New computational methods for NLO and NNLO calculations in QCD

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I: **Techniques already encountered at LO**

II: **Methods at NLO**

III: **Steps towards NNLO**

Part I: Prelude

Physics is about numbers

Monte Carlo integration

We are interested in multi-dimensional integrals:

$$I = \int_{[0,1]^n} d^n u \, f(u_1, \ldots, u_n)$$

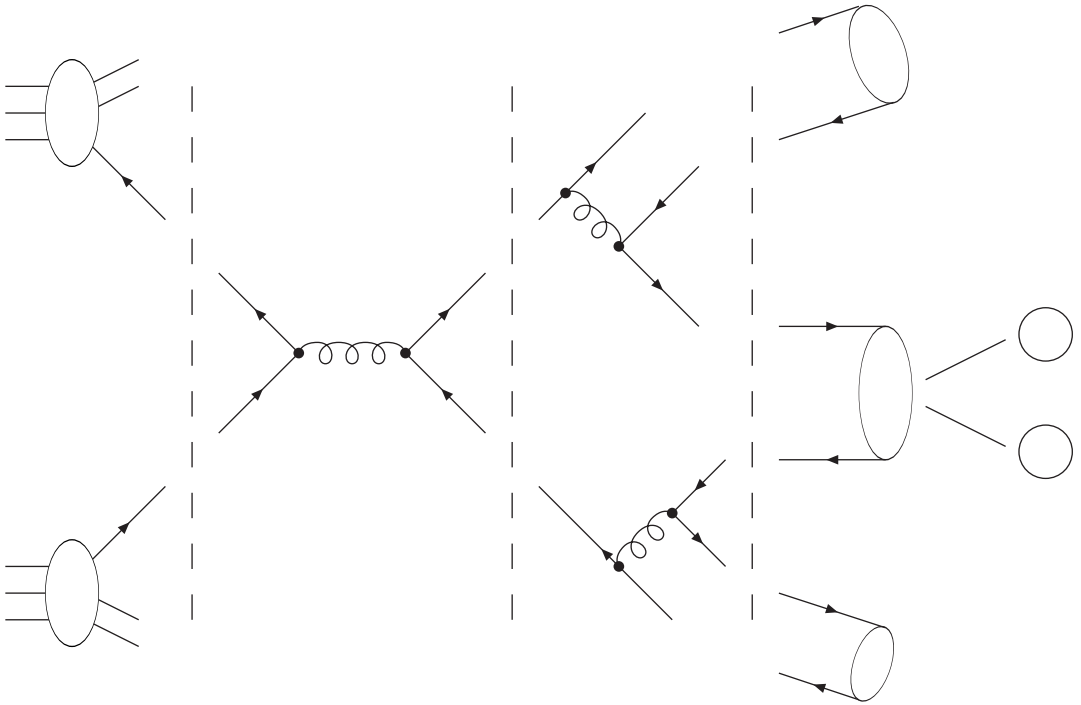
Evaluate the integrand at N random points $\vec{u}_j = (u_{j,1}, \ldots, u_{j,n})$.

$$I = \frac{1}{N} \sum_{j=1}^{N} f(\vec{u}_j)$$

Error scales as

$$\sigma \sim \frac{1}{\sqrt{N}}$$

Simulation of scattering events

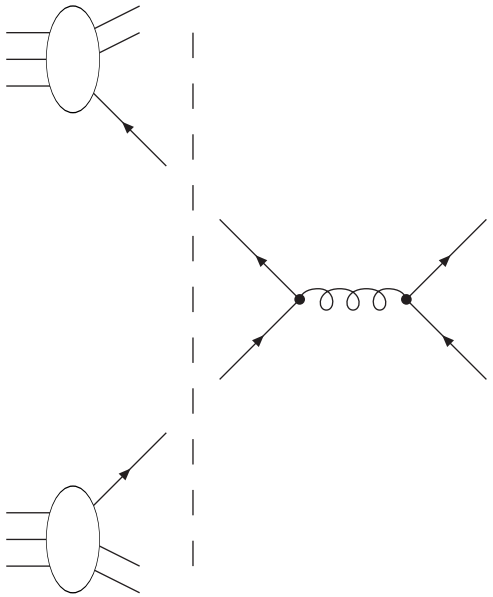


Underlying event: Interactions of the proton remnants.

Multiple interactions: more than one pair of partons undergo hard scattering

Pile-up events: more than one hadron-hadron scattering within a bunch crossing

Fixed-order calculations



pdf's

hard scattering

Done at the parton level with quarks and gluons.

Usually only a few partons in the final state.

Amplitudes calculated in perturbation theory.

Method of choice to describe well-separated jets.

The master formula for the calculation of observables

$$\langle O \rangle = \sum_{a,b} \underbrace{\int dx_1\, f_a(x_1) \int dx_2\, f_b(x_2)}_{\text{pdf's}} \underbrace{\frac{1}{2K(\hat{s})}}_{\text{flux factor}} \underbrace{\frac{1}{n_a^{\text{spin}} n_b^{\text{spin}} n_a^{\text{colour}} n_b^{\text{colour}}}}_{\text{average over initial spins and colours}}$$

$$\times \sum_n \underbrace{\int d\phi_n}_{\text{integral over phase space}} \underbrace{O(p_1, \ldots, p_n)}_{\text{observable}} \underbrace{|\mathcal{A}_{n+2}|^2}_{\text{amplitude}}$$

We will discuss:

- Required properties of observables
- Calculation of the amplitude
- Integration over the phase space

Part I

Infrared-safe observables

Soft and collinear particles

A particle detector has a finite resolution.

- Finite angular resolution: A pair of particles moving in (almost) the same direction can not be resolved below a certain angle.

  We call these particles a pair of collinear particles.

  Example: An electron and a photon not resolved by the electromagnetic calorimeter.

- Detection only above a certain threshold: A particle with an energy below a certain threshold will not be detected.

  We call this particle a soft particle.

  Example: A low-energy photon.

Infrared-safe observables

Observables which do not depend on long-distance behaviour, are called infrared-safe observables and can reliably be calculated in perturbation theory.

In particular, it is required that they do not change value, if infinitessimal soft or collinear particles are added.
For example:

$$\text{collinear}: \quad \lim_{p_i \| p_j} O_n(p_1, \ldots, p_i, \ldots, p_j, \ldots, p_n) = O_{n-1}(p_1, \ldots, p_{ij}, \ldots, p_n)$$

$$\text{soft}: \quad \lim_{p_j \to 0} O_n(p_1, \ldots, p_j, \ldots, p_n) = O_{n-1}(p_1, \ldots, p_{j-1}, p_{j+1}, \ldots, p_n)$$

Event shapes

Event shapes are observables calculated from all particles in an event.

Typical examples of infrared-safe event shapes in electron-positron annihilation are thrust, heavy jet mass, wide jet broadening, total jet broadening, C parameter, etc.

Definition: Thrust

$$T = \max_{\hat{n}} \frac{\sum_i |\vec{p}_i \cdot \hat{n}|}{\sum_i |\vec{p}_i|}$$

For two particles back-to-back one has

$$T = 1$$

For many particles, isotropically distributed we have

$$T = \frac{1}{2}$$

Spherocity versus sphericity

Spherocity:

$$S = \left(\frac{4}{\pi}\right)^2 \min_{\hat{n}} \left(\frac{\sum_i |\vec{p}_i^{\perp}|}{\sum_i |\vec{p}_i|}\right)^2$$

Sphericity:

$$\left(\frac{4}{\pi}\right)^2 \min_{\hat{n}} \frac{\sum_i |\vec{p}_i^{\perp}|^2}{\sum_i |\vec{p}_i|^2}$$

Sphericity is not infrared-safe ! (Altarelli, Phys. Rept. 1981)

... however this does not stop experimentalists from measuring it ... (Aleph 1990)

Jet algorithms

The most fine-grained look at hadronic events consistent with infrared safety is given by classifying the particles into jets.

Ingredients for a sequential recombination algorithm:

- a resolution variable y_{ij} where a smaller y_{ij} means that particles i and j are "closer";

$$y_{ij}^{\mathrm{Durham}} \quad = \quad \frac{2(1-\cos\theta_{ij})}{Q^2}\,\min(E_i^2, E_j^2)$$

- a combination procedure which combines two four-momenta into one;

$$p_{(ij)}^{\mu} \quad = \quad p_i^{\mu} + p_j^{\mu}.$$

- a cut-off y_{cut} which provides a stopping point for the algorithm.

Jet algorithms

- In electron-positron annihilation one uses mainly exclusive jet algorithms, where each particle in an event is assigned uniquely to one jet.

- In hadron-hadron collisions one uses mainly inclusive jet algorithms, where each particle is either assigned uniquely to one jet or to no jet at all.

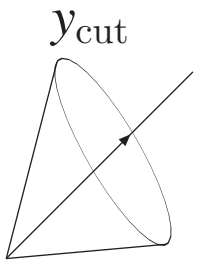
- One distinguishes further sequential recombination algorithm and cone algorithms. Infrared-safe cone algorithm: SISCone.

- Once jets are defined we can look at cross sections, $p_\perp$ distributions, rapidity distributions, etc.

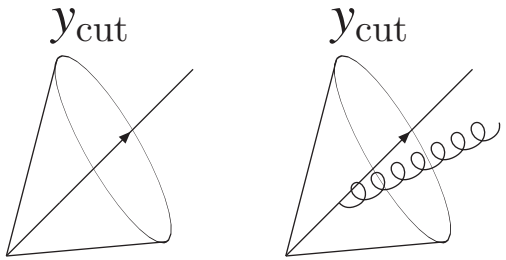
Modeling of jets

In a perturbative calculation jets are modeled by only a few partons. This improves with the order to which the calculation is done.

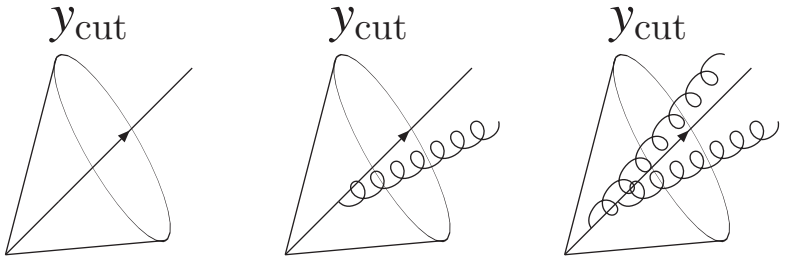
At leading order:



At next-to-leading order:



At next-to-next-to-leading order:



Part I

Amplitudes

Quantum chromodynamics

QCD describes quarks and gluons. The gauge group is the non-Abelian group $SU(3)$.

$$\mathcal{L}_{\mathrm{QCD}} = -\frac{1}{4}F^a_{\mu\nu}F^{a\mu\nu} + \sum_{\mathrm{quarks}} \bar{\psi}(i\partial\!\!\!/ + g\gamma^\mu T^a A^a_\mu - m_q)\psi$$

Field strength:

$$F^a_{\mu\nu} = \partial_\mu A^a_\nu - \partial_\nu A^a_\mu + g f^{abc} A^b_\mu A^c_\nu$$

$SU(3)$ matrices:

$$\left[T^a, T^b\right] = i f^{abc} T^c$$

If we neglect quark masses, then QCD depends on one parameter

$$\alpha_s = \frac{g^2}{4\pi}$$

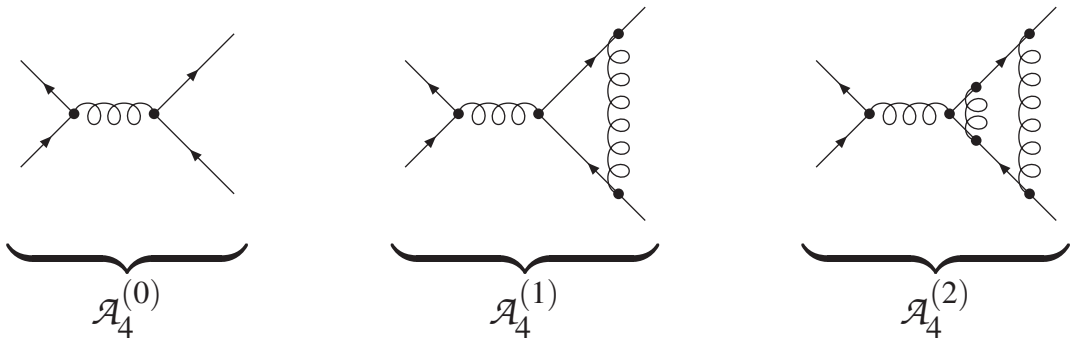
Perturbation theory

Due to the smallness of the coupling constants α_s at high energies, we may compute the amplitude reliable in perturbation theory,

$$\mathcal{A}_n \quad = \quad g^{n-2}\left(\mathcal{A}_n^{(0)} + g^2\mathcal{A}_n^{(1)} + g^4\mathcal{A}_n^{(2)} + g^6\mathcal{A}_n^{(3)} + \ldots\right).$$

$\mathcal{A}_n^{(l)}$: amplitude with n external particles and l loops.

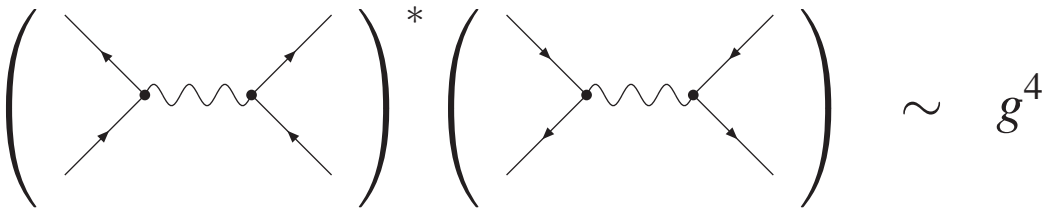
Some examples of diagrams:



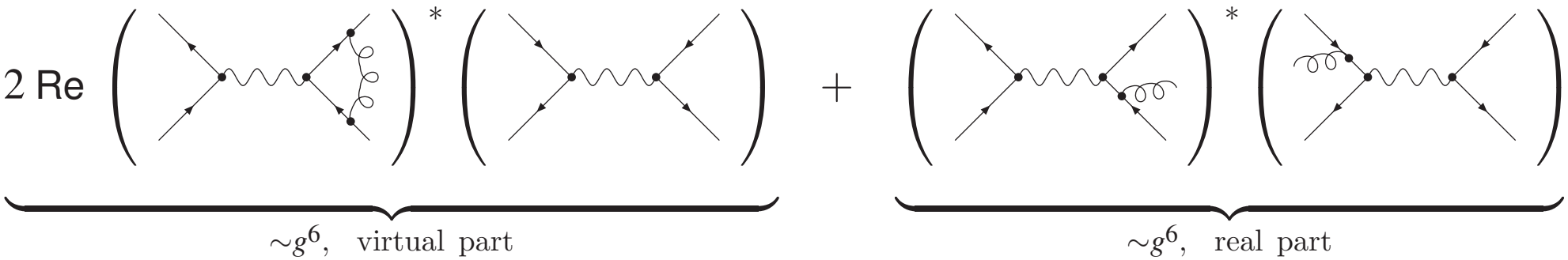
Perturbation theory

We need the amplitude squared:

At leading order (LO) only Born amplitudes contribute:



At next-to-leading order (NLO): One-loop amplitudes and Born amplitudes with an additional parton.



Real part contributes whenever the additional parton is not resolved.

Perturbation theory

Perturbative expansion of the amplitude squared (LO, NLO, NNLO):

$$|\mathcal{A}_n|^2 = g^{2n-4} \underbrace{\left|\mathcal{A}_n^{(0)}\right|^2}_{\text{Born}} + g^{2n-2} \underbrace{2\,\text{Re}\;\mathcal{A}_n^{(0)\,*}\,\mathcal{A}_n^{(1)}}_{\text{virtual}} + g^{2n} \underbrace{\left(\left|\mathcal{A}_n^{(1)}\right|^2 + 2\,\text{Re}\;\mathcal{A}_n^{(0)\,*}\,\mathcal{A}_n^{(2)}\right)}_{\text{one-loop squared and two-loop}}$$

$$|\mathcal{A}_{n+1}|^2 = g^{2n-2} \underbrace{\left|\mathcal{A}_{n+1}^{(0)}\right|^2}_{\text{real}} + g^{2n} \underbrace{2\,\text{Re}\;\mathcal{A}_{n+1}^{(0)\,*}\,\mathcal{A}_{n+1}^{(1)}}_{\text{loop+unresolved}}$$

$$|\mathcal{A}_{n+2}|^2 = g^{2n} \underbrace{\left|\mathcal{A}_{n+2}^{(0)}\right|^2}_{\text{double unresolved}}$$

Feynman rules

Each piece of a Feynman diagram corresponds to a mathematical expression:

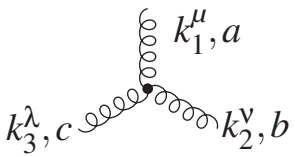
External edge:

$$= \quad \varepsilon^a_\mu(k)$$

Internal edge:

$$= \quad \frac{i}{k^2}\left(-g_{\mu\nu} + (1-\xi)\frac{k_\mu k_\nu}{k^2}\right)\delta^{ab}$$

Vertex:



$$= \quad g f^{abc}\left[g^{\mu\nu}\left(k_1^\lambda - k_2^\lambda\right) + g^{\nu\lambda}\left(k_2^\mu - k_3^\mu\right) + g^{\lambda\mu}\left(k_3^\nu - k_1^\nu\right)\right]$$

Inconveniences we know to handle

- Loop amplitudes may have ultraviolet and infrared (soft and collinear) divergences.
- Dimensional regularisation is the method of choice for the regularisation of loop integrals.
- Ultraviolet divergences are removed by renormalisation.
- Phase space integration for the real emission diverges in the soft or collinear region.
- Unitarity requires the same regularisation (i.e. dimensional regularisation) for these divergences.
- Infrared divergences cancel between real and virtual contribution, or with an additional collinear counterterm in the case of initial-state partons.

The textbook method

- The amplitude is given as a sum of Feynman diagrams.
- Squaring the amplitude implies summing over spins and colour.
- One-loop tensor integrals can always be reduced to scalar integrals (Passarino-Veltman).
- All one-loop scalar integrals are known.
- Phase space slicing or subtraction method to handle infrared divergences.

Works in principle, but not in practice ...

An analogy: Testing prime numbers

To check if an integer N is prime,

- For $2 \leq j \leq \sqrt{N}$ check if j divides N.
- If such a j is found, N is not prime.
- Otherwise N is prime.

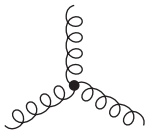
Works in principle, but not in practice ...

Brute force

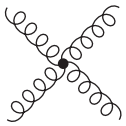
Number of Feynman diagrams contributing to $gg \to ng$ at tree level:

2	4
3	25
4	220
5	2485
6	34300
7	559405
8	10525900

Feynman rules:



$$= g f^{abc} \left[(k_2 - k_3)_\mu g_{\nu\lambda} + (k_3 - k_1)_\nu g_{\lambda\mu} + (k_1 - k_2)_\lambda g_{\mu\nu} \right]$$



$$= -ig^2 \left[f^{abe} f^{ecd} \left(g_{\mu\lambda} g_{\nu\rho} - g_{\mu\rho} g_{\nu\lambda} \right) + f^{ace} f^{ebd} \left(g_{\mu\nu} g_{\lambda\rho} - g_{\mu\rho} g_{\lambda\nu} \right) + f^{ade} f^{ebc} \left(g_{\mu\nu} g_{\lambda\rho} - g_{\mu\lambda} g_{\nu\rho} \right) \right]$$

Feynman diagrams are not the method of choice !

Helicity amplitudes

Suppose that an amplitude is given as the sum of N Feynman diagrams.
To calculate the amplitude squared à la Bjorken-Drell:
Sum over all spins and use

$$\begin{aligned}
\sum_\lambda \varepsilon_\mu^*(k,\lambda)\varepsilon_\nu(k,\lambda) &= -g_{\mu\nu} + \frac{k_\mu n_\nu + n_\mu k_\nu}{kn}, \\
\sum_\lambda u(p,\lambda)\bar{u}(p,\lambda) &= \not{p} + m, \\
\sum_\lambda v(p,\lambda)\bar{v}(p,\lambda) &= \not{p} - m.
\end{aligned}$$

This gives of the order N^2 terms.

Better: For each spin configuration evaluate the amplitude to a complex number. Taking the norm of a complex number is a cheap operation.

Spinors

Spinors are solutions of the Dirac equation.

For massless particles two-component Weyl spinors are a convenient choice:

$$|p+\rangle = \frac{1}{\sqrt{|p_+|}} \begin{pmatrix} -p_{\perp^*} \\ p_+ \end{pmatrix} \qquad |p-\rangle = \frac{1}{\sqrt{|p_+|}} \begin{pmatrix} p_+ \\ p_\perp \end{pmatrix}$$

$$\langle p+| = \frac{1}{\sqrt{|p_+|}} (-p_\perp, p_+) \qquad \langle p-| = \frac{1}{\sqrt{|p_+|}} (p_+, p_{\perp^*})$$

Light-cone coordinates: $p_+ = p_0 + p_3$, $p_- = p_0 - p_3$, $p_\perp = p_1 + ip_2$, $p_{\perp^*} = p_1 - ip_2$

Spinor products:

$$\langle pq \rangle = \langle p - | q + \rangle , \qquad [qp] = \langle q + | p - \rangle .$$

The spinor products are anti-symmetric.

Bra-ket notation versus dotted-undotted indices

Two different notations for the same thing:

$$|p+\rangle = p_B \qquad\qquad \langle p+| = p_{\dot{A}}$$

$$|p-\rangle = p^{\dot{B}} \qquad\qquad \langle p-| = p^A$$

The spinor helicity method

Gluon polarisation vectors:

$$\varepsilon_\mu^+(k,q) = \frac{\langle k+|\gamma_\mu|q+\rangle}{\sqrt{2}\langle q-|k+\rangle}, \qquad \varepsilon_\mu^-(k,q) = \frac{\langle k-|\gamma_\mu|q-\rangle}{\sqrt{2}\langle k+|q-\rangle}$$

q is an arbitrary light-like reference momentum. Dependency on q drops out in gauge invariant quantities.

Berends, Kleiss, De Causmaecker, Gastmans and Wu; Xu, Zhang and Chang;

Kleiss and Stirling; Gunion and Kunszt

Integration over helicity angles

Example: For $gg \to 7g$ we have $N = 559405$ Born diagrams.

- Helicity amplitudes reduce the complexity from

$$N^2 = 312933954025 \text{ terms}$$
$$\text{to } 2^n \cdot N = 512 \cdot 559405 \text{ terms.}$$

- Factor $2^n = 2^9 = 512$ from sum over all helicities.

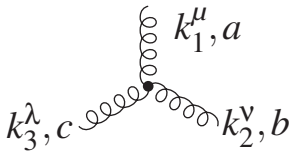
- Replace sum over helicities by Monte Carlo integration over helicity angles:
  P. Draggiotis, R. Kleiss, C. Papadopoulos, '98

$$\sum_{\lambda=\pm} \varepsilon_\mu^{\lambda\,*} \varepsilon_\nu^\lambda \quad = \quad \frac{1}{2\pi} \int_0^{2\pi} d\phi\, \varepsilon_\mu(\phi)^* \varepsilon_\nu(\phi), \qquad \varepsilon_\mu(\phi) = e^{i\phi} \varepsilon_\mu^+ + e^{-i\phi} \varepsilon_\mu^-.$$

- Monte Carlo error is independent of the number of dimensions,
  this removes the factor 2^n.

Colour decomposition

Each Feynman rule has a colour part and a kinematical part:



$$= g \underbrace{f^{abc}}_{\text{colour}} \underbrace{\left[g^{\mu\nu}\left(k_1^\lambda - k_2^\lambda\right) + g^{\nu\lambda}\left(k_2^\mu - k_3^\mu\right) + g^{\lambda\mu}\left(k_3^\nu - k_1^\nu\right)\right]}_{\text{kinematic}}$$

In an amplitude collect all terms with the same colour structure.

Example: The n-gluon amplitude:

$$\mathcal{A}_n^{(0)}(g_1, g_2, \ldots, g_n) = g^{n-2} \sum_{\sigma \in S_n/Z_n} \underbrace{2\,\mathrm{Tr}\left(T^{a_{\sigma(1)}} \ldots T^{a_{\sigma(n)}}\right)}_{\text{colour factors}} \underbrace{A_n^{(0)}\left(g_{\sigma(1)}, \ldots, g_{\sigma(n)}\right)}_{\text{partial amplitudes}}.$$

The partial amplitudes do not contain any colour information and are gauge-invariant.
Each partial amplitude has a fixed cyclic order of the external legs.

P. Cvitanovic, P. G. Lauwers, and P. N. Scharbach; F. A. Berends and W. Giele; M. L. Mangano, S. J. Parke, and Z. Xu; D. Kosower, B.-H. Lee, and V. P. Nair; Z. Bern and D. A. Kosower.

Colour decomposition

Lie algebra of $SU(N)$:

$$\left[T^a, T^b\right] = i f^{abc} T^c, \qquad \text{Tr}\left(T^a T^b\right) = \frac{1}{2}\delta^{ab}$$

Multiply commutator relation by T^d and take the trace:

$$i f^{abc} \;=\; 2\text{Tr}\left(T^a T^b T^c\right) - 2\text{Tr}\left(T^b T^a T^c\right)$$

Fierz identities:

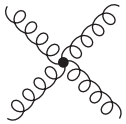
$$\begin{aligned}
\text{Tr}\left(T^a X\right)\text{Tr}\left(T^a Y\right) &= \frac{1}{2}\left[\text{Tr}\left(XY\right) - \frac{1}{N}\text{Tr}\left(X\right)\text{Tr}\left(Y\right)\right], \\
\text{Tr}\left(T^a X T^a Y\right) &= \frac{1}{2}\left[\text{Tr}\left(X\right)\text{Tr}\left(Y\right) - \frac{1}{N}\text{Tr}\left(XY\right)\right].
\end{aligned}$$

Improvement due to the colour decomposition

Number of Feynman diagrams contributing to $gg \to ng$ at tree level:

n	2	3	4	5	6	7	8
unordered	4	25	220	2485	34300	559405	10525900
cyclic ordered	3	10	36	133	501	1991	7335

Feynman rules: Four-gluon vertex



Traditional (unordered):

$$-ig^2\left[f^{abe}f^{ecd}\left(g^{\mu\lambda}g^{\nu\rho}-g^{\mu\rho}g^{\nu\lambda}\right)+f^{ace}f^{ebd}\left(g^{\mu\nu}g^{\lambda\rho}-g^{\mu\rho}g^{\lambda\nu}\right)+f^{ade}f^{ebc}\left(g^{\mu\nu}g^{\lambda\rho}-g^{\mu\lambda}g^{\nu\rho}\right)\right]$$

Colour-stripped and cyclic ordered:

$$i\left(2g^{\mu\lambda}g^{\nu\rho}-g^{\mu\nu}g^{\lambda\rho}-g^{\mu\rho}g^{\nu\lambda}\right)$$

The $U(1)$-gluon

Fierz identities for $SU(N)$:

$$\begin{aligned}
\mathrm{Tr}\,(T^a X)\,\mathrm{Tr}\,(T^a Y) &= \frac{1}{2}\mathrm{Tr}\,(XY) - \frac{1}{2N}\mathrm{Tr}\,(X)\,\mathrm{Tr}\,(Y)\,, \\
\mathrm{Tr}\,(T^a X T^a Y) &= \frac{1}{2}\mathrm{Tr}\,(X)\,\mathrm{Tr}\,(Y) - \frac{1}{2N}\mathrm{Tr}\,(XY)\,.
\end{aligned}$$

Fierz identities for $U(N)$:

$$\begin{aligned}
\mathrm{Tr}\,(T^a X)\,\mathrm{Tr}\,(T^a Y) &= \frac{1}{2}\mathrm{Tr}\,(XY)\,, \\
\mathrm{Tr}\,(T^a X T^a Y) &= \frac{1}{2}\mathrm{Tr}\,(X)\,\mathrm{Tr}\,(Y)\,.
\end{aligned}$$

Can think of an $SU(N)$-gauge theory as an $U(N)$-gauge theory where the additional $U(1)$-degree of freedom is subtracted out.

Leading colour approximation: Ignore terms suppressed by $1/N$.

The double line notation

Replace a colour index in the adjoint representation by two indices in the fundamental representation:

$$V^a E^a \quad = \quad = \left(\sqrt{2} T^a_{ij} V^a\right) \left(\sqrt{2} T^b_{ji} E^b\right).$$

Then split a $SU(N)$ gluon into an $U(N)$-part and an $U(1)$-part:

$$U(N): \quad \begin{matrix} i & & l \\ j & & k \end{matrix} \quad = \quad \delta_{il}\delta_{kj},$$

$$U(1): \quad \begin{matrix} i & & l \\ j & & k \end{matrix} \quad = \quad -\frac{1}{N}\delta_{ij}\delta_{kl}.$$

One can show that the $U(1)$ gluon couples only to quarks.

The colour-flow basis

Colour decomposition of the Born n-gluon amplitude in the double-line notation:

$$\mathcal{A}_n^{(0)}(g_1, g_2, \ldots, g_n) = \left(\frac{g}{\sqrt{2}}\right)^{n-2} \sum_{\sigma \in S_n/Z_n} \underbrace{\delta_{i_{\sigma_1} j_{\sigma_2}} \delta_{i_{\sigma_2} j_{\sigma_3}} \ldots \delta_{i_{\sigma_n} j_{\sigma_1}}}_{\text{closed string}} A_n^{(0)}(g_{\sigma_1}, \ldots, g_{\sigma_n})$$

Colour decomposition of a Born amplitude with a pair of quarks:

$$\mathcal{A}_n^{(0)}(q, g_1, \ldots, g_{n-2}, \bar{q}) = \left(\frac{g}{\sqrt{2}}\right)^{n-2} \sum_{S_{n-2}} \underbrace{\delta_{i_q j_{\sigma_1}} \delta_{i_{\sigma_1} j_{\sigma_2}} \ldots \delta_{i_{\sigma_{n-2}} j_{\bar{q}}}}_{\text{open string}} A_n^{(0)}(q, g_{\sigma_1}, \ldots, g_{\sigma_{n-2}}, \bar{q})$$

Kronecker-delta's describe how the colour flows.

Symmetric phase space integration

Example: $q\bar{q} \to ng$ with colour decomposition:

$$\mathcal{A}_{n+2}^{(0)}(q, g_1, \ldots, g_n, \bar{q}) = g^n \sum_{\sigma \in S_n} \left(T^{a_{\sigma(1)}} \ldots T^{a_{\sigma(n)}}\right)_{i_q j_{\bar{q}}} A_n^{(0)}\left(q, g_{\sigma(1)}, \ldots, g_{\sigma(n)}, \bar{q}\right) = g^n \sum_{i=1}^{n!} C_i \, A_{n,i}^{(0)}.$$

There are $n!$ partial amplitudes.

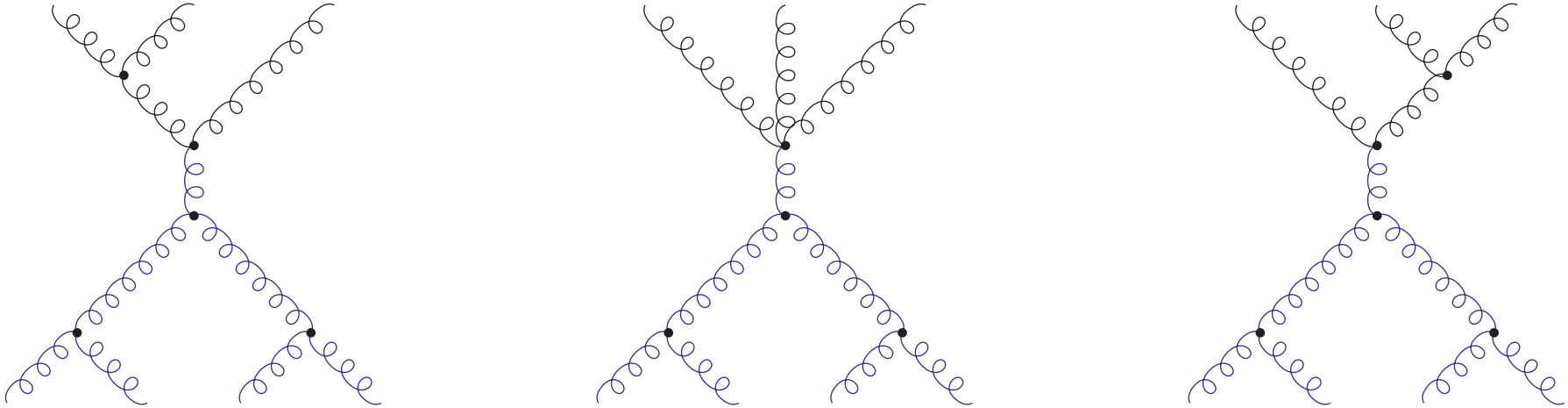
Leading colour contribution:

$$\left|\mathcal{A}_{n+2}^{(0)}\right|^2_{\text{lc}} \quad = \quad g^{2n} \sum_{i=1}^{n!} \left(C_i^\dagger C_i\right) \left|A_{n,i}^{(0)}\right|^2.$$

Phase space integration is symmetric, can remove sum with $n!$ terms:

$$\int d\phi_n O_n \left|\mathcal{A}_{n+2}^{(0)}\right|^2_{\text{lc}} \quad = \quad n! \, g^{2n} \left(C_1^\dagger C_1\right) \int d\phi_n O_n \left|A_{n,1}^{(0)}\right|^2.$$

How to avoid to compute the same sub-expression again and again

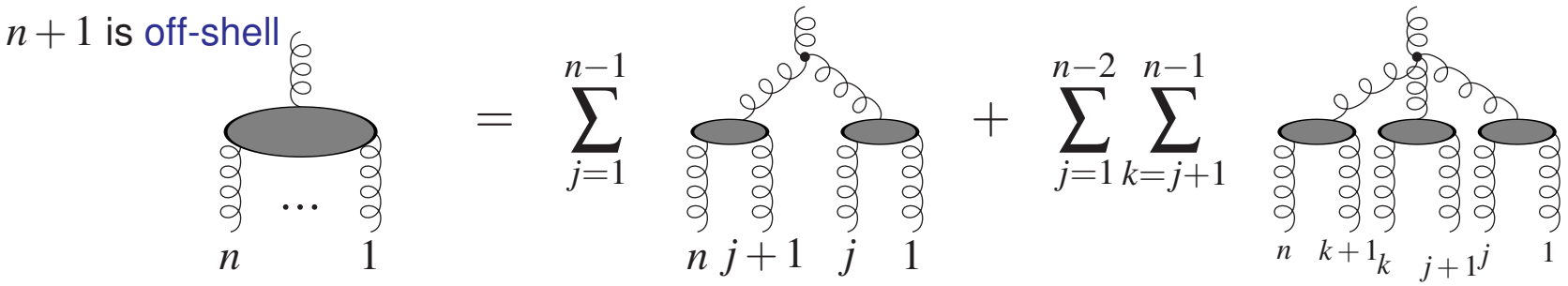


Lower part identical in all three diagrams.

Strategy: Compute this sub-expression once and store the result.

Recurrence relations

Off-shell currents $J^\mu(g_1,\ldots,g_n)$ provide an efficient way to calculate amplitudes:



Momentum conservation: $p_{n+1} = p_1 + p_2 + \ldots + p_n$.

On-shell condition for particles 1 to n: $p_j^2 = m_j^2$.

Recursion start: $J^\mu(g_1) = \varepsilon_1^\mu$.

No Feynman diagrams are calculated in this approach !

F. A. Berends and W. T. Giele,

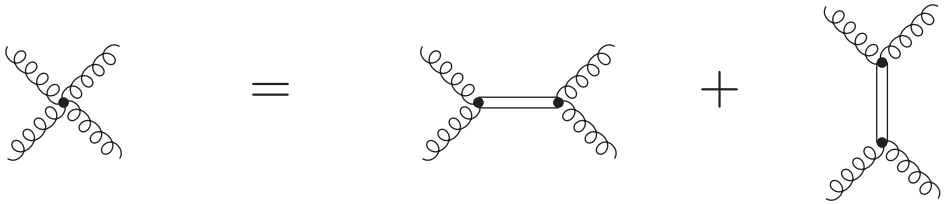
D. A. Kosower.

Computational costs

Born amplitudes with n particles and three- and four-valent vertices scale as n^4.

Can replace four-gluon vertex by a tensor particle, obtain only three-valent vertices:

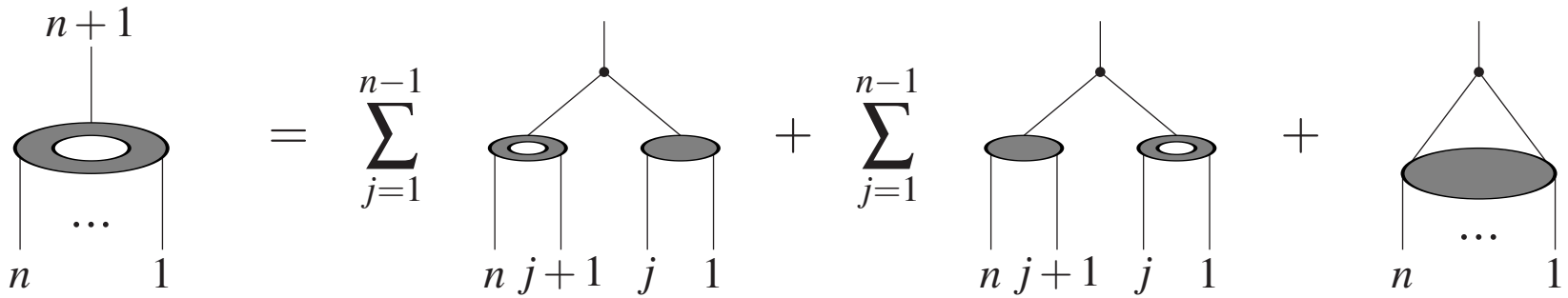
P. Draggiotis, R. Kleiss, C. Papadopoulos, '02; C. Duhr, S. Höche, F. Maltoni, '06



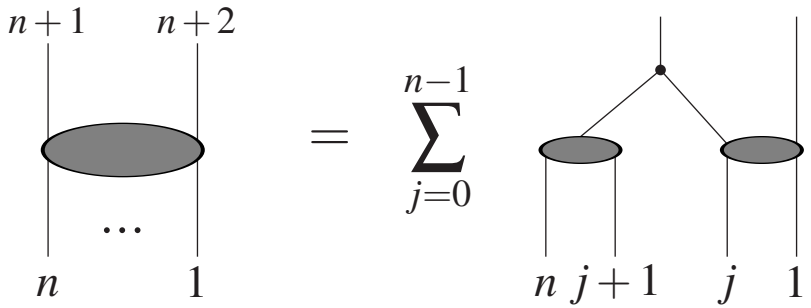
Scaling reduced to n^3.

Recurrence relations at one-loop

With only three-valent vertices we have for the integrand of a one-loop amplitude:



Recurrence relation for new tree-like object with two legs off-shell:



Part I

Phase space integration

Integration over the phase space

Recall the master formula:

$$\langle O \rangle = \sum_{a,b} \int dx_1 \, f_a(x_1) \int dx_2 \, f_b(x_2) \quad \frac{1}{2K(\hat{s})} \quad \frac{1}{n_a^{\text{spin}} n_b^{\text{spin}} n_a^{\text{colour}} n_b^{\text{colour}}} \sum_n \int d\phi_n O(p_1, \ldots, p_n) \quad |\mathcal{A}_{n+2}|^2$$

The phase space measure:

$$d\phi_n \quad = \quad \frac{1}{n!} \prod_{i=1}^{n} \frac{d^3 p_i}{(2\pi)^3 2E_i} (2\pi)^4 \delta^4 \left(p_a + p_b - \sum_{i=1}^{n} p_i \right)$$

Integration over $(3n-4)$ dimensions.

Goal: Once we have calculated the matrix element squared $|\mathcal{A}_{n+2}|^2$ for a given process, we would like to get predictions for different observables related to this process.

Solution: Numerical integration over the phase space with Monte Carlo techniques.

Integration over the phase space

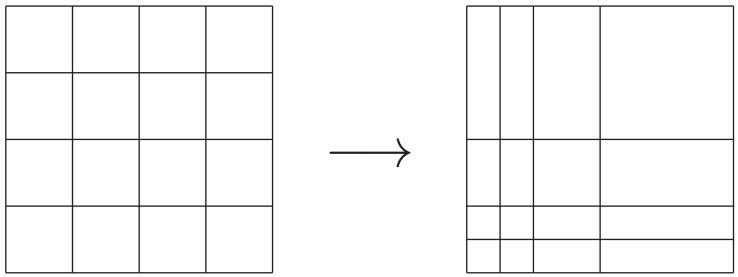
Change integration variables such that the phase space integral becomes an integral over the unit hypercube $[0,1]^{(3n-4)}$.

This is a high dimensional integral. For numerical integration in more than two dimensions Monte Carlo techniques are usually better suited then quadrature rules.

Error estimate of Monte Carlo integration is independent of the number of dimensions, scales like $1/\sqrt{N_{\mathrm{eval}}}$.

Can use variance-reducing techniques like importance sampling.

VEGAS: Integration over the unit hypercube with importance sampling.



Adapts where the integrand is largest and “learns” about the integrand as it proceeds.

Histograms

Suppose we would like to calculate for the process $pp \to 2$ jets

- the cross section,
- the $p_\perp$-distributions of the jets,
- the rapidity distributions of the jets.

Can do it in one Monte Carlo run:

- Set up the calculation for the cross section
- For every event put the corresponding weight in the appropriate bin of the histogram.

Attention: When using Vegas, we need to know the Vegas weight.

Phase space generators

The concrete form of the change of variables from $d\phi_n$ to the unit hypercube affects the error of the Monte Carlo integration.

Several possibilities:

- Sequential generator: Based on successive two-body decays. Phase space weight varies from event to event.
- RAMBO: Constant weight for every phase space point.
- Generators based on QCD radiation pattern: Peak structure of the matrix element squared absorbed into the phase space weight.
- Generators mapping a Breit-Wigner shape, essential for electro-weak physics.

Part II

NLO corrections

Motivation for higher order corrections

- For precision physics a leading-order calculation is not sufficient.

  In perturbation theory: Better precision is reached by including higher order.

- In particular: LO jet rate $pp \to n$ jets proportional to $(\alpha_s(\mu))^n$.

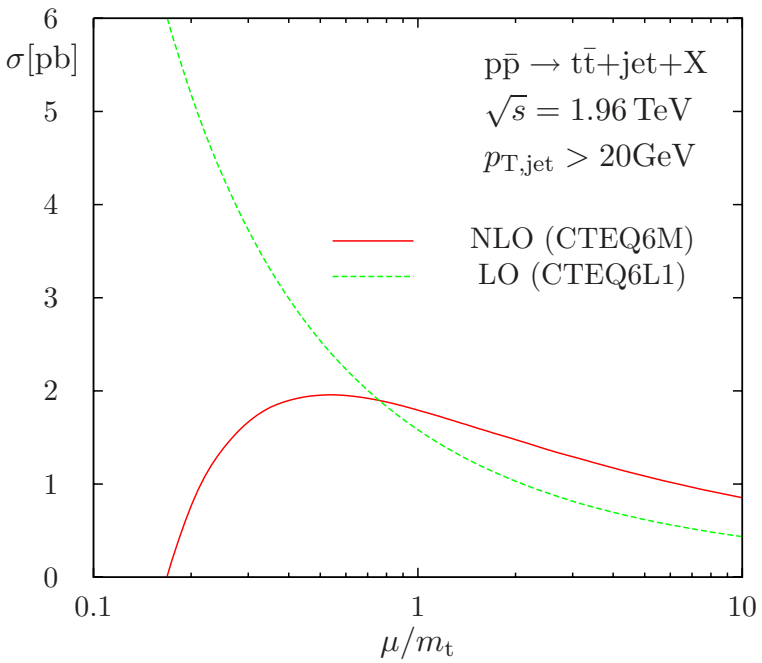
  Strong dependence on the renormalisation scale μ.
  Scale dependence is reduced by including higher order corrections.

Dependence on renormalisation and factorisation scales

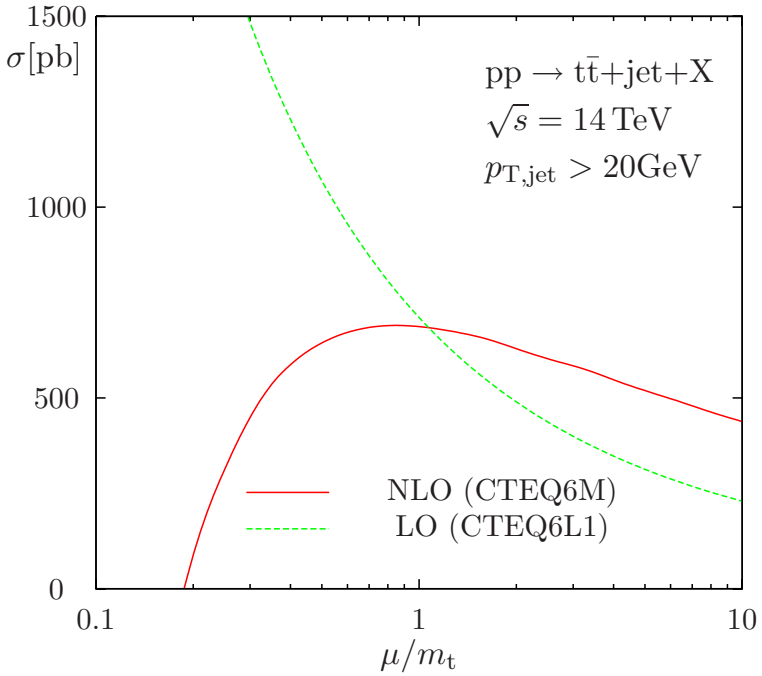
Example: $pp \to t\bar{t} + \text{jet}$.

Leading order is proportional to α_s^3 !

Tevatron:



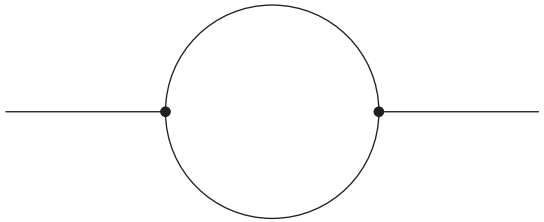
LHC:



S. Dittmaier, P. Uwer and S.W.

Quantum loop corrections

Loop diagrams are divergent !



$$\int \frac{d^4k}{(2\pi)^4}\frac{1}{(k^2)^2} = \frac{1}{(4\pi)^2}\int_0^\infty dk^2 \frac{1}{k^2} = \frac{1}{(4\pi)^2}\int_0^\infty \frac{dx}{x}$$

This integral diverges at

- $k^2 \to \infty$ (UV-divergence) and at
- $k^2 \to 0$ (IR-divergence).

Use dimensional regularisation to regulate UV- and IR-divergences.

Regularisation and renormalisation

Dimensional regularisation: Integrals are performed in $D = 4 - 2\varepsilon$ dimensions instead of four dimensions:

$$\int \frac{d^D k}{(2\pi)^D} \frac{1}{(k^2)^2} = \frac{1}{(4\pi)^{2-\varepsilon}} \frac{1}{\Gamma(2-\varepsilon)} \int_0^\infty dx\, x^{-1-\varepsilon}$$

Divergences are transformed into poles in ε and for $\varepsilon \neq 0$ the integral is well-defined.

Renormalisation: Parameters appearing in the Lagrangian are not observed quantities, but "bare" quantities.
UV-divergences are absorbed into universal renormalisation constants:

$$g_{\text{bare}} = Z_g \cdot g_{\text{renorm}}$$

$$Z_g = 1 - \frac{1}{2}\beta_0 \frac{g^2}{(4\pi)^2} \frac{1}{\varepsilon} + \ldots, \qquad \beta_0 = \frac{11}{3} C_A - \frac{4}{3} T_R N_f$$

The Kinoshita-Lee-Nauenberg theorem

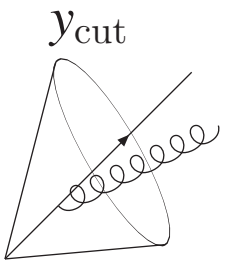
- The phase space integration over the unresolved region diverges, need a regulator.
- Unitarity requires the same regulator as in the virtual part, therefore use dimensional regularisation.
- Nature ensures that the amplitudes have a nice behaviour in the soft and collinear limits,
  physicists have to ensure that also the observables have a nice behaviour in these limits:
  Restriction to infrared-safe observables.
- For infrared-safe observables infrared divergences cancel in the sum of real and virtual corrections.
  This is the Kinoshita-Lee-Nauenberg theorem: Any infrared-safe observable, summed over all states degenerate according to some resolution criteria, will be finite.

Part II: NLO corrections

Real corrections

The real correction

- Born matrix element $|\mathcal{A}_{n+1}^{(0)}|^2$ with $(n+1)$ partons.
- Contributes whenever the additional parton is below y_{cut} and is not resolved.
- In particular this is the case in the soft and collinear region.
- Phase space integration over soft and collinear region diverges.



Factorisation in the soft region

In the soft limit:

$$\lim_{p_j \to 0} \mathcal{A}_{n+1}^{(0)} \quad = \quad g\mu^{\varepsilon} \varepsilon_{\mu}(p_j)\, \mathbf{J}^{\mu}\, \mathcal{A}_n^{(0)}, \qquad \mathbf{J}^{\mu} = \sum_{i=1}^{n} \mathbf{T}_i \frac{p_i^{\mu}}{p_i \cdot p_j}.$$

$\mathbf{J}^{\mu}$ is called the eikonal current.

Squaring the amplitude one finds

$$\lim_{p_j \to 0} \left| \mathcal{A}_{n+1}^{(0)} \right|^2 = -4\pi\alpha_s \mu^{2\varepsilon} \sum_{i=1}^{n} \sum_{k=1, k\neq i}^{n} \mathcal{A}_n^{(0)*} \mathbf{T}_i \cdot \mathbf{T}_k \left[\frac{p_i \cdot p_k}{(p_i \cdot p_j)(p_j \cdot p_k)} \right] \mathcal{A}_n^{(0)}.$$

This is not a complete factorisation, the colour charge operators $\mathbf{T}_i \cdot \mathbf{T}_k$ lead to colour correlations.

The soft limit is independent of spins or helicities.

Factorisation in the collinear region

In the collinear limit we parametrise the momenta of the partons i and j as

$$p_i = zp + k_\perp - \frac{k_\perp^2}{z}\frac{n}{2pn}, \qquad p_j = (1-z)p - k_\perp - \frac{k_\perp^2}{1-z}\frac{n}{2pn}, \qquad n^2 = 2pk_\perp = 2nk_\perp = 0$$

Factorisation in the collinear limit:

$$\lim_{p_i||p_j} \mathcal{A}_{n+1}^{(0)} \quad = \quad g\mu^\varepsilon \sum_\lambda \text{Split}^\lambda(p_i,p_j)\, \mathbf{T}_{(ij)\to i+j}\, \mathcal{A}_n^{(0)}(\ldots,p_{(ij)}^\lambda,\ldots).$$

where the sum is over all polarisations of the intermediate particle (ij).

Colour charge operators: $\mathbf{T}_{q\to qg} = \mathbf{T}_q$, $\mathbf{T}_{g\to gg} = \mathbf{T}_g$ and

$$\mathbf{T}_{g\to q\bar{q}}\mathcal{A}\left(\ldots g^b \ldots\right) \quad = \quad \left(T_{ij}^b\right)\mathcal{A}\left(\ldots g^b \ldots\right).$$

Factorisation in the collinear region

Squaring the amplitude:

$$\lim_{p_i||p_j} \left|\mathcal{A}_{n+1}^{(0)}\right|^2 = 4\pi\alpha_s\mu^{2\varepsilon} \sum_{\lambda,\lambda'} \mathcal{A}_n^{\lambda\,(0)^*} P^{\lambda\lambda'}_{(ij)\to i+j} \mathcal{A}_n^{\lambda'\,(0)}.$$

$\mathcal{A}_n^{\lambda\,(0)}$ is the amplitude with polarisation vector of particle (ij) removed.

$P^{\lambda\lambda'}_{(ij)\to i+j}$ is called the Altarelli-Parisi splitting function.

$$\begin{aligned}
P^{\lambda\lambda'}_{q\to qg} &= C_F \frac{2}{2p_i\cdot p_j} p\!\!\!/ \left[\frac{2z}{1-z} + (1-\varepsilon)(1-z)\right], \\
P^{\lambda\lambda'}_{g\to gg} &= C_A \frac{2}{2p_i\cdot p_j} \left[-g^{\mu\nu}\left(\frac{2z}{1-z} + \frac{2(1-z)}{z}\right) - 4(1-\varepsilon)z(1-z)\frac{k_\perp^\mu k_\perp^\nu}{k_\perp^2}\right], \\
P^{\lambda\lambda'}_{g\to q\bar{q}} &= T_R \frac{2}{2p_i\cdot p_j} \left[-g^{\mu\nu} + 4z(1-z)\frac{k_\perp^\mu k_\perp^\nu}{k_\perp^2}\right].
\end{aligned}$$

This is not a complete factorisation, the sum over λ and λ' leads to spin correlations.

The collinear limit is independent of colour.

Summary on factorisation in soft and collinear limits

- In the soft limit, amplitudes factorise completely in spin space, but colour correlations remain.

- In the collinear limit, amplitudes factorise completely in colour space, but spin correlations remain.

How to handle correlations: Use colour decomposition and helicity amplitudes.

The cancellation of infrared divergences in practise

- The real contribution has $(n+1)$ particles in the final state.
  In four space-time dimensions, the phase space integral is a $3(n+1)-4=3n-1$ dimensional integral.

- In $D=4-2\varepsilon$ space-time dimensions, the phase space integral is a

$$(D-1)(n+1)-D=3n-1-2n\varepsilon$$

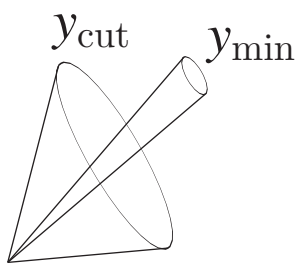
  dimensional integral.

- We want to perform the phase space integration by Monte Carlo techniques in four space-time dimensions.

Phase space slicing

Splits the integration of the real emission contribution into a region $y > y_{\min}$ and a region $y < y_{\min}$.

The former is free of singularities and the integration can be performed numerically there.
In the latter the matrix element is approximated and the integration over the one-parton phase space is performed analytically.



- Introduces an error of order $y_{\min}$.
- The first region gives a contribution of the form

$$a \ln^2 y_{\min} + b \ln y_{\min} + c$$

  The logarithms $\ln^2 y_{\min}$ and $\ln y_{\min}$ cancel against the contribution from the second region.
- But: Cancelation happens only numerically!

The subtraction method

The NLO cross section is rewritten as

$$\begin{aligned}\sigma^{NLO} &= \int_{n+1} d\sigma^R + \int_n d\sigma^V \\ &= \int_{n+1} \left(d\sigma^R - d\sigma^A\right) + \int_n \left(d\sigma^V + \int_1 d\sigma^A\right)\end{aligned}$$

The approximation $d\sigma^A$ has to fulfill the following requirements:

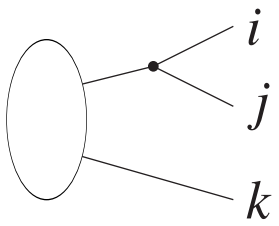
- $d\sigma^A$ must be a proper approximation of $d\sigma^R$ such as to have the same pointwise singular behaviour in D dimensions as $d\sigma^R$ itself. Thus, $d\sigma^A$ acts as a local counterterm for $d\sigma^R$ and one can safely perform the limit $\varepsilon \to 0$.

- Analytic integrability in D dimensions over the one-parton subspace leading to soft and collinear divergences.

The dipole subtraction terms

The approximation term $d\sigma^A$ is given as a sum over dipoles:

$$d\sigma^A = \sum_{\text{pairs } i,j} \sum_{k \neq i,j} \mathcal{D}_{ij,k}.$$



Each dipole contribution has the following form:

$$\mathcal{D}_{ij,k} = -\frac{1}{2p_i \cdot p_j} \mathcal{A}_n^{\lambda\,(0)\,*}\left(p_1,\ldots,\tilde{p}_{(ij)},\ldots,\tilde{p}_k,\ldots\right) \frac{\mathbf{T}_k \cdot \mathbf{T}_{ij}}{\mathbf{T}_{ij}^2} V_{ij,k}^{\lambda\lambda'} \mathcal{A}_n^{\lambda'\,(0)}\left(p_1,\ldots,\tilde{p}_{(ij)},\ldots,\tilde{p}_k,\ldots\right)$$

- Colour correlations through $\mathbf{T}_k \cdot \mathbf{T}_{ij}$.
- Spin correlations through $V_{ij,k}^{\lambda\lambda'}$.

The dipoles have the correct soft and collinear limit.

Momentum mapping

The amplitudes $\mathcal{A}_n^{\lambda\,(0)}\left(\ldots,\tilde{p}_{(ij)},\ldots,\tilde{p}_k,\ldots\right)$ in the subtraction terms depend on n external momenta.

Need a mapping from a $(n+1)$-parton configuration to a n-parton configuration.

The mapping has to respect:

- Momentum conservation
- On-shell conditions

$$\begin{aligned}\tilde{p}_{ij} &= p_i + p_j - \frac{y}{1-y}p_k, \qquad y = \frac{s_{ij}}{s_{ijk}},\\ \tilde{p}_k &= \frac{1}{1-y}p_k.\end{aligned}$$

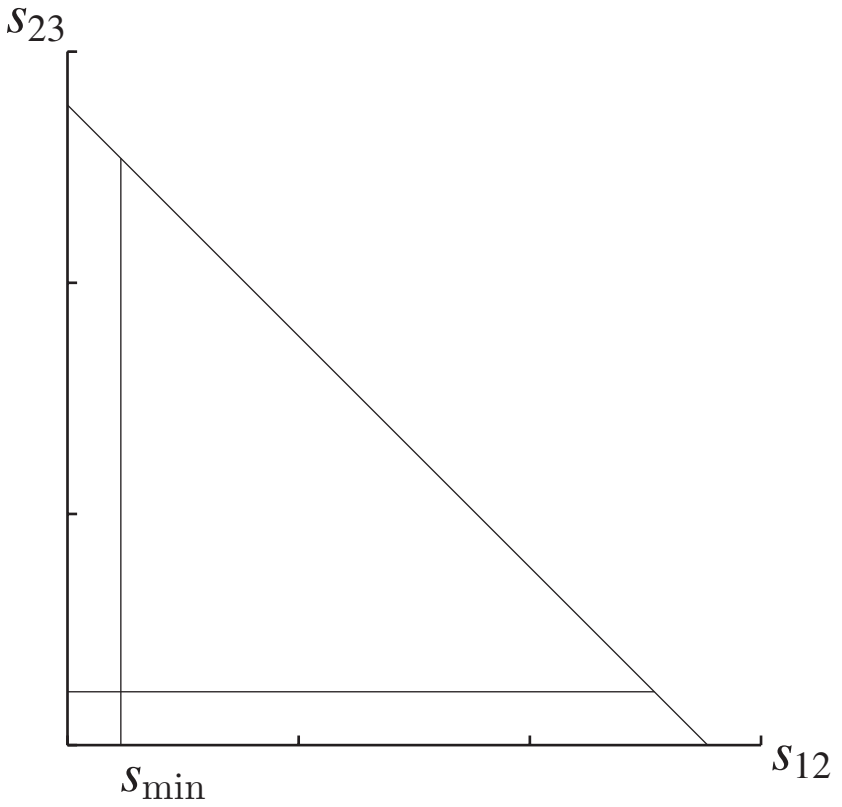
An example: $e^+e^- \to$ 2 jets at NLO

The matrix element squared for $\gamma^* \to qg\bar{q}$:

$$M_3 = 8(1-\varepsilon)\left[2\frac{s_{123}^2}{s_{12}s_{23}} - 2\frac{s_{123}}{s_{12}} - 2\frac{s_{123}}{s_{23}} + (1-\varepsilon)\frac{s_{23}}{s_{12}} + (1-\varepsilon)\frac{s_{12}}{s_{23}} - 2\varepsilon\right]$$

The dipole subtraction terms:

$$\mathcal{D}_{12,3} + \mathcal{D}_{32,1} = 8(1-\varepsilon)$$
$$\left\{\left[2\frac{s_{123}^2}{s_{12}(s_{12}+s_{23})} - 2\frac{s_{123}}{s_{12}} + (1-\varepsilon)\frac{s_{23}}{s_{12}}\right]\right.$$
$$\left. + \left[2\frac{s_{123}^2}{s_{23}(s_{12}+s_{23})} - 2\frac{s_{123}}{s_{23}} + (1-\varepsilon)\frac{s_{12}}{s_{23}}\right]\right\}$$

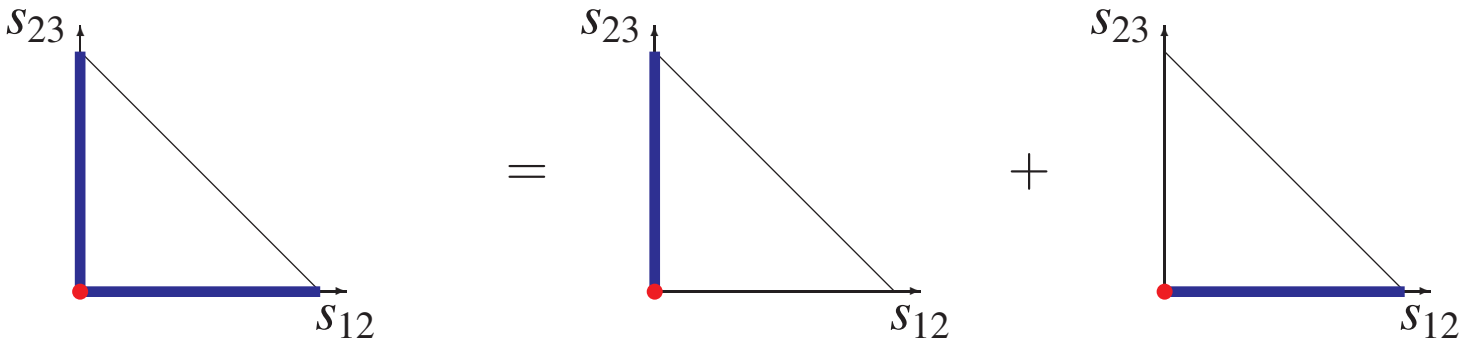


The antenna subtraction term:

$$\mathcal{A}_{123} = \mathcal{D}_{12,3} + \mathcal{D}_{32,1}$$

Singular regions in the Dalitz plot

$$\mathcal{A}_{123} = \mathcal{D}_{12,3} + \mathcal{D}_{32,1}$$



$$\frac{1}{s_{12}s_{23}} = \frac{1}{s_{12}\left(s_{12}+s_{23}\right)} + \frac{1}{s_{23}\left(s_{12}+s_{23}\right)}$$

Summary on the subtraction method

In electron-positron annihilation we have:

$$\sigma^{NLO} = \int_{n+1} \left(d\sigma^R - d\sigma^A\right) + \int_n \left(d\sigma^V + \int_1 d\sigma^A \right)$$

With hadrons in the initial state:

$$\sigma^{NLO} = \int_{n+1} \left(d\sigma^R - d\sigma^A\right) + \int_n \left(d\sigma^V + d\sigma^C + \int_1 d\sigma^A \right)$$

$d\sigma^C$ subtracts initial state collinear singularities.

Variants of the subtraction method

The singular part of the subtraction terms is fixed, the finite part can be chosen freely.

- Residue subtraction: Frixione, Kunszt and Signer, '95; Del Duca, Somogyi, Trócsányi, '05; Frixione, '11
- Dipole subtraction: Catani and Seymour '96; Phaf and S.W. '01; Catani, Dittmaier, Seymour and Trócsányi '02; Dittmaier and Kasprzik, '08; Czakon, Papadopoulos and Worek, '09; Götz, Schwan, S.W., '12
- Antenna subtraction: Kosower, '97; Gehrmann-De Ridder, Gehrmann, Glover, '05; Daleo, Gehrmann, Maitre, '06; Gehrmann-De Ridder, Ritzmann, '09
- Nagy-Soper subtraction (modified dipole subtraction) Nagy and Soper, '07; Chung, Kramer and Robens, '10; Chung and Robens, '12; Bevilacqua, Czakon, Kubocz and Worek, '13

Real emission (minus the subtraction terms) can be automated.

S.W., '05, T. Gleisberg and F. Krauss, '07, M. Seymour and C. Tevlin, '08, K. Hasegawa, S. Moch and P. Uwer, '08, R. Frederix, T. Gehrmann and N. Greiner, '08, M. Czakon, C. Papadopoulos and M. Worek, '09.

Part II: NLO corrections

Virtual corrections

The virtual correction

- Tensor reduction technique:

  - At one-loop can always reduce tensor integrals to scalar integrals
  - Avoid Gram determinants
  - Recursive techniques can be used through open loops

- Cut-based techniques:

  - Scalar integrals are known, need only the coefficients of these integrals
  - Coefficients can be obtained by calculating tree-like objects
  - Have to solve a linear system of equations numerically
  - Need also rational terms not accompagnied by a scalar integral

- Numerical integration with subtraction and contour deformation:

  - Integrand is simple close to singular regions
  - Fast, scales like a Born calculation
  - Monte Carlo error depends on the chosen contour

Reduction of tensor integrals

The Passarino-Veltman algorithm:

$$\int \frac{d^D k}{i\pi^{D/2}} \frac{k_\mu k_\nu}{(k^2 - m_1^2)((k-p_1)^2 - m_2^2)((k-p_1-p_2)^2 - m_3^2)}$$
$$= \quad p_1^\mu p_1^\nu C_{21} + p_2^\mu p_2^\nu C_{22} + (p_1^\mu p_2^\nu + p_1^\nu p_2^\mu) C_{23} + g^{\mu\nu} C_{24}.$$

Inverting the linear system of equations introduces Gram determinants:

$$\Delta \quad = \quad \begin{vmatrix} p_1^2 & p_1 \cdot p_2 \\ p_1 \cdot p_2 & p_2^2 \end{vmatrix}.$$

Improved algorithms avoid these Gram determinants!

A. Denner and S. Dittmaier,

T. Binoth, J.-Ph. Guillet, G. Heinrich, E. Pilon, C. Schubert,

F. del Aguila and R. Pittau,

A. van Hameren, J. Vollinga and S.W.,

F. Cascioli, P Maierhöfer, S. Pozzorini

Reduction of scalar integrals

Finite one-loop integrals with more than four propagators can always be reduced to integrals with maximally four propagators.

Melrose (1965)

Basic idea: In a space of dimension four there can be no more than four linear independet vectors.

The proof can be extended towards integrals computed within dimensional regularization.

Reduction of scalar integrals

Reduction of pentagons (W. van Neerven and J. Vermaseren; Z. Bern, L. Dixon, and D. Kosower):

$$I_5 = \sum_{i=1}^{5} b_i I_4^{(i)} + O(\varepsilon).$$

Reduction of hexagons (T. Binoth, J. P. Guillet, and G. Heinrich):

$$I_6 = \sum_{i=1}^{6} b_i I_5^{(i)}.$$

Reduction of scalar integrals with more than six propagators (G. Duplancic and B. Nizic):

$$I_n = \sum_{i=1}^{n} r_i I_{n-1}^{(i)}.$$

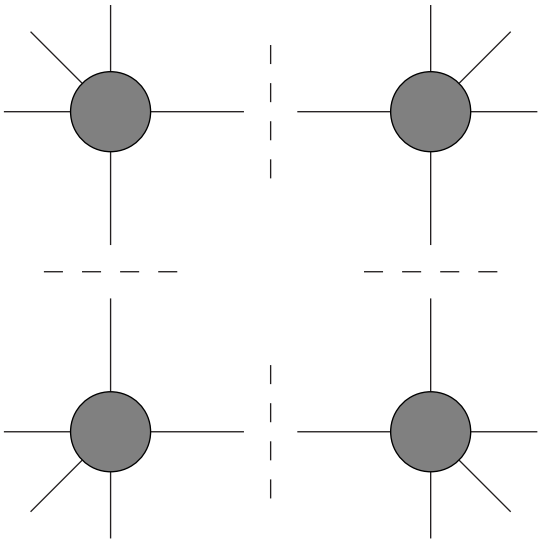
Here, the decomposition is no longer unique.

Cut techniques

Scalar integrals are known, need only the coefficients in front and the rational part R_n:

$$A_n^{(1)} = \sum_{i,j,k,l} c_{ijkl} I_{ijkl}^{\text{Box}} + \sum_{i,j,k} c_{ijk} I_{ijk}^{\text{Triangle}} + \sum_{i,j} c_{ij} I_{ij}^{\text{Bubble}} + R_n$$

- Box coefficients from quadruple cuts.
- Triangle coefficients from triple cuts, after box contribution has been subtracted out.
- Bubble coefficients from double cuts, after box and triangle have been subtracted out.
- Rational part from cuts in D dimensions.



R. Britto, F. Cachazo, B. Feng; D. Forde; G. Ossola, C. Papadopoulos, R. Pittau; Anastasiou, Britto, Feng, Kunszt, Mastrolia; Ellis, Giele, Kunszt, Melnikov; Badger, Sattler, Yundin; ...

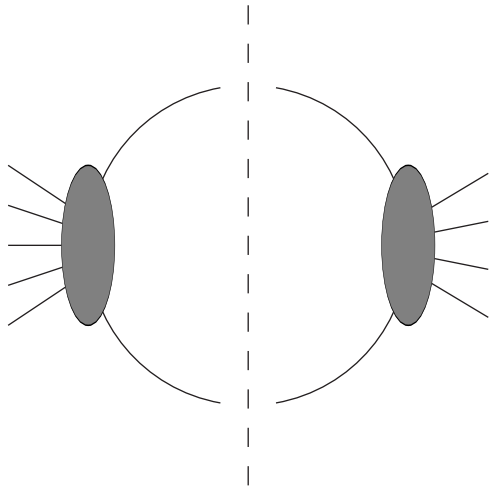
Cut techniques

Prehistoric version of the cut technique: Cutkosky rules

Cutkosky, '60

Medieval version of the cut technique:

$$A^{(1)} = \int \frac{d^D k}{(2\pi)^D} \frac{1}{k_1^2 + i\varepsilon} \frac{1}{k_2^2 + i\varepsilon} A_L^{(0)} A_R^{(0)} + \text{cut free pieces}$$



Bern, Dixon, Dunbar and Kosower, '94; Bern, Morgan, '95

Numerical integration: Never change a winning team

Do the loop integrals numerically with Monte Carlo techniques !

- Can combine phase space integration ($3n-4$ dimensions) with loop integration (4 dimensions) in one Monte Carlo integration.
- Monte Carlo integration error scales with $1/\sqrt{N}$, independent of the dimension.

But: Loop integrals are divergent and need regularization. They are therefore calculated in $D = 4 - 2\varepsilon$ dimensions

$$\int d^{4-2\varepsilon}k \;\; f(k) \quad = \quad \frac{c_2}{\varepsilon^2} + \frac{c_1}{\varepsilon} + c_0 + O(\varepsilon)$$

Idea: Subtraction method.

$$\int d^{4-2\varepsilon}k \;\; f(k) \quad = \quad \underbrace{\int d^{4-2\varepsilon}k \;\; [f(k)-g(k)]}_{\text{convergent}} + \underbrace{\int d^{4-2\varepsilon}k \;\; g(k)}_{\text{simple}}$$

Subtraction method for loop integrals

Use subtraction also for the virtual part:

$$\int_{n+1} d\sigma^R + \int_n d\sigma^V = \underbrace{\int_{n+1} \left(d\sigma^R - d\sigma^A\right)}_{\text{convergent}} + \underbrace{\int_n (\mathbf{I}+\mathbf{L}) \otimes d\sigma^B}_{\text{finite}} + \underbrace{\int_n \left(d\sigma^V - d\sigma^{A'}\right)}_{\text{convergent}}$$

- In the last term $d\sigma^V - d\sigma^{A'}$ the Monte Carlo integration is over a phase space integral of n final state particles plus a 4-dimensional loop integral.
- All explicit poles cancel in the combination $\mathbf{I}+\mathbf{L}$.
- Divergences of one-loop amplitudes related to IR-divergences (soft and collinear) and to UV-divergences.

M. Assadsolimani, S. Becker, D. Götz, Ch. Reuschle, Ch. Schwan, S.W.

Numerical NLO QCD calculations

Proceed through the following steps:

1. Local subtraction terms for soft, collinear and ultraviolet singular part of the integrand of one-loop amplitudes

2. Contour deformation for the 4-dimensional loop integral.

3. Numerical Monte Carlo integration over phase space and loop momentum.

Not a new idea: Nagy and Soper proposed in '03 this method, working graph by graph.
(see also: Soper; Krämer, Soper; Catani, Gleisberg, Krauss, Rodrigo, Winter; Kilian, Kleinschmidt)

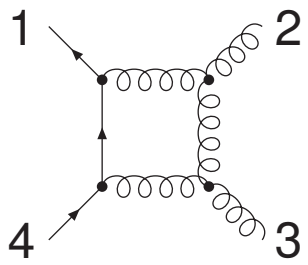
What is new: The IR-subtraction terms can be formulated at the level of amplitudes, no need to work graph by graph.

The IR-subtraction terms are universal and amasingly simple.

Primitive amplitudes

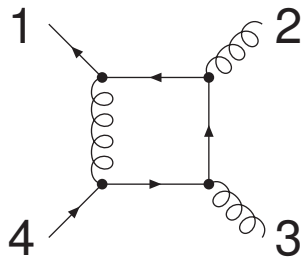
Colour-decomposition of one-loop amplitudes:

$$\mathcal{A}^{(1)} = \sum_j C_j A_j^{(1)}.$$



Primitive amplitudes distinguished by:

- fixed cyclic ordering
- definite routing of the fermion lines
- particle content circulating in the loop

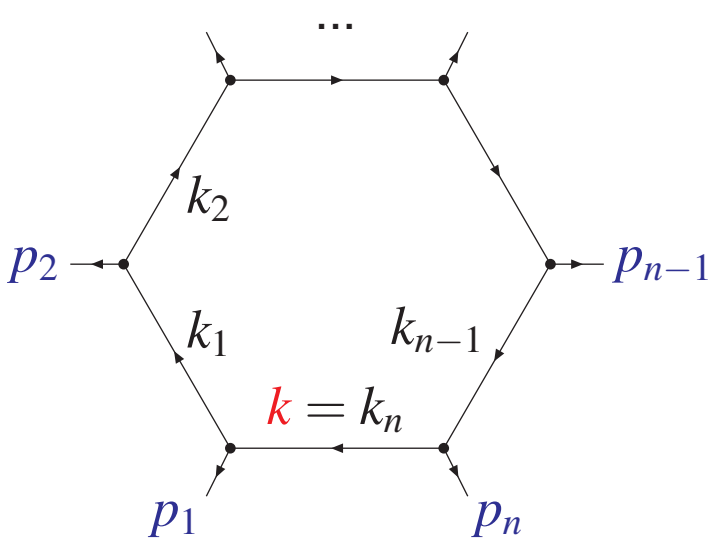


Z. Bern, L. Dixon, D. Kosower, '95

Notation and kinematics

All momenta specified by p_1, ..., p_n and k:

$$k_i \quad = \quad k - (p_1 + \ldots + p_i)$$



For cyclic ordered amplitudes we have only n different propagators.

Write primitive one-loop amplitude as

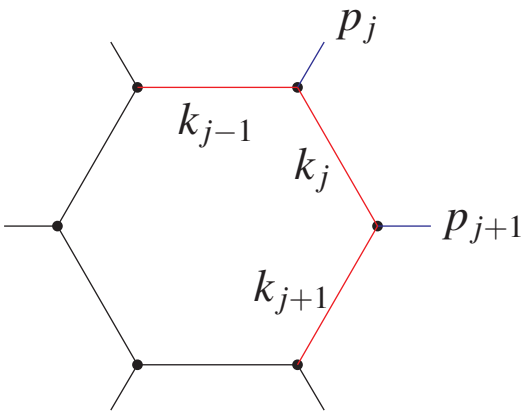
$$A^{(1)}_{\text{bare}} = \int \frac{d^D k}{(2\pi)^D} G^{(1)}_{\text{bare}}, \qquad G^{(1)}_{\text{bare}} = P(k) \prod_{i=1}^{n} \frac{1}{k_i^2 - m_i^2 + i\delta}.$$

$P(k)$ is a polynomial in k.
Integrand can be calculated efficiently using recursion relations.

The origin of infrared divergences

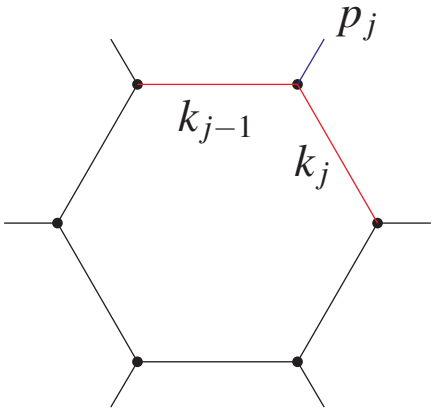
Soft singularities: 3 propagators on-shell

$$k_j \sim 0 \quad \text{and} \quad m_j = 0, \quad p_j^2 = m_{j-1}^2, \quad p_{j+1}^2 = m_{j+1}^2.$$



Collinear singularities: 2 propagators on-shell

$$k_{j-1} \sim x p_j, \quad \text{and} \quad p_j^2 = 0, \quad m_{j-1} = 0, \quad m_j = 0.$$



Infrared structure of one-loop amplitudes

General formula for the infrared poles of a one-loop amplitude:

$$\mathcal{A}_n^{(1)} = \mathbf{I}^{(1)}\,\mathcal{A}_n^{(0)} + \mathcal{F}_n^{(1)},$$

$$\mathbf{I}^{(1)} = \frac{\alpha_s}{2\pi}\frac{1}{2}\frac{e^{\varepsilon\gamma_E}}{\Gamma(1-\varepsilon)}\sum_i\left(\frac{1}{\varepsilon^2}+\frac{\gamma_i}{\mathbf{T}_i^2}\frac{1}{\varepsilon}\right)\sum_{j\neq i}\mathbf{T}_i\mathbf{T}_j\left(\frac{-2p_ip_j}{\mu^2}\right)^{-\varepsilon},$$

$$\mathbf{T}_q^2 = C_F, \quad \mathbf{T}_g^2 = C_A, \quad \gamma_q = \frac{3}{2}C_F, \quad \gamma_g = \frac{\beta_0}{2}.$$

$\mathbf{I}^{(1)}$ contains all infrared poles, $\mathcal{F}_n^{(1)}$ is a finite remainder.

Colour charge operators:

$$\mathbf{T}_q\mathcal{A}(\ldots q_j\ldots) = \left(T_{ij}^a\right)\mathcal{A}(\ldots q_j\ldots),$$

$$\mathbf{T}_g\mathcal{A}\left(\ldots g^b\ldots\right) = \left(if^{cab}\right)\mathcal{A}\left(\ldots g^b\ldots\right).$$

The infrared subtraction terms for the virtual corrections

Local unintegrated form:

$$G^{(1)}_{\text{soft+coll}} = -4\pi\alpha_s i \sum_{i\in I_g} \left(\frac{4p_i p_{i+1}}{k_{i-1}^2 k_i^2 k_{i+1}^2} - 2\frac{S_i g^{UV}_{i-1,i}}{k_{i-1}^2 k_i^2} - 2\frac{S_{i+1} g^{UV}_{i,i+1}}{k_i^2 k_{i+1}^2} \right) A_i^{(0)}.$$

with $S_q = 1$, $S_g = 1/2$. The function $g^{UV}_{i,j}$ provides damping in the UV-region:

$$\lim_{k\to\infty} g^{UV}_{i,j} = O\left(k^{-2}\right), \qquad \lim_{k_i||k_j} g^{UV}_{i,j} = 1.$$

Integrated form:

$$S_\varepsilon^{-1}\mu^{2\varepsilon}\int \frac{d^Dk}{(2\pi)^D} G^{(1)}_{\text{soft+coll}} = \frac{\alpha_s}{4\pi}\frac{e^{\varepsilon\gamma_E}}{\Gamma(1-\varepsilon)} \sum_{i\in I_g} \left[\frac{2}{\varepsilon^2}\left(\frac{-2p_i\cdot p_{i+1}}{\mu^2}\right)^{-\varepsilon} + \frac{2}{\varepsilon}(S_i+S_{i+1})\left(\frac{\mu^2_{\text{UV}}}{\mu^2}\right)^{-\varepsilon} \right] A_i^{(0)} + O(\varepsilon),$$

M. Assadsolimani, S. Becker, S.W., '09

UV-subtraction terms

In a fixed direction in loop momentum space the amplitude has up to quadratic UV-divergences.

Only the integration over the angles reduces this to a logarithmic divergence.

For a local subtraction term we have to match the quadratic, linear and logarithmic divergence.

The subtraction terms have the form of counter-terms for propagators and vertices.

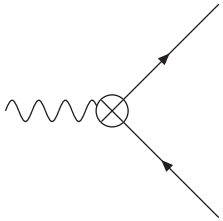
The complete UV-subtraction term can be calculated recursively.

S. Becker, Ch. Reuschle, S.W., JHEP 1012 (2010), 013, arxiv:1010.4187

UV-subtraction terms

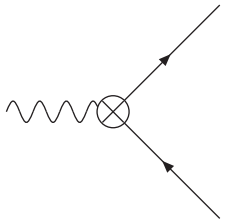
Example: The quark-gluon vertex.

Local unintegrated form:



$$= \quad ig^3 S_\varepsilon^{-1} \mu^{4-D} \int \frac{d^D k}{(2\pi)^D i} \frac{2(1-\varepsilon)\bar{k}\!\!\!/\gamma^\mu \bar{k}\!\!\!/ + 4\mu_{UV}^2 \gamma^\mu}{\left(\bar{k}^2 - \mu_{UV}^2\right)^3}$$

Integrated form:



$$= \quad i\frac{g^3}{(4\pi)^3}\gamma^\mu (-1)\left(\frac{1}{\varepsilon} - \ln\frac{\mu_{UV}^2}{\mu^2}\right) + O(\varepsilon)$$

We can ensure that the integrated expression is proportional to the Born.

Contour deformation

With the subtraction terms for UV- and IR-singularities one removes

- UV divergences
- Pinch singularities due to soft or collinear partons

Still remains:

- Singularities in the integrand, where a deformation into the complex plane of the contour is possible.
- Pinch singularities for exceptional configurations of the external momenta (thresholds, anomalous thresholds ...), integrable over phase space and loop space.

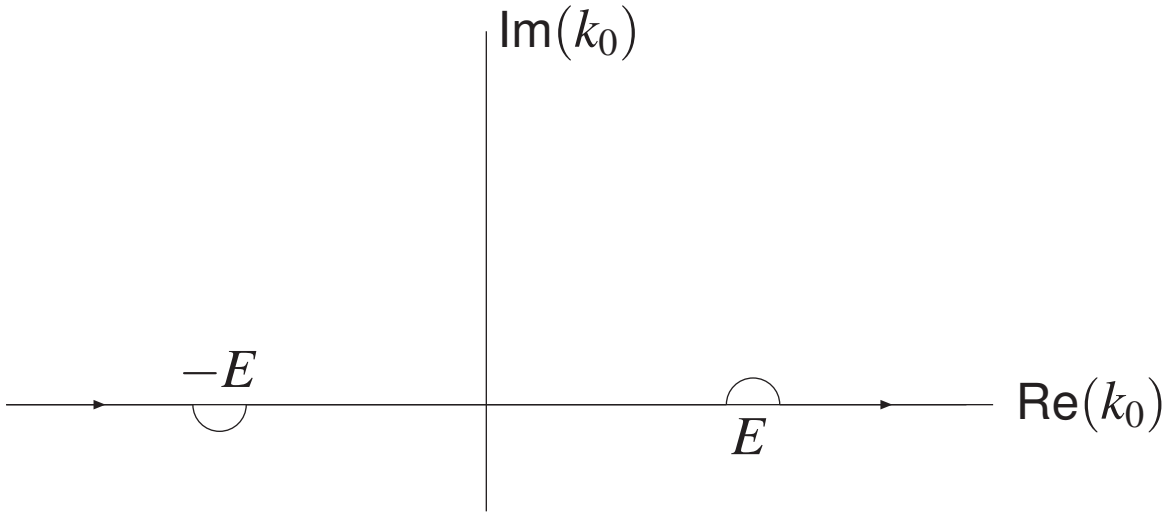
Contour deformation

$$I = \int d^4k \underbrace{[f(k) - g(k)]}_{h(k)}$$

$h(k)$ meromorphic function of four complex variables k_0, k_1, k_2, k_3.

Integration over a surface of (real) dimension 4 in $\mathbb{C}^4$.

I independent of the choice of the surface, as long as no poles are crossed.



What is the best choice for the surface, in order to minimize Monte Carlo integration errors ?

Contour deformation

We work with two methods for the contour deformation:

- Direct deformation, entirely in the space of the loop momentum.
  Integration is over the loop momentum k.
  At present only for massless particles.

  Gong, Nagy, Soper, '09; Becker, Reuschle, S.W., '12

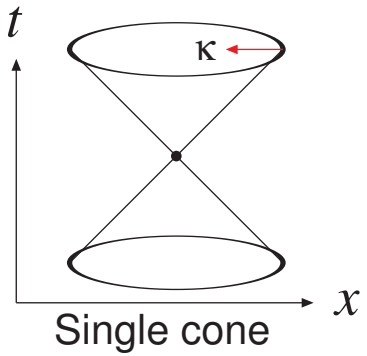
- Additional Feynman parameters.
  Integration is over the loop momentum k and the Feynman parameters α.
  General, but slightly less efficient.

  Nagy, Soper, '06; Anastasiou, Beerli, Daleo, '07; Becker, Reuschle, S.W., '10

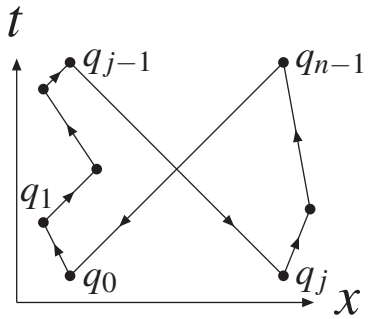
Direct contour deformation

Deformation of the loop momentum:

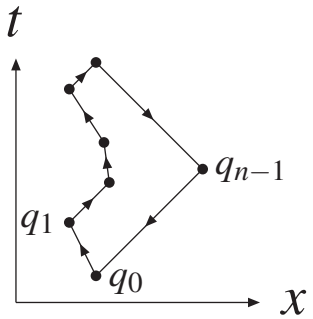
$$k_{\mathbb{C}} \quad = \quad k_{\mathbb{R}} + i\kappa$$



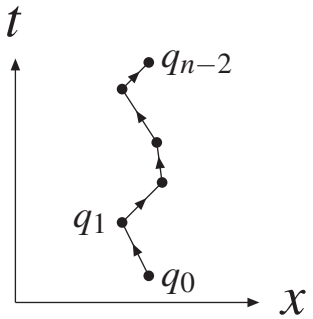
For n cones draw only the origins of the cones:



generic with 2 initial partons



initial partons adjacent



no initial partons

Efficiency

With the local subtraction terms and the contour deformation we obtain an integral, where the loop integration can – in principle – be performed with Monte Carlo methods.

However, the integrand is oscillating:

$$I = \int_0^1 dx \, [c + A \sin(2\pi x)], \qquad A \gg c$$

This leads to large Monte Carlo integration errors.

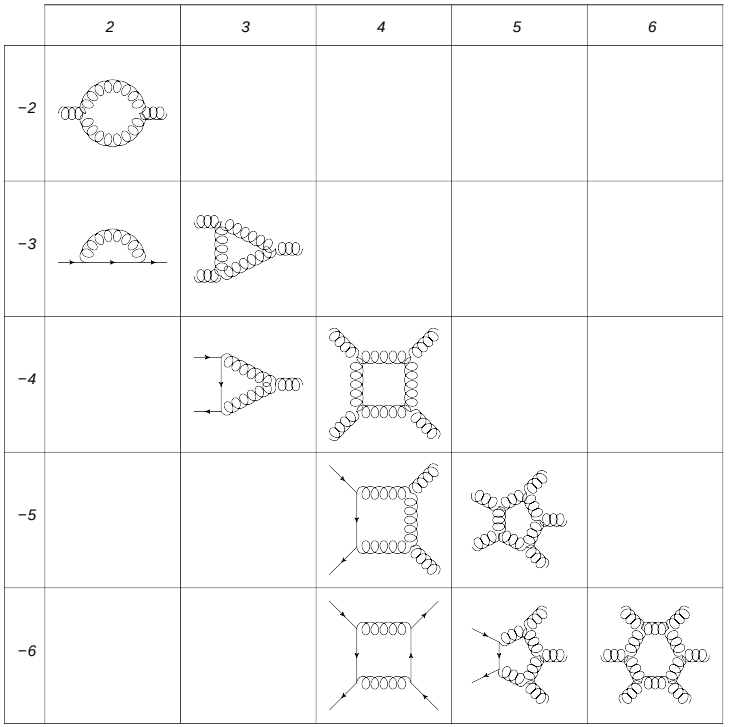
Solution: Antithetic variates: Evaluate the integrand at x and $(1-x)$.

UV improvement

Ultraviolet behaviour of some example diagrams:

To the right: number of external particles

In the vertical:
leading power of the large $|k|$-behaviour



UV-finiteness requires fall off like $|k|^{-5}$.

$|k|^{-5}$ contribution is odd under $k \to -k$ and integrates to zero.

However, $|k|^{-5}$ term gives a large contribution to the Monte Carlo error.

UV improvement

- Split the integration holomorphic into two channels:

$$1 \quad = \quad \left[\prod_{j=1}^{n} \frac{k_j^2 - m_j^2}{\bar{k}^2 - \mu_{\mathrm{UV}}^2}\right] + \left[1 - \prod_{j=1}^{n} \frac{k_j^2 - m_j^2}{\bar{k}^2 - \mu_{\mathrm{UV}}^2}\right]$$

  First channel: simple pole structure, can be evaluated with a simple contour. Second channel: Integrand falls off with two additional powers of $|k|$ in the ultraviolet.

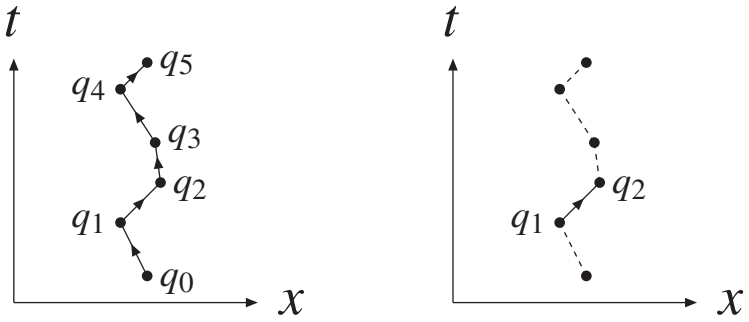
- Improvement of the counterterms for the propagators and three-valent vertices from $|k|^{-5}$ to $|k|^{-7}$.

- Use antithetic Monte Carlo integration technique: Evaluate k and $(-k)$ together.

Infrared channels

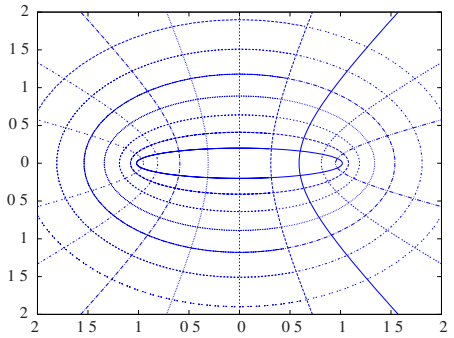
Non-holomorphic splitting:

$$I_{\text{int}} = \sum_i \int \frac{d^4k}{(2\pi)^4} w_i(k) f(k),$$



Weights:

$$w_i(k) = \frac{\left(\frac{1}{|k_i^2||k_{i+1}^2|}\right)^{\alpha}}{\sum_j \left(\frac{1}{|k_j^2||k_{j+1}^2|}\right)^{\alpha}},$$



Coordinate system, where a line segment $[q_i, q_{i+1}]$ is singled out:
Generalised elliptical coordinates

Use technique of antithetic variates in these coordinates.

Part III

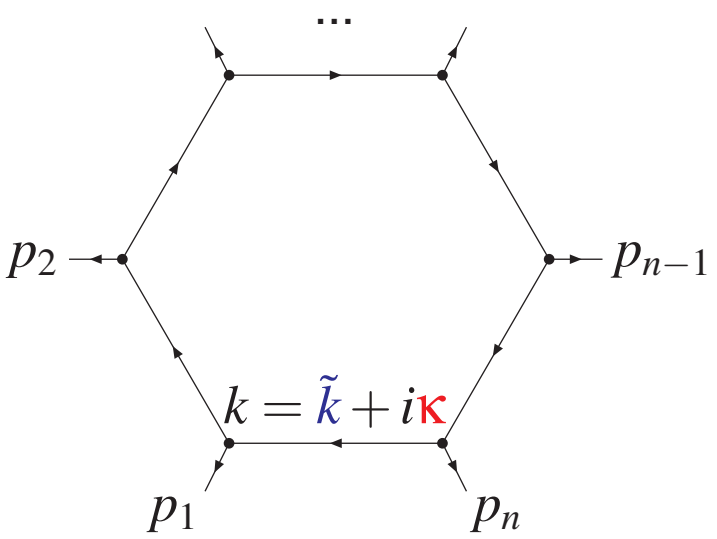
Steps towards NNLO

Extension to higher orders

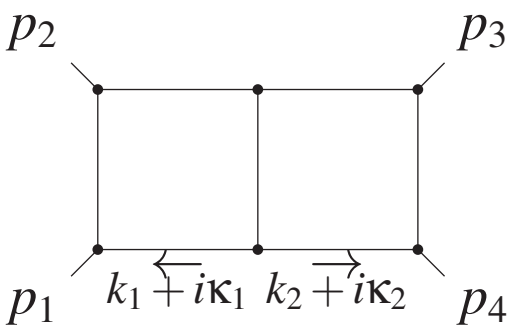
- Subtraction terms
- Contour deformation

$$\int \frac{d^4k}{(2\pi)^4} f(k) \quad = \quad \int \frac{d^4\tilde{k}}{(2\pi)^4} \left| \frac{\partial k^\mu}{\partial \tilde{k}^\nu} \right| f(k(\tilde{k}))$$

κ vanishes whenever one loop momentum becomes soft.



Beyond one-loop

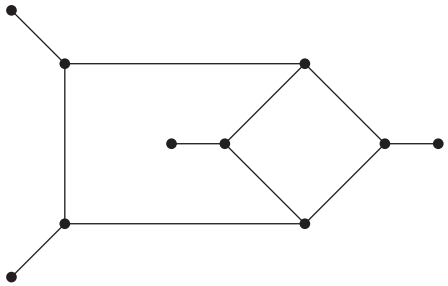


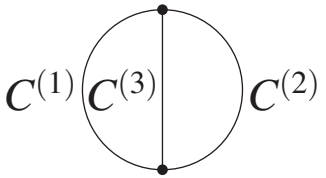
We have:

- 2 independent loop momenta
- 3 inequivalent cycles

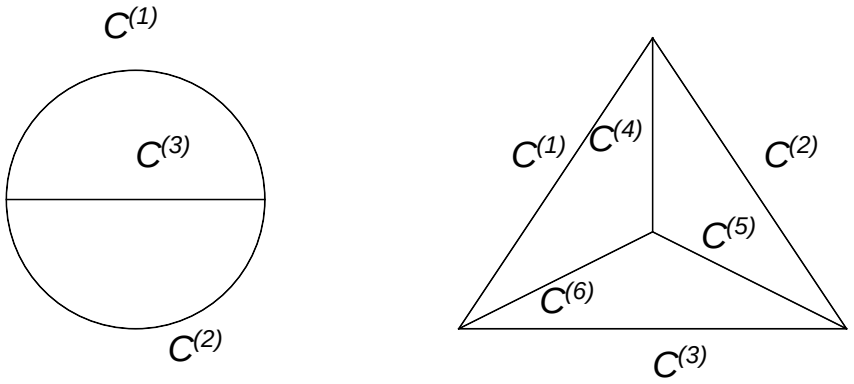
Chain diagrams

The momenta of the propagators in the same chain differ only by a linear combination of the external momenta.





Two and three loop chain diagrams

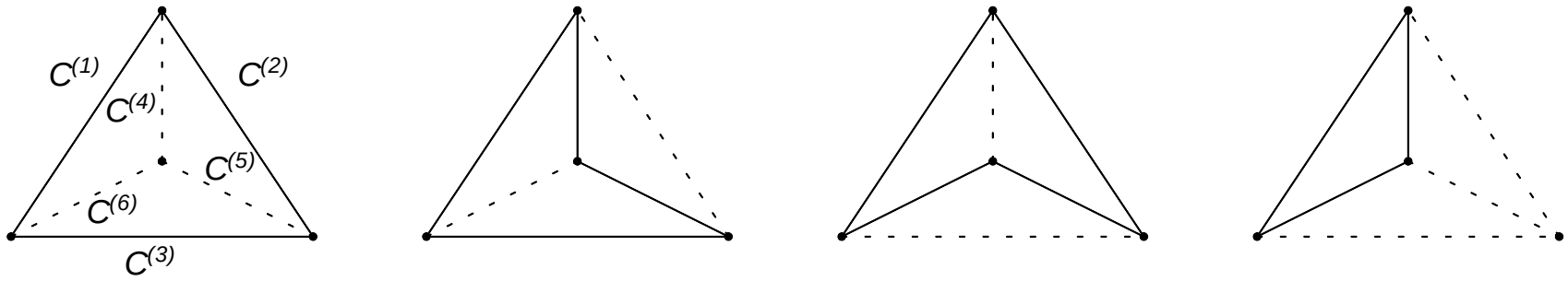


κ_i obtained as the sum of all deformation vectors for cycles containing propagator i.

Two-loop example:

$$\begin{aligned} \kappa_1 &= \kappa^{(12)} + \kappa^{(13)}, \\ \kappa_2 &= \kappa^{(12)} + \kappa^{(23)}, \end{aligned}$$

Three loops



$$
\begin{aligned}
\kappa_1 &= \kappa^{(123)} + \kappa^{(146)} + \kappa^{(1256)} + \kappa^{(1345)}, \\
\kappa_2 &= \kappa^{(123)} + \kappa^{(245)} + \kappa^{(1256)} + \kappa^{(2346)}, \\
\kappa_3 &= \kappa^{(123)} + \kappa^{(356)} + \kappa^{(1345)} + \kappa^{(2346)}.
\end{aligned}
$$

Verification and results

Comparison with analytical result (no internal masses, external legs off-shell):

- two- and three-loop propagator corrections
- two- and three-loop vertex functions (planar and non-planar)
- ladder diagrams (double box, triple box)

In addition:

- Two-loop six-point functions