

# Overview of NNLO QCD subtraction schemes

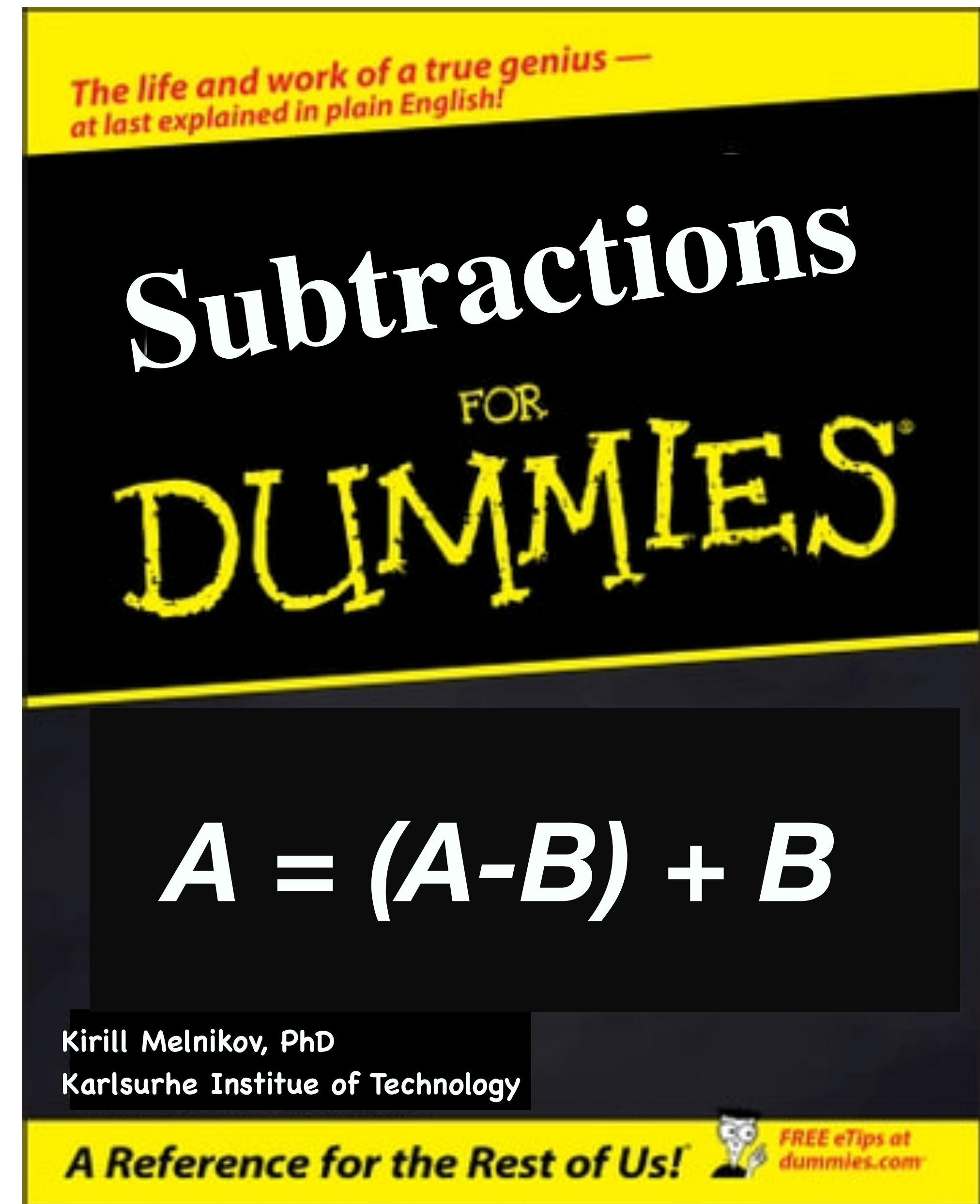
Kirill Melnikov

TTP KIT

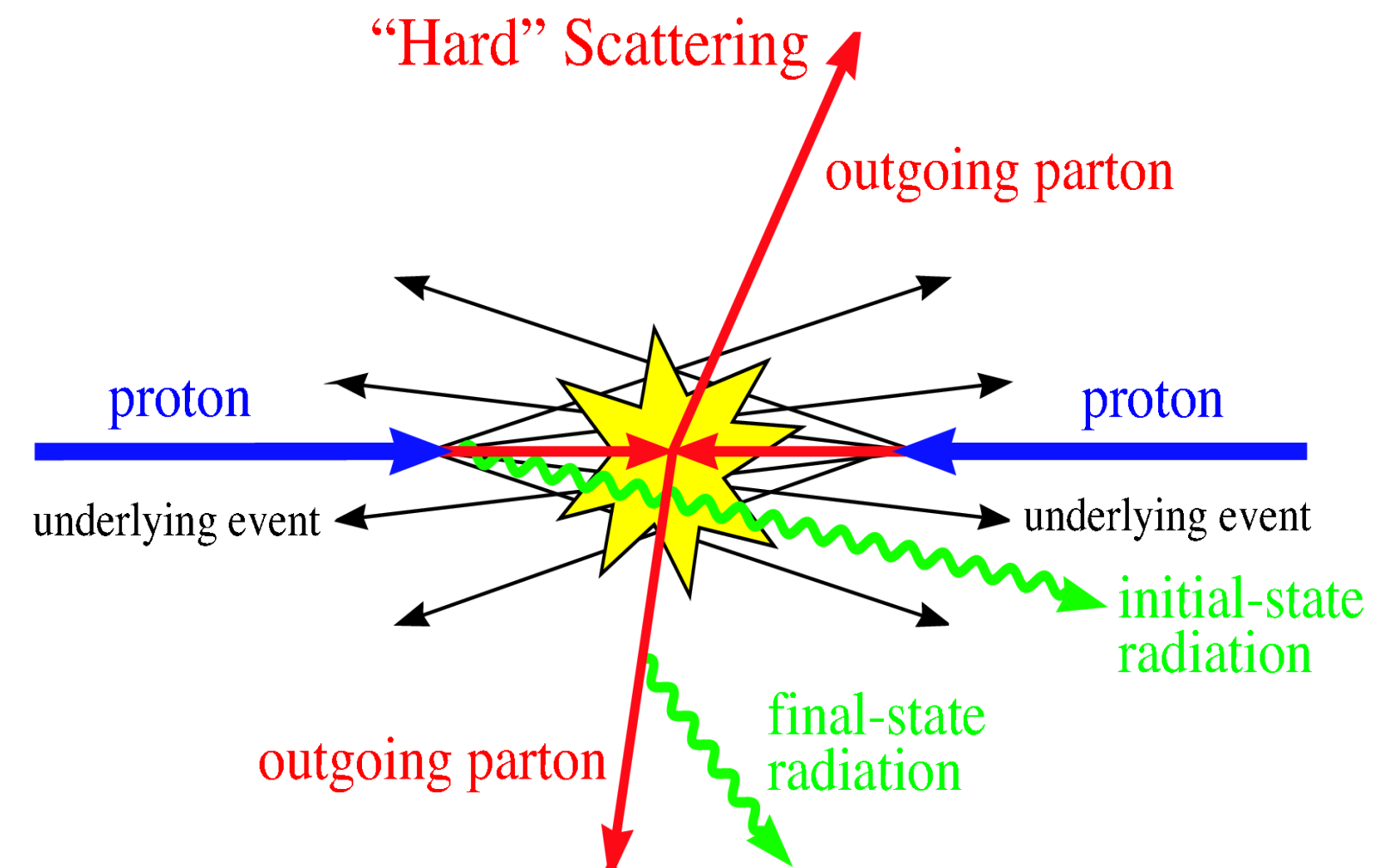
HP2 conference, September 18-22 2022, Newcastle

In this talk I would like to discuss

- universal principles behind the existing subtraction schemes;
- their similarities and differences at the technical and the conceptual levels;
- prospects for their further developments;

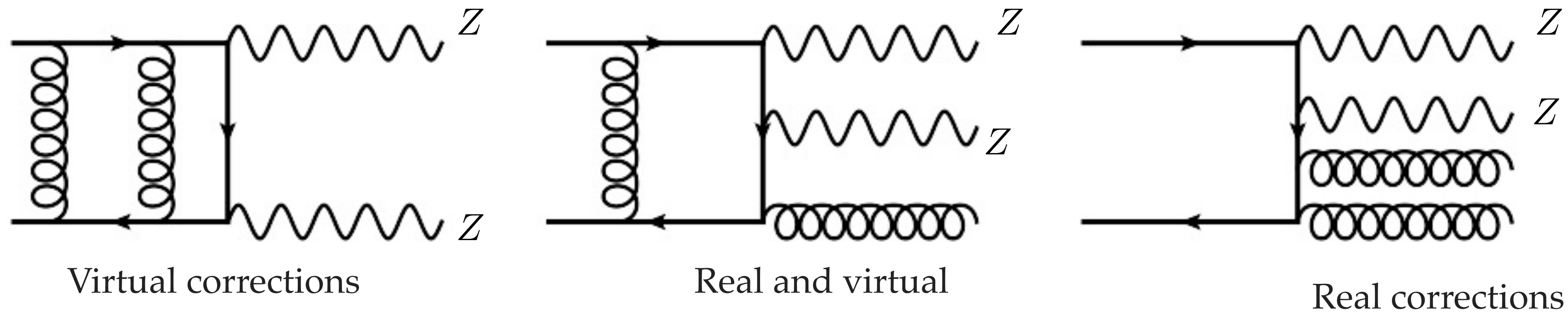


To describe processes which occur when two protons collide and large momentum is being exchanged between them, we need to compute partonic cross sections in QCD perturbation theory.



$$d\sigma_{pp \rightarrow X} = \sum_{ij} \int dx_1 dx_2 f_i(x_1) f_j(x_2) d\sigma_{ij \rightarrow X}(x_1 P_1, x_2 P_2) F_J$$

At next-to-next-to-leading order, we need to account for double-virtual, real-virtual and double-real corrections.



$$d\sigma_{pp \rightarrow X} = \sum_{ij} \int dx_1 dx_2 f_i(x_1) f_j(x_2) d\sigma_{ij \rightarrow X}(x_1 P_1, x_2 P_2) F_J$$

Loop integrations produce explicit divergences

$$|\mathcal{M}_2\rangle = I^{(2)} |\mathcal{M}_0\rangle + I^{(1)} |\mathcal{M}_1\rangle$$

$$I^{(2)} \sim \frac{1}{\epsilon^4} \quad I^{(1)} \sim \frac{1}{\epsilon^2}$$

Real emission contributions are finite in the bulk of the phase space.

Integration is not an option because we aim at fully-differential predictions.



There are two main approaches to extracting the singular contributions and making observable- and process-dependent contributions integrable.

**Slicing** 
$$\int |\mathcal{M}|^2 F_J d\phi_d = \int_0^\delta [|\mathcal{M}|^2 F_J d\phi_d]_{\text{simp}} + \int_\delta^1 |\mathcal{M}|^2 F_J d\phi_d + \mathcal{O}(\delta)$$

- conceptually simple, straightforward to implement (bulk is NLO);
- non-local in phase space;
- strong dependence on the slicing parameter and large cancellations between singular and regular terms;
- “easy” generalization to N3LO;

**Subtraction** 
$$\int |\mathcal{M}|^2 F_J d\phi_d = \int [|\mathcal{M}|^2 F_J - S] d\phi_d + \int S d\phi_d$$

- more difficult conceptually;
- local in phase space;
- potentially, offers better numerical stability and scalability than slicing;
- at least for now, every step to yet higher order (e.g. N2LO  $\rightarrow$  N3LO) is a challenge.

***Subtraction***

$$\int |\mathcal{M}|^2 F_J \, \mathrm{d}\phi_d = \int [|\mathcal{M}|^2 F_J - S] \, \mathrm{d}\phi_4 + \int S \mathrm{d}\phi_d$$

**Subtraction**

$$\int |\mathcal{M}|^2 F_J \, d\phi_d = \int [|\mathcal{M}|^2 F_J - S] \, d\phi_d + \int S d\phi_d$$

A construction of a subtraction scheme involves several well-defined steps.

We need to:

- find regions of phase space which lead to non-integrable singularities of the matrix elements;
- define simplified versions of the matrix element squared to be used in the subtraction terms;
- understanding how to deal with multiple radiators....
- ....and overlapping singularities (first time at NNLO);
- define simplified expressions of a phase space in the subtraction terms;
- find a way to integrate the subtraction terms in d-dimensions;

## **Subtraction**

$$\int |\mathcal{M}|^2 F_J d\phi_d = \int [|\mathcal{M}|^2 F_J - S] d\phi_d + \int S d\phi_d$$

A construction of a subtraction scheme involves several well-defined steps. We need to:

- find regions of phase space which lead to non-integrable singularities of the matrix elements;
- define simplified versions of the matrix element squared used in the singular limits;
- understanding how to deal with multiple singularities....
- ....and overlapping singularities (important at NNLO);
- define simplified expressions for a phase space in the singular limits;
- find a way to express the subtraction terms in d-dimensions;

Choices made for all of these points define a subtraction scheme

“Sector-improved residue subtraction” [M. Czakon et al.]  
“Nested Soft-Collinear subtraction scheme” [F. Caola et al.]  
“Local analytic subtraction” [L. Magnea et al.];  
“Geometric” [F. Herzog]  
“Colourful subtraction” [Z. Troscanyi et al.]  
“Antenna subtraction” [Th. Gehrmann et al. ]  
“Projection-to-Born” [M. Cacciari et al.]



## ***Multiple singular limits of scattering amplitudes***

One has to recognise that amplitudes for multi-particle final states are too complicated objects to be dealt in their entirety. Hence, we try to split it into simpler “building blocks” and deal with them separately. Two ways of doing this exist:

- partition the phase space into sectors such that at each one has to deal with an “elementary” singularity structure (at NLO this is Frixione-Kunszt-Signer subtraction scheme);

“Sector-improved residue subtraction” [M. Czakon et al.]

“Nested Soft-Collinear subtraction scheme” [F. Caola et al.]

“Local analytic subtraction” [L. Magnea];

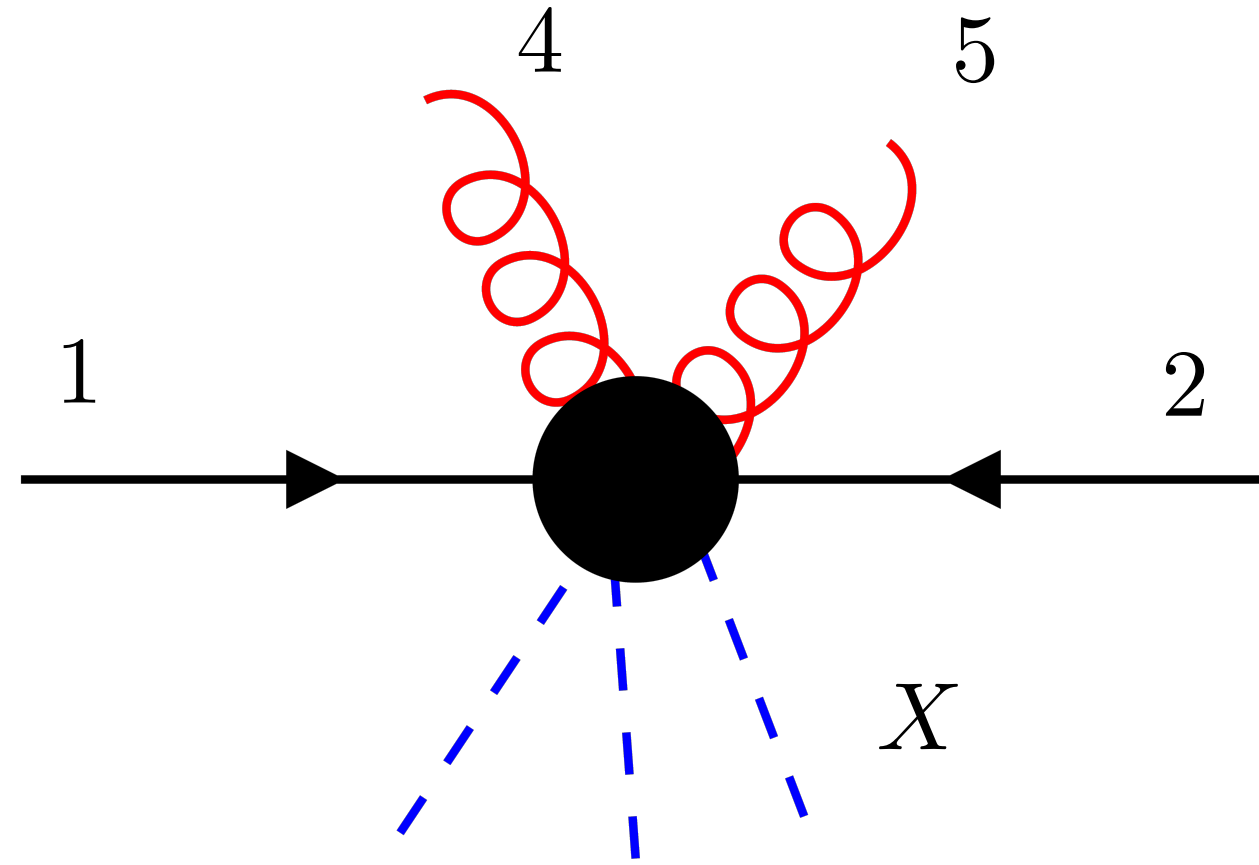
“Geometric” [F. Herzog]

- make use of the properties of the amplitudes themselves to address this point (at NLO this is similar to Catani-Seymour subtraction scheme);

“Antenna subtraction” [Gehrmann et al.]

“Colourful subtraction” [Z. Troscanyi]

**FKS-like subtractions** introduce explicit partition functions that remove all but the minimal number of singularities. Partitions should be constructed in such a way that in the singular limits they simplify.



$$\int d\phi |\mathcal{M}|^2(1, 2, 4, 5) = \sum_{\alpha, \beta} d\sigma^{\alpha, \beta}$$

$$d\sigma^{\alpha, \beta} = \int d\phi |\mathcal{M}|^2(1, 2, 4, 5) w^{\alpha, \beta}$$

$$1 = w^{14,15} + w^{24,25} + w^{14,25} + w^{15,24}$$

$$w^{14,15} = \frac{\rho_{24}\rho_{25}}{d_4 d_5} \left( 1 + \frac{\rho_{14}}{d_{4521}} + \frac{\rho_{15}}{d_{4512}} \right)$$

$\Rightarrow$  singular when the gluons 4 and 5 are collinear to 1 or to each other;

$$w^{24,25} = \frac{\rho_{14}\rho_{15}}{d_4 d_5} \left( 1 + \frac{\rho_{25}}{d_{4521}} + \frac{\rho_{24}}{d_{4512}} \right)$$

$\Rightarrow$  singular when the gluons 4 and 5 are collinear to 2 or to each other;

$$w^{14,25} = \frac{\rho_{24}\rho_{15}\rho_{45}}{d_4 d_5 d_{4512}}, \quad w^{24,15} = \frac{\rho_{14}\rho_{25}\rho_{45}}{d_4 d_5 d_{4521}}$$

$\Rightarrow$  singular when the gluon 4 is collinear to 1 and the gluon 5 is collinear to the gluon 2 and vice versa;

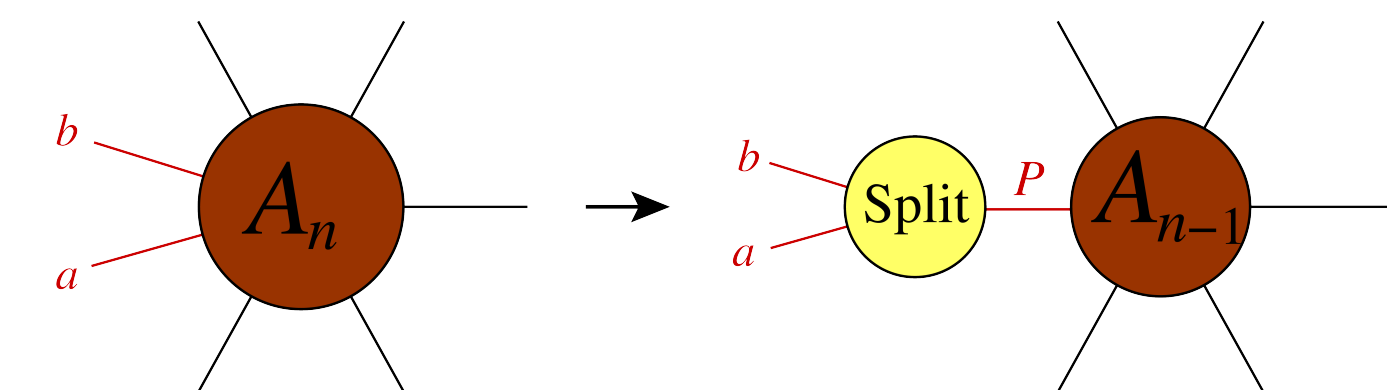
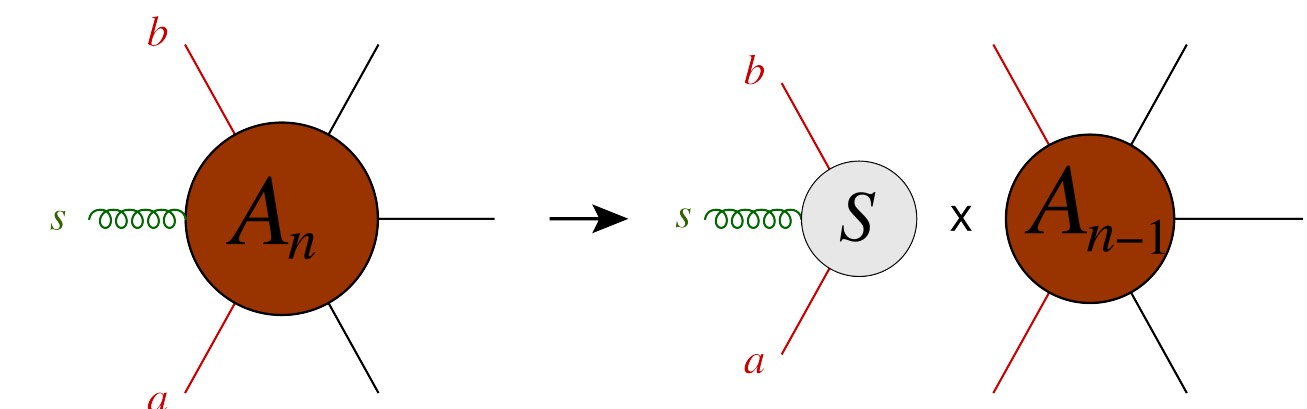
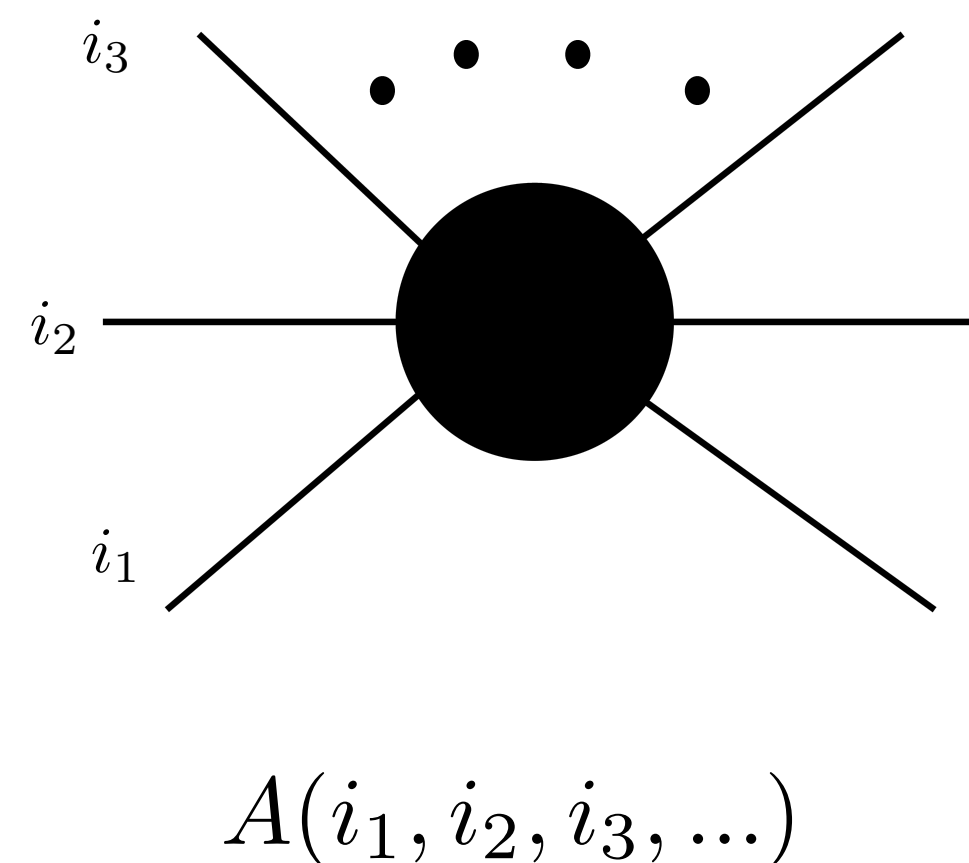
$$\rho_{ij} = 1 - \vec{n}_i \cdot \vec{n}_j \quad d_{i=4,5} = \rho_{1i} + \rho_{2i} = 2, \quad d_{4521} = \rho_{45} + \rho_{42} + \rho_{51}, \quad d_{4512} = \rho_{45} + \rho_{41} + \rho_{52}.$$

In case of the [antenna subtraction](#), no partitioning is introduced. Instead, color ordering is employed to rewrite a general scattering amplitude through “partial amplitudes”.

The most important property of a color-ordered amplitude is that a particle can only be emitted off its neighbours (at least as far as singular contributions are concerned).

The “elementary blocks” in this case are 3- and 4-particle sub-amplitudes of the color-ordered amplitudes; for particular kinematic configurations, these blocks contain all the relevant singularities and other particles in the amplitude are just “spectators”.

$$\mathcal{A}(1, 2, 3, \dots, N) = \sum_{\sigma_p} C_{i_2, \dots, i_N} \mathcal{A}(1, i_2, i_3, i_4, \dots, i_N)$$



**From lectures by L. Dixon**



## ***Singular regions and singular limits***

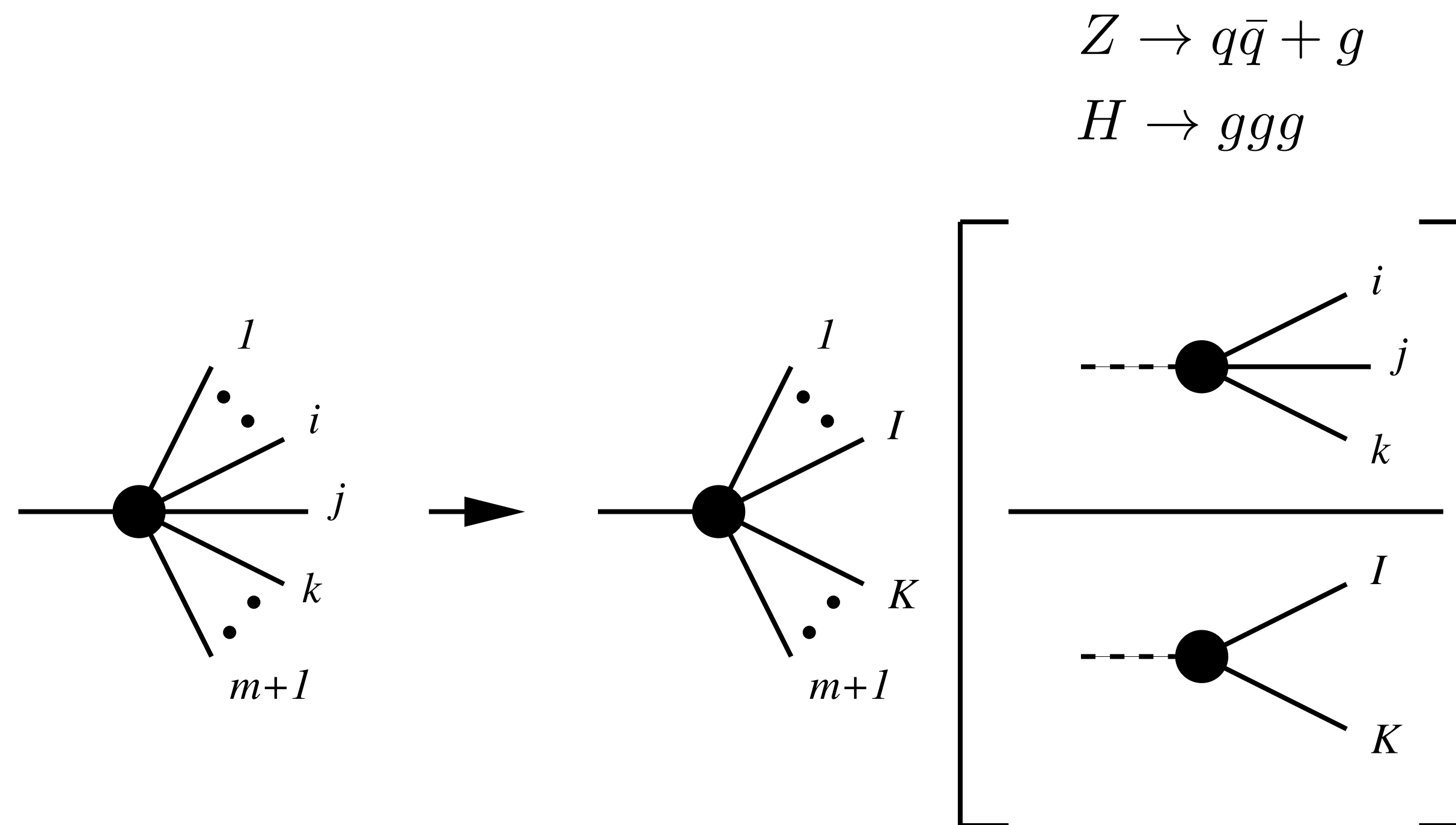
I remark that multiple infrared configurations which are not soft-collinear can contribute to QCD cross sections beyond next-to-leading order.

S. Frixione, A general approach to jet cross sections in QCD, 1997.

- it was not obvious that **independent soft and collinear subtractions are sufficient** and that no nontrivial correlations between (small) energies and (collinear) angles exist;
- in fact, such correlations do exist in individual Feynman diagrams but they appear to be absent in gauge-invariant amplitudes;
- this fact led to a confusion in early formulations of the FKS-like subtraction schemes.

For the antenna subtraction, one uses [exact matrix elements for simple processes](#) (e.g.  $Z \rightarrow qq+gg$ ,  $H \rightarrow gg+gg$ , etc.) to define the antenna functions; no singular limits are taken.

This sidesteps the problem of defining the singular regions etc. since they are fully included in physical matrix elements. The price to pay — not all spin correlations are correctly accounted for.



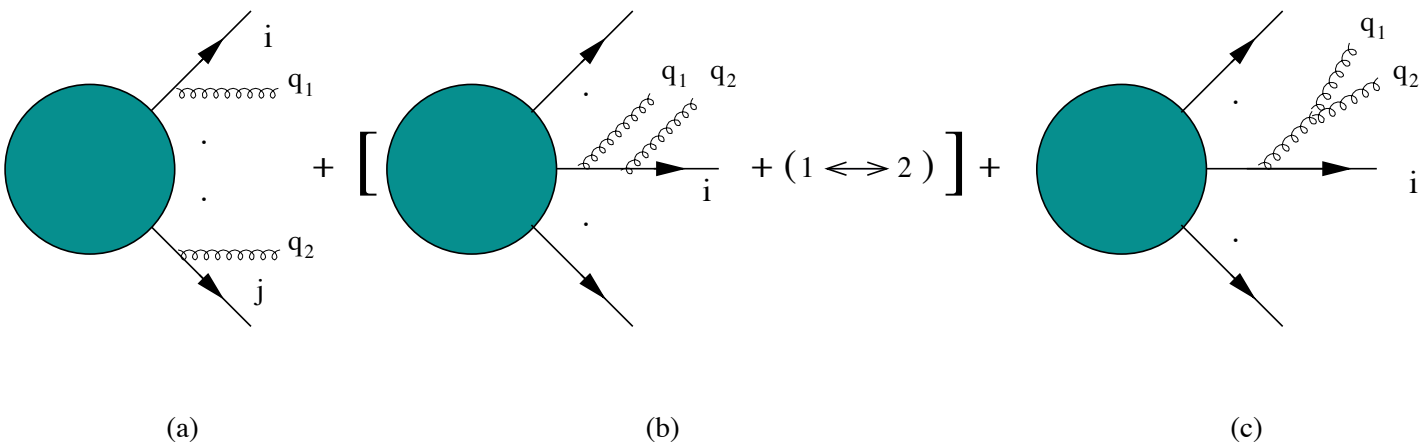
**Gehrmann et al.**

For FKS-like subtractions, the realisation that **independent** soft and collinear limits are sufficient to describe all singularities of the matrix elements is crucial as all these limits are known.

$$\int |\mathcal{M}|^2 \mathcal{F}_J d\phi_d = \int [|\mathcal{M}|^2 \mathcal{F}_J - \mathcal{S}] d\phi_4 + \int \mathcal{S} d\phi_d$$

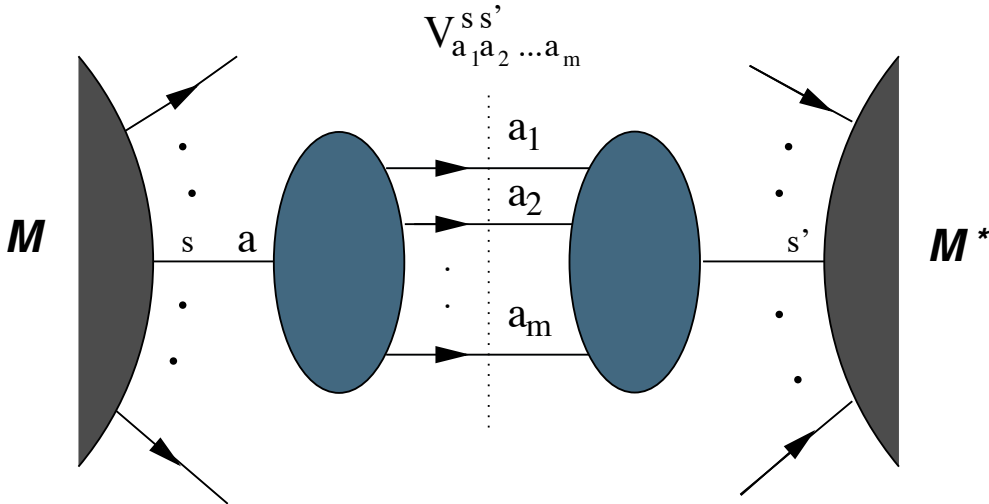
Soft limits, single and double:

$$\lim_{k_{1,2} \rightarrow 0} |\mathcal{M}|^2_{n+2}(\{p\}, k_1, k_2) \approx \text{Eik}(\{p\}, k_1, k_2) |M_n(\{p\})|^2$$



Collinear, double and triple:

$$\lim_{k_1 || k_2 || p_j} |\mathcal{M}_{n+2}|^2(\{p\}, k_1, k_2) \approx \frac{1}{s_{jk_1 k_2}^2} P(z_1, z_2, k_\perp) \otimes |\mathcal{M}_n(p_j k_1 k_2, \dots)|^2$$

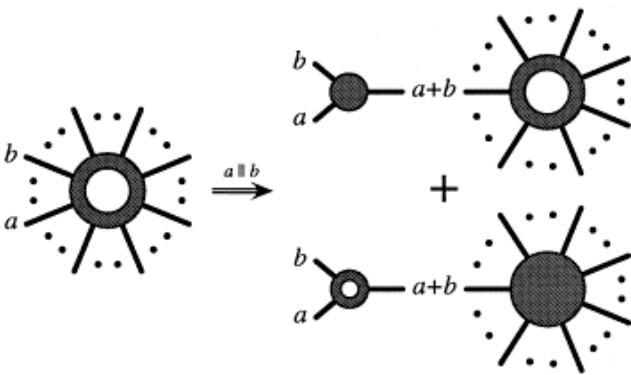


Soft limits of one-loop

$$\text{[Diagram: A shaded circle with a vertical rectangle attached to its right side. The rectangle has three horizontal lines extending to the right, labeled l, i, and j from top to bottom. A wavy line labeled q is attached to the top line l.]}$$

$$- \left( \text{[Diagram: A shaded circle with a vertical rectangle attached to its right side. The rectangle has three horizontal lines extending to the right, labeled i, j, and j from top to bottom. A wavy line labeled q is attached to the top line i.]} + \text{[Diagram: A shaded circle with a vertical rectangle attached to its right side. The rectangle has three horizontal lines extending to the right, labeled i, j, and j from top to bottom. A wavy line labeled q is attached to the top line i.]} \right) \times J^{(0)}(q)$$

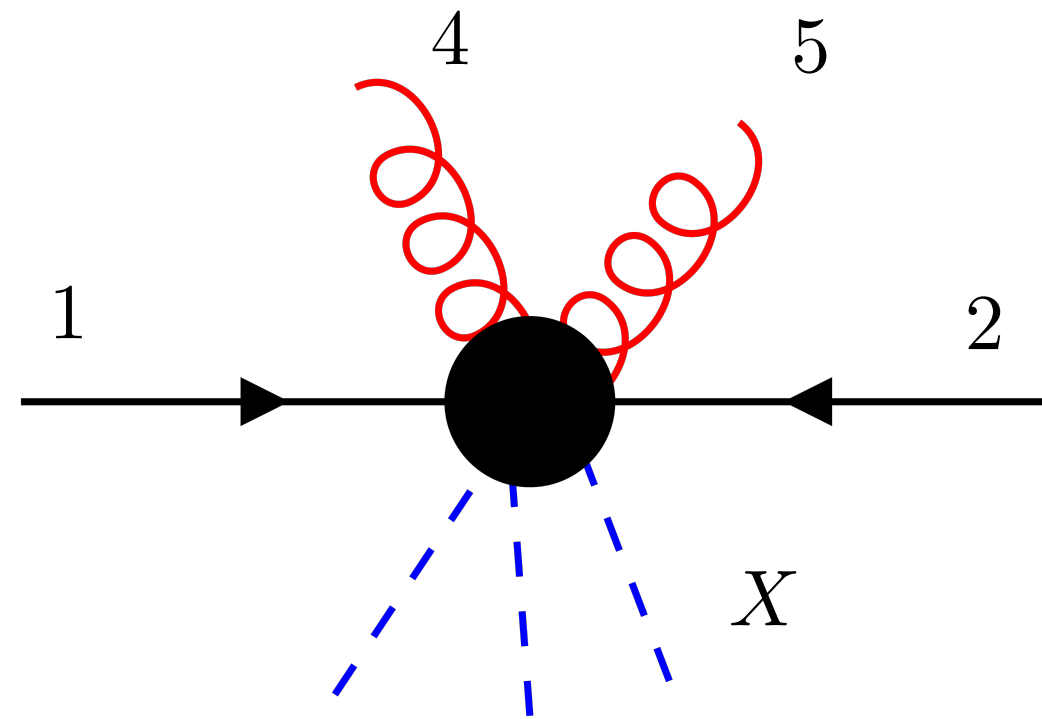
Collinear limits, one-loop



**Catani, Grazzini, Glover, Campbell, Kosower, Uwer, Czakon, Mitov**



These limits can be used for a straightforward definition of the subtraction terms, through an iterated subtraction of infra-red and collinear singularities. The action of operators on the matrix elements and the phase space requires explicit phase space parameterisation. If chosen properly, the operators commute.


 $\mathcal{S}$ 

Double-soft:  $E_4, E_5 \rightarrow 0$

 $S_5$ 

Single-soft:  $E_5 \rightarrow 0$

 $\mathcal{C}_{1,2}$ 

Triple-collinear:  $4||5||1$  and  $4||$

 $C_{4i}, C_{5i}$ 

Double-collinear  $4||i, 5||i, i=1,2$

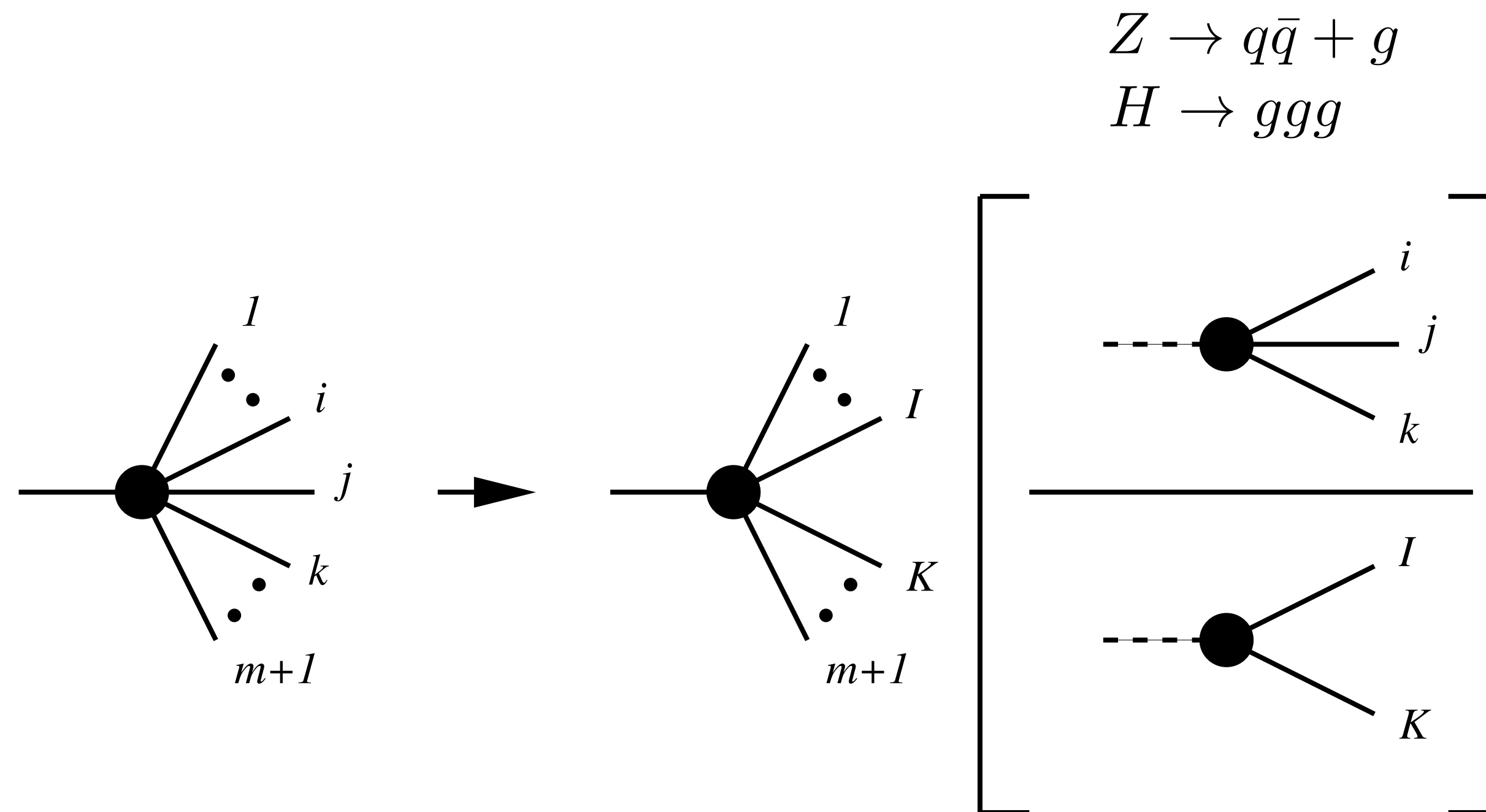
 $C_{45}$ 

Double-collinear  $4||5$

$$\begin{aligned}
 d\hat{\sigma}_{1245,f_a f_b}^{\text{NNLO}} = & \sum_{(ij) \in dc} \left\langle \left[ (I - C_{5j})(I - C_{4i}) \right] [I - \mathcal{S}] [I - S_5] \times \right. \\
 & \left. \times [df_4][df_5] w^{4i,5j} F_{\text{LM},f_a f_b}(1, 2, 4, 5) \right\rangle \\
 & + \sum_{i \in tc} \left\langle \left[ \theta^{(a)} [I - \mathcal{C}_i] [I - C_{5i}] + \theta^{(b)} [I - \mathcal{C}_i] [I - C_{45}] \right. \right. \\
 & \left. \left. + \theta^{(c)} [I - \mathcal{C}_i] [I - C_{4i}] + \theta^{(d)} [I - \mathcal{C}_i] [I - C_{45}] \right] \right. \\
 & \left. \times [I - \mathcal{S}] [I - S_5] [df_4][df_5] w^{4i,5i} F_{\text{LM},f_a f_b}(1, 2, 4, 5) \right\rangle.
 \end{aligned}$$

***Phase space in the singular limits and in the subtraction terms***

The antenna subtraction uses **exact**  $1 \rightarrow 3$  and  $1 \rightarrow 4$  phase spaces (NLO and NNLO, respectively) to integrate **exact** matrix elements used as subtraction terms.



**Gehrmann et al.**

For FKS-like subtraction schemes, phase spaces in the subtraction terms are usually simplified.

However, there is a lore that says that admissible simplifications are subtle, that Lorentz-invariant factorisation is important and that analytic integration of the subtraction terms is essential.



Is the **analytic** integration of the subtraction terms important ?

The answer, of course, is no. What we need is an integration **in d-dimensions**, but such an integration can be performed **both analytically and numerically**.

For a numerical integration in d-dimensions, one needs to find a parametrisation of the phase space which factorises all the singularities explicitly. Such a parametrisation is known.

$$\begin{aligned}
 d\Omega_{45}^{(a,c)} &= \frac{d\Omega_b^{(d-2)} d\Omega_a^{(d-3)}}{2^{6\epsilon} (2\pi)^{2d-2}} \frac{dx_3}{x_3^{1+2\epsilon}} \frac{dx_4}{x_4^{1+\epsilon}} \frac{d\lambda}{(\lambda(1-\lambda))^{1/2+\epsilon}} F_\epsilon^{-\epsilon} F_0 x_3^2 x_4 = \\
 &= \left[ \frac{1}{8\pi^2} \frac{(4\pi)^\epsilon}{\Gamma(1-\epsilon)} \right]^2 \left[ \frac{\Gamma^2(1-\epsilon)}{\Gamma(1-2\epsilon)} \right] \left[ \frac{d\Omega_{d-2}^{(b)}}{\Omega_{d-2}} \frac{d\Omega_{d-3}^{(a)}}{\Omega_{d-3}} \right] \times \\
 &\quad \times \frac{dx_3}{x_3^{1+2\epsilon}} \frac{dx_4}{x_4^{1+\epsilon}} \frac{d\lambda}{\pi(\lambda(1-\lambda))^{1/2+\epsilon}} (256 F_\epsilon)^{-\epsilon} 4 F_0 x_3^2 x_4. \\
 F_\epsilon &= \frac{(1-x_3)(1-x_3 x_4/2)(1-x_4/2)^2}{2N(x_3, x_4/2, \lambda)^2}, \quad F_0 = \frac{(1-x_4/2)}{2N(x_3, x_4/2, \lambda)},
 \end{aligned}$$

**M. Czakon et al.**

$$F(x_3, x_4) = x_3^2 x_4 |\mathcal{M}|^2(x_3, x_4)$$

$$\begin{aligned}
 \int_0^1 \frac{dx_3}{x_3^{1+2\epsilon}} \frac{dx_4}{x_4^{1+\epsilon}} F(x_3, x_4) &= \frac{1}{2\epsilon^2} F(0, 0) \\
 &- \frac{1}{\epsilon} \int_0^1 \frac{dx_3}{x_3} (F(x_3, 0) - F(0, 0)) \\
 &- \frac{1}{2\epsilon} \int_0^1 \frac{dx_4}{x_4} (F(0, x_4) - F(0, 0)) + \dots
 \end{aligned}$$

## Does one need Lorentz-invariant phase-space factorisation for an analytic integration?

The answer is again no. Lorentz invariance helps, of course, but it is definitely not necessary. In fact, modern methods for multi-loop computations and reverse unitarity allows us to perform complex computations even in predefined and not optimal reference frames.

$$\mathfrak{S}_{ij}^{(gg)} = \int [dk_4][dk_5] \theta(E_{\max} - k_4^0) \theta(k_4^0 - k_5^0) \widetilde{S}_{ij}(k_4, k_5),$$

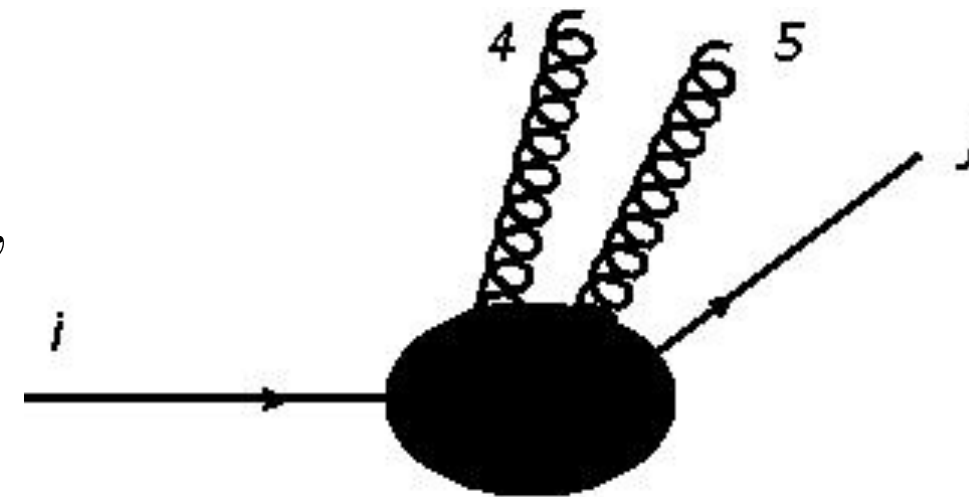
$$\widetilde{S}_{ij}(k_4, k_5) = 2S_{ij}(k_4, k_5) - S_{ii}(k_4, k_5) - S_{jj}(k_4, k_5),$$

$$S_{ij}(k) = \frac{p_i \cdot p_j}{(p_i \cdot k)(p_j \cdot k)},$$

$$S_{ij}(k_4, k_5) = S_{ij}^{\text{so}}(k_4, k_5) - \frac{2p_i \cdot p_j}{k_4 \cdot k_5 [p_i \cdot (k_4 + k_5)] [p_j \cdot (k_4 + k_5)]} \\ + \frac{(p_i \cdot k_4)(p_j \cdot k_5) + (p_i \cdot k_5)(p_j \cdot k_4)}{[p_i \cdot (k_4 + k_5)] [p_j \cdot (k_4 + k_5)]} \left[ \frac{(1 - \epsilon)}{(k_4 \cdot k_5)^2} - \frac{1}{2} S_{ij}^{\text{so}}(k_4, k_5) \right]$$

$$\text{Ci}_n(z) = \frac{(\text{Li}_n(e^{iz}) + \text{Li}_n(e^{-iz}))}{2}, \quad \text{Si}_n(z) = \frac{(\text{Li}_n(e^{iz}) - \text{Li}_n(e^{-iz}))}{2i}$$

**M. Delto et al.**



$$\mathfrak{S}_{ij}^{(gg)} = (2E_{\max})^{-4\epsilon} \left[ \frac{1}{8\pi^2} \frac{(4\pi)^\epsilon}{\Gamma(1 - \epsilon)} \right]^2 \left\{ \frac{1}{2\epsilon^4} + \frac{1}{\epsilon^3} \left[ \frac{11}{12} - \ln(s^2) \right] \right. \\ + \frac{1}{\epsilon^2} \left[ 2\text{Li}_2(c^2) + \ln^2(s^2) - \frac{11}{6} \ln(s^2) + \frac{11}{3} \ln 2 - \frac{\pi^2}{4} - \frac{16}{9} \right] \\ + \frac{1}{\epsilon} \left[ 6\text{Li}_3(s^2) + 2\text{Li}_3(c^2) + \left( 2\ln(s^2) + \frac{11}{3} \right) \text{Li}_2(c^2) - \frac{2}{3} \ln^3(s^2) \right. \\ + \left( 3\ln(c^2) + \frac{11}{6} \right) \ln^2(s^2) - \left( \frac{22}{3} \ln 2 + \frac{\pi^2}{2} - \frac{32}{9} \right) \ln(s^2) \\ \left. - \frac{45}{4} \zeta_3 - \frac{11}{3} \ln^2 2 - \frac{11}{36} \pi^2 - \frac{137}{18} \ln 2 + \frac{217}{54} \right] \\ + 4\text{G}_{-1,0,0,1}(s^2) - 7\text{G}_{0,1,0,1}(s^2) + \frac{22}{3} \text{Ci}_3(2\delta) + \frac{1}{3 \tan(\delta)} \text{Si}_2(2\delta) \\ + 2\text{Li}_4(c^2) - 14\text{Li}_4(s^2) + 4\text{Li}_4 \left( \frac{1}{1+s^2} \right) - 2\text{Li}_4 \left( \frac{1-s^2}{1+s^2} \right) \\ + 2\text{Li}_4 \left( \frac{s^2-1}{1+s^2} \right) + \text{Li}_4(1-s^4) + \left[ 10\ln(s^2) - 4\ln(1+s^2) \right. \\ \left. + \frac{11}{3} \right] \text{Li}_3(c^2) + \left[ 14\ln(c^2) + 2\ln(s^2) + 4\ln(1+s^2) + \frac{22}{3} \right] \text{Li}_3(s^2) \\ \left. + 4\ln(c^2) \text{Li}_3(-s^2) + \frac{9}{2} \text{Li}_2^2(c^2) - 4\text{Li}_2(c^2) \text{Li}_2(-s^2) + \left[ 7\ln(c^2) \ln(s^2) \right] \right\}$$

$$\delta = \frac{\theta_{ij}}{2} \\ s = \sin \frac{\theta_{ij}}{2} \\ c = \cos \frac{\theta_{ij}}{2}$$

***Slicing***

$$\int |\mathcal{M}|^2 F_J \, \mathrm{d}\phi_d = \int_0^\delta [|\mathcal{M}|^2 F_J \, \mathrm{d}\phi_d]_{\text{simp}} + \int_\delta^1 |\mathcal{M}|^2 F_J \, \mathrm{d}\phi_4 + \mathcal{O}(\delta)$$

***Slicing***

$$\int |\mathcal{M}|^2 F_J \, \mathrm{d}\phi_d = \int_0^\delta [|\mathcal{M}|^2 F_J \, \mathrm{d}\phi_d]_{\text{simp}} + \int_\delta^1 |\mathcal{M}|^2 F_J \, \mathrm{d}\phi_4 + \mathcal{O}(\delta)$$

**Not Cool**

***Slicing***

$$\int |\mathcal{M}|^2 F_J d\phi_d = \int_0^\delta [|\mathcal{M}|^2 F_J d\phi_d]_{\text{simp}} + \int_\delta^1 |\mathcal{M}|^2 F_J d\phi_d + \mathcal{O}(\delta)$$



One of the main reasons for the slicing comeback is the increase in computing power available for such computations.

## **Slicing**

$$\int |\mathcal{M}|^2 F_J d\phi_d = \int_0^\delta [|\mathcal{M}|^2 F_J d\phi_d]_{\text{simp}} + \int_\delta^1 |\mathcal{M}|^2 F_J d\phi_4 + \mathcal{O}(\delta)$$

“q<sub>t</sub> slicing” [S. Catani and M. Grazzini]

“Jettiness slicing” [R. Boughezal et al., J. Gaunt et al.]

Modern slicing parameters:

- 1) transverse momentum of a colorless or colored (but massive) system;
- 2) jettiness;

$$\tau_N = \sum_i \min \left\{ \frac{2q_a k_i}{Q^2}, \frac{q_b k_i}{Q^2}, \dots, \frac{2q_N k_i}{Q^2} \right\}$$

Computation of singular contribution is helped by an understanding how the cross sections behave in the limit of small slicing parameter.

$$\lim_{\tau \rightarrow 0} d\sigma_{pp \rightarrow X} \approx B \otimes B \otimes S \otimes H \otimes J \otimes d\sigma_{pp \rightarrow X}^{\text{LO}}$$

Jettiness is applicable to final states with jets; beam and jet functions are universal and known, soft functions are always challenging.

q<sub>t</sub> slicing is venturing in the direction of jet physics using new interpretation of the slicing parameter.

**L. Buonocore et al.**

Transverse momentum slicing does not receive linear corrections in the slicing parameter if done properly.

**L. Buonocore et al.**



## **Slicing**

$$\int |\mathcal{M}|^2 F_J d\phi_d = \int_0^\delta [|\mathcal{M}|^2 F_J d\phi_d]_{\text{simp}} + \int_\delta^1 |\mathcal{M}|^2 F_J d\phi_4 + \mathcal{O}(\delta)$$

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The slicing schemes can be generalised to N3LO in a straightforward way; many ingredients are known and many calculations for  $2 \rightarrow 1$  have been done (Drell-Yan, Higgs).

Similar to NNLO with multi-jets, [calculation of jettiness soft functions](#) is an obstacle for extending the N3LO slicing computations to final states with jets.

## Summary:

- fixed order computations in general and NNLO QCD computations in particular are very important for the LHC physics program;
- there exists a large number of working NNLO QCD subtraction and slicing schemes;
- some of these schemes can do (more or less) everything that we can dream of, in the context of the LHC physics and a recent computation of NNLO QCD corrections to 3-jet production at the LHC is a clear confirmation of this point;
- in spite of the differences in details, existing subtraction schemes are based on similar ideas and principles;
- it seems that none of the newly proposed subtraction schemes has been a game-changer;
- analytic refinements of the subtraction schemes and their improvements are probably less important than their efficient implementations in numerical programs. In my opinion, this is what will make the difference in the future.