the underlying event (and of small- $p_T$  stuff in general) is a serious one, owing to

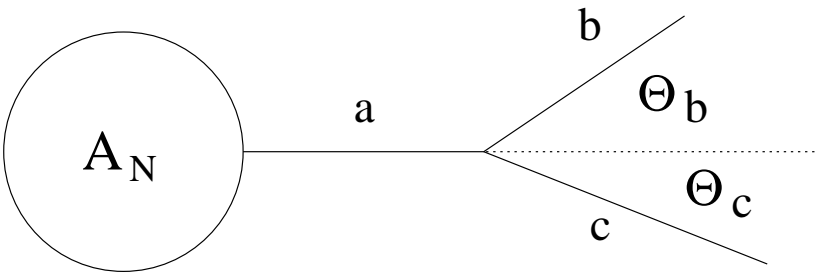
- ▶ its importance for all kind of physics simulations
- ▶ the still-poor theoretical understanding of its mechanisms

The process of checking the predictions of and of improving the models for the underlying event is a constant effort at colliders

There is a lot of ongoing activity on this issue, which I won't report

Let's start by ignoring the problem of soft singularities

Collinear kinematics



$$\begin{aligned}
 z &= E_b/E_a; \quad t = k_a^2 \\
 \Theta &= \Theta_b + \Theta_c \\
 &= \frac{\Theta_b}{1-z} = \frac{\Theta_c}{z} \\
 &= \frac{1}{E_a} \sqrt{\frac{t}{z(1-z)}}
 \end{aligned}$$

Work in axial gauges

$$\begin{aligned}
 d\sigma_{N+1} &= d\sigma_N \frac{dt}{t} \frac{d\phi}{2\pi} dz \frac{\alpha_s}{2\pi} |K_{ba}(z)|^2 \\
 d\bar{\sigma}_{N+1} &= d\bar{\sigma}_N \frac{dt}{t} dz \frac{\alpha_s}{2\pi} P_{ba}(z)
 \end{aligned}$$

which is the known result

In the phase space,  $\phi$  can be conveniently identified with the azimuthal angle between the plane of branching and the polarization of  $a$



It is easy to iterate the branching process (splittings are called branchings in this context)

$$a(t) \longrightarrow b(z) + c, \quad b(t') \longrightarrow d(z') + e$$
$$d\bar{\sigma}_{N+2} = d\bar{\sigma}_N \frac{dt}{t} dz \frac{dt'}{t'} dz' \left( \frac{\alpha_s}{2\pi} \right)^2 P_{ba}(z) P_{db}(z')$$

This is a *Markov process*, ie a random process in which the probability of the next step only depends on the present values of the random variables. In formulae

$$\tau_1 < \dots < \tau_n \implies$$
$$P\left(x(\tau_n) < x_n | x(\tau_{n-1}), \dots, x(\tau_1)\right) = P(x(\tau_n) < x_n | x(\tau_{n-1}))$$

In our case, the probability of each branching depends on the type of splitting ( $g \rightarrow gg, \dots$ ), the virtuality  $t$ , and the energy fraction  $z$

Following a given line in a branching tree, it is clear that enhanced contributions will be due to the strongly-ordered region

$$Q^2 \gg t_1 \gg t_2 \gg \dots t_N \gg Q_0^2$$
$$\sigma_N \propto \sigma_0 \alpha_S^N \int_{Q_0^2}^{Q^2} \frac{dt_1}{t_1} \int_{Q_0^2}^{t_1} \frac{dt_2}{t_2} \dots \int_{Q_0^2}^{t_{N-1}} \frac{dt_N}{t_N} = \sigma_0 \frac{\alpha_S^N}{N!} \left( \log \frac{Q^2}{Q_0^2} \right)^N$$

Denote by

$$\Phi_a[E, Q^2]$$

the ensemble of parton cascades initiated by a parton  $a$  of energy  $E$  emerging from a hard process with scale  $Q^2$ . Also, denote by

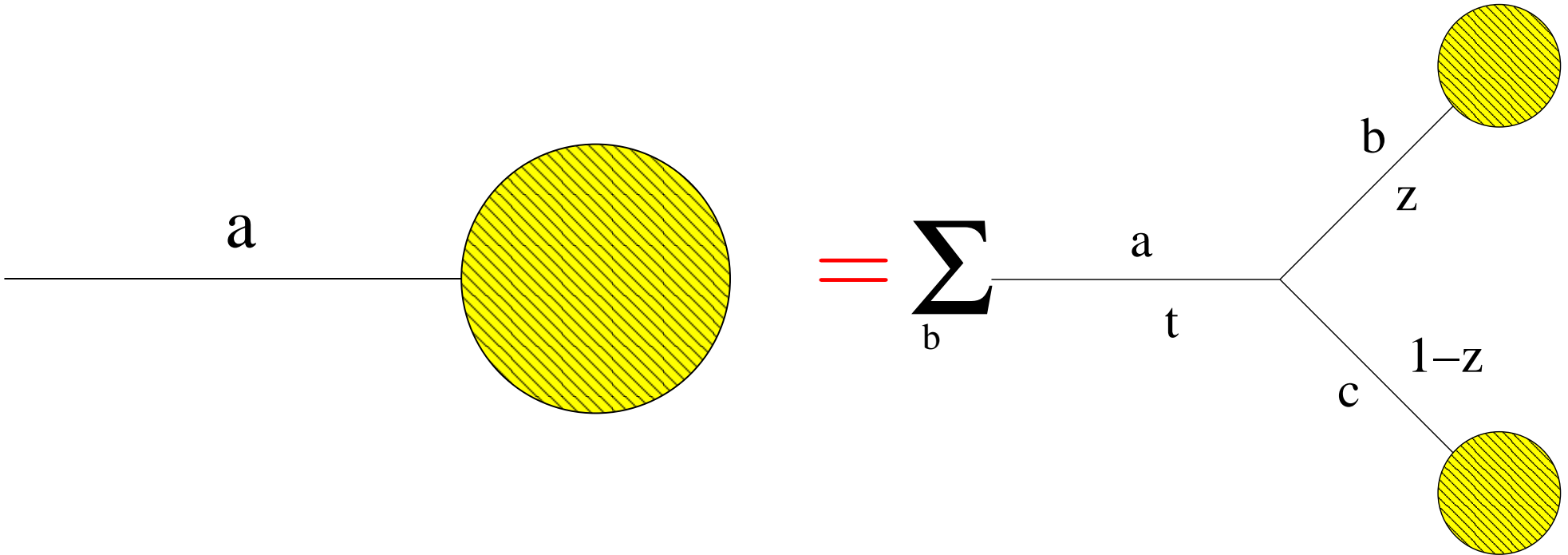
$$\Delta_a(Q_1^2, Q_2^2)$$

the probability that  $a$  **does not branch** for virtualities  $Q_2^2 < t < Q_1^2$

With this, it is easy to write a formula that takes into account all the branches in a branching tree:

$$\begin{aligned} \Phi_a[E, Q^2] &= \Delta_a(Q^2, Q_0^2) \Phi_a[E, Q_0^2] \\ &+ \int_{Q_0^2}^{Q^2} \frac{dt}{t} \Delta_a(Q^2, t) \sum_b \int dz \frac{\alpha_s}{2\pi} P_{ba}(z) \Phi_b[zE, t] \Phi_c[(1-z)E, t] \end{aligned}$$

which has an immediate pictorial representation



Now simply impose that no information is lost during the parton shower: the sum of all the probabilities associated with the branchings of partons must be one. Therefore

$$1 = \Delta_a(Q^2, Q_0^2) + \int_{Q_0^2}^{Q^2} \frac{dt}{t} \Delta_a(Q^2, t) \sum_b \int dz \frac{\alpha_s}{2\pi} P_{ba}(z)$$

which can be solved:

$$\Delta_a(Q^2, Q_0^2) = \exp \left( - \int_{Q_0^2}^{Q^2} \frac{dt}{t} \sum_b \int dz \frac{\alpha_s}{2\pi} P_{ba}(z) \right)$$

## Note

- ▶ This Sudakov form factor looks familiar to those who know resummation techniques
- ▶ *Some* virtual corrections must be included, otherwise unitarity couldn't be imposed!

It's clear that a Sudakov must appear: resummation and parton shower describe the same physics

## Double logs

Keep in mind: this treatment is valid only in the collinear limit. Choices which affect the behaviour away from this limit are equivalent

For example, the choice of the shower variable  $t$  affects the double-log structure

$$\begin{aligned} t \equiv Q^2 &= z(1-z)\theta^2 E^2 \quad (\text{virtuality}) &\implies & \frac{1}{2} \log^2 \frac{t}{E^2} \\ t \equiv p_T^2 &= z^2(1-z)^2 \theta^2 E^2 \quad (p_T^2) &\implies & \frac{1}{4} \log^2 \frac{t}{E^2} \\ t \equiv \tilde{t} &= \theta^2 E^2 \quad (\text{angle} \times \text{energy}) &\implies & \log \frac{t}{\Lambda} \log \frac{E}{\Lambda} \end{aligned}$$

owing to soft divergences. Note in fact that:

$$\frac{d\theta^2}{\theta^2} = \frac{dQ^2}{Q^2} = \frac{dp_T^2}{p_T^2} = \frac{d\tilde{t}}{\tilde{t}}$$

So the study of soft emission may give extra information on the proper choice for  $t$

## Soft emissions

Re-use the formulae derived before (with  $\mathbf{T}_p \equiv \vec{Q}_p$  to avoid confusions with virtuality)

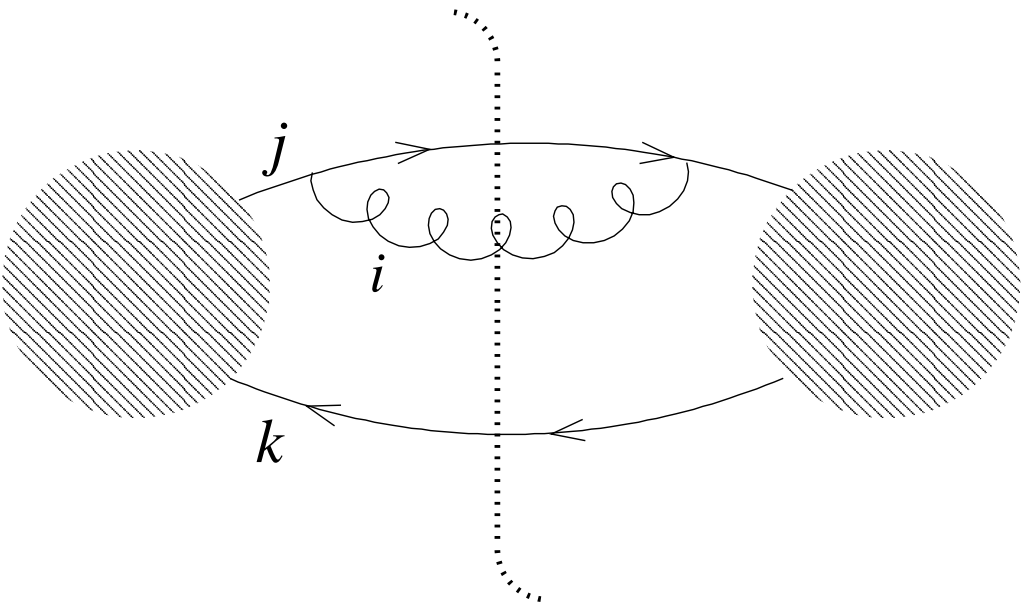
$$d\bar{\sigma}_{N+1} = -d\bar{\sigma}_N \frac{dE_i}{E_i} \frac{d\Omega_i}{2\pi} \frac{\alpha_S}{2\pi} \sum_{jk} \mathbf{T}_j \cdot \mathbf{T}_k \frac{\zeta_{jk}}{\zeta_{ij}\zeta_{ik}}$$

Gluon  $i$  has collinear singularities to  $j$  and  $k$

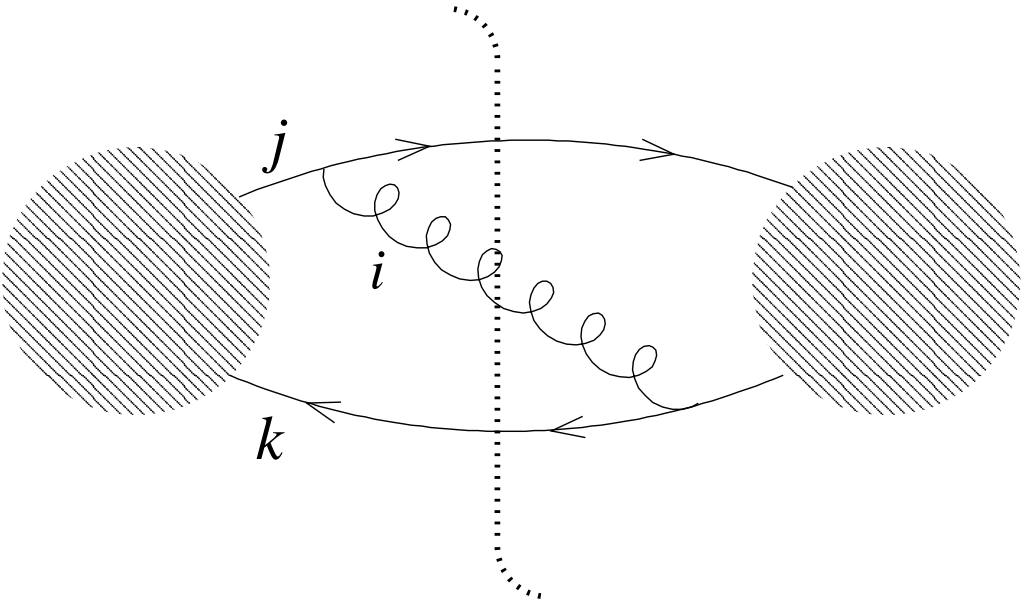
$$\zeta_{ab} = \frac{k_a \cdot k_b}{E_a E_b} = 1 - \cos \theta_{ab}$$
$$\mathbf{T}_g^2 = C_A, \quad \mathbf{T}_q^2 = C_F$$

When iterating this formula to the next emission, one gets

- ▶ A non-positive definite expression (owing to interference)
- ▶ A non-Markovian structure (step 2 depends on step 1 and 0)



Collinear



Soft

## Manipulate the radiation function

$$W_{jk} = \frac{\zeta_{jk}}{\zeta_{ij}\zeta_{ik}} = W_{jk}^{[j]} + W_{jk}^{[k]}$$
$$W_{jk}^{[j]} = \frac{1}{2} \left( \frac{\zeta_{jk}}{\zeta_{ij}\zeta_{ik}} + \frac{1}{\zeta_{ij}} - \frac{1}{\zeta_{ik}} \right)$$

This decomposition has two remarkable properties

- ▶ It disentangles the collinear singularities  $i \parallel j$  and  $i \parallel k$
- ▶ It has *angular ordering*

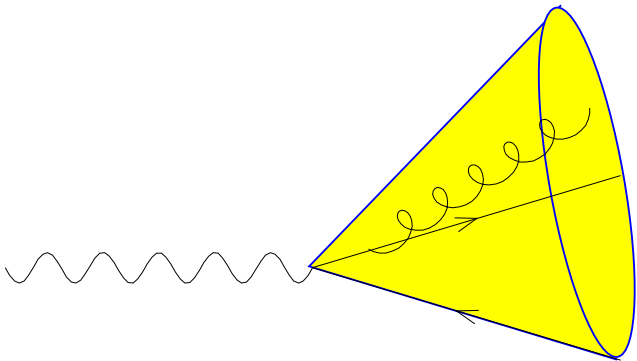
$$\int_0^{2\pi} d\phi_{ij} W_{jk}^{[j]} = \begin{cases} 1/\zeta_{ij} & \zeta_{ij} < \zeta_{jk} \\ 0 & \zeta_{ij} > \zeta_{jk} \end{cases}$$

Angular ordering is a manifestation of (destructive) interference effects present in gauge theories – eg in QED

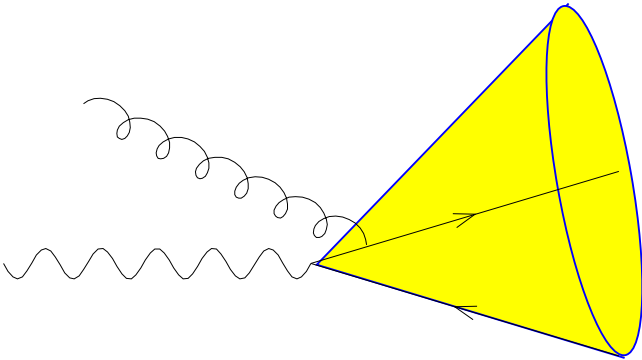


The radiation of a soft gluon is confined in the cone defined by the two partons that “exchange” the gluon

This is how one can depict it:



Allowed



Suppressed

Remember the general property of soft-gluon emissions:

$$\widehat{\mathcal{A}}^{(n+1)}(\dots k_k, k, k_l, \dots) \xrightarrow{k \rightarrow 0} g^2 \left( \frac{k_l \cdot \epsilon}{k_l \cdot k} - \frac{k_k \cdot \epsilon}{k_k \cdot k} \right) \widehat{\mathcal{A}}^{(n)}(\dots k_k, k_l, \dots)$$

In this case, there is a unique colour flow at the Born level, hence this property applies to the whole amplitude

The radiation of a soft gluon is confined in the cone defined by the two partons that “exchange” the gluon

This looks like a frame-dependent statement, but it is not

In the rest frame of the emitting dipole, the emitters are back to back, and the gluon can be emitted at any angle

Now if a boost is performed, the emitters and the gluon will all be squeezed in the boost direction

This is equivalent to considering a soft emission in the boosted frame, where the angle between the two emitters is small

Angular ordering implies that after azimuthal average we have

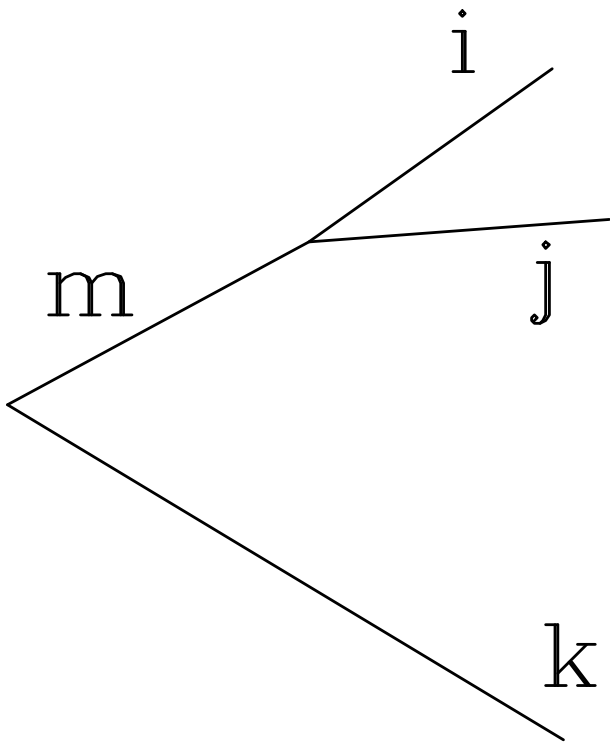
$$d\bar{\sigma}_{N+1} = -d\bar{\sigma}_N \frac{dE_i}{E_i} \frac{\alpha_S}{2\pi} \sum_{jk} 2\mathbf{T}_j \cdot \mathbf{T}_k \int_0^{\zeta_{jk}} \frac{d\zeta_{ij}}{\zeta_{ij}}$$

This looks promising: may be interpreted as

$$\dots \longrightarrow j + k; \quad j \longrightarrow i + j' \dots$$

The process is fully symmetric in  $j \longleftrightarrow k$

In order to study the emission pattern in more details, we must at least consider the next branching



Consider the emission of a soft gluon from the *colour singlet* formed by the three partons  $i$ ,  $j$  and  $k$

The radiation pattern will be obtained by attaching a soft gluon to the three external legs  $i$ ,  $j$ ,  $k$

$$W_{ijk} = -\mathbf{T}_i \cdot \mathbf{T}_j W_{ij} - \mathbf{T}_j \cdot \mathbf{T}_k W_{jk} - \mathbf{T}_i \cdot \mathbf{T}_k W_{ik}$$

Assuming that  $\theta_{mk} \gg \theta_{ij}$  one gets

$$W_{ijk} = \mathbf{T}_i^2 W_{ij}^{[i]} + \mathbf{T}_j^2 W_{ij}^{[j]} + \mathbf{T}_k^2 W_{km}^{[k]} + \mathbf{T}_m^2 W_{km}^{[m]} \Theta(\theta_{mg} > \theta_{ij})$$

- ▶ Inside the cone  $(ij)$ , the gluon is emitted by two independent charges  $\mathbf{T}_i^2$  and  $\mathbf{T}_j^2$
- ▶ Outside of this cone, the gluon cannot resolve  $i$  and  $j$ , and only "sees"  $\mathbf{T}_m^2 = (\mathbf{T}_i + \mathbf{T}_j)^2$

⇒ A Markov structure has emerged:  $(ijk) \equiv ((i+j)k) + (ij)$

Indeed, we can obtain

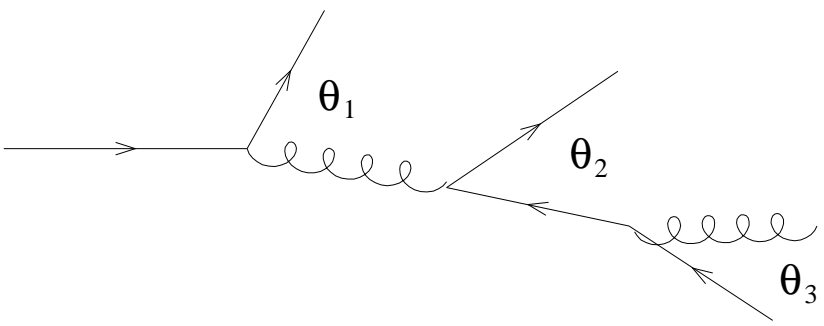
$$W_{ijk} = \mathbf{T}_i^2 W_{ij}^{[i]} + \mathbf{T}_j^2 W_{ij}^{[j]} + \mathbf{T}_k^2 W_{km}^{[k]} + \mathbf{T}_m^2 W_{km}^{[m]} \Theta(\theta_{mg} > \theta_{ij})$$

as a two-step branching process. First, attach the soft gluon to the pair  $(mk)$ , ie

$$\mathbf{T}_k^2 W_{km}^{[k]} + \mathbf{T}_m^2 W_{km}^{[m]}$$

Note that  $m$  is on shell!. Next, after the branching  $m \rightarrow ij$  with  $\theta_{ij} < \theta_{mg}$ , attach the soft gluon to the pair  $(ij)$ , ie

$$\mathbf{T}_i^2 W_{ij}^{[i]} + \mathbf{T}_j^2 W_{ij}^{[j]}$$



Angular ordering

$$\theta_1 > \theta_2 > \theta_3$$

We have therefore obtained that, after an azimuthal average, soft emissions can be treated as a Markov process with probability

$$dP_i = 2\mathbf{T}_i^2 \frac{\alpha_S}{2\pi} \frac{d\zeta}{\zeta} \frac{dE_i}{E_i}$$

with the pre-factor of 2 coming from the symmetrization over eikonals in the original formula

Defining  $z$  such that

$$\frac{dE_i}{E_i} = \frac{dz}{z}$$

one observes that  $2\mathbf{T}_i^2/z$  is the leading-soft behaviour of the relevant Altarelli-Parisi kernel. This is all we need to guess the branching probability which describes soft **and/or** collinear emissions

# Coherent branching

What done above can be combined with the collinear branching stuff. One arrives at a coherent branching formalism, which correctly incorporates collinear *and* soft enhancements to all orders

The most straightforward approach is that of replacing the shower variable  $t$  with  $\zeta = 1 - \cos \theta$ , and impose  $\zeta_{n+1} < \zeta_n$ . Iterated cross section formulae now read

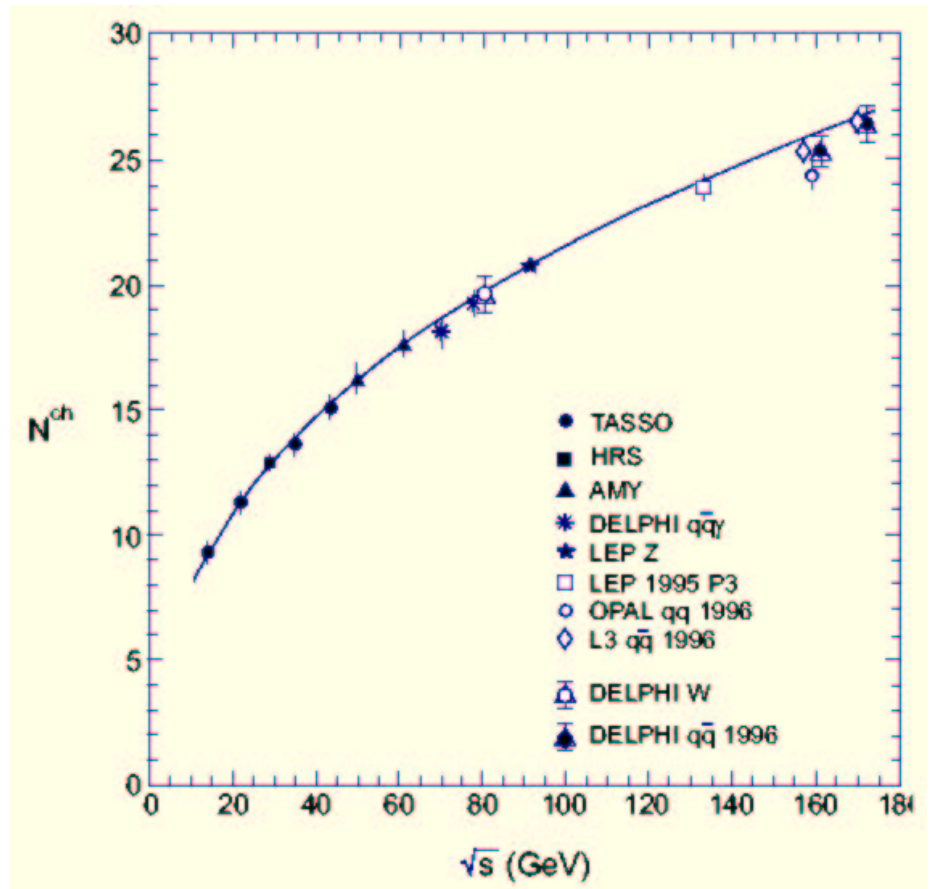
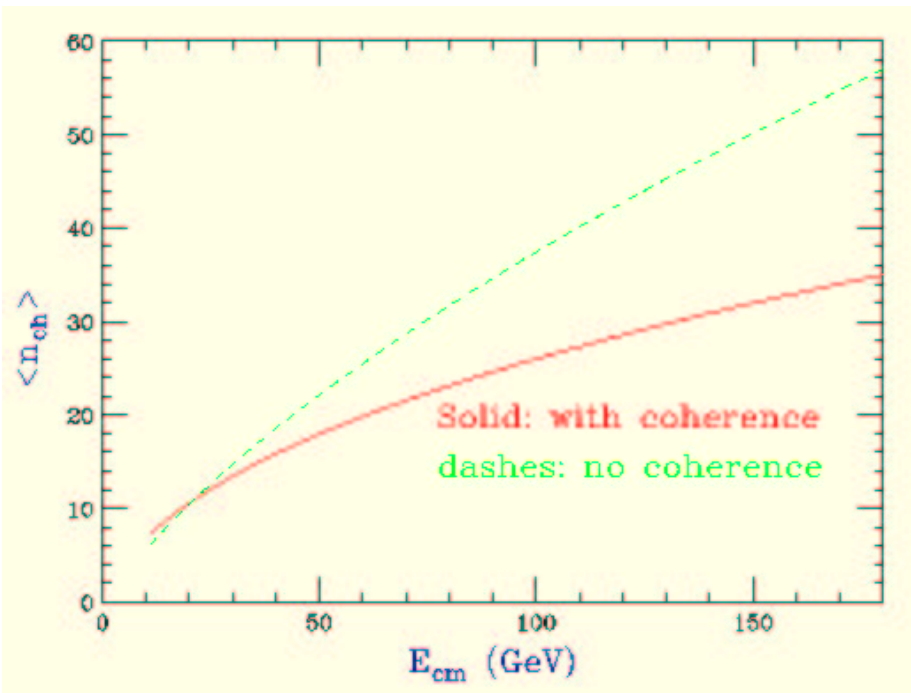
$$d\bar{\sigma}_{N+1} = d\bar{\sigma}_N \frac{d\zeta}{\zeta} dz \frac{\alpha_s}{2\pi} P_{ba}(z)$$

In practice, to take into account emission from non-zero-mass lines, it's more convenient to use as shower variable for  $a \rightarrow bc$  (HERWIG)

$$Q_a^2 = E_a^2 \zeta_a; \quad \zeta_a > \zeta_b \implies Q_b^2 < z_b^2 Q_a^2$$

There are non-accessible kinematic regions (dead zones)





Coherence can be seen in data

Note that coherence reduces the multiplicity wrt to what one would get from fully incoherent radiation

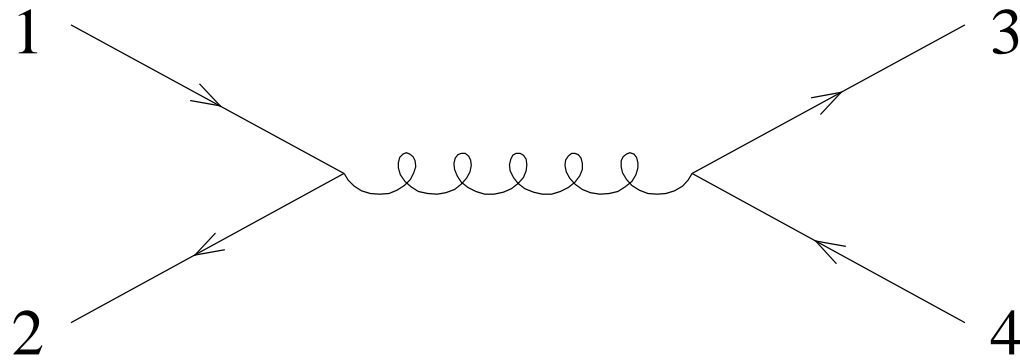
Parton showers are based on a probabilistic and Markovian interpretation of the branching process

Soft emissions are neither positive-definite, nor Markovian, which implies the necessity of non-trivial manipulations in order to be able to take them correctly into account, via angular ordering

It must be kept in mind that angular ordering is exact only  
after azimuthal integration

The simplicity of the case seen so far hides the fundamental question:  
which is the angle that defines the radiation cone?

Suppose one wants to emit a gluon from leg #1:

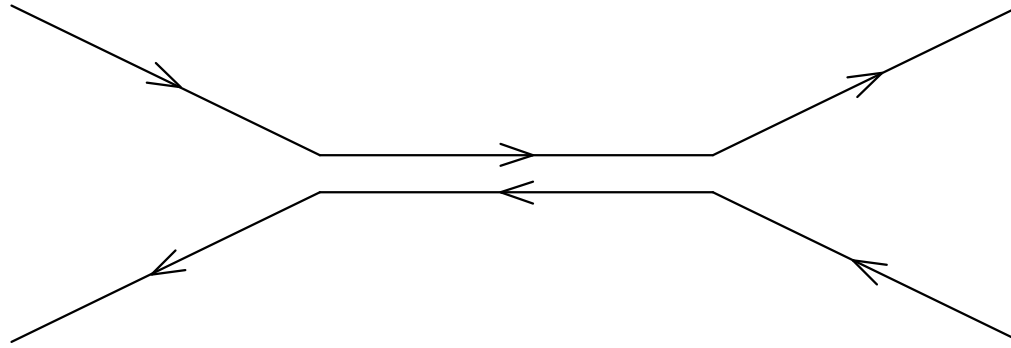


Should one impose  $\theta_{g1} \leq \theta_{12}$ , or  $\theta_{g1} \leq \theta_{13}$ , or  $\theta_{g1} \leq \theta_{14}$ ?

To find the answer, one should keep in mind that at the amplitude level, the dominant contributions are determined by the colour connections of dual amplitudes, and that dual amplitudes are orthogonal at the leading order in  $N$

Hence, the pattern of radiation is driven by the colour connections present in the process before the radiation takes place

Therefore, one draws the colour flow:



Quark #1 is colour-connected with quark #3, hence the radiation will be limited by  $\theta_{13}$

- ▶ The picture is valid at the leading order in  $N$ . It works fairly well
- ▶ A gluon has two colour patterns – choose one of them at random
- ▶ In the case of processes with several colour flows, one of them is picked at random, using  $N \rightarrow \infty$  weights

## Different choices of variables led to:

HERWIG(++)

$t \simeq \text{angle}$

hardest not first

coherent

dead zones

ISR easy

kinematics: difficult

cluster hadr

PYTHIA/SHERPA

$t = \text{virtuality}$

hardest first

coherence forced

no dead zones

ISR easy

kinematics: easy

string/cluster hadr

ARIADNE

$t = p_T^2$

hardest first

coherent

no dead zones

ISR difficult

kinematics: easy

string hadr

- Since 2006 PYTHIA has also  $p_T$ -ordered evolution (PYTHIA8 is only  $p_T$ -ordered). SHERPA will also abandon virtuality order

## Summary of Event Generators

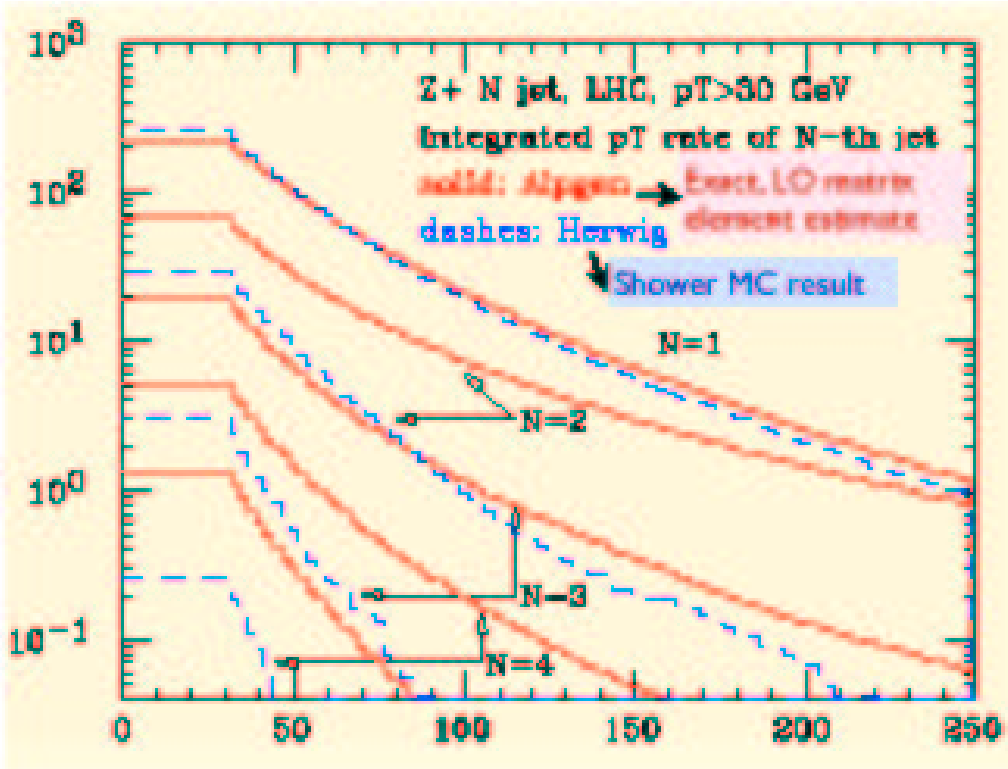
- 0) Start from a *leading order* hard subprocess
- 1) Let initial- and final-state partons branch
- 2) Iterate 1) (ie shower) till reaching a small scale  $Q_0$
- 3) For final-state partons, use a model to convert partons into hadrons; for initial-state partons, force further branchings till valence flavours are generated, and fold with  $f(x, Q_0)$
- 4) Add low- $p_T$  stuff (underlying event, ...)

Given the approximations involved, it is sort of surprising that Event Generators work amazingly well

Sooner or later, however, they will run out of steam

The probability that this happens at the LHC is, unfortunately, not negligible

Plot: M. Mangano



LHC physics is a multi-jet physics

New-physics signal may easily have 5-10 jets (e.g. fully hadronic SUSY Higgs,  $T \rightarrow tW$ , heavy sparticle pair production, ...)

- ▶ MCs are simply unable to reliably simulate these multi-jet events
- ▶ The reason behind this failure is obvious. The parton shower is inherently collinear. The probability associated with well-separated final-state particles is largely underestimated



The message is then:

- ◆ At the LHC, standard MCs are either incapable of describing hard processes, or they do so at the price of rendering it impossible the study of uncertainties

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## The message is then:

- ◆ At the LHC, standard MCs are either incapable of describing hard processes, or they do so at the price of rendering it impossible the study of uncertainties
- ◆ In the context of a reliable computation, the assessment of the theoretical uncertainty is a well defined procedure
- ◆ Hence, what one should do is to give MCs more **predictive power**. This should not and will not *turn them into discovery tools*, but will rather help:
  - ▶ Obtain state-of-the-art simulations of backgrounds
  - ▶ Reduce theory bias on search strategies
  - ▶ Better discriminate among BSM scenarios

## MCs: always keep in mind

Parton Shower Monte Carlos are very flexible, essential tools for experimental physics. But:

- ◆ Each emission in a shower is based on a **collinear approximation**; matrix elements are **leading order**
- ◆ No  $K$  factors, no hard emissions
- ◆ Very good in peak regions, ie the bulk of the cross section
- ◆ Fairly poor in large- $p_T$  tails, ie rare events

It is left to you to determine whether you are using an MC outside the range of validity of its approximation. It is a very common mistake to abuse of this freedom