Calculations beyond one loop: more methods, tools and applications

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I.: **Introduction**

II.: **Loop amplitudes: The analytical approach**

III: **Loop amplitudes: The numerical approach**

It's all about precision

Theoretical prediction for an infrared-safe observable:

$$\langle O \rangle \quad \sim \quad \sum_n \int d\phi_{n-2}\, O_n\, |\mathcal{A}_n|^2$$

Higher precision $\Rightarrow$ include higher orders in perturbation theory!

We want flexibilty on the observable: Phase-space integration performed numerically by Monte-Carlo methods in four space-time dimensions.

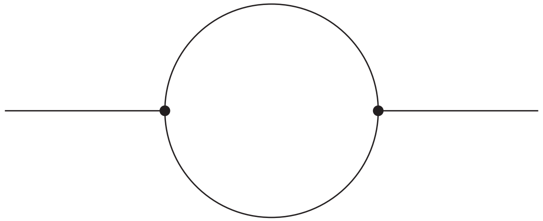
Amplitudes $\mathcal{A}_n$ calculated in perturbation theory ($\mathcal{G}_n^{(l)}$ denotes the integrand of the l-loop amplitude):

$$\mathcal{A}_n \quad = \quad \mathcal{G}_n^{(0)} + \int d^D k_1\, \mathcal{G}_n^{(1)} + \int d^D k_1 \int d^D k_2\, \mathcal{G}_n^{(2)} + \dots$$

There are two integrations: Phase space integration
Loop integration

Quantum corrections

Loop integrals and phase space integrals for unresolved particles 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).

Dimensional regularisation (setting $D = 4 - 2\varepsilon$) has become a standard to regulate UV- and IR-divergences.

Part I

Loop amplitudes: The analytical approach

I.1: **Multiple polylogarithms**

I.2: **Elliptic generalisations**

One-loop amplitudes

All one-loop amplitudes can be expressed as a sum of algebraic functions of the spinor products and masses times two transcendental functions, whose arguments are again algebraic functions of the spinor products and the masses.

The two transcendental functions are the logarithm and the dilogarithm:

$$
\begin{aligned}
\mathrm{Li}_1(x) &= -\ln(1-x) = \sum_{n=1}^{\infty} \frac{x^n}{n} \\
\mathrm{Li}_2(x) &= \sum_{n=1}^{\infty} \frac{x^n}{n^2}
\end{aligned}
$$

Generalisations of the logarithm

Beyond one-loop, at least the following generalisations occur:

Polylogarithms:

$$\mathrm{Li}_m(x) = \sum_{n=1}^{\infty} \frac{x^n}{n^m}$$

Multiple polylogarithms (Goncharov 1998):

$$\mathrm{Li}_{m_1,m_2,...,m_k}(x_1,x_2,...,x_k) = \sum_{n_1>n_2>...>n_k>0}^{\infty} \frac{x_1^{n_1}}{n_1^{m_1}} \cdot \frac{x_2^{n_2}}{n_2^{m_2}} \cdot \ldots \cdot \frac{x_k^{n_k}}{n_k^{m_k}}$$

Iterated integrals

Define the functions G by

$$G(z_1,...,z_k;y) = \int\limits_0^y \frac{dt_1}{t_1 - z_1} \int\limits_0^{t_1} \frac{dt_2}{t_2 - z_2} ... \int\limits_0^{t_{k-1}} \frac{dt_k}{t_k - z_k}.$$

Scaling relation:

$$G(z_1,...,z_k;y) = G(xz_1,...,xz_k;xy)$$

Short hand notation:

$$G_{m_1,...,m_k}(z_1,...,z_k;y) = G(\underbrace{0,...,0}_{m_1-1},z_1,...,z_{k-1},\underbrace{0...,0}_{m_k-1},z_k;y)$$

Conversion to multiple polylogarithms:

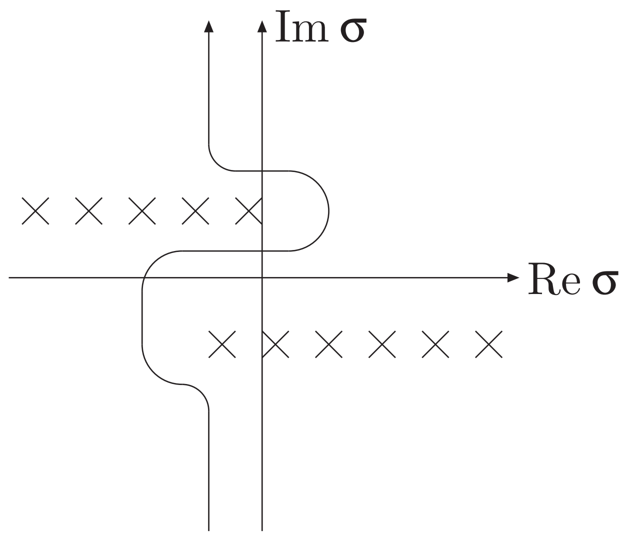
$$\text{Li}_{m_1,...,m_k}(x_1,...,x_k) = (-1)^k G_{m_1,...,m_k}\left(\frac{1}{x_1}, \frac{1}{x_1 x_2}, ..., \frac{1}{x_1 ... x_k}; 1\right).$$

Mellin-Barnes

Mellin-Barnes transformation:

$$(A_1 + A_2)^{-c} =$$

$$\frac{1}{\Gamma(c)} \frac{1}{2\pi i} \int_{-i\infty}^{i\infty} d\sigma \, \Gamma(-\sigma)\Gamma(\sigma + c) \, A_1^{\sigma} A_2^{-\sigma - c}$$



The contour is such that the poles of $\Gamma(-\sigma)$ are to the right and the poles of $\Gamma(\sigma + c)$ are to the left.

Converts a sum into products and is therefore the “inverse” of Feynman parametrisation.

Smirnov; Tausk; Davydychev; Bierenbaum, S.W.; Czakon; Kosower; Anastasiou, Daleo; Gluza, Kajda, Riemann;

Higher transcendental functions

The following sums of residues can be converted to multiple polylogarithms:

- Type A: $$\sum_{i=0}^{\infty} \frac{\Gamma(i+a_1)...\Gamma(i+a_k)}{\Gamma(i+a'_1)...\Gamma(i+a'_k)}\, x^i$$

  Example: Hypergeometric functions ${}_{J+1}F_J$ (up to prefactors).

- Type B: $$\sum_{i=0}^{\infty}\sum_{j=0}^{\infty} \frac{\Gamma(i+a_1)...\Gamma(i+a_k)}{\Gamma(i+a'_1)...\Gamma(i+a'_k)} \frac{\Gamma(j+b_1)...\Gamma(j+b_l)}{\Gamma(j+b'_1)...\Gamma(j+b'_l)} \frac{\Gamma(i+j+c_1)...\Gamma(i+j+c_m)}{\Gamma(i+j+c'_1)...\Gamma(i+j+c'_m)}\, x^i y^j$$

  Example: First Appell function F_1.

- Type C: $$\sum_{i=0}^{\infty}\sum_{j=0}^{\infty} \binom{i+j}{j} \frac{\Gamma(i+a_1)...\Gamma(i+a_k)}{\Gamma(i+a'_1)...\Gamma(i+a'_k)} \frac{\Gamma(i+j+c_1)...\Gamma(i+j+c_m)}{\Gamma(i+j+c'_1)...\Gamma(i+j+c'_m)}\, x^i y^j$$

  Example: Kampé de Fériet function S_1.

- Type D: $$\sum_{i=0}^{\infty}\sum_{j=0}^{\infty} \binom{i+j}{j} \frac{\Gamma(i+a_1)...\Gamma(i+a_k)}{\Gamma(i+a'_1)...\Gamma(i+a'_k)} \frac{\Gamma(j+b_1)...\Gamma(j+b_l)}{\Gamma(j+b'_1)...\Gamma(j+b'_l)} \frac{\Gamma(i+j+c_1)...\Gamma(i+j+c_m)}{\Gamma(i+j+c'_1)...\Gamma(i+j+c'_m)}\, x^i y^j$$

  Example: Second Appell function F_2.

provided all a, b, c's are of the form "integer $+$ const $\cdot\, \varepsilon$".

Moch, Uwer, S.W.

Differential equations for Feynman integrals

If it is not feasible to compute the integral directly:

Pick one variable t from the set s_{jk} and m_i^2.

1. Find a differential equation for the Feynman integral.

$$\sum_{j=0}^{r} p_j(t) \frac{d^j}{dt^j} I_G(t) = \sum_i q_i(t) I_{G_i}(t)$$

   Inhomogeneous term on the rhs consists of simpler integrals I_{G_i}.

   $p_j(t)$, $q_i(t)$ polynomials in t.

2. Solve the differential equation.

Kotikov; Remiddi, Gehrmann; Laporta; Argeri, Mastrolia; S. Müller-Stach, S.W., R. Zayadeh; Henn; ...

The canonical form of the differential equation for Feynman integrals evaluating to multiple polylogarithms

Can always convert a differential equation of order r to a system of r first-order differential equations.

Canonical form:

$$\frac{d}{dt}\vec{I} = \varepsilon \left(\sum_j \frac{1}{t - z_j} C_j \right) \vec{I}$$

- Explicit factor of ε on the r.h.s.
- C_j are matrices with constant entries.
- Singularities of the differential equation captured by $1/(t - z_j)$.

The canonical form is easily integrated to give multiple polylogarithms.

Henn, 2013

Numerical evaluations of multiple polylogarithms

Multiple polylogarithms have branch cuts.

Numerical evaluation of multiple polylogarithms $\text{Li}_{m_1,m_2,...,,m_k}(x_1,x_2,...,x_k)$ as a function of k complex variables x_1, x_2, ..., x_k:

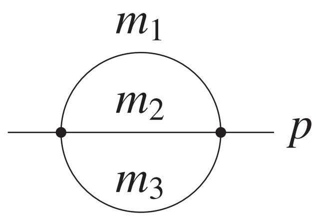
- Use truncated sum representation within its region of convergence.
- Use integral representation to map arguments into this region.
- Some tricks to speed up the computation.

Implementation in GiNaC, using arbitrary precision arithmetic in C++.

J. Vollinga, S.W., (2004)

Beyond multiple polylogarithms: The two-loop sunset integral

$$S\left(p^2, m_1^2, m_2^2, m_3^2\right) \quad = $$



- Two-loop contribution to the self-energy of massive particles.

- Sub-topology for more complicated diagrams.

Well-studied in the literature:

Broadhurst, Fleischer, Tarasov, Bauberger, Berends, Buza, Böhm, Scharf, Weiglein, Caffo, Czyz, Laporta, Remiddi, Groote, Körner, Pivovarov, Bailey, Borwein, Glasser, Adams, Bogner, Müller-Stach, S.W, Zayadeh, Bloch, Vanhove, Tancredi, Pozzorini, Gunia, ...

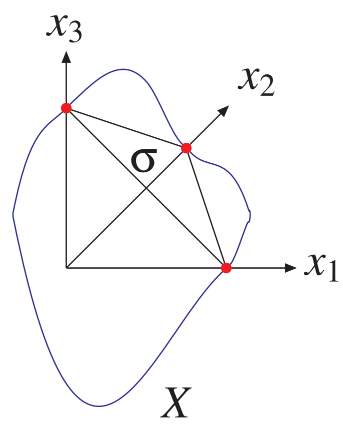
but still room for further investigations ...

Elliptic generalisations of multiple polylogarithms

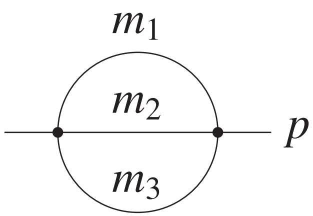
The two-loop sunrise integral with non-zero masses is the first integral, which cannot be expressed in terms of multiple polylogarithms.

In two dimensions: Sunset integral is finite.
Integrand depends only on one graph polynomial.

Graph polynomial corresponds to an elliptic curve.



$$S(t) \quad = $$



$$= \int\limits_{x_j \geq 0} d^3x \, \delta\left(1 - \sum x_j\right) \frac{1}{\mathcal{F}},$$

$$\mathcal{F} \quad = \quad -x_1 x_2 x_3 t + \left(x_1 m_1^2 + x_2 m_2^2 + x_3 m_3^2\right)\left(x_1 x_2 + x_2 x_3 + x_3 x_1\right), \qquad t = p^2$$

The elliptic dilogarithm

Recall the definition of the classical polylogarithms:

$$\mathrm{Li}_n(x) = \sum_{j=1}^{\infty} \frac{x^j}{j^n}.$$

Generalisation, the two sums are coupled through the variable q:

$$\mathrm{ELi}_{n;m}(x;y;q) = \sum_{j=1}^{\infty} \sum_{k=1}^{\infty} \frac{x^j}{j^n} \frac{y^k}{k^m} q^{jk}.$$

Elliptic dilogarithm:

$$\mathrm{E}_{2;0}(x;y;q) = \frac{1}{i}\left[\frac{1}{2}\mathrm{Li}_2(x) - \frac{1}{2}\mathrm{Li}_2\left(x^{-1}\right) + \mathrm{ELi}_{2;0}(x;y;q) - \mathrm{ELi}_{2;0}\left(x^{-1};y^{-1};q\right)\right].$$

(Slightly) different definitions of elliptic polylogarithms can be found in the literature

Beilinson ’94, Levin ’97, Brown, Levin ’11, Wildeshaus ’97.

The result for $D = 2$ in terms of elliptic dilogarithms

The result for the two-loop sunset integral in two space-time dimensions with arbitrary masses:

$$S = \underbrace{\frac{4}{\left[\left(t-\mu_1^2\right)\left(t-\mu_2^2\right)\left(t-\mu_3^2\right)\left(t-\mu_4^2\right)\right]^{\frac{1}{4}}}}_{\text{algebraic prefactor}} \underbrace{\frac{K(k)}{\pi}}_{\text{elliptic integral}} \underbrace{\sum_{j=1}^{3} \mathrm{E}_{2;0}\left(w_j;-1;-q\right)}_{\text{elliptic dilogarithms}}$$

t	momentum squared
μ_1, μ_2, μ_3	pseudo-thresholds
μ_4	threshold
$K(k)$	complete elliptic integrals of the first kind
k, q	modulus and nome
w_1, w_2, w_3	points in the Jacobi uniformization

Elliptic generalisations

In order to express the (equal mass) sunrise integral to all orders in ε introduce

$$\mathrm{ELi}_{n_1,...,n_l;m_1,...,m_l;2o_1,...,2o_{l-1}}\left(x_1,...,x_l;y_1,...,y_l;q\right) =$$

$$= \sum_{j_1=1}^{\infty} ... \sum_{j_l=1}^{\infty} \sum_{k_1=1}^{\infty} ... \sum_{k_l=1}^{\infty} \frac{x_1^{j_1}}{j_1^{n_1}} ... \frac{x_l^{j_l}}{j_l^{n_l}} \frac{y_1^{k_1}}{k_1^{m_1}} ... \frac{y_l^{k_l}}{k_l^{m_l}} \frac{q^{j_1k_1+...+j_lk_l}}{\prod\limits_{i=1}^{l-1} \left(j_ik_i+...+j_lk_l\right)^{o_i}}.$$

Integral representation:

$$\mathrm{ELi}_{n_1,...,n_l;m_1,...,m_l;2,2o_2,...,2o_{l-1}}\left(x_1,...,x_l;y_1,...,y_l;q\right) =$$

$$= \int \frac{dq}{q} \mathrm{ELi}_{n_1;m_1}\left(x_1;y_1;q\right) \mathrm{ELi}_{n_2,...,n_l;m_2,...,m_l;2o_2,...,2o_{l-1}}\left(x_2,...,x_2;y_1,...,y_l;q\right).$$

The all-order in ε result for the equal mass case

Taylor expansion around $D = 2 - 2\varepsilon$:

$$S = \frac{\psi_1}{\pi} \sum_{j=0}^{\infty} \varepsilon^j E^{(j)}$$

Each term in the ε-series is of the form

$$E^{(j)} \sim \text{linear combination of } \mathrm{ELi}_{n_1,...,n_l;m_1,...,m_l;2o_1,...,2o_{l-1}} \text{ and } \mathrm{Li}_{n_1,...,n_l}$$

Using dimensional-shift relations this translates to the expansion around $4 - 2\varepsilon$.

$\Rightarrow$ The multiple polylogarithms extended by $\mathrm{ELi}_{n_1,...,n_l;m_1,...,m_l;2o_1,...,2o_{l-1}}$ are the class of functions to express the equal mass sunrise graph to all orders in ε.

Adams, Bogner, S.W.

Part II

Loop amplitudes: The numerical approach

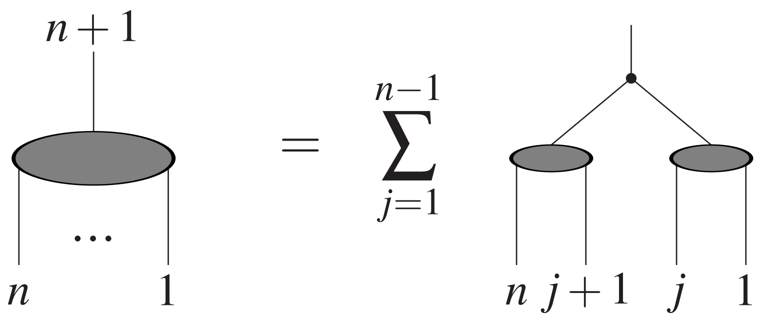
I.1: **Direct numerical integration**

I.2: **Contour deformation**

I.3: **Cancellations at the integrand level**

Recurrence relations

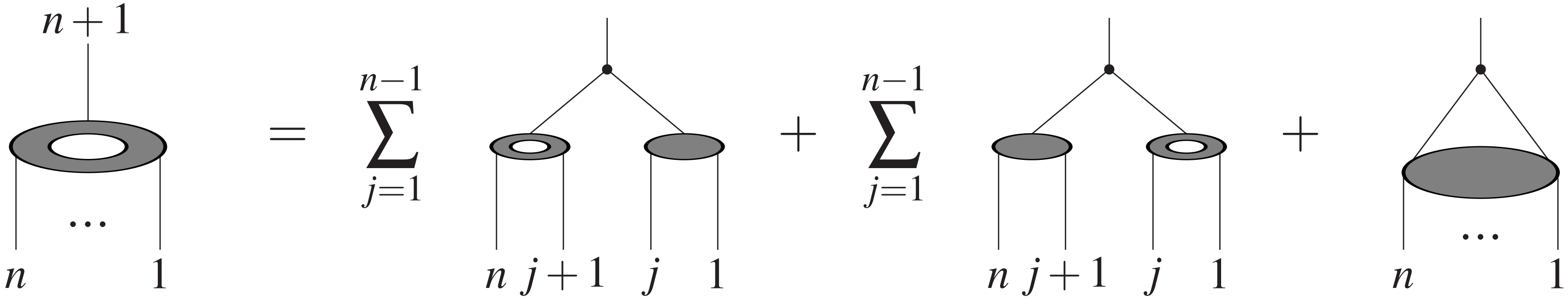
Off-shell currents provide an efficient way to calculate amplitudes:



Computational cost grows like n^3.

Berends and Giele, '88

The integrand of a loop amplitude is a rational function. Can use recurrence relations:



Draggiotis et al., '06; van Hameren, '09; Becker, Reuschle, S.W., '10; Cascioli, Maierhöfer, Pozzorini, '11

Numerical NLO QCD calculations

Use subtraction also for the virtual part:

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

- In the last term $d\sigma^{\mathrm{V}} - d\sigma^{\mathrm{A}}_{\mathrm{V}}$ 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.

- The IR-subtraction terms can be formulated at the level of amplitudes.

Z. Nagy, D. Soper, ’03; M. Assadsolimani, S. Becker, D. Götz, Ch. Reuschle, Ch. Schwan, S.W., ’09

Contour deformation

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

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

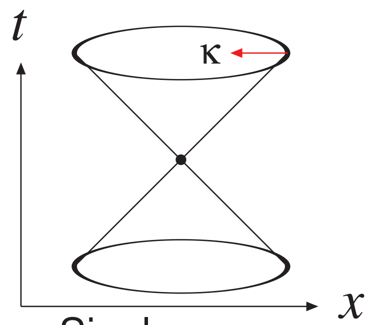
Still remains:

- 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 ...)

Contour deformation

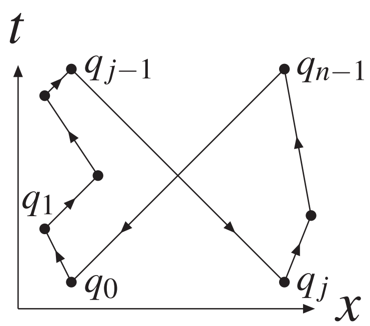
Deformation of the loop momentum:

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

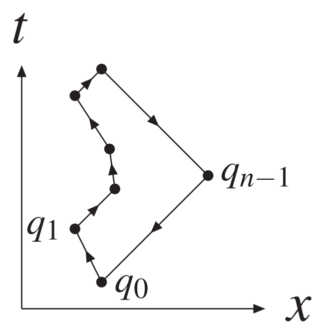


Single cone

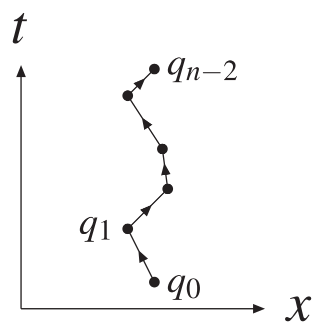
For n cones draw only the origins of the cones:



generic with 2 initial partons



initial partons adjacent

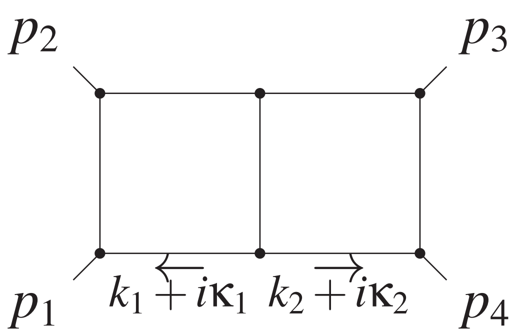


no initial partons

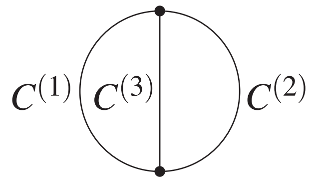
Gong, Nagy, Soper, ’08; Becker, Reuschle, S.W., ’12

Contour deformation beyond one-loop

Feynman diagram:



Chain diagram:



We have:

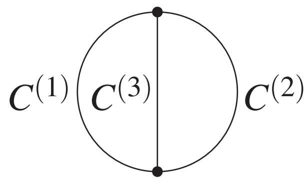
- 2 independent loop momenta
- 3 inequivalent cycles

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

Kinoshita, '62

Multi-loop contour deformation

The contour deformation for a multi-loop integral can be obtained from the contour deformation for one-loop integrals:



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

Two-loop example:

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

Becker, S.W., '12

Cancellations at the integrand level

$$\int_{n+1} d\sigma^{\mathrm{R}} + \int_{n} d\sigma^{\mathrm{V}} = \int_{n+1} \left(d\sigma^{\mathrm{R}} - d\sigma^{\mathrm{A}}_{\mathrm{R}}\right) + \underbrace{\int_{n} (\mathbf{I}+\mathbf{L}) \otimes d\sigma^{B}}_{\text{numerical integrable?}} + \int_{n+\mathrm{loop}} \left(d\sigma^{\mathrm{V}} - d\sigma^{\mathrm{A}}_{\mathrm{V}}\right)$$

- At NLO both $d\sigma^{\mathrm{A}}_{\mathrm{R}}$ and $d\sigma^{\mathrm{A}}_{\mathrm{V}}$ are easily integrated analytically.
- This is no longer true at NNLO and beyond.

$$\int_{n} (\mathbf{I}+\mathbf{L}) = \int_{n} \left[\int_{1} d\sigma^{\mathrm{A}}_{\mathrm{R}} + \int_{\mathrm{loop}} d\sigma^{\mathrm{A}}_{\mathrm{V}} + d\sigma^{\mathrm{V}}_{\mathrm{CT}} + d\sigma^{\mathrm{C}}\right].$$

- Unresolved phase space is $(D-1)$-dimensional.
- Loop momentum space is D-dimensional
- $d\sigma^{\mathrm{V}}_{\mathrm{CT}}$ counterterm from renormalisation
- $d\sigma^{\mathrm{C}}$ counterterm from factorisation

Loop-tree duality

A cyclic-ordered one-loop amplitude

$$A_n = \int \frac{d^D k}{(2\pi)^D} \frac{P(k)}{\prod_{j=1}^{n} \left(k_j^2 - m_j^2 + i\delta\right)}.$$

can be written with Cauchy's theorem as

$$A_n = -i \sum_{i=1}^{n} \int \frac{d^{D-1} k}{(2\pi)^{D-1}\, 2k_i^0} \frac{P(k)}{\prod_{\substack{j=1 \\ j\neq i}}^{n} \left[k_j^2 - m_j^2 - i\delta \left(k_j^0 - k_i^0\right)\right]} \Bigg|_{k_i^0 = \sqrt{\vec{k}_i^2 + m_i^2}},$$

Note the modified $i\delta$-prescription!

Catani, Gleisberg, Krauss, Rodrigo, Winter, ’08

Maps

We need to relate the real unresolved phase space and the loop integration in the loop-tree duality approach:

Given a set $\{p_1, p_2, ..., p_n\}$ of external momenta and an on-shell loop momentum k there is an invertible map

$$\{p_1, p_2, ..., p_n\} \times \{k\} \quad \to \quad \{p'_1, p'_2, ..., p'_n, p'_{n+1}\}$$

Remark:

$$\{p'_1, p'_2, ..., p'_n, p'_{n+1}\} \quad \to \quad \{p_1, p_2, ..., p_n\}$$

is the standard Catani-Seymour projection.

Sborlini, Driencourt-Mangin, Hernandez-Pinto, German; Seth, S.W.

Collinear singularities

Problem with collinear singularities:

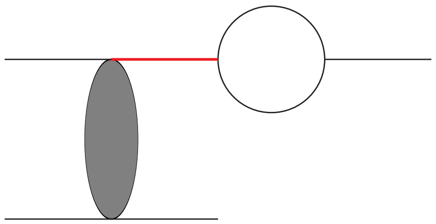
$d\sigma_{\mathrm{R}}^{\mathrm{A}}$: both partons have transverse polarisations,
divergence in $g \to q\bar{q}$,

$d\sigma_{\mathrm{V}}^{\mathrm{A}}$: one parton has longitudinal polarisation,
no divergence in $g \to q\bar{q}$.

Solution: Take field renormalisation constants into account:

$$
\begin{aligned}
Z_2 &= 1 = 1 + \frac{\alpha_s}{4\pi} C_F \left(\frac{1}{\varepsilon_{\mathrm{IR}}} - \frac{1}{\varepsilon_{\mathrm{UV}}} \right) \\
Z_3 &= 1 = 1 + \frac{\alpha_s}{4\pi} (2C_A - \beta_0) \left(\frac{1}{\varepsilon_{\mathrm{IR}}} - \frac{1}{\varepsilon_{\mathrm{UV}}} \right)
\end{aligned}
$$

Field renormalisation

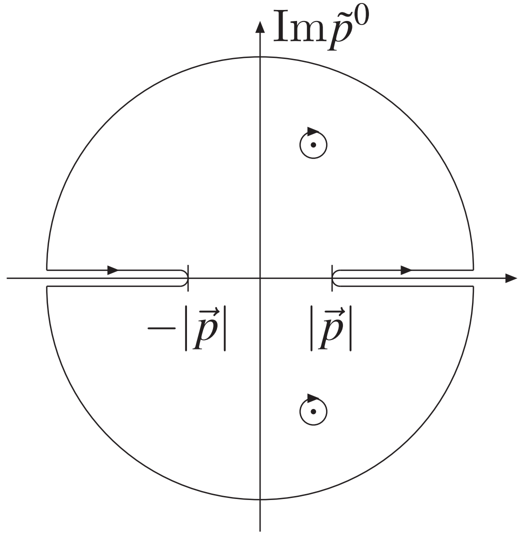


Field renormalisation constants derived from self-energies.

Problem: Internal on-shell propagator.

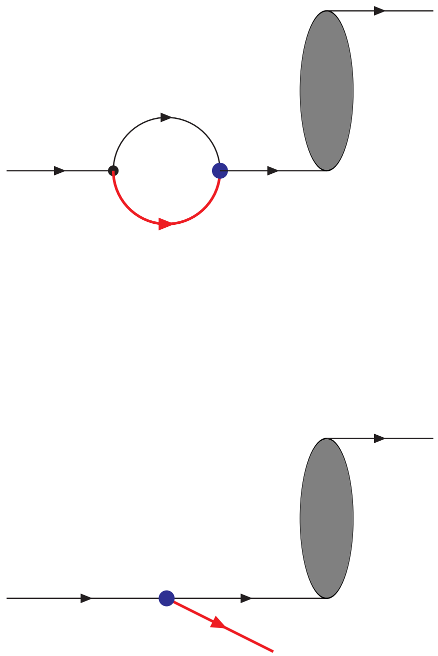
Solution: Use dispersion relation.

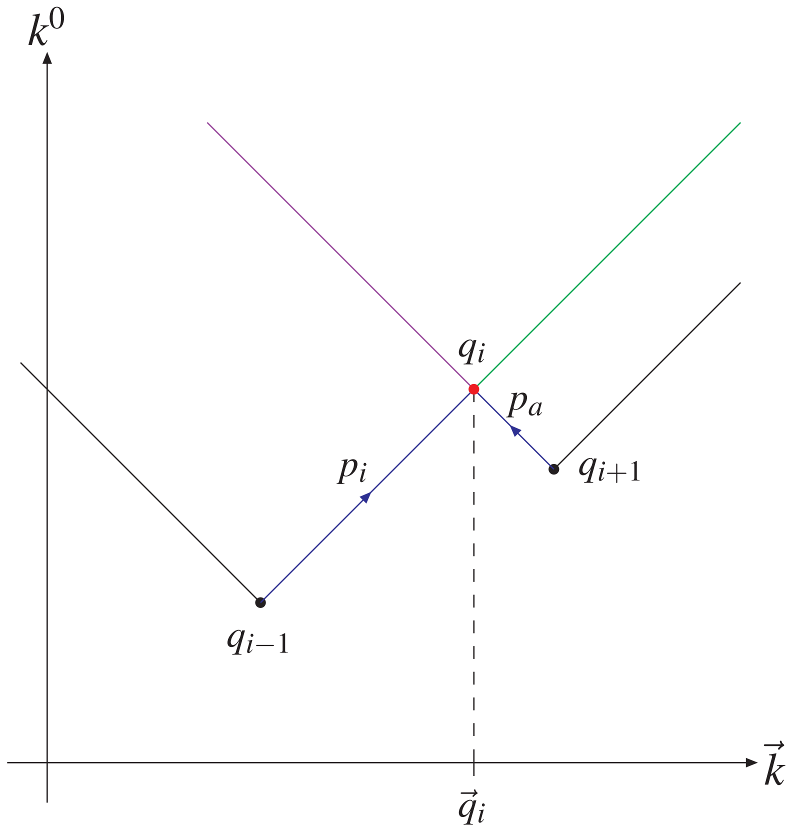
Soper, '01; Seth, S.W., '16



Initial-state collinear singularities

Problem: For initial-state collinear singularities the regions do not match.





Initial-state collinear singularities

We still have to include the counterterm from factorisation.

$$d\sigma^{\mathrm{C}} = \frac{\alpha_s}{4\pi} \int_0^1 dx_a \frac{2}{\varepsilon} \left(\frac{\mu_F^2}{\mu^2} \right)^{-\varepsilon} P^{a'a}(x_a)\, d\sigma^{\mathrm{B}}(\ldots, x_a p'_a, \ldots) .$$

Example of splitting function:

$$P^{gg} = 2C_A \left[\left. \frac{1}{1-x} \right|_+ + \frac{1-x}{x} - 1 + x(1-x) \right] + \frac{\beta_0}{2} \delta(1-x) .$$

Solution: Unintegrated representation of the collinear subtraction term $d\sigma^{\mathrm{C}}$.

- x-dependent part matches on real contribution
- end-point part matches on virtual contribution

Comment on remaining analytic integrals

Does the numerical approach eliminate the need of any analytic calculation of an integral?

- No analytic integral required where divergences cancel (i.e. final-state soft or collinear)
- But: UV divergences removed by renormalisation, initial-state collinear divergences by factorisation, this introduces a scheme dependence.
- Have to reproduce the finite terms associated to a given renormalisation scheme / factorisation scheme ($\overline{\text{MS}}$-scheme,...)
- Need simple integrals analytically

$$\text{Renormalisation}: \int \frac{d^D k}{(2\pi)^D} \frac{1}{(k^2 - m)^\nu}, \qquad \text{Factorisation}: \int_0^1 dx\, x^{\nu-\varepsilon} (1-x)^{-\varepsilon}.$$

Conclusions

- The analytical approach:
  - Multiple polylogarithms
  - Elliptic generalisations
- The numerical approach:
  - Contour deformation
  - Cancellations at the integrand level

"Zwei Seelen wohnen, ach! in meiner Brust ...", J. W. von Goethe