Infrared finite cross sections at NNLO

Stefan Weinzierl

Max-Planck-Institut für Physik München

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The need for NNLO calculations

Hunting for the Higgs and other yet-to-be-discovered particles requires a better knowledge of the theoretical cross section.

The strong coupling constant α_s is one fundamental parameter of the theory and its precise value affects the magnitude of many (background) processes.

The next generation of colliders will increase the experimental precision. This has to be matched by an improvement in the accuracy of theoretical predictions.

Theoretical predictions are calculated as a power expansion in the coupling. Higher precision is reached by including the next higher term in the perturbative expansion.

What is necessary:

NNLO calculations

Perturbative NNLO calculations

The experimental needs are numerical programs which yield predictions for a wide range of observables.

Fully differential NNLO programs for

- Bhabha scattering
- $pp \to 2$ jets
- $e^+e^- \to 3$ jets

which allow the calculation of any infrared safe observable.

Infrared safe at NNLO:

$$\begin{aligned} \text{Single unresolved}: \quad & \mathcal{O}_{n+1}(p_1, ..., p_{n+1}) \quad \to \quad \mathcal{O}_n(p_1', ..., p_n'), \\ \text{Double unresolved}: \quad & \mathcal{O}_{n+2}(p_1, ..., p_{n+2}) \quad \to \quad \mathcal{O}_n(p_1', ..., p_n'). \end{aligned}$$

Necessary ingredients for a NNLO calculation

- Calculation of the (two-loop) amplitudes.

  Requires: Two-loop integrals and tensor reduction.

- Cancellation of IR divergences has to be done before any Monte Carlo integration.

  Requires: Extension of the subtraction or slicing method to NNLO.

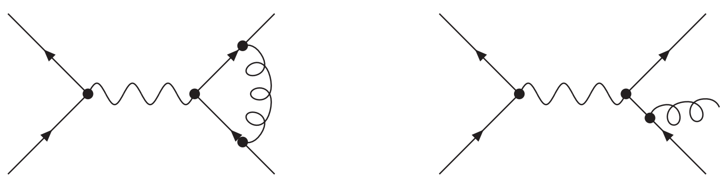
- The final numerical computer program.

  Requires: Stable and efficient numerical methods.

Infrared divergences and the Kinoshita-Lee-Nauenberg theorem

In addition to ultraviolet divergences, loop integrals can have infrared divergences.

For each IR divergence there is a corresponding divergence with the opposite sign in the real emission amplitude, when particles becomes soft or collinear (e.g. unresolved).



The Kinoshita-Lee-Nauenberg theorem: Any observable, summed over all states degenerate according to some resolution criteria, will be finite.

General methods at NLO

Fully differential NLO Monte Carlo programs need a general method to handle the cancelation of infrared divergencies.

- Phase space slicing
  - e^+e^-: W. Giele and N. Glover, (1992)
  - initial hadrons: W. Giele, N. Glover and D.A. Kosower, (1993)
  - massive partons, fragmentation: S. Keller and E. Laenen, (1999)

- Subtraction method
  - residue approach: S. Frixione, Z. Kunzst and A. Signer, (1995)
  - dipole formalism: S. Catani and M. Seymour, (1996)
  - massive partons: L. Phaf and S.W. (2001),
    S. Catani, S. Dittmaier, M. Seymour and Z. Trócsányi, (2002)

The dipole formalism at NLO

The dipole formalism is based on 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 subtraction method at NNLO

- Singular behaviour
  - Factorization of tree amplitudes in double unresolved limits, Berends, Giele, Cambell, Glover, Catani, Grazzini, Del Duca, Frizzo, Maltoni, Kosower '99
  - Factorization of one-loop amplitudes in single unresolved limits, Bern, Del Duca, Kilgore, Schmidt, Kosower, Uwer, Catani, Grazzini, '99

- Interpolation and construction of subtraction terms, Kosower '03, S.W. '03, Kilgore '04

- Integration, either analytically or by sector decomposition, S.W. '03, Anastasiou, Melnikov, Petriello '03, Gehrmann-De Ridder, Gehrmann, Heinrich '03, Binoth, Heinrich '04, Gehrmann-De Ridder, Gehrmann, Glover '04

- Applications:
  - $pp \to W$, Anastasiou, Dixon, Melnikov, Petriello '03,
  - $e^+e^- \to$ 2 jets, Anastasiou, Melnikov, Petriello '04,

The subtraction method at NNLO

Contributions at NNLO:

$$
\begin{aligned}
d\sigma_{n+2}^{(0)} &= \left({\mathcal{A}_{n+2}^{(0)}}^* \mathcal{A}_{n+2}^{(0)} \right) d\phi_{n+2}, \\
d\sigma_{n+1}^{(1)} &= \left({\mathcal{A}_{n+1}^{(0)}}^* \mathcal{A}_{n+1}^{(1)} + {\mathcal{A}_{n+1}^{(1)}}^* \mathcal{A}_{n+1}^{(0)} \right) d\phi_{n+1}, \\
d\sigma_{n}^{(2)} &= \left({\mathcal{A}_{n}^{(0)}}^* \mathcal{A}_{n}^{(2)} + {\mathcal{A}_{n}^{(2)}}^* \mathcal{A}_{n}^{(0)} + {\mathcal{A}_{n}^{(1)}}^* \mathcal{A}_{n}^{(1)} \right) d\phi_{n},
\end{aligned}
$$

Adding and subtracting:

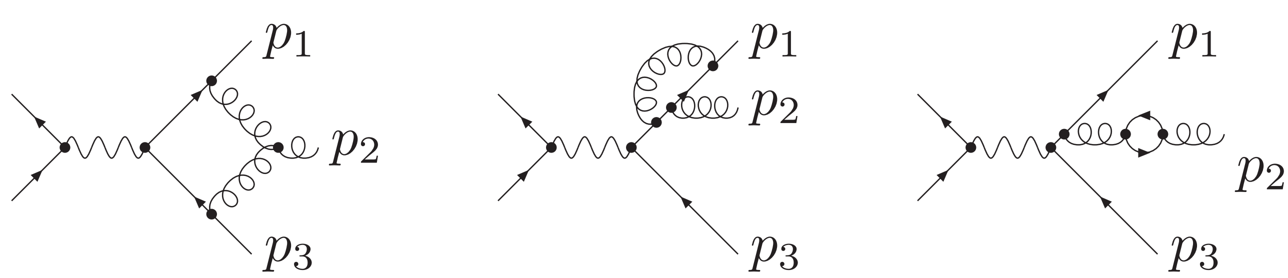
$$
\begin{aligned}
\langle \mathcal{O} \rangle_n^{NNLO} &= \int \left(\mathcal{O}_{n+2}\, d\sigma_{n+2}^{(0)} - \mathcal{O}_{n+1} \circ d\alpha_{n+1}^{(0,1)} - \mathcal{O}_{n} \circ d\alpha_{n}^{(0,2)} \right) \\
&\quad + \int \left(\mathcal{O}_{n+1}\, d\sigma_{n+1}^{(1)} + \mathcal{O}_{n+1} \circ d\alpha_{n+1}^{(0,1)} - \mathcal{O}_{n} \circ d\alpha_{n}^{(1,1)} \right) \\
&\quad + \int \left(\mathcal{O}_{n}\, d\sigma_{n}^{(2)} + \mathcal{O}_{n} \circ d\alpha_{n}^{(0,2)} + \mathcal{O}_{n} \circ d\alpha_{n}^{(1,1)} \right).
\end{aligned}
$$

Colour disentanglement

Full QCD amplitudes do not factorize in the singular limits, but primitive amplitudes do.

Primitive amplitudes distinguished by:

- fixed cyclic ordering of the QCD partons
- definite routing of the external fermion lines through the diagram
- particle content circulating in the loop



The leading singular behaviour

Factorization of one-loop amplitudes in single unresolved limits:

$$A_n^{(1)} \;=\; \text{Sing}^{(0,1)} \cdot A_{n-1}^{(1)} + \text{Sing}^{(1,1)} \cdot A_{n-1}^{(0)},$$

Z. Bern, Del Duca, W. Kilgore, C. Schmidt, D. Kosower, P. Uwer, S. Catani, M. Grazzini

Factorization of tree amplitudes in double unresolved limits:

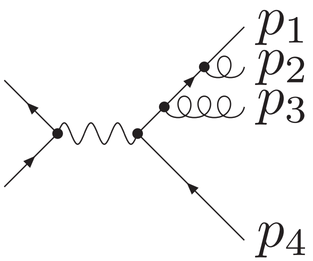
$$A_n^{(0)} \;=\; \text{Sing}^{(0,2)} \cdot A_{n-2}^{(0)},$$

F. Berends, W. Giele, J. Cambell, N. Glover, S. Catani, M. Grazzini, V. Del Duca, A. Frizzo, F. Maltoni, D. Kosower

For the subtraction method one needs also the subleading singular behaviour !

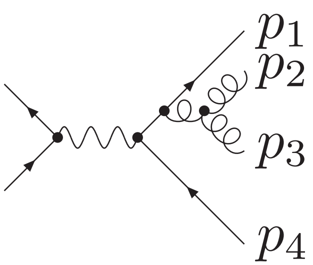
An example involving double unresolved configurations

The leading-colour contributions to $e^+e^- \to qgg\bar{q}$.



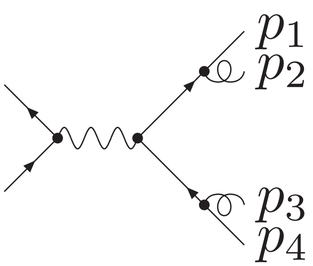
Double unresolved configurations:

- Two pairs of separately collinear particles
- Three particles collinear
- Two particles collinear and a third soft particle
- Two soft particles
- Coplanar degeneracy



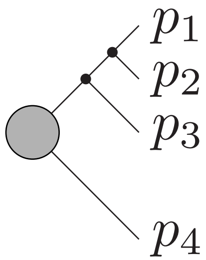
Single unresolved configurations:

- Two collinear particles
- One soft particle



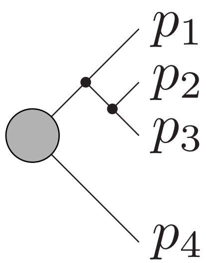
NNLO subtraction terms

The $(n+2)$-parton contribution:



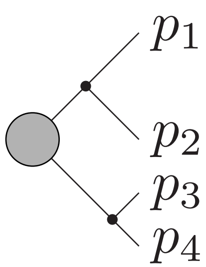
$$\int \left(\mathcal{O}_{n+2}\, d\sigma_{n+2}^{(0)} - \mathcal{O}_{n+1} \circ d\alpha_{n+1}^{(0,1)} - \mathcal{O}_n \circ d\alpha_n^{(0,2)} \right)$$

The NNLO subtraction term is written as



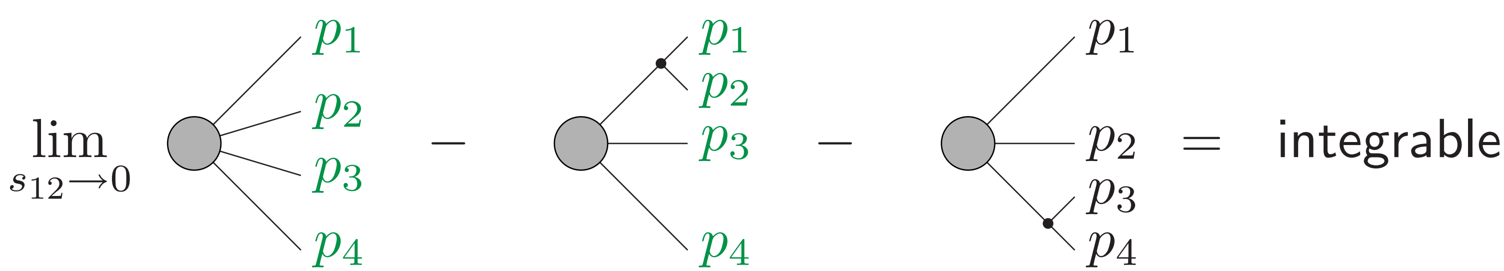
$$d\alpha_n^{(0,2)} \quad = \quad \sum_T \left(\mathcal{D}_{(0,0)n}^{(0,2)} - \mathcal{D}_{(0,1)n}^{(0,2)} \right),$$

where $\sum_T \mathcal{D}_{(0,0)n}^{(0,2)}$ approximates $d\sigma_{n+2}^{(0)}$ and
$\sum_T \mathcal{D}_{(0,1)n}^{(0,2)}$ approximates $d\alpha_{n+1}^{(0,1)}$.

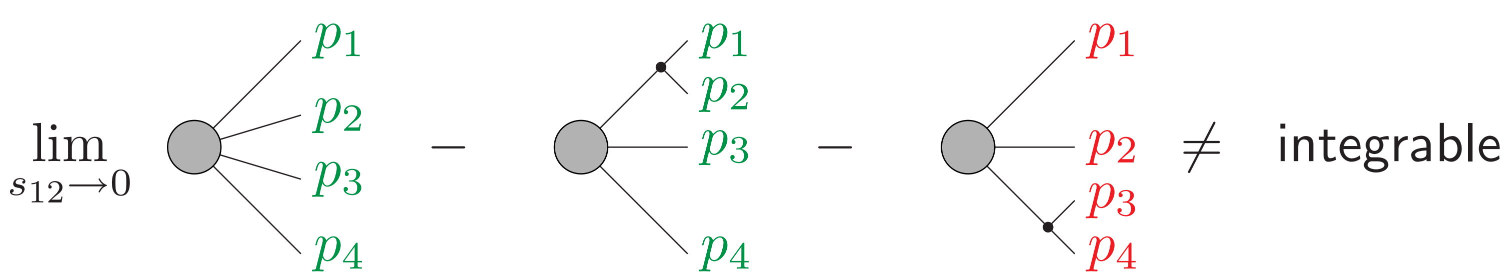


Single unresolved contributions

For an observable, which vanishes on n-parton configurations:

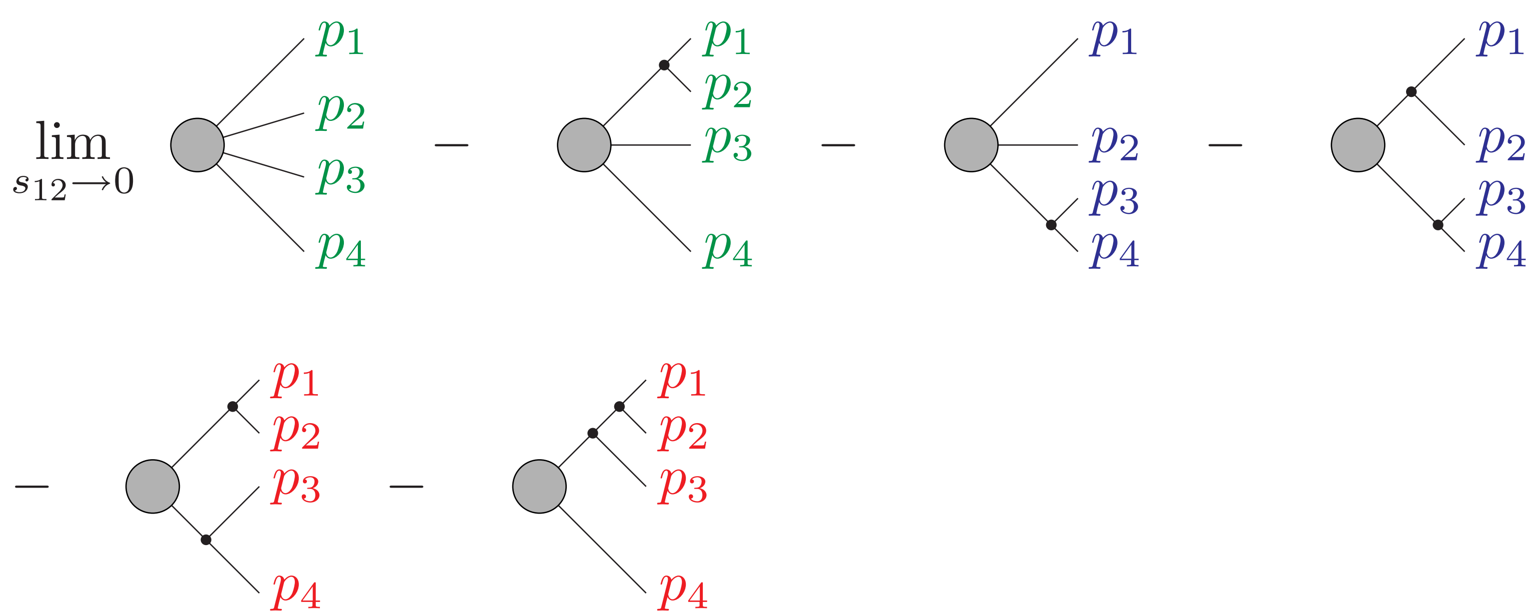


For an observable, which does not vanish on n-parton configurations:



Single unresolved contributions

The subtraction terms are subtracted over the complete phase space. The integrand has to be finite also in single unresolved limits !



Checks

The subtracted matrix element with $(n+2)$-parton kinematics

$$\int \left(\mathcal{O}_{n+2}\, d\sigma^{(0)}_{n+2} - \mathcal{O}_{n+1} \circ d\alpha^{(0,1)}_{n+1} - \mathcal{O}_{n} \circ d\alpha^{(0,2)}_{n} \right)$$

has to be integrable. This has been checked for all double and single unresolved limits.

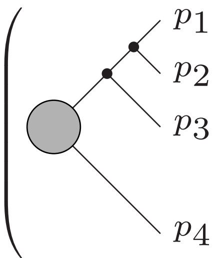
The subtracted matrix element with $(n+1)$-parton kinematics

$$\int \left(\mathcal{O}_{n+1}\, d\sigma^{(1)}_{n+1} + \mathcal{O}_{n+1} \circ d\alpha^{(0,1)}_{n+1} - \mathcal{O}_{n} \circ d\alpha^{(1,1)}_{n} \right)$$

has to be integrable over single unresolved limits. In addition, explicit poles in ε have to cancel.

Results

$$\mathcal{P}^{(0,2)}_{(0,0)\; q\to qgg}\left(\right.$$



$$\left.\right) = \not{p}_e^{(2)} \frac{4}{s_{1234}^2}\frac{1}{x_1^2}\left\{ \frac{1}{y_1\left(y_1+\bar{y}_1\bar{z}_1\right)}\left[\frac{2}{\left(y_1+\bar{y}_1\bar{z}_1\right)x_1+\bar{y}_1x_2}+\frac{2}{y_1x_1+u}\right.\right.$$

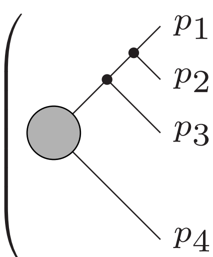
$$\left.+\frac{u}{\left(y_1+\bar{y}_1\bar{z}_1\right)x_1+\bar{y}_1x_2}\left(-2+(1-\varepsilon)u\right)+\frac{\bar{y}_1x_2}{u}\left(-2+(1-\varepsilon)\bar{y}_1x_2\right)\right]$$

$$+\frac{1}{y_1}\left[\frac{2}{u\left[\left(y_1+\bar{y}_1\bar{z}_1\right)x_1+\bar{y}_1x_2\right]}+\frac{1}{x_1+\bar{y}_1x_2}\left(-2+(1-\varepsilon)u\right)-\frac{4}{u}+(1-\varepsilon)\frac{\bar{y}_1x_2}{u}-\frac{\bar{y}_1x_2}{u}\left(-2+(1-\varepsilon)\bar{y}_1x_2\right)\right.$$

$$\left.+\varepsilon(1-\varepsilon)u-\varepsilon(1-\varepsilon)\bar{y}_1x_2-1+3\varepsilon\right]+(1-\varepsilon)^2\frac{\bar{y}_1\bar{z}_1}{y_1}+3-4\varepsilon+\varepsilon^2+\frac{x_1}{y_1}\left[-\varepsilon\left(\frac{2}{y_1+\bar{y}_1\bar{z}_1}-2+(1-\varepsilon)\bar{y}_1\bar{z}_1\right)\right.$$

$$\left.\left.+\frac{2}{u}-(1-\varepsilon)\left(\frac{x_1}{u}-2\bar{y}_1z_1+(1-\varepsilon)\bar{y}_1z_1x_1\right)+\frac{1}{u\left(y_1+\bar{y}_1\bar{z}_1\right)}\left(-2+(1-\varepsilon)x_1\right)\right]\right\}$$

$$\mathcal{P}^{(0,2)}_{(0,1)\; q\to qgg}\left(\right.$$



$$\left.\right) = \not{p}_e^{(2)} \frac{4}{s_{1234}^2}\frac{1}{x_1^2}\left[\frac{2}{x_1+x_2}-2+(1-\varepsilon)\,x_2-\varepsilon x_1\right]$$

$$\times\frac{1}{y_1}\left[\frac{2}{1-z_1(1-y_1)}-2+(1-\varepsilon)\,(1-y_1)(1-z_1)\right]$$

One-loop amplitudes with one unresolved parton

Slightly simpler than double unresolved configurations are the subtraction terms for one-loop amplitudes with one unresolved parton.

- Colour correlation due to soft gluons.
- The subtraction terms in electron-positron annihilation.
- Technique for the integration over the unresolved phase space.
- Results of the integration.

$$\int \left(\mathcal{O}_{n+1}\, d\sigma^{(1)}_{n+1} + \mathcal{O}_{n+1} \circ d\alpha^{(0,1)}_{n+1} - \mathcal{O}_{n} \circ d\alpha^{(1,1)}_{n} \right),$$

$$d\alpha^{(1,1)}_{n} = d\alpha^{(1,1)}_{(1,0)\ n} + d\alpha^{(1,1)}_{(0,1)\ n}$$

The soft current

In the soft limit, one-loop amplitudes factorize as (Catani, Grazzini)

$$\left|\mathcal{M}_{n+1}^{(1)}\right\rangle = \sqrt{4\pi\alpha_s}\, S_\varepsilon^{-1/2} \varepsilon^\mu(p_j) \left[\mathbf{J}_\mu^{(0)}(p_j) \left|\mathcal{M}_n^{(1)}\right\rangle + \left(\frac{\alpha_s}{2\pi}\right) \mathbf{J}_\mu^{(1)}(p_j) \left|\mathcal{M}_n^{(0)}\right\rangle \right],$$

with the soft currents

$$\mathbf{J}_\mu^{a\,(0)}(p_j) = \sum_i \mathbf{T}_i^a \frac{p_i^\mu}{p_i \cdot p_j},$$

$$\mathbf{J}_\mu^{a\,(1)}(p_j) = -\frac{S_\varepsilon^{-1} c_\Gamma}{\varepsilon^2} \Gamma(1+\varepsilon)\Gamma(1-\varepsilon) \frac{1}{2} i f^{abc} \sum_{i \neq k} \mathbf{T}_i^b \mathbf{T}_k^c \left(\frac{\mu^2(-s_{ik})}{(-s_{ij})(-s_{jk})} \right)^\varepsilon \left(\frac{p_i^\mu}{p_i \cdot p_j} - \frac{p_k^\mu}{p_k \cdot p_j} \right) - \frac{\beta_0}{2\varepsilon} \mathbf{J}_\mu^{a\,(0)}(p_j).$$

In general, this leads to colour-correlations between three hard partons:

$$i f^{abc}\, \mathbf{T}_i^a \mathbf{T}_k^b \mathbf{T}_l^c.$$

For processes with three hard partons these correlations vanish due to colour conservation.

The subtraction terms for one-loop amplitudes with one unresolved parton

Example: The splitting $q \to qg$.

$$\mathcal{P}^{(1,1)}_{(1,0)\; q \to qg, lc, corr} = S_\varepsilon^{-1} c_\Gamma \left(\frac{-s_{ijk}}{\mu^2} \right)^{-\varepsilon} y^{-\varepsilon}$$

$$\times \left\{ g_{1,corr}(y,z) \; \mathcal{P}^{(0,1)}_{q \to qg} + f_2 \frac{2}{s_{ijk}} \frac{1}{y} \not{p}_e \left[1 - \rho\varepsilon (1-y)(1-z) \right] \right\} - \frac{11}{6\varepsilon} \mathcal{P}^{(0,1)}_{q \to qg},$$

$$\mathcal{P}^{(1,1)}_{(1,0)\; q \to qg, nf} = \frac{1}{3\varepsilon} \mathcal{P}^{(0,1)}_{q \to qg},$$

$$\mathcal{P}^{(1,1)}_{(1,0)\; q \to qg, sc} = S_\varepsilon^{-1} c_\Gamma \left(\frac{-s_{ijk}}{\mu^2} \right)^{-\varepsilon} y^{-\varepsilon}$$

$$\times \left\{ \left[-\frac{1}{\varepsilon^2} - g_{1,intr}(y, 1-z) \right] \; \mathcal{P}^{(0,1)}_{q \to qg} + f_2 \; \frac{2}{s_{ijk}} \frac{1}{y} \not{p}_e \left[1 - \rho\varepsilon (1-y)(1-z) \right] \right\}.$$

with

$$g_{1,intr}(y,z) = -\frac{1}{\varepsilon^2} \left[\Gamma(1+\varepsilon)\Gamma(1-\varepsilon) \left(\frac{z}{1-z} \right)^{\varepsilon} + 1 - (1-y)^{\varepsilon} z^{\varepsilon} \; {}_2F_1\left(\varepsilon, \varepsilon, 1+\varepsilon; (1-y)(1-z) \right) \right].$$

Integration over the unresolved phase space

Reduction to basic integrals:

$$\int\limits_0^1 dy\, y^a (1-y)^{1+c+d} \int\limits_0^1 dz\, z^c (1-z)^d \left[1 - z(1-y)\right]^e {}_2F_1\left(\varepsilon, \varepsilon; 1+\varepsilon; (1-y)z\right) =$$

$$\frac{\Gamma(1+a)\Gamma(1+d)\Gamma(2+a+d+e)\Gamma(1+\varepsilon)}{\Gamma(2+a+d)\Gamma(\varepsilon)\Gamma(\varepsilon)} \sum_{j=0}^{\infty} \frac{\Gamma(j+\varepsilon)\Gamma(j+\varepsilon)\Gamma(j+1+c)}{\Gamma(j+1)\Gamma(j+1+\varepsilon)\Gamma(j+3+a+c+d+e)},$$

Result proportional to hypergeometric functions ${}_4F_3$ with unit argument.

These sums are then expanded into a Laurent series in ε with the help of Z-sums (S. Moch, P. Uwer, S.W.).

Simplifications: Relations among multiple-zeta values.

$$\zeta_2 = \frac{\pi^2}{6}, \quad \zeta_4 = \frac{\pi^4}{90}, \quad \zeta_{1,2} = \zeta_3, \quad \zeta_{1,3} = \frac{\pi^4}{360}, \quad \zeta_{2,2} = \frac{\pi^4}{120}, \quad \zeta_{1,1,2} = \frac{\pi^4}{90}.$$

Results for one-loop amplitudes with one unresolved parton

$\mathcal{V}^{(1,1)}$ defined by

$$8\pi^2 S_\varepsilon^{-1}\mu^{2\varepsilon}\int d\phi_{unresolved}\,\mathcal{P}^{(1,1)} \quad = \quad \frac{S_\varepsilon^{-2}(4\pi)^{2\varepsilon}}{\Gamma(1-\varepsilon)^2}\left(\frac{s_{ijk}}{\mu^2}\right)^{-2\varepsilon}\,\mathcal{T}\,\mathcal{V}^{(1,1)}.$$

For the splitting $q \to qg$ one finds with $L = \ln(s_{ijk}/\mu^2)$:

$$\begin{aligned}
\mathcal{V}^{(1,1)}_{(1,0)\,q\to qg,lc,intr} = & -\frac{1}{4\varepsilon^4} - \frac{31}{12\varepsilon^3} + \left(-\frac{51}{8} - \frac{1}{4}\rho + \frac{5}{12}\pi^2 - \frac{11}{6}L\right)\frac{1}{\varepsilon^2} + \left(-\frac{151}{6} - \frac{55}{24}\rho + \frac{145}{72}\pi^2 + \frac{15}{2}\zeta_3 - \frac{11}{4}L - \frac{11}{12}L^2\right)\frac{1}{\varepsilon} \\
& -\frac{1663}{16} - \frac{233}{24}\rho + \frac{107}{16}\pi^2 + \frac{5}{12}\rho\pi^2 + \frac{356}{9}\zeta_3 - \frac{1}{72}\pi^4 - \frac{187}{24}L - \frac{11}{12}\rho L + \frac{55}{72}\pi^2 L - \frac{11}{8}L^2 - \frac{11}{36}L^3 \\
& +i\pi\left[-\frac{1}{4\varepsilon^3} - \frac{3}{4\varepsilon^2} + \left(-\frac{29}{8} - \frac{1}{4}\rho + \frac{\pi^2}{3}\right)\frac{1}{\varepsilon} - \frac{139}{8} - \frac{11}{8}\rho + \pi^2 + \frac{15}{2}\zeta_3\right] + \mathcal{O}(\varepsilon), \\
\mathcal{V}^{(1,1)}_{(1,0)\,q\to qg,nf} = & \frac{1}{3\varepsilon^3} + \left(\frac{1}{2} + \frac{1}{3}L\right)\frac{1}{\varepsilon^2} + \left(\frac{17}{12} + \frac{1}{6}\rho - \frac{5}{36}\pi^2 + \frac{1}{2}L + \frac{1}{6}L^2\right)\frac{1}{\varepsilon} + \frac{33}{8} + \frac{7}{12}\rho - \frac{5}{24}\pi^2 - \frac{23}{9}\zeta_3 \\
& +\frac{17}{12}L + \frac{1}{6}\rho L - \frac{5}{36}\pi^2 L + \frac{1}{4}L^2 + \frac{1}{18}L^3 + \mathcal{O}(\varepsilon), \\
\mathcal{V}^{(1,1)}_{(1,0)\,q\to qg,sc} = & \left(\frac{5}{8} - \frac{\pi^2}{6}\right)\frac{1}{\varepsilon^2} + \left(\frac{35}{8} + \frac{3}{8}\rho - \frac{\pi^2}{4} - 7\zeta_3\right)\frac{1}{\varepsilon} + 25 + \frac{15}{4}\rho - \frac{35}{24}\pi^2 - \frac{1}{12}\rho\pi^2 - \frac{21}{2}\zeta_3 - \frac{17}{90}\pi^4 \\
& +i\pi\left[\left(\frac{5}{8} - \frac{\pi^2}{6}\right)\frac{1}{\varepsilon} + \frac{35}{8} + \frac{3}{8}\rho - \frac{\pi^2}{4} - 7\zeta_3\right] + \mathcal{O}(\varepsilon).
\end{aligned}$$

Introducing nested sums

$$Z(n; m_1, ..., m_k; x_1, ..., x_k) = \sum_{n \geq i_1 > i_2 > ... > i_k > 0} \frac{x_1^{i_1}}{i_1^{m_1}} \frac{x_2^{i_2}}{i_2^{m_2}} ... \frac{x_k^{i_k}}{i_k^{m_k}}.$$

- Multiple polylogarithms are a special subset
- Euler-Zagier sums are a special subset
- The nested sums form a Hopf algebra

$$\frac{1}{\Gamma\left(\frac{1}{2}\right)} \sum_{n=1}^{\infty} \frac{\Gamma\left(n+\frac{1}{2}\right)}{\Gamma(n+1)} \frac{x^n}{n^2} = 2\left[\ln 2 \ln\left(1+\sqrt{1-x}\right) + \ln 2 \ln\left(1-\sqrt{1-x}\right) - \text{Li}_{11}\left(-\sqrt{1-x}, 1\right) - \text{Li}_{11}\left(\sqrt{1-x}, -1\right) - \text{Li}_2(-1) - (\ln 2)^2\right],$$

$$\Gamma\left(\frac{1}{2}\right) \sum_{n=1}^{\infty} \frac{\Gamma(n+1)}{\Gamma\left(n+\frac{1}{2}\right)} \frac{x^n}{n^2} = -\text{Li}_{11}(\chi, 1) + \text{Li}_{11}(\chi, -1) - \text{Li}_{11}(-\chi, 1) + \text{Li}_{11}(-\chi, -1),$$

where $\chi = \sqrt{-x/(1-x)}$.

Outlook

Extension of the subtraction method to NNLO.

Already done:

- Construction of the subtraction terms
  $\longrightarrow$ Subtracted matrix elements can be integrated numerically !

- Integration of the subtraction terms for one-loop amplitudes with one unresolved parton.

To be done:

- Analytic integration over the unresolved phase space for double unresolved terms.