Non-Perturbative Aspects of Event Simulation

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Set of 2 Lectures for Graduate Students in Particle Physics

1. Non-Perturbative aspects of Event Simulation in *ee* Collisions

2. Non-Perturbative aspects of Event Simulation in *pp* Collisions

(+ optionally: PYTHIA tutorial)

THE ROYAL SOCIETY
THE UNIVERSITY OF WARWICK
Australian Government
Australian Research Council
MCnet

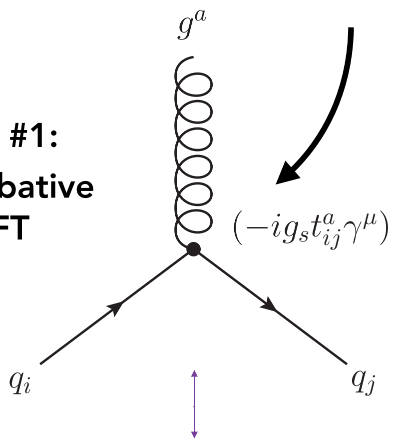
The Problem

Theory Goal: Use LHC measurements to test hypotheses about Nature

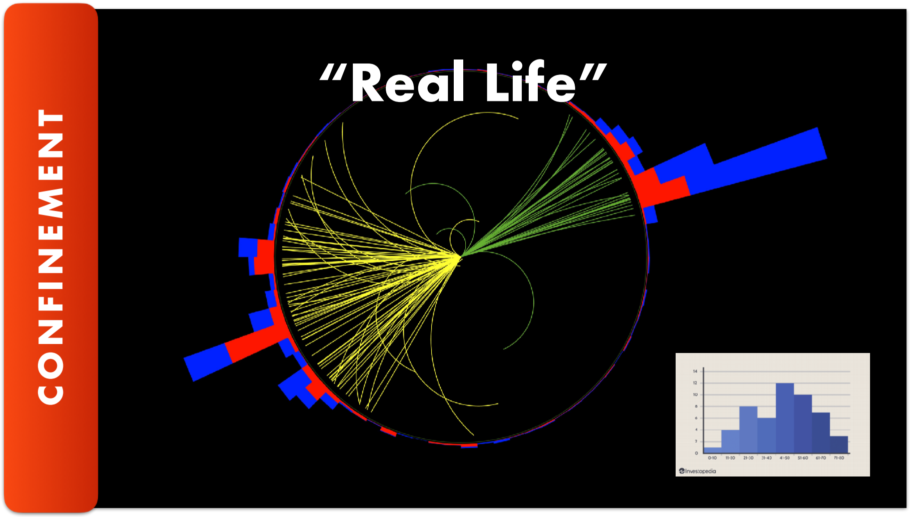
Problem #1: have no exact solutions to QFT for the SM or Beyond
How to make predictions to form (reliable) conclusions?

Elementary Fields, Symmetries, and Interactions

Tool #1: Perturbative QFT



"Fundamental" parameters



Problem #2: we are colliding — and observing — hadrons
Strongly bound states of quarks and gluons.

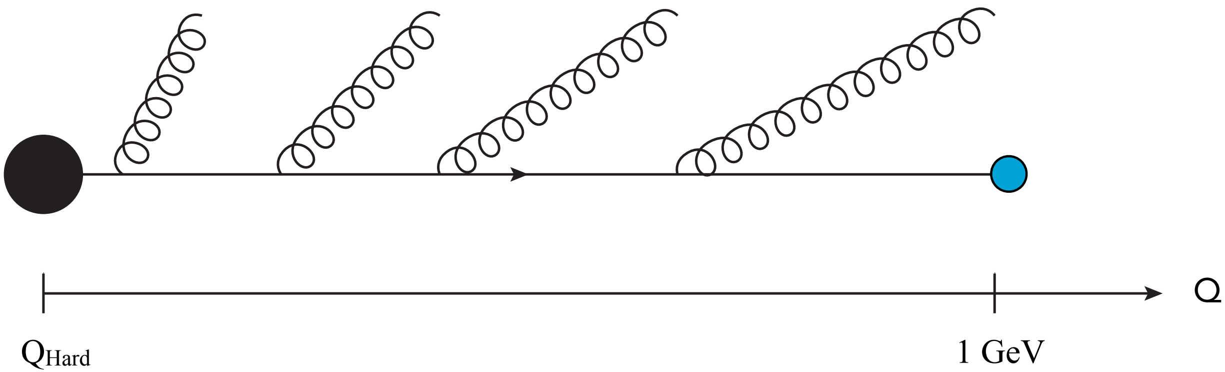
From Partons to Pions

Consider a parton emerging from a hard scattering (or decay) process

Hard means:
Large momentum transfer
$Q_{\text{Hard}} \gg 1\,\text{GeV}$

It showers
(bremsstrahlung)

It ends up
at a low effective
factorization scale
$Q_{\text{Hadronization}} \sim m_\rho \sim 1\,\text{GeV}$



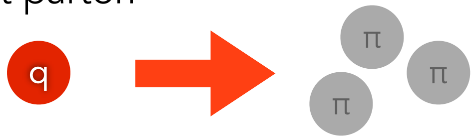
How about I just call it a hadron?
→ "Local Parton-Hadron Duality"

Local Parton Hadron Duality ↔ "Independent Fragmentation"

***L**ocal*
***P**arton*
***H**adron*
***D**uality*

Fast parton

Hadrons



$Q_{\mathrm{Factorization}}$

Momentum fractions $\{x\}$

"Fragmentation Function" $F_{\pi/q}(Q_F, x)$

⬍

Late 70s MC models: Independent Fragmentation

E.g., PYTHIA (then called JETSET) anno 1978

LU TP 78-18 November, 1978

A Monte Carlo Program for Quark Jet Generation

T. Sjöstrand, B. Söderberg

A Monte Carlo computer program is presented, that simulates the **fragmentation of a fast parton into a jet of mesons.** It uses an iterative scaling scheme and is compatible with the jet model of Field and Feynman.

Field-Feynman was an early fragmentation model.

```
      SUBROUTINE JETGEN(N)
      COMMON /JET/ K(100,2), P(100,5)
      COMMON /PAR/ PUD, PS1, SIGMA, CX2, EBEG, WFIN, IFLBEG
      COMMON /DATA1/ MESO(9,2), CMIX(6,2), PMAS(19)
      IFLSGN=(10-IFLBEG)/5
      W=2.*EBEG
      I=0
      IPD=0
C 1 FLAVOUR AND PT FOR FIRST QUARK
      IFL1=IABS(IFLBEG)
      PT1=SIGMA*SQRT(-ALOG(RANF(0)))
      PHI1=6.2832*RANF(0)
      PX1=PT1*COS(PHI1)
      PY1=PT1*SIN(PHI1)
  100 I=I+1
C 2 FLAVOUR AND PT FOR NEXT ANTIQUARK
      IFL2=1+INT(RANF(0)/PUD)
      PT2=SIGMA*SQRT(-ALOG(RANF(0)))
      PHI2=6.2832*RANF(0)
      PX2=PT2*COS(PHI2)
      PY2=PT2*SIN(PHI2)
C 3 MESON FORMED, SPIN ADDED AND FLAVOUR MIXED
      K(I,1)=MESO(3*(IFL1-1)+IFL2,IFLSGN)
      ISPIN=INT(PS1+RANF(0))
      K(I,2)=1+9*ISPIN+K(I,1)
      IF(K(I,1).LE.6) GOTO 110
      TMIX=RANF(0)
      KM=K(I,1)-6+3*ISPIN
      K(I,2)=8+9*ISPIN+INT(TMIX+CMIX(KM,1))+INT(TMIX+CMIX(KM,2))
C 4 MESON MASS FROM TABLE, PT FROM CONSTITUENTS
  110 P(I,5)=PMAS(K(I,2))
      P(I,1)=PX1+PX2
      P(I,2)=PY1+PY2
      PMTS=P(I,1)**2+P(I,2)**2+P(I,5)**2
C 5 RANDOM CHOICE OF X=(E+PZ)MESON/(E+PZ)AVAILABLE GIVES E AND PZ
      X=RANF(0)
      IF(RANF(0).LT.CX2) X=1.-X**(1./3.)
      P(I,3)=(X*W-PMTS/(X*W))/2.
      P(I,4)=(X*W+PMTS/(X*W))/2.
C 6 IF UNSTABLE, DECAY CHAIN INTO STABLE PARTICLES
  120 IPD=IPD+1
      IF(K(IPD,2).GE.8) CALL DECAY(IPD,I)
      IF(IPD.LT.I.AND.I.LE.96) GOTO 120
C 7 FLAVOUR AND PT OF QUARK FORMED IN PAIR WITH ANTIQUARK ABOVE
      IFL1=IFL2
      PX1=-PX2
      PY1=-PY2
C 8 IF ENOUGH E+PZ LEFT, GO TO 2
      W=(1.-X)*W
      IF(W.GT.WFIN.AND.I.LE.95) GOTO 100
      N=I
      RETURN
      END
```

Colour Neutralization

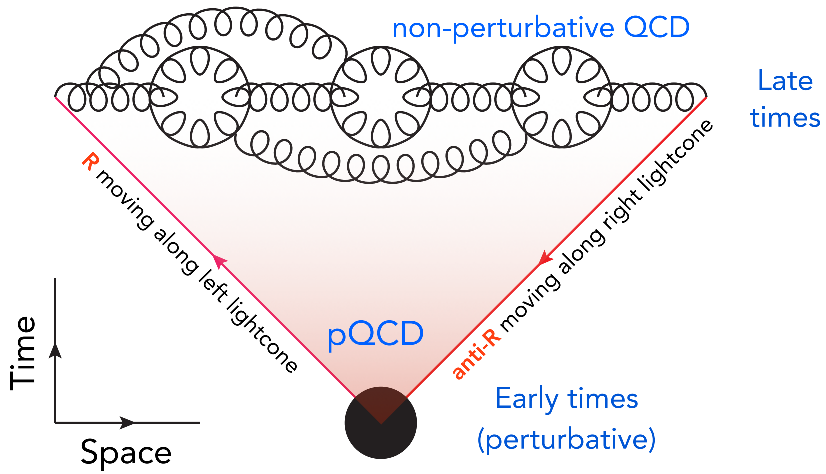
As a **physical** model, however, LPHD is a not a good starting point

The point of confinement is that partons are **coloured**.

A physical hadronization model

Should involve at least **two** partons, with opposite colour charges

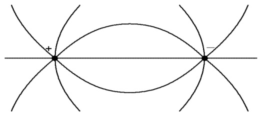
A strong **confining field** emerges between the two when their separation ≳ 1fm



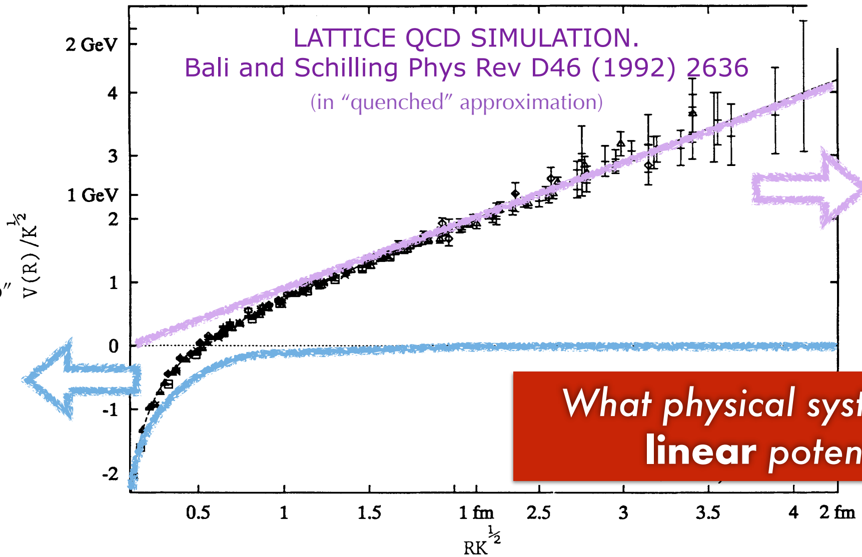
Two Partons: Linear Confinement

In lattice QCD, one can compute the potential energy of a colour-singlet $q\bar{q}$ state, as a function of the distance, r, between the q and $\bar{q}$

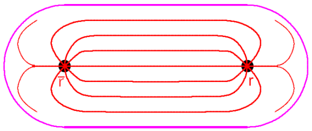
Short Distances ~ "Coulomb"



"Free" Partons



Long Distances ~ Linear Potential



"Confined" Partons
(a.k.a. Hadrons)

"Cornell Potential" fit: $V(r) = -\frac{a}{r} + \kappa r$ with $\kappa \sim 1\ \mathrm{GeV/fm}$ (→ could lift a 16-ton truck)

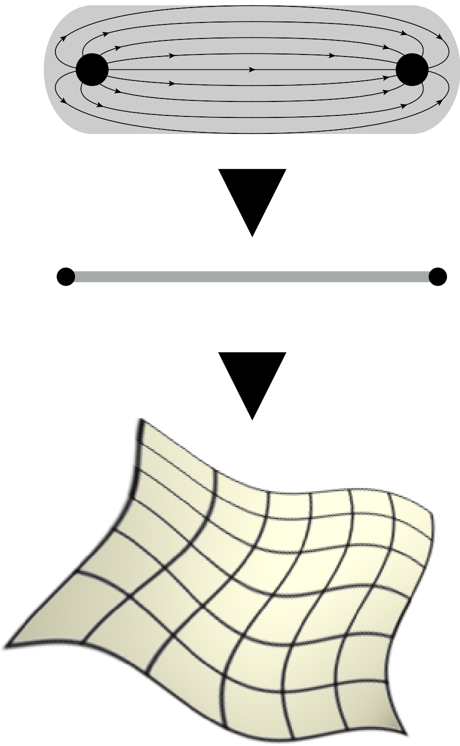
From Partons to Strings

Linear Potential motivates a Model:

Let colour field between each pair of "colour-connected" partons collapse into a **narrow flux tube**

For $|p_z| \gg \Lambda_{\mathrm{QCD}}$: flux tube → much "longer" than "wide"

Limit: infinitely narrow → Relativistic 1+1 dimensional worldsheet — String



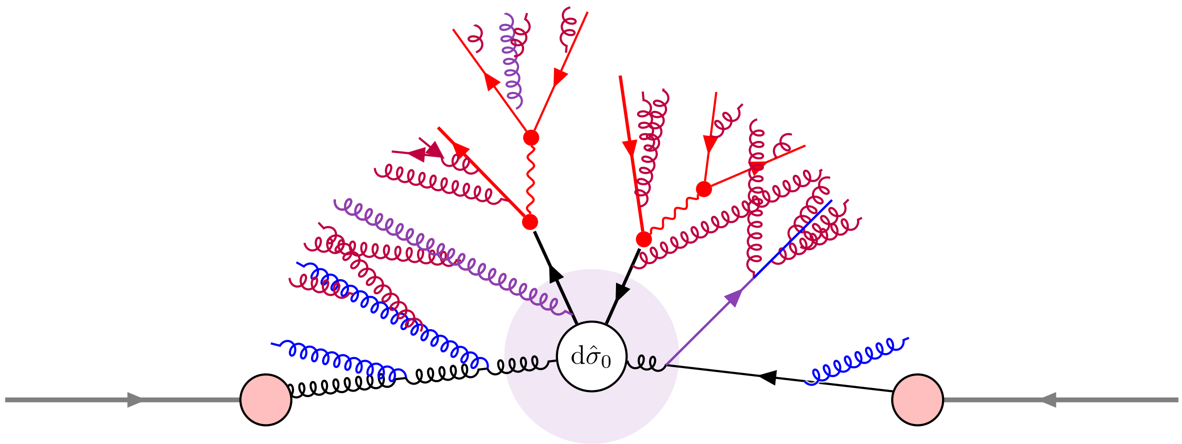
Uniform energy density κ ~ 1 GeV / fm

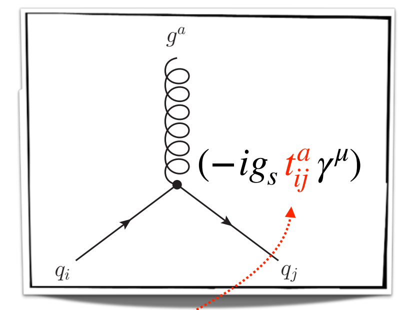
(Neglecting Coulomb effects near endpoints)

What does it mean that two partons are “colour connected”?

Between *which* partons should confining potentials form?

E.g., if we have events with lots of quarks and gluons





Complication:

Every quark-gluon vertex contains an SU(3) Gell-Mann matrix in colour space!

(And $g \to gg$ vertices contain further complicated structures)

➤ **Who ends up confined with whom?**

Colour Tracing

Colour Flow in Event Generators

Event Generators use simplified **"colour flow"** — to trace colour correlations through hard processes & showers ➤ determine which partons end up "colour connected"

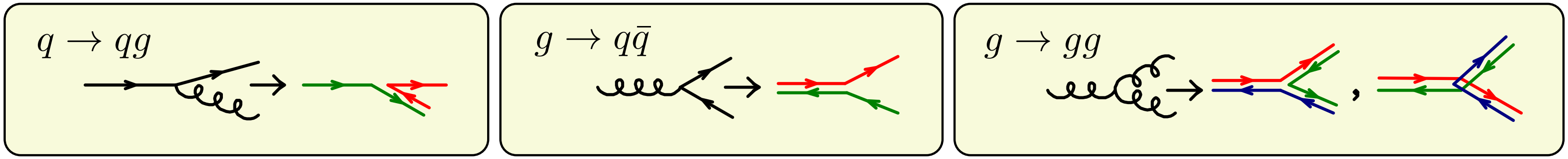
Based on SU(N) group product: $N \otimes \bar{N} = (N^2 - 1) \oplus 1$

- N: Fundamental representation (**quarks**)
- $\bar{N}$: Antifundamental representation (**antiquarks**)
- $(N^2 - 1)$: Adjoint Representation (**gluons**)
- 1: Singlet (becomes irrelevant for large N)

Thus, for large N ("leading colour"), we can approximate $(N^2 - 1) \sim N \otimes \bar{N}$

LC: gluons → direct products of colour and anticolour; for SU(3) this is valid to ~ $1/N_C^2$ ~ 10%

⇛ Rules for colour flow (= colour-space vertices) in MC Event Generators:

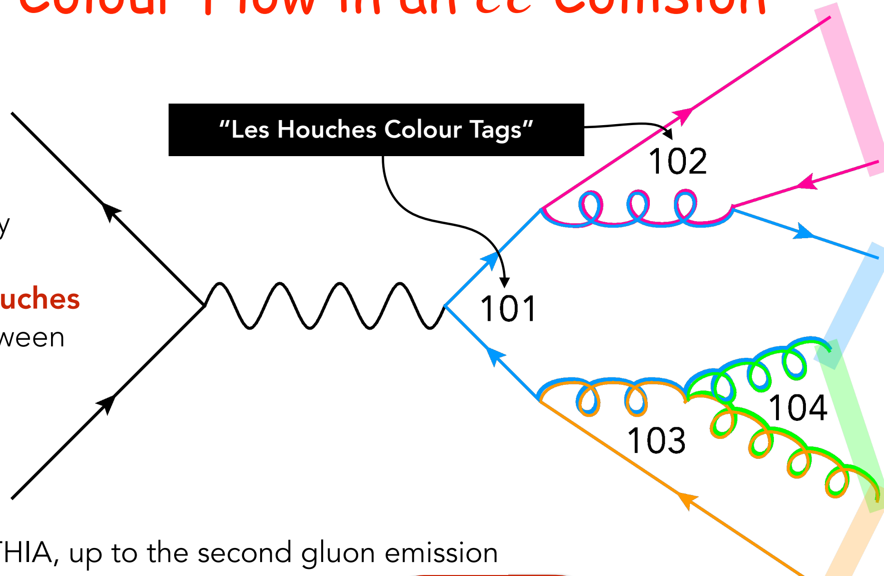


(Note: the "colour dipoles" in dipole and antenna showers are also based on these rules)

LC Colour Flow in an *ee* Collision

MCs: $N_C \to \infty$ limit formalised by letting **each "colour line"** be represented by a **unique Les Houches colour tag**† (no interference between different colour lines in this limit)

†: hep-ph/0109068; hep-ph/0609017



A corresponding event record from PYTHIA, up to the second gluon emission

#	id	name	status	mothers		daughters		colours		p_x	p_y	p_z	e	m
5	23	(Z0)	-22	3	4	6	7			0.000	0.000	0.000	91.188	91.188
6	3	(s)	-23	5	0	10	0	101	0	-12.368	16.523	40.655	45.594	0.000
7	-3	(sbar)	-23	5	0	8	9	0	101	12.368	-16.523	-40.655	45.594	0.000
8	21	(g)	-51	7	0	13	0	103	101	9.243	-9.146	-29.531	32.267	0.000
9	-3	sbar	51	7	0			0	103	3.084	-7.261	-10.973	13.514	0.000
10	3	(s)	-52	6	0	11	12	101	0	-12.327	16.406	40.505	45.406	0.000
11	21	g	-51	10	0			101	102	-2.834	-2.408	1.078	3.872	0.000
12	3	s	51	10	0			102	0	-10.246	17.034	38.106	42.979	0.000
13	21	g	52	8	0			103	101	9.996	-7.366	-28.211	30.823	0.000

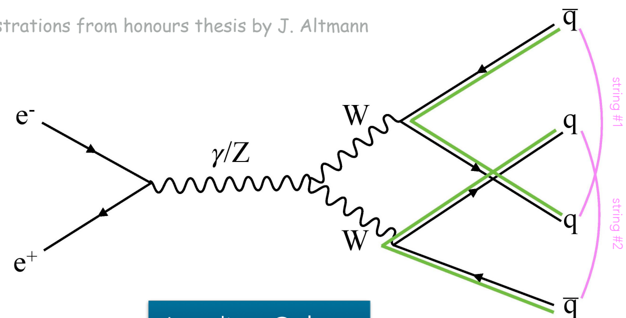
Colour Reconnections? (CR)

NB: much more important in LHC collisions ➜ next lecture

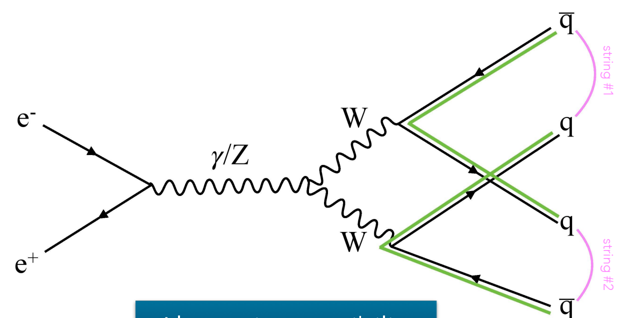
Consider two (uncorrelated) parton systems

Textbook example: $e^+e^- \to W^+W^- \to \text{hadrons}$

Illustrations from honours thesis by J. Altmann



Leading Colour



Alternative possibility

Probability for uncorrelated $q\bar{q}$ pair to **accidentally** be in colour-singlet state follows from $3 \otimes \bar{3} = 8 \oplus 1$ ☛ 1 in 9 ☚ $= 1/N_C^2$

With a probability of 1/9, both options should be possible (remaining 8/9 allow LC only)

Choose "lowest-energy" one (cf action principle) (assuming genuine quantum superpositions to be rare.)

➜ small shift in W mass ("string drag") (➜ now important for top quark mass at LHC)

LEP-2: No-CR excluded at 99.5% CL [Phys.Rept. 532 (2013) 119; arXiv:1302.3415]

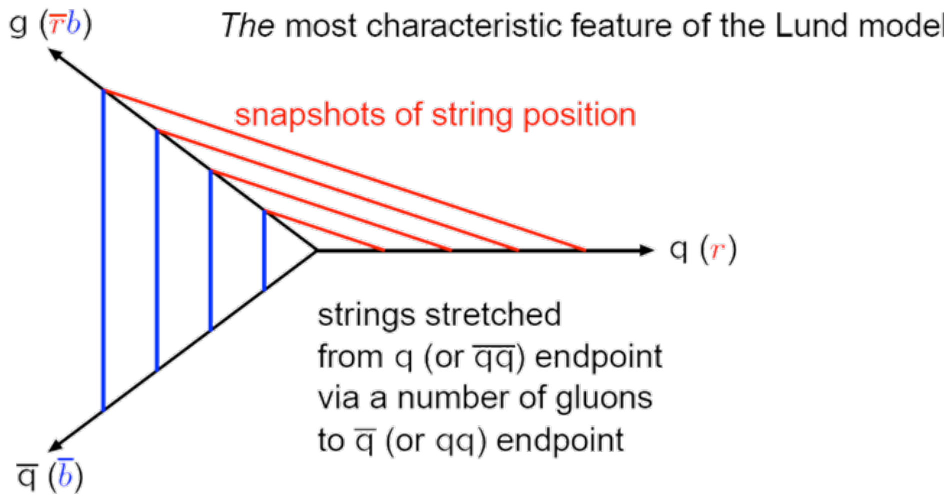
Measurements consistent with $\sim 1/N_C^2$ expectation but not much detailed information.

From Partons to Strings

Map:

Quarks → String Endpoints

Gluons → Transverse Excitations (kinks)



Gluon = kink on string, carrying energy and momentum

Physics then in terms of string worldsheet evolving in spacetime

"Nambu-Goto action" $\Longrightarrow$ Area Law.
(Classically equivalent to Polyakov Action)

Fundamental concepts in string theory. Beyond scope of these lectures.

The motion of strings

In Spacetime:

$$\left|\frac{dE}{dz}\right| = \left|\frac{dp_z}{dz}\right| = \left|\frac{dE}{dt}\right| = \left|\frac{dp_z}{dt}\right| = \kappa$$

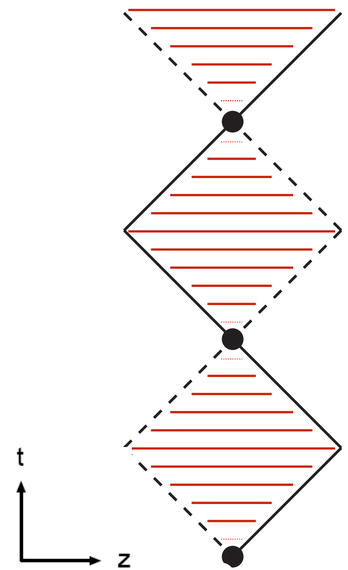
String tension ≈ 1 GeV/fm

→ a 10-GeV quark can travel 10 fm before all its kinetic energy is transformed to potential energy in the string.

Then it must start moving the other way.

For small kinetic energies ($\lesssim$ 1 GeV)

→ "yo-yo" model of mesons: ⟶



$$t = \frac{2\sqrt{s}}{\kappa}$$

$$t = \frac{\sqrt{s}}{\kappa}$$

$$t = \frac{\sqrt{s}}{2\kappa}$$

$$t = 0$$

For larger kinetic energies

String breaks → several mesons

→ String Fragmentation

(Note: formulated in momentum space, not spacetime)

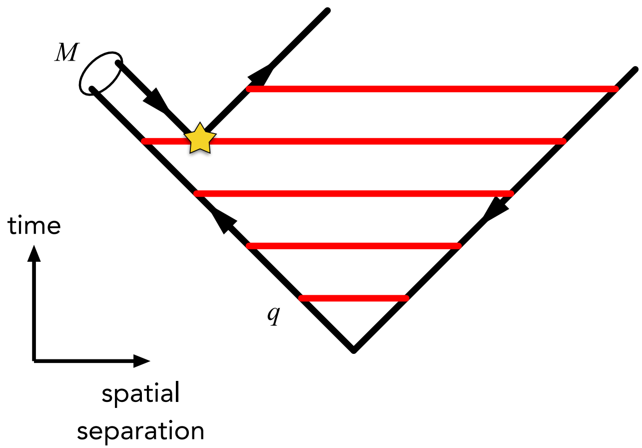
String Breaking

In "unquenched" QCD

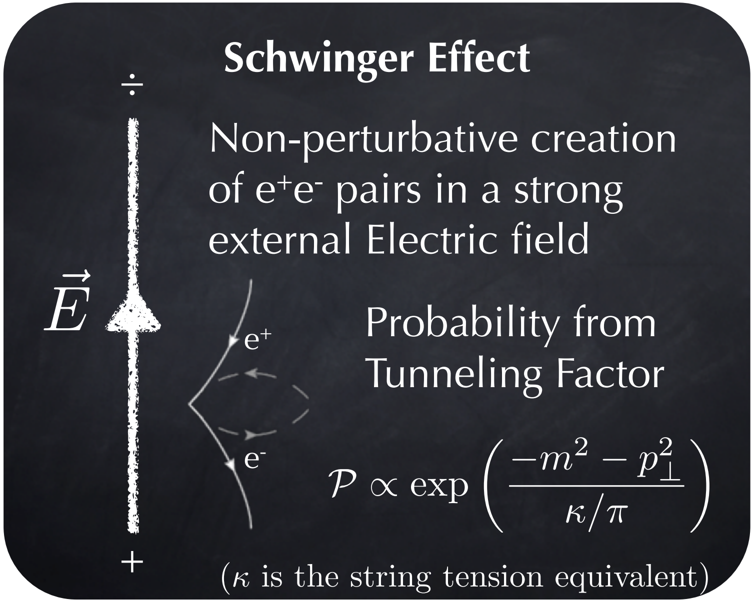
$g \to q\bar{q} \implies$ The strings will "break"

Non-perturbative so can't use $P_{g\to q\bar{q}}(z)$

Our model: Schwinger mechanism →



J. Schwinger, Phys. Rev. **82** (1951) 664



→ Gaussian suppression of high $m_\perp = \sqrt{m_q^2 + p_\perp^2}$

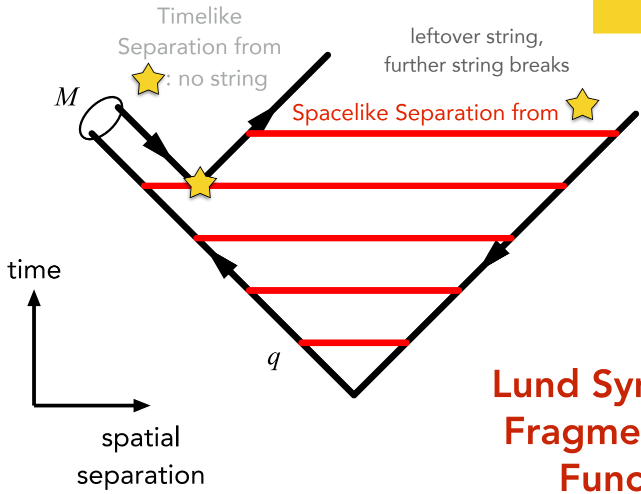
Assume probability of string break constant per unit world-sheet area

The String Fragmentation Function (in momentum space)

Consider a string break ⭐, producing a meson M, and a leftover string piece

The meson M takes a fraction z of the quark momentum,

Probability distribution in $z \in [0,1]$ parametrised by **Fragmentation Function**, $f(z, Q^2_{\mathrm{HAD}})$



Observation: All string breaks are **causally disconnected**

Lorentz invariance $\Longrightarrow$ string breaks can be considered in *any order*. Imposes "left-right symmetry" on the **FF**

$\Longrightarrow$ **FF** constrained to a form with **two free parameters**, a & b: constrained by fits to measured hadron spectra

Lund Symmetric Fragmentation Function

$$f(z) \propto \frac{1}{z}(1-z)^a \exp\left(-\frac{b(m_h^2 + p_{\perp h}^2)}{z}\right)$$

Supresses high-z hadrons (↑ a)

Supresses low-z hadrons (↑ b)

Will return to illustrations of these parameters later (tuning)

The Lund Symmetric Fragmentation Function

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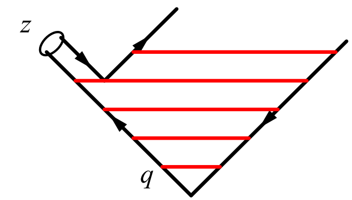
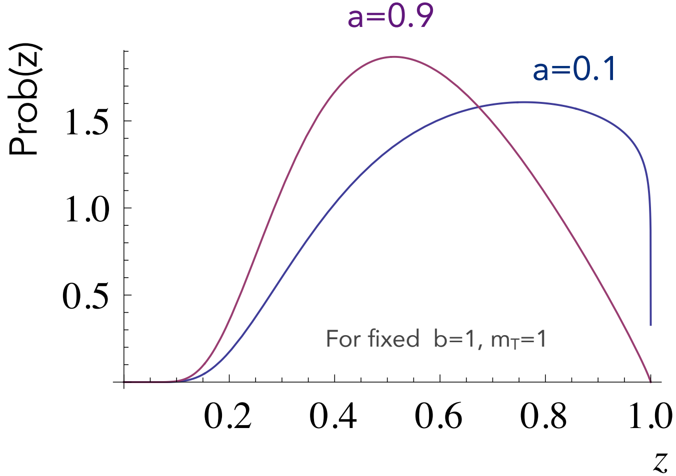
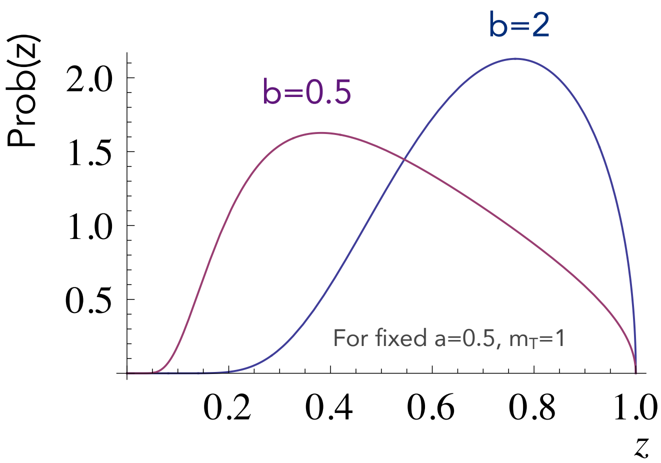






Note: In principle, a can be flavour-dependent. In practice, we usually only distinguish between baryons and mesons

Demonstration

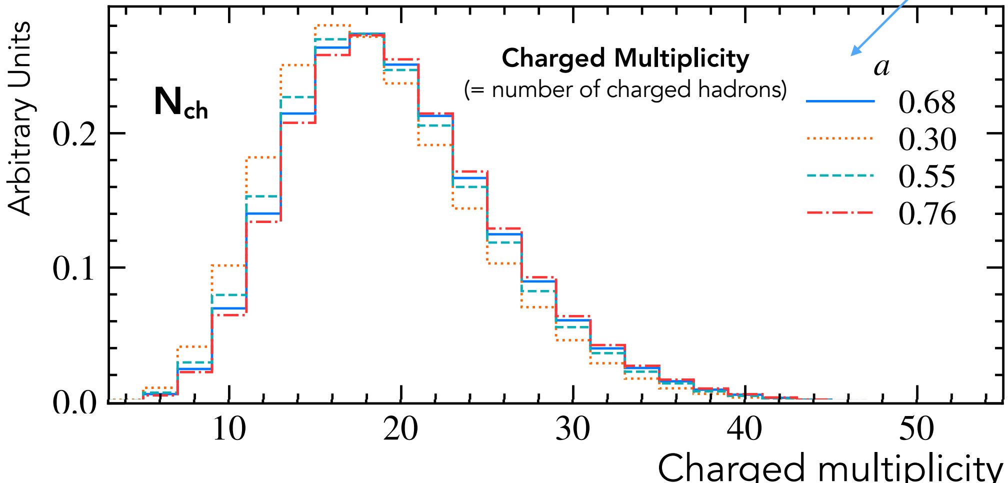
[*Reweighting MC Predictions & Automated Fragmentation Variations in Pythia 8*, 2308.13459]

Example: Varying the a Parameter (Lund Symmetric FF)

$f(z)$ ~ **scaled light-cone hadron momentum fraction** $\propto \frac{1}{z^{1+r_Q b m_Q^2}}(1-z)^a \exp\left(-\frac{b m_\perp^2}{z}\right)$

variations

Probability Distribution

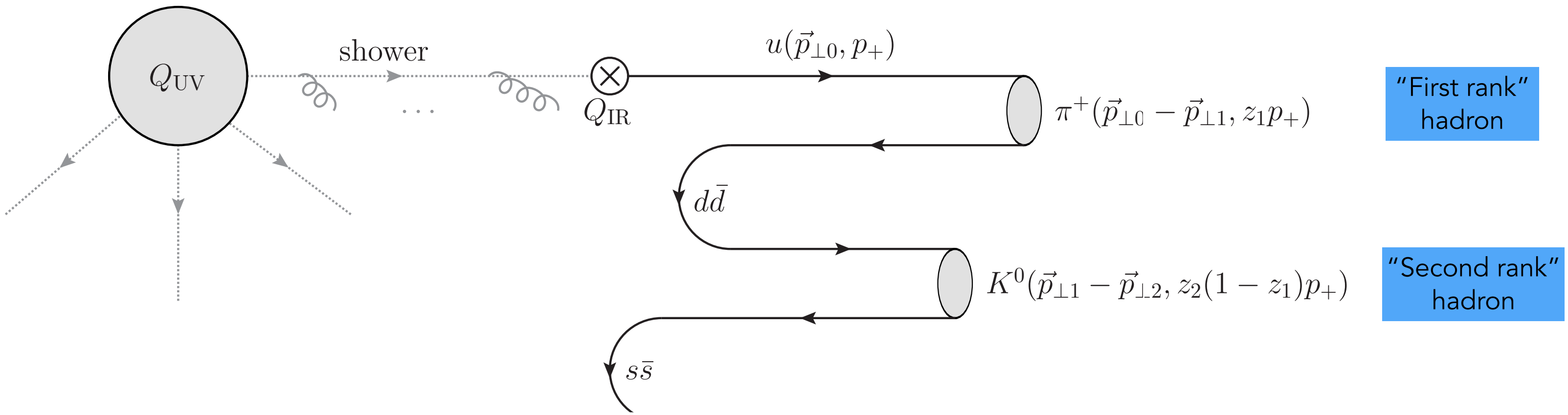


Question:
Why small a $\Rightarrow$ fewer hadrons?

Iterative String Breaks (in momentum space)

Recall: String breaks are causally disconnected → **May iterate from outside-in**

Note: using light-cone momentum coordinates: $p_+ = E + p_z$



On average, expect energy* of n[th] "rank" hadron to scale like ~

$$E_n \sim \langle z \rangle (1 - \langle z \rangle)^{n-1} E_0$$

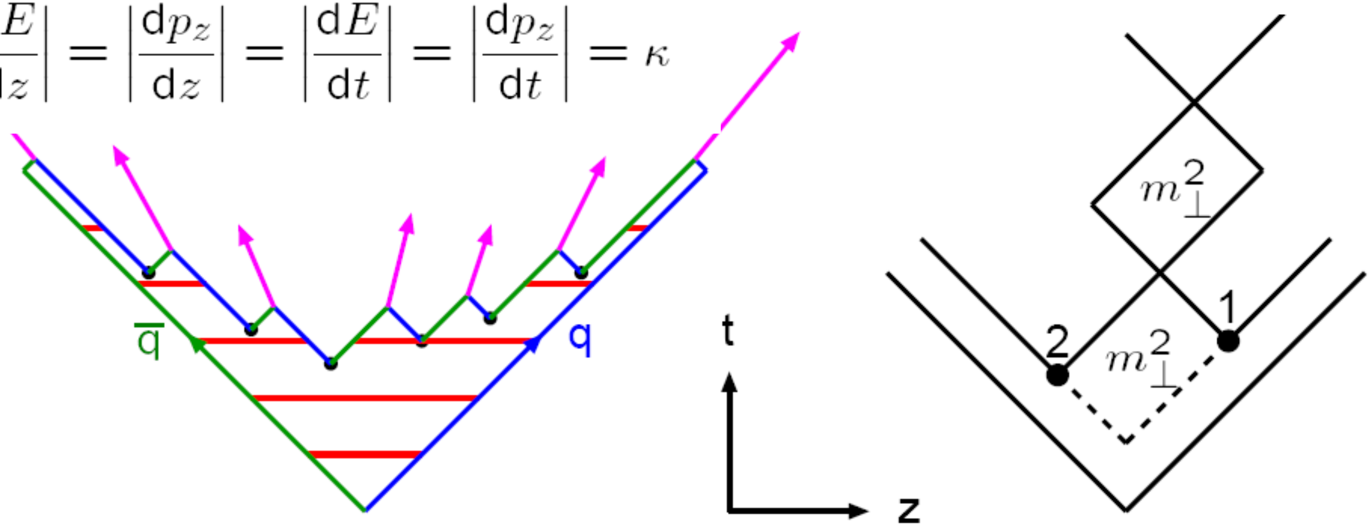
*) more correctly, the p_+ light-cone momentum coordinate

Breakup of a String System (in spacetime)

Illustrations by T. Sjöstrand

Repeat for large system → Lund Model

$$\left|\frac{\mathrm{d}E}{\mathrm{d}z}\right| = \left|\frac{\mathrm{d}p_z}{\mathrm{d}z}\right| = \left|\frac{\mathrm{d}E}{\mathrm{d}t}\right| = \left|\frac{\mathrm{d}p_z}{\mathrm{d}t}\right| = \kappa$$



A simple prediction: constant rapidity density of hadrons along string

Rapidity

$$y = \frac{1}{2}\ln\left(\frac{E+p_z}{E-p_z}\right) = \frac{1}{2}\ln\left(\frac{(E+p_z)^2}{E^2-p_z^2}\right) \to \ln\left(\frac{2E}{m_\perp}\right)$$

(in limit of small $m_\perp = \sqrt{m^2+p_\perp^2} \ll E$)

Recall: **expect energy of n^th^ "rank" hadron** $E_n \sim \langle z \rangle (1 - \langle z \rangle)^{n-1} E_0$

$$\implies y_n \sim y_1 + (n-1)\ln\left(1-\langle z\rangle\right)$$

Rapidity difference between two adjacent hadrons:

$$\Delta y = y_{n+1} - y_n \sim \ln\left(1-\langle z\rangle\right)$$

$\longleftarrow$ Constant, independent of n (and of E_0)

Predicts a flat (uniform) rapidity "plateau" (along the string axis):

Also called **"Lightcone scaling";** this is exactly what is observed in practice.

The Rapidity Plateau

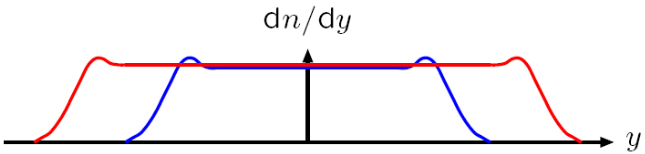
Expect ~ flat Rapidity Plateau along string axis

Estimate of rapidity range for fixed E_q:

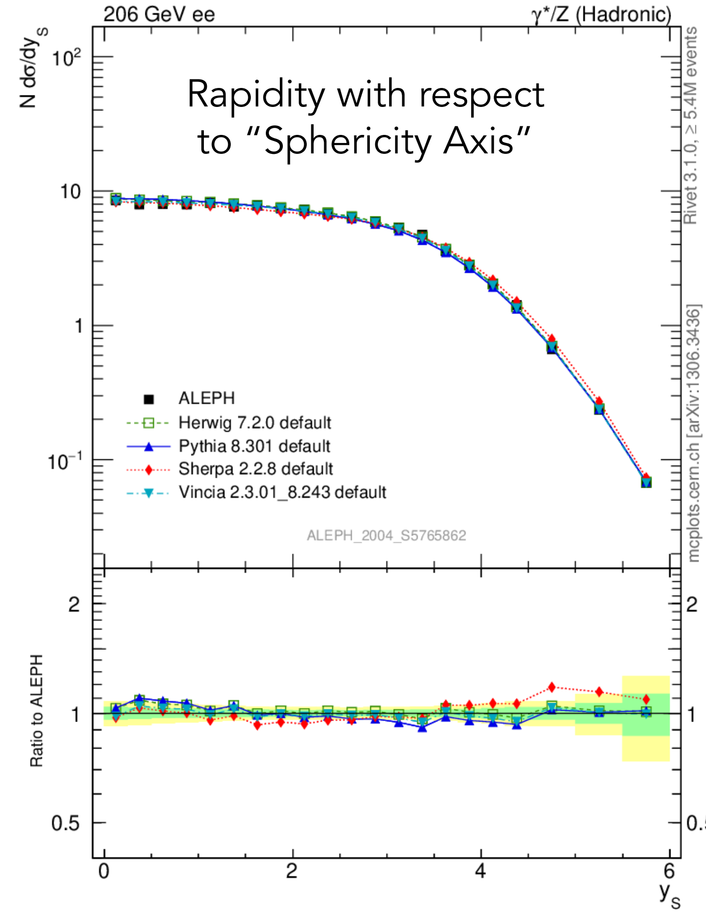
$$\langle y \rangle_1 \sim \ln \left(\frac{2 \langle z \rangle E_q}{\langle m_\perp \rangle} \right)$$

~ 5 for $E_q \sim$ 100 GeV, <z> ~ 0.5, and $\langle m_\perp \rangle \sim 0.5$ GeV

Changing $E_q \Longrightarrow$ logarithmic change in rapidity range:



$\langle n_{ch} \rangle \approx c_0 + c_1 \ln E_{cm}$, ~ Poissonian multiplicity distribution



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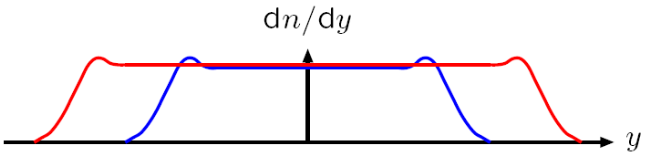

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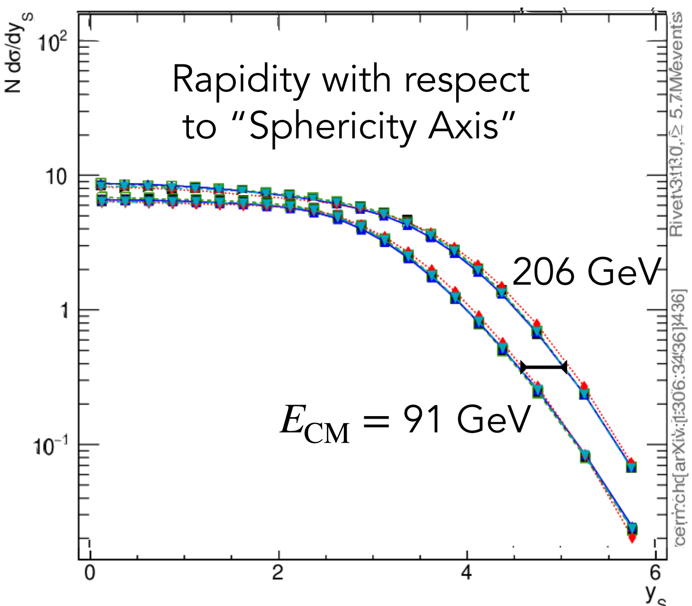


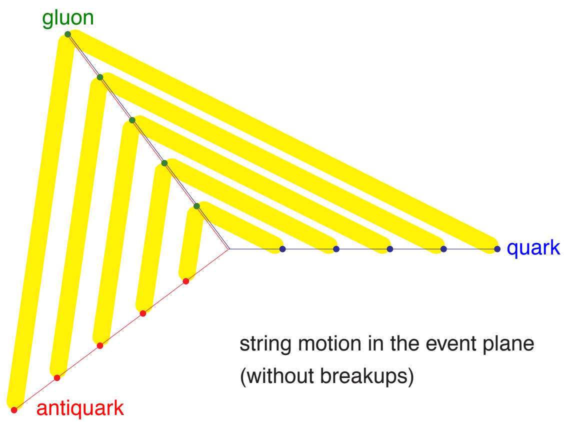
$$\ln\left(\frac{206}{91}\right) = 0.8$$

Actual difference is smaller $\longmapsto \sim 0.5$

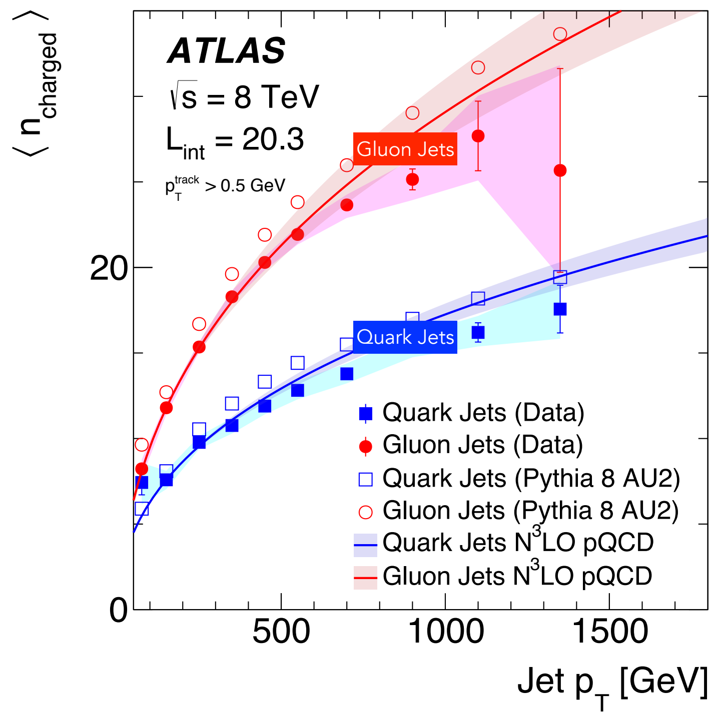
(some energy also goes to increase particle production in the central region, **3-jet events**)

Gluon Kinks: The Signature Feature of the Lund Model

Gluons are connected to two string pieces



ATLAS, Eur.Phys.J. C76 (2016) no.6, 322



Each quark connected to **one** string piece

Expect factor ~ $2 \sim C_A/C_F$ more particles in gluon jets

Important for discriminating new-physics signals

Decays to **quarks** vs decays to **gluons**,

vs composition of **background** and **bremsstrahlung** combinatorics

See also
Larkoski et al., JHEP 1411 (2014) 129
Thaler et al., Les Houches, arXiv:1605.04692

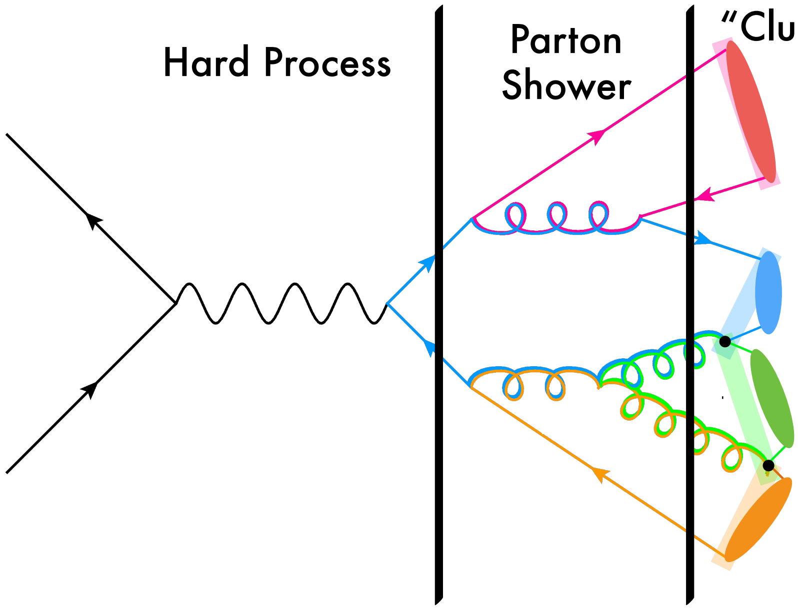
(Alternative: **The Cluster Model** — Used in Herwig and Sherpa)

In "unquenched" QCD

$g \to q\bar{q} \implies$ The strings will "break"

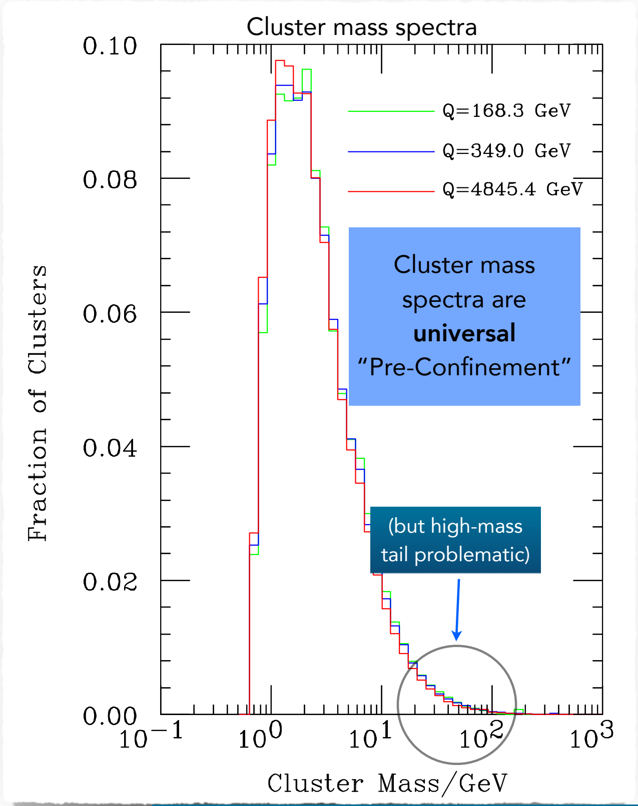
Non-perturbative so can't use $P_{g\to q\bar{q}}(z)$

Alternative: **force** $g \to q\bar{q}$ at end of shower



Isotropic 2-body decays to hadrons

According to phase space



Large clusters → string-like splittings

Next Lecture: LHC collisions

Hard Process
- Hard Interaction
- Resonance Decays
- MECs, Matching & Merging

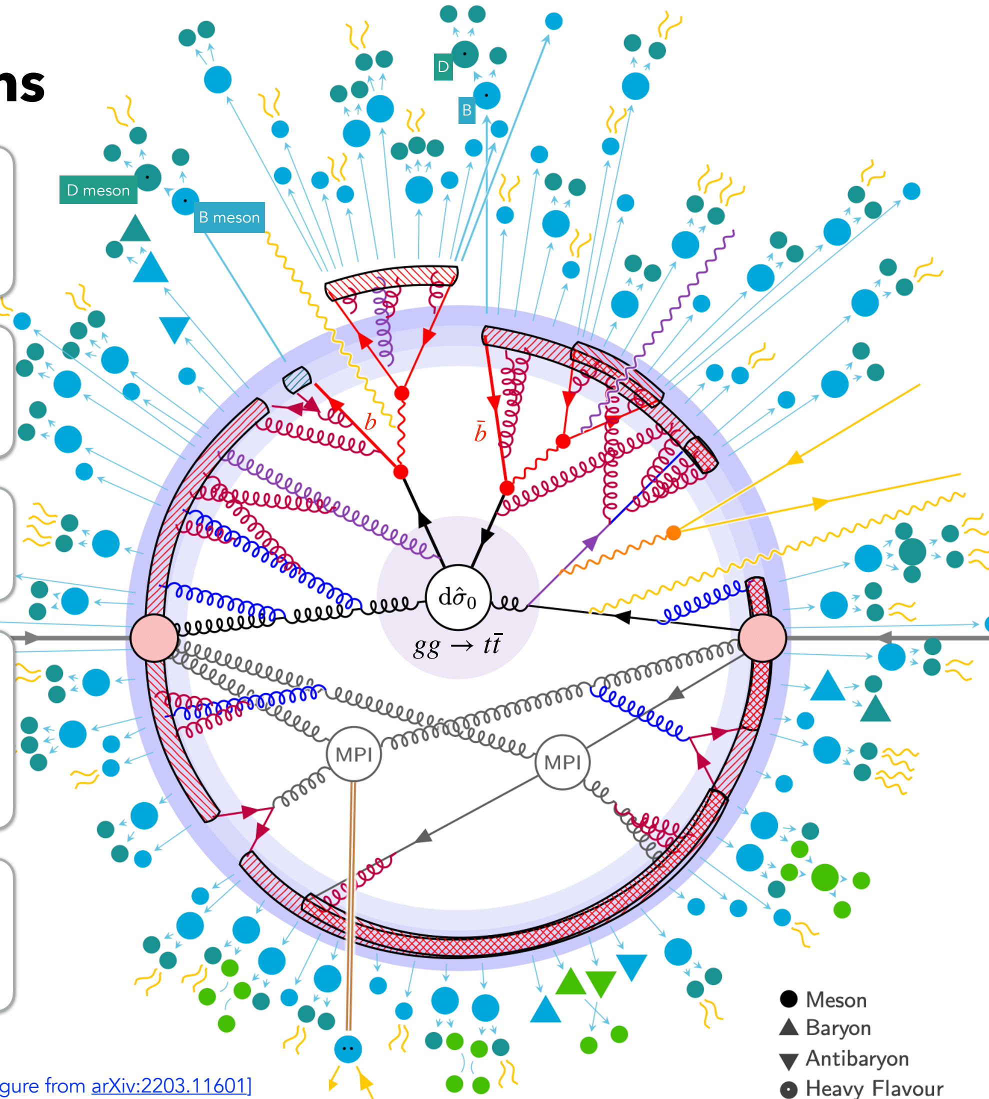
Parton Showers
- QCD Final-State Radiation
- QCD Initial-State Radiation*
- Electroweak Radiation

Underlying Event
- Multiparton Interactions
- Beam Remnants*

Hadronization
- Strings
- Colour Reconnections
- String Interactions
- Bose-Einstein & Fermi-Dirac

Hadron (& τ) Decays
- Primary Hadrons
- Secondary Hadrons
- Hadronic Reinteractions

(: incoming lines are crossed)*



[Figure from arXiv:2203.11601]

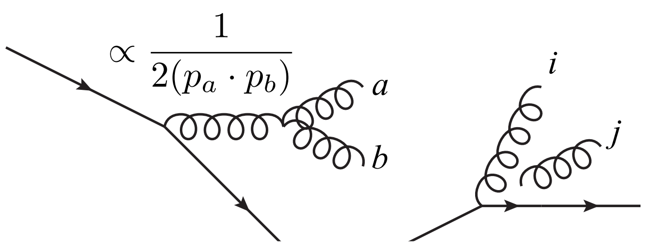
Extra Slides

Parton Showers: Theory

see e.g PS, *Introduction to QCD*, TASI 2012, arXiv:1207.2389

Most bremsstrahlung is driven by divergent propagators → simple structure

Mathematically, **gauge amplitudes factorize** in **singular limits**



Partons ab → **collinear**:

$$|\mathcal{M}_{F+1}(\ldots,a,b,\ldots)|^2 \overset{a||b}{\rightarrow} g_s^2 \mathcal{C} \frac{P(z)}{2(p_a \cdot p_b)} |\mathcal{M}_F(\ldots,a+b,\ldots)|^2$$

$P(z)$ = **DGLAP splitting kernels**", with $z = E_a/(E_a + E_b)$

Gluon j → **soft**:

$$|\mathcal{M}_{F+1}(\ldots,i,j,k\ldots)|^2 \overset{j_g \to 0}{\rightarrow} g_s^2 \mathcal{C} \frac{(p_i \cdot p_k)}{(p_i \cdot p_j)(p_j \cdot p_k)} |\mathcal{M}_F(\ldots,i,k,\ldots)|^2$$

Coherence → Parton j really emitted by (i,k) "dipole" or **"antenna" (eikonal factors)**

These are the **building blocks of parton showers** (DGLAP, dipole, antenna, ...)

(+ running coupling, unitarity, and explicit energy-momentum conservation.)

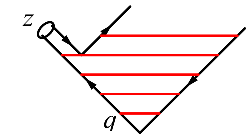
The same event, including all four branchings that were shown in the figure

no	id	name	status	mothers		daughters		colours		p_x	p_y	p_z	e	m
0	90	(system)	-11							0.000	0.000	0.000	91.188	91.188
1	11	(e-)	-12			3	0			0.000	0.000	45.594	45.594	0.001
2	-11	(e+)	-12			4	0			0.000	0.000	-45.594	45.594	0.001
3	11	(e-)	-21	1	0	5	0			0.000	0.000	45.594	45.594	0.000
4	-11	(e+)	-21	2	0	5	0			0.000	0.000	-45.594	45.594	0.000
5	23	(Z0)	-22	3	4	6	7			0.000	0.000	0.000	91.188	91.188
6	3	(s)	-23	5	0	10	0	101	0	-12.368	16.523	40.655	45.594	0.000
7	-3	(sbar)	-23	5	0	8	9	0	101	12.368	-16.523	-40.655	45.594	0.000
8	21	(g)	-51	7	0	13	0	103	101	9.243	-9.146	-29.531	32.267	0.000
9	-3	sbar	51	7	0			0	103	3.084	-7.261	-10.973	13.514	0.000
10	3	(s)	-52	6	0	11	12	101	0	-12.327	16.406	40.505	45.406	0.000
11	21	(g)	-51	10	0	16	0	101	102	-2.834	-2.408	1.078	3.872	0.000
12	3	(s)	-51	10	0	19	0	102	0	-10.246	17.034	38.106	42.979	0.000
13	21	(g)	-52	8	0	14	15	103	101	9.996	-7.366	-28.211	30.823	0.000
14	21	g	51	13	0			122	101	0.503	0.347	-5.126	5.162	0.000
15	21	g	51	13	0			103	122	8.892	-7.272	-23.060	25.763	0.000
16	21	(g)	-52	11	0	17	18	101	102	-2.234	-2.848	1.053	3.769	0.000
17	-1	dbar	51	16	0			0	102	-0.471	-0.509	-0.471	0.839	0.000
18	1	d	51	16	0			101	0	-1.894	-2.119	2.015	3.484	0.000
19	3	s	52	12	0			102	0	-10.114	16.815	37.615	42.426	0.000

Parameters (in PYTHIA): String Tuning

Hadron energy fractions

Fragmentation Function



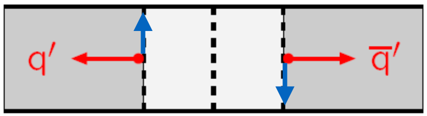
The "Lund a and b parameters"

Or use a and $\langle z \rangle$ instead (less correlated) A. Jueid et al., *JCAP* 05 (2019) 007

$+ \Delta a_{\mathrm{diquark}}$ for baryons

p_T in string breaks

Scale of string-breaking process



Shower cutoff and $\langle p_\perp \rangle$ in string breaks

Meson Multiplets

Mesons

Strangeness suppression, **Vector/Pseudoscalar**, η, η′, …

Baryon Multiplets

Baryons

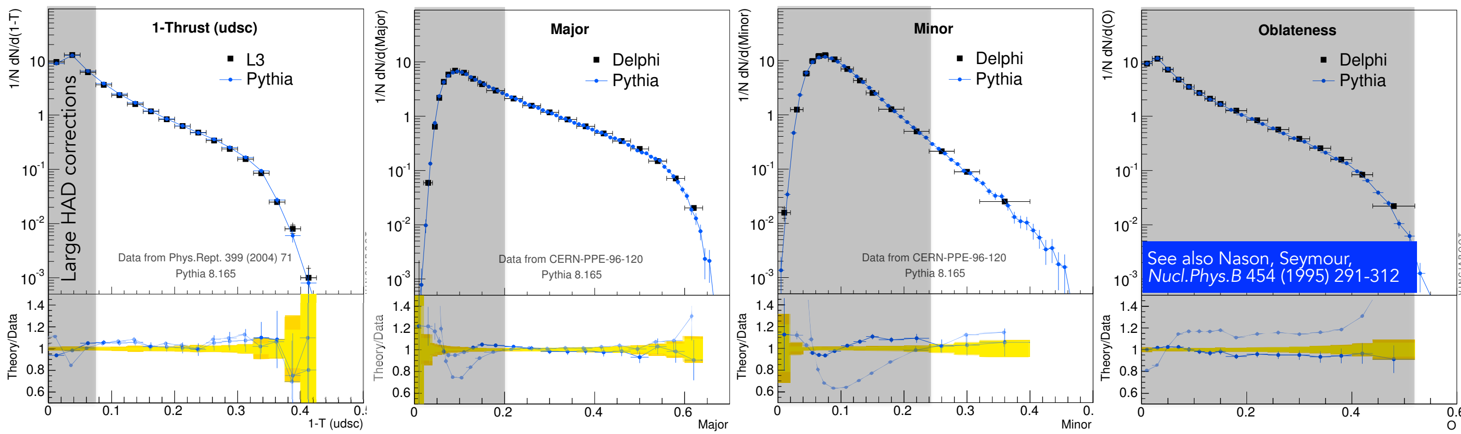
Baryon-to-meson ratios, **Spin-3/2 vs Spin-1/2**, "popcorn", colour reconnections (junctions), … ?

IR Safe Observables: Sensitivity to Hadronization Parameters

PYTHIA 8 (hadronization on) **Vs** (hadronization off)

Important point: These observables are **IR safe ➜ minimal hadronisation corrections**

Big differences in **how** sensitive each of these are to hadronisation & over what **range**



The shaded bins provide constraints for the non-perturbative tuning stage.

You want your hadronization power corrections to do the "right thing" eg at low Thrust.

Hadronization Corrections: Fragmentation Tuning

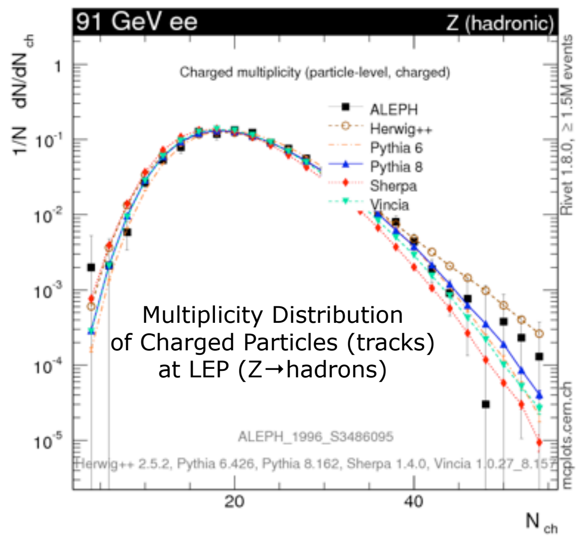
Now use infrared **sensitive** observables - sensitive to hadronization +
first few bins of previous (IR safe) ones

Longitudinal FF parameters *a* and *b*.

Transverse p_T broadening in string breaks (curtails high-N tail, and significantly affects event shapes)

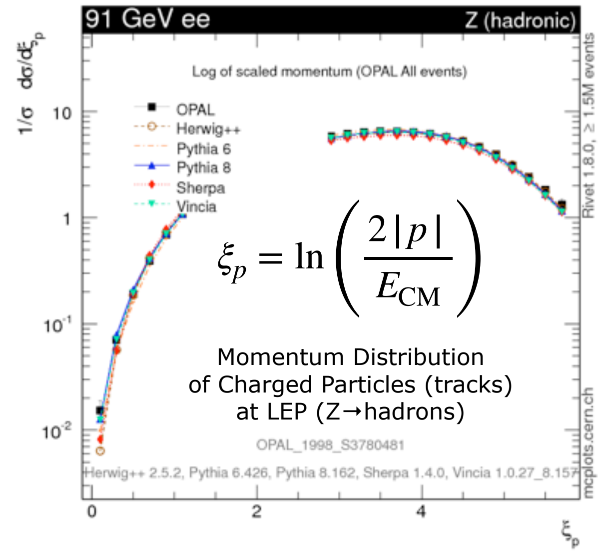
Further parameter $a_{diquark}$ requires looking at a baryon spectrum

How many hadrons do you get?



$\langle N_{ch}(M_Z) \rangle \sim 21$

And how much momentum do they carry?



Fragmentation Tuning — Know what Physics Goes In

Somewhat sensitive to particle composition:
heavier hadrons are harder!

$$f(z) \propto \frac{1}{z}(1-z)^{a}\exp\left(-\frac{b(m_h^2 + p_{\perp h}^2)}{z}\right)$$

+ particle decays

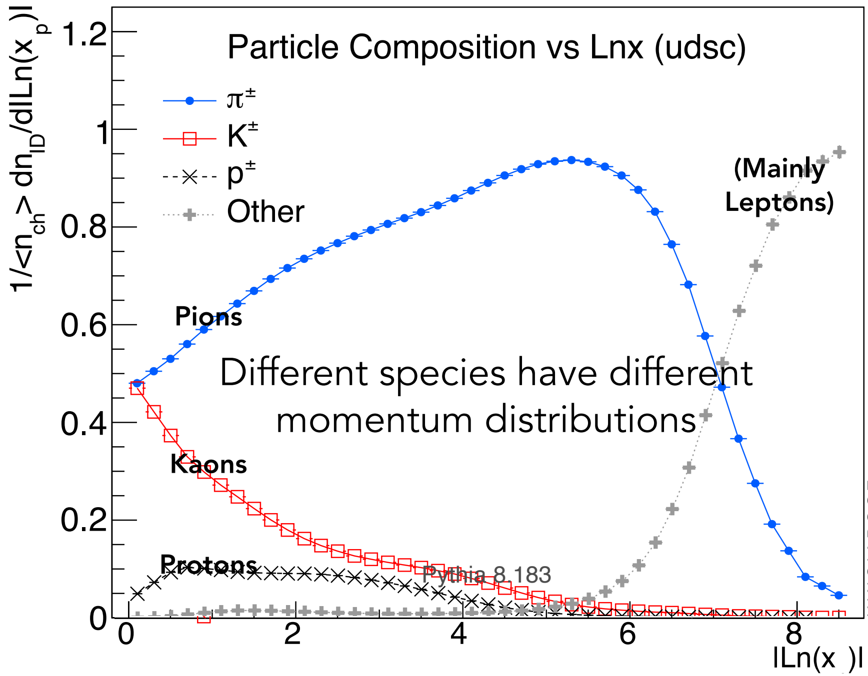
→ effects of feed-down!

$\rho \to \pi\pi$

$K^* \to K\pi$

$\eta \to \pi\pi\pi$

…



Meson and Baryon Rates and Ratios

From PS et al., "Tuning PYTHIA 8.1: the Monash 2013 Tune", Eur.Phys.J.C 74 (2014) 8