Introduction to Quantum Chromodynamics

Lecture 2

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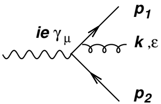
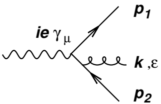
GEFÖRDERT VOM
Bundesministerium
für Bildung
und Forschung

Infrared Singularities

IR singularities: Soft & collinear emissions

consider real-emission correction to $\gamma^* \to q\bar{q}$, i.e. $\gamma^* \to q\bar{q}g$

$\mathcal{M}_{q\bar{q}g} =$ 

$+$ 

$$= -\bar{u}_a(p_1) i g_s \not{\epsilon} t^A_{ab} \frac{i(\not{p}_1 + \not{k})}{(p_1+k)^2} i e_q \gamma_\mu v_b(p_2) + \bar{u}_a(p_1) i e_q \gamma_\mu \frac{i(\not{p}_2 + \not{k})}{(p_2+k)^2} i g_s \not{\epsilon} t^A_{ab} v_b(p_2)$$

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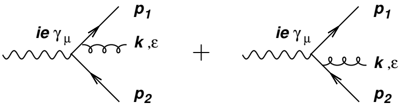

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assume gluon is soft, i.e. $k^0 \ll p_1^0, p_2^0$, ignore terms suppressed by powers of k

$$\mathcal{M}_{q\bar{q}g} \simeq \bar{u}_a(p_1) i e_q \gamma_\mu t^A_{ab} v_b(p_2)\, g_s \left(\frac{p_1 \cdot \epsilon}{p_1 \cdot k} - \frac{p_2 \cdot \epsilon}{p_2 \cdot k} \right)$$

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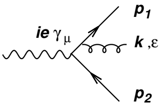
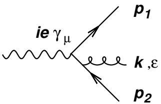
$\mathcal{M}_{q\bar{q}g} =$ 

$+$ 

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$$|\mathcal{M}_{q\bar{q}g}|^2 \simeq \sum_{A,a,b,\mathrm{pol}} \left| \bar{u}_a(p_1) i e_q \gamma_\mu {t^A}_{ab} v_b(p_2)\, g_s \left(\frac{p_1 \cdot \epsilon}{p_1 \cdot k} - \frac{p_2 \cdot \epsilon}{p_2 \cdot k} \right) \right|^2$$

$$= |M^2_{q\bar{q}}| C_F g_s^2 \frac{2 p_1 \cdot p_2}{(p_1 \cdot k)(p_2 \cdot k)}$$ $\rightsquigarrow$ squared amplitude factorises

IR singularities: Soft & collinear emissions

consider phase-space factor $d\Phi_{q\bar{q}g} \simeq d\Phi_{q\bar{q}} \frac{d^3\vec{k}}{2E(2\pi)^3} = d\Phi_{q\bar{q}} \frac{E^2 dE \sin\theta d\theta d\phi}{2E(2\pi)^3}$
[factorizes as well]

$$|\mathcal{M}_{q\bar{q}g}|^2 d\Phi_{q\bar{q}g} \simeq |\mathcal{M}_{q\bar{q}}|^2 d\Phi_{q\bar{q}} d\mathcal{S}$$

$\rightsquigarrow$ factorization into hard $q\bar{q}$ piece & soft-gluon emission probability $d\mathcal{S}$

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$$\begin{aligned} d\mathcal{S} &= EdE\, d\cos\theta \frac{d\phi}{2\pi} \frac{2\alpha_s C_F}{\pi} \frac{2p_1 \cdot p_2}{(2p_1 \cdot k)(2p_2 \cdot k)} \\ &= \frac{2\alpha_s C_F}{\pi} \frac{dE}{E} \frac{d\theta}{\sin\theta} \frac{d\phi}{2\pi}, \quad \text{with } \theta = \theta_{p_1 k} \,\&\, \phi \text{ azimuth} \end{aligned}$$

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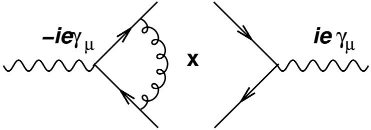
gluon-emission singularity structure (universal/process independent)

- diverges for $E \to 0$ aka infrared/soft singularity
- diverges for $\theta \to 0$ and $\theta \to \pi$ aka collinear singularity

IR singularities: Real–virtual cancellation

$\mathcal{O}(\alpha_s)$ correction to total cross section, sum of real & virtual contributions

$V \supset$ 

Total cross section must be finite. If real part is divergent, so must the virtual!

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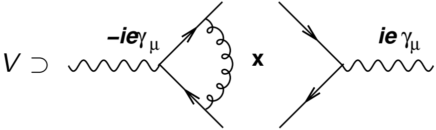

Total cross section must be finite. If real part is divergent, so must the virtual!

$$\sigma_{tot} = \sigma_{q\bar{q}} \left(1 + \frac{2\alpha_s C_F}{\pi} \int \frac{dE}{E} \int \frac{d\theta}{\sin\theta} R\left(\frac{E}{Q},\theta\right) - \frac{2\alpha_s C_F}{\pi} \int \frac{dE}{E} \int \frac{d\theta}{\sin\theta} V\left(\frac{E}{Q},\theta\right)\right)$$

- $R(E/Q,\theta)$ parametrizes full real-emission matrix element ($E \gg 0$)

$$\lim_{E\to 0} R(E/Q,\theta) = 1$$

- $V(E/Q,\theta)$ parametrizes virtual corrections for all momenta
- for every divergence $R(E/Q,\theta)$ and $V(E/Q,\theta)$ cancel

$$\lim_{E\to 0}(R - V) = 0 \quad \text{and} \quad \lim_{\theta\to 0,\pi}(R - V) = 0$$

IR singularities: Soft & collinear emissions

I) soft/collinear gluon emission cross section factorizes

$$|\mathcal{M}_{q\bar{q}g}|^2 d\Phi_{q\bar{q}g} \simeq |\mathcal{M}_{q\bar{q}}|^2 d\Phi_{q\bar{q}} d\mathcal{S}$$

where

$$d\mathcal{S} = \frac{2\alpha_s C_F}{\pi} \frac{dE}{E} \frac{d\theta}{\sin\theta} \frac{d\phi}{2\pi}$$

$\rightsquigarrow$ divergent as $E \to 0$ and/or $\theta \to 0, \pi$

II) very singularities cancel between real & virtual parts

$$\sigma_{tot}(e^+e^- \to q\bar{q}) = \sigma_{q\bar{q}} \left(\underbrace{1}_{\text{LO}} + \underbrace{C_1 \frac{\alpha_s(Q^2)}{\pi}}_{\text{NLO}} + \underbrace{\ldots}_{\text{higher orders}} \right)$$

$\rightsquigarrow$ perturbation theory works well for inclusive cross sections

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$\leadsto$ perturbation theory works well for inclusive cross sections

$\leadsto$ **let's look a little more exclusive now**

$\leadsto$ **estimate the number of emitted gluons**

IR singularities: Multiple gluon emissions

Let's try to integrate emission probability to estimate mean number of gluon emissions off a quark with energy $\sim Q$

$$\langle N_g \rangle \simeq \frac{2\alpha_s C_F}{\pi} \int^Q \frac{dE}{E} \int^{\pi/2} \frac{d\theta}{\theta} \Theta(E\theta > Q_0)$$

- diverges for $E \to 0$ & $\theta \to 0$
- cut out transverse momenta ($k_t \simeq E\theta$) smaller than $Q_0 \sim \Lambda_{\mathrm{QCD}}$
  $\rightsquigarrow$ below that the language of quarks & gluons loses its meaning

$$\langle N_g \rangle \simeq \frac{\alpha_s C_F}{\pi} \ln^2 \frac{Q}{Q_0} + \mathcal{O}\left(\alpha_s \ln \frac{Q}{Q_0}\right)$$

assume $Q = 200$ GeV & $Q_0 = 1$ GeV $\rightsquigarrow \ln^2 \frac{Q}{Q_0} \approx 30$

$\rightsquigarrow$ simple expansion in α_s spoiled by large logarithms, $\langle N_g \rangle > 1$

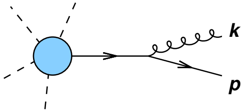
Is 1st order perturbation theory useless beyond total cross sections?

- Could try to calculate next order, and see what happens!
- Can try to approximate higher-order contributions!
- Look for better behaved final-state observables!

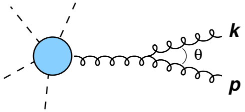
IR singularities: Multiple gluon emissions

Once a gluon is emitted it can itself emit further gluons

- consider collinear (& soft) emissions only [logarithmically enhanced]
- in the small angle limit ($\theta \ll 1$) emissions factorize



$$\simeq \quad \frac{2\alpha_s C_F}{\pi} \frac{dE}{E} \frac{d\theta}{\theta}$$



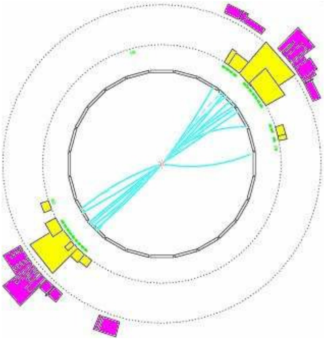
$$\simeq \quad \frac{2\alpha_s C_A}{\pi} \frac{dE}{E} \frac{d\theta}{\theta}$$

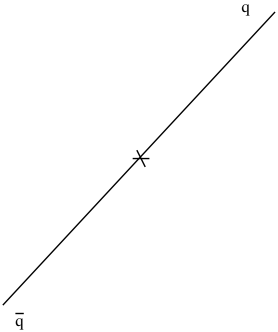
- same divergence structure, independent of who emits
- only difference being the colour factor ($C_F = 4/3,\ C_A = 3$)

  $\rightsquigarrow$ gluons emit more
- expect 1st-order structure ($\alpha_s \ln^2 Q/Q_0$) to appear at each new order

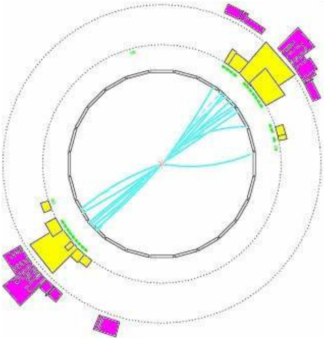
IR singularities: Multiple gluon emissions

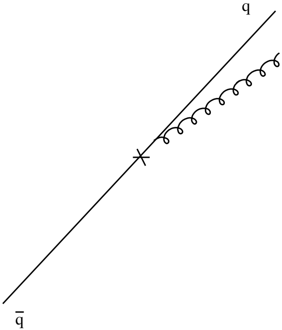
Start out with the $q\bar{q}$ system



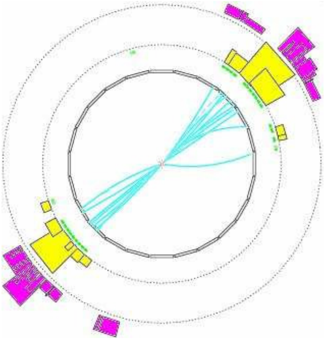


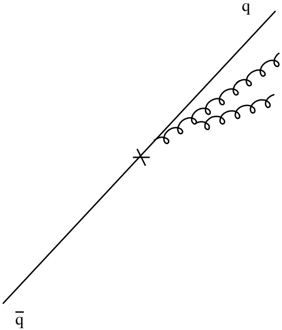
Quark emits small angle gluon





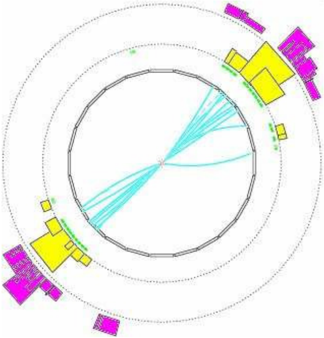
Gluon radiates a further gluon

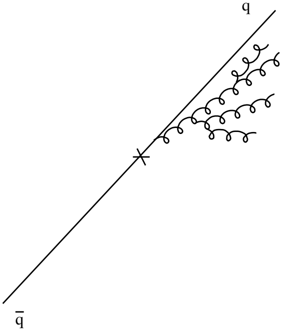




IR singularities: Multiple gluon emissions

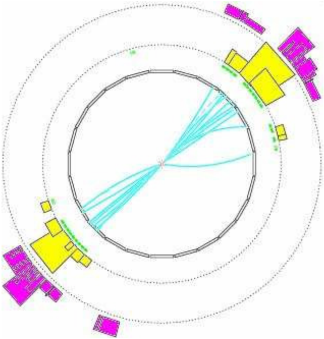
And so on and so forth ...

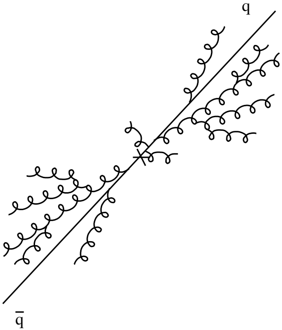




IR singularities: Multiple gluon emissions

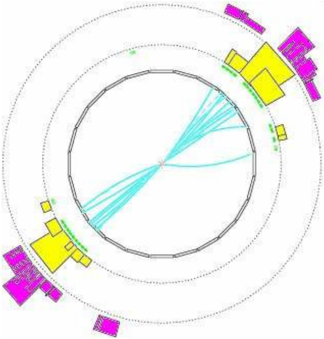
Meanwhile the same happend on the other side

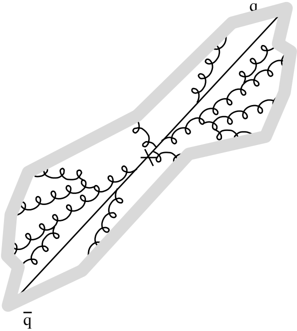




IR singularities: Multiple gluon emissions

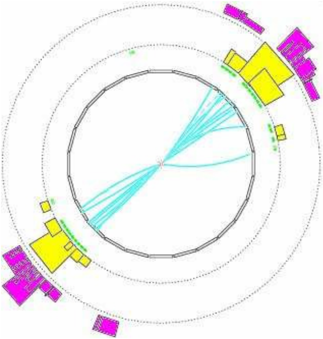
At some point a non-perturbative transition happens

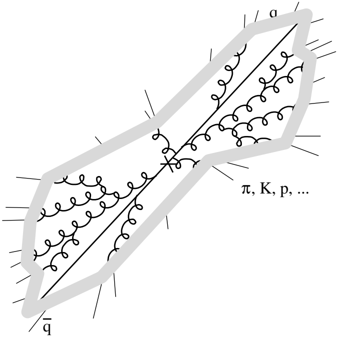




IR singularities: Multiple gluon emissions

Resulting in a pattern of collimated hadrons [at small angles wrt to the quarks]





IR singularities: Gluon vs. Hadron multiplicity

gluon multiplicity can be calculated by summing all orders of perturbation theory (n):

$$\langle N_g \rangle \sim \frac{C_F}{C_A} \sum_{n=1}^{\infty} \frac{1}{(n!)^2} \left(\frac{C_A}{2\pi b_0^2 \alpha_s} \right)^n$$

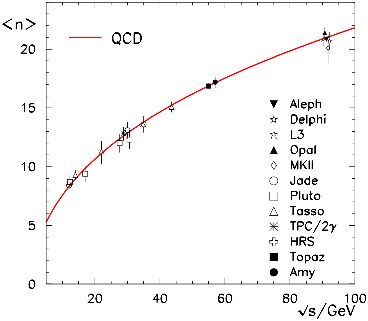
$$\sim \frac{C_F}{C_A} \exp\left(\sqrt{\frac{2C_A}{\pi b_0^2 \alpha_s(Q)}} \right)$$

interprete as a function of $Q \equiv \sqrt{s}$

direct comparison suggests

$$\langle N_{\rm had} \rangle = c_{\rm fit} \langle N_g \rangle$$

charged hadron multiplicity in e^+e^- collisions



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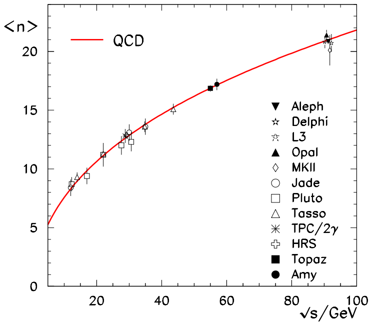

Seems like perturbative QCD can get us quite far!

Resummation of large logarithms

Appearance of large logarithms spoils pure power series in α_s

- restrictions on real-emission phase space can induce large logarithms

$$L \equiv \ln(Q/Q_0) \propto \ln(1/v) \quad \text{[with } v \in [0,1] \text{ some observable value]}$$

$\rightsquigarrow$ enhanced terms $\mathcal{O}(\alpha_s^n L^m)$ in multi-emission cross sections

$\rightsquigarrow$ factorization of amplitudes and phase space might allow for resummation

simplified sketch of LL resummation

$$\begin{aligned} \sigma(v) &\propto c_{\mathrm{LL}}\alpha_s L^2 + \frac{c_{\mathrm{LL}}^2}{2!}\alpha_s^2 L^4 + \ldots \\ &\propto \sum_{n=1}^{\infty} \frac{c_{LL}^n}{n!}\alpha_s^n L^{2n} \end{aligned}$$

$\rightsquigarrow$ fixed order reliable only when $\alpha_s \ln^2(1/v) \ll 1$, note $\ln^2(1/0.05) \approx 9$

$\rightsquigarrow$ involves observable specific coefficient functions, here sketched by c_{LL}

Resummation of large logarithms

consider cummulant distribution

$$\Sigma(v) = \int_0^v dv \frac{1}{\sigma}\frac{d\sigma}{dv}$$

$\rightsquigarrow$ resummation yields for small v

$$\Sigma(v) = C(\alpha_s)\exp\left(G(\alpha_s, L)\right) + \underbrace{D(\alpha_s, v)}_{\to 0 \text{ for } v\to 0}$$

with

$$\begin{aligned} C(\alpha_s) &= 1 + \sum_{n=1}^{\infty} C_n \alpha_s^n \\ G(\alpha_s, L) &= \sum_{n=1}^{\infty}\sum_{m=1}^{n+1} G_{nm}\alpha_s^n L^m \\ &= \underbrace{Lg_1(\alpha_s L)}_{\text{LL}} + \underbrace{g_2(\alpha_s L)}_{\text{NLL}} + \underbrace{\alpha_s g_3(\alpha_s L)}_{\text{NNLL}} + \dots \end{aligned}$$

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$$= \underbrace{L g_1(\alpha_s L)}_{\text{LL}} + \underbrace{g_2(\alpha_s L)}_{\text{NLL}} + \underbrace{\alpha_s g_3(\alpha_s L)}_{\text{NNLL}} + \ldots$$

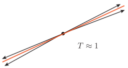
LL good when $\alpha_s L^2 \lesssim 1$

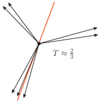
NLL needed when $\alpha_s L \lesssim 1$

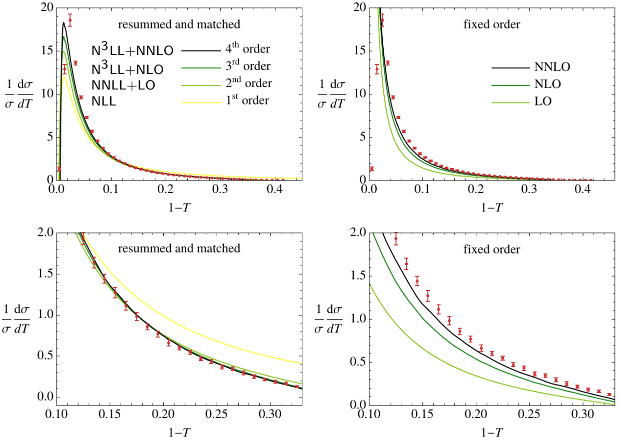
Resummation of large logarithms

An example: the thrust distribution in e^+e^- annihilation

$$T = \max_{\vec{n}} \frac{|\vec{p}_i \cdot \vec{n}|}{\sum_i |\vec{p}_i|} = \max_{\vec{n}} \frac{|\vec{p}_i \cdot \vec{n}|}{Q} \;\rightsquigarrow\; v \equiv \tau = 1 - T$$







[Becher, Schwartz JHEP **0807** (2008) 034, data from ALEPH]

Using the soft/collinear approximation we can make predictions for events' detailed partonic structure, when supplemented with a model for hadronization for hadronic final states even.

However, we cannot perform analytic calculations for every observable ever be measured. [too many experimenters, too many observables, too few theorists]

The solution: Parton-Shower simulations

- implement space-time picture of parton evolution [limited to leading logarithms]
- successive parton emissions for arbitrary processes
- Markov-chain Monte Carlo process describing the parton proliferation
- observable/process independent

$\rightsquigarrow$ cornerstone of Monte-Carlo event generators, see MC lectures

NLO QCD predictions

Hard Processes at Next-to-Leading Order QCD

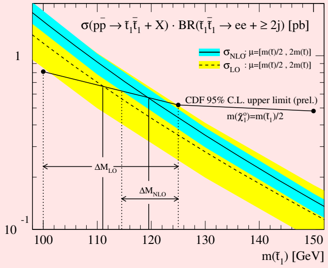
The need for higher precision

- derive exclusion bounds from a given measurement
  - non-observation of a given hypothesis, e.g. heavy Higgs, BSM model
  - crucial to know the corresponding production cross sections precisely
  - derive limits on particle masses, model parameters
- counting experiments to extract certain parameters, couplings

$\rightsquigarrow$ at hadron colliders α_S corrections indispensible, need one-loop QCD

stop mass bounds from Tevatron

[from the early days, T. Plehn private communication]



Higgs coupling extraction

- $\sigma(gg \to h \to \gamma\gamma) \sim \frac{\Gamma_g \Gamma_\gamma}{\Gamma}$
- $\sigma(gg \to h \to WW^*) \sim \frac{\Gamma_g \Gamma_W}{\Gamma}$
- $\sigma(qq \to qqh,\ h \to \tau\tau) \sim \frac{\Gamma_W \Gamma_\tau}{\Gamma}$
- ...

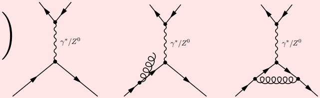
$\rightsquigarrow$ $\Gamma_i \sim g_{iih}$, $\Gamma_g \sim g_{tth}$

$\rightsquigarrow$ theoretical uncertainties dominate

$\rightsquigarrow$ systematics reduced for σ ratios

Anatomy of NLO QCD calculations

$$|\mathcal{M}|^2 = |\mathcal{M}_B|^2 + \alpha_S \left(|\mathcal{M}_R|^2 + 2\Re(\mathcal{M}_B \mathcal{M}_V^\dagger) \right)$$



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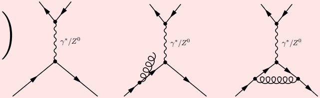

$$\sigma^{NLO}_{2\to n} = \int_n \mathrm{d}^{(4)}\sigma^B + \underbrace{\int_{n+1} \mathrm{d}^{(d)}\sigma^R + \int_n \mathrm{d}^{(d)}\sigma^V}_{\alpha_S \text{ real \& virtual corrections}}$$

Hard Processes at Next-to-Leading Order QCD

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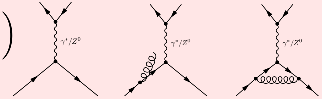

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- real-emission σ^R

  $\rightsquigarrow$ IR divergence for soft/collinear emission
- (UV renormalized) virtual-corrections σ^V

  $\rightsquigarrow$ IR divergent when propagator goes on-shell
- divergences manifest in dimensional regularisation, $d = 4 - 2\epsilon$

  $\rightsquigarrow$ occurence of single & double poles, i.e. $1/\epsilon$, $1/\epsilon^2$
- for IR safe observables poles cancel, the sum is finite [Kinoshita '62; Lee, Nauenberg '64]

Infrared & Collinear safe observables

- interested in observable-independent formulation

$$\begin{aligned}
\mathcal{O}^{\mathrm{B}} &= \int |\mathcal{M}_{\mathrm{B}}^{(n)}|^2 \, d\Phi_n \Theta^{(n)}(\mathcal{O}, \{p_n\}) \\
\mathcal{O}^{\mathrm{R}} &= \int |\mathcal{M}_{\mathrm{R}}^{(n+1)}|^2 \, d\Phi_{n+1} \Theta^{(n+1)}(\mathcal{O}, \{p_{n+1}\}) \\
\mathcal{O}^{\mathrm{V}} &= \int 2\Re(\mathcal{M}_{\mathrm{B}} \mathcal{M}_{\mathrm{V}}^{\dagger}) \, d\Phi_n \Theta^{(n)}(\mathcal{O}, \{p_n\})
\end{aligned}$$

with $d\Phi_{n/n+1}$ the $n/n+1$ particle phase space, $\Theta^{(n/n+1)}$ obs. measure function

Hard Processes at Next-to-Leading Order QCD

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with $\mathrm{d}\Phi_{n/n+1}$ the $n/n+1$ particle phase space, $\Theta^{(n/n+1)}$ obs. measure function

- formal requirements on the measurement function:

$$\begin{aligned}
\Theta^{(n+1)}(p_1,\ldots,p_i=\lambda q,\ldots,p_{n+1}) &\to \Theta^{(n)}(p_1,\ldots,p_{n+1}) \\
\text{for } \lambda \to 0 & \qquad \text{soft limit} \\
\Theta^{(n+1)}(p_1,\ldots,p_i,\ldots,p_j,\ldots,p_{n+1}) &\to \Theta^{(n)}(p_1,\ldots,p,\ldots,p_{n+1}) \\
\text{for } p_i \to zp\,,\ \ p_j=(1-z)p & \qquad \text{collinear limit}
\end{aligned}$$

simply remove (soft) parton i, or replace collinear pair $\{p_i, p_j\}$ by $p = p_i + p_j$

$\rightsquigarrow$ definition of infrared & collinear safe observables

Anatomy of NLO QCD calculations cont'd

$$\sigma_{2\to n}^{NLO} = \int_n \mathrm{d}^{(4)}\sigma^B + \underbrace{\int_{n+1} \mathrm{d}^{(d)}\sigma^R + \int_n \mathrm{d}^{(d)}\sigma^V}_{\alpha_S \text{ real \& virtual corrections}}$$

- finite corrections for IR safe observables
- analytical integration with cuts in d-dim infeasible for high-multi final states
- we are interested in fully-differential answer, use of MC integration methods
  however, both terms σ^R & σ^V exhibit divergences, i.e. are unbound
  σ^R in $(n+1)$-particle phase space, σ^V in n-particle phase space

Anatomy of NLO QCD calculations cont'd

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Subtraction methods

- attempt to devise local *subtraction term* such that both integrals are separately finite and can be performed as ordinary multi-dimensional phase-space integrals

  $\rightsquigarrow$ based on universality of QCD IR divergences

  $\rightsquigarrow$ aim for IR regularisation at integrand level

Subtraction methods cont'd

- subtraction terms provide local approximation for the real-emission process

$$\int_{n+1} \mathrm{d}^{(d)}\sigma^{\mathrm{A}} = \int_n \int_1 \mathrm{d}^{(d)}\sigma^{\mathrm{A}}$$

$\hookrightarrow$ captures soft & collinear limits of amplitudes [$1/\epsilon$ and $1/\epsilon^2$ poles]

$\hookrightarrow$ analytically integrable (d-dim) over one-parton emission phase space

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↪ analytically integrable (d-dim) over one-parton emission phase space

- add & subtract from NLO differential cross section

$$\sigma^{NLO}_{2\to n} = \int_{n+1}\left[\mathrm{d}^{(4)}\sigma^{\mathrm{R}} - \mathrm{d}^{(4)}\sigma^{\mathrm{A}}\right] + \int_{n}\left[\mathrm{d}^{(4)}\sigma^{\mathrm{B}} + \int_{\mathrm{loop}} \mathrm{d}^{(d)}\sigma^{\mathrm{V}} + \int_{1} \mathrm{d}^{(d)}\sigma^{\mathrm{A}}\right]_{\epsilon=0}$$

Subtraction methods cont'd

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  $\rightsquigarrow$ separately finite phase-space integrals (4-dim)

  $\rightsquigarrow$ can be performed by means of MC integration

  $\rightsquigarrow$ no ambiguous or unphysical cut-offs/scales get introduced

Hard Processes at Next-to-Leading Order QCD

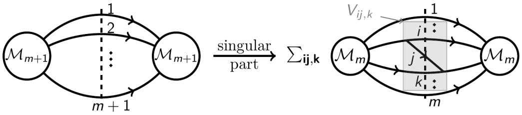
Dipole subtraction method [Catani, Seymour Nucl. Phys. B **485** (1997) 291]

- Catani & Seymour presented general expression for $\mathrm{d}^{(d)}\sigma^{\mathrm{A}}$ (known as the dipole factorisation formula)
- constructed from Born process using universal dipole terms

$$\int_{n+1} \mathrm{d}^{(d)}\sigma^{\mathrm{A}} = \sum_{\mathrm{dipoles}} \int_{n} \mathrm{d}^{(d)}\sigma^{\mathrm{B}} \otimes \int_{1} \mathrm{d}^{(d)} V_{\mathrm{dipole}} = \int_{m} \left[\mathrm{d}^{(d)}\sigma^{\mathrm{B}} \otimes I \right]$$

spin- & color correlations ⟵ ⟶ universal dipole terms

- sum over dipoles contains all real-emission soft/collinear divergences
- suited for any process with massless partons (0, 1, 2 initial-state hadrons)
- generalisation to massive partons [Catani, Dittmaier, Seymour, Trocsanyi Nucl. Phys. B **627** (2002) 189]



Dipole subtraction method cont'd

- subtraction method for arbitrary observables (IRC safe)

$$
\begin{aligned}
\mathcal{O}^{\mathrm{B}} &= \int |\mathcal{M}_{\mathrm{B}}^{(n)}|^2 \, \mathrm{d}\Phi_n \Theta^{(n)}(\mathcal{O},\{p_n\}) \\
\mathcal{O}^{\mathrm{RS}} &= \int \mathrm{d}\Phi_{n+1} \Big[|\mathcal{M}_{\mathrm{R}}^{(n+1)}(\{p_n\})|^2 \, \Theta^{(n+1)}(\mathcal{O},\{p_{n+1}\}) \\
&\qquad - \sum_{i\neq j\neq k} \mathcal{D}_{ij,k}(\{p_n\}) \;\; \Theta^{(n)}(\mathcal{O},p_1,..,\tilde{p}_{ij},\tilde{p}_k,..,p_{n+1}\}) \Big] \\
\mathcal{O}^{\mathrm{VI}} &= \int \mathrm{d}\Phi_n \left[2\Re(\mathcal{M}_{\mathrm{B}}\mathcal{M}_{\mathrm{V}}^{\dagger}) + \int_1 [\mathrm{d}\tilde{p}]\mathcal{D}_{ij,k} \right] \Theta^{(n)}(\mathcal{O},\{p_n\})
\end{aligned}
$$

- $[\mathrm{d}\tilde{p}]$ phase-space element of one-parton
- such, differential & integrated subtraction terms cancel exactly

  ↪ requires mapping of $(n+1) \to n$ configuration

  ↪ need to distinguish different dipole types

Dipole subtraction method cont'd

- dipoles involve three partons, splitting particles i, j and spectator k
- distinguish initial- & final-state splitter/spectator
- all contributions known, suitable for automated evaluation

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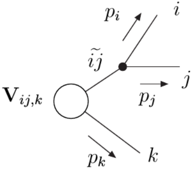

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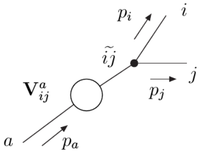

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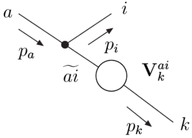

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