

On phase-space integrals with Heaviside functions

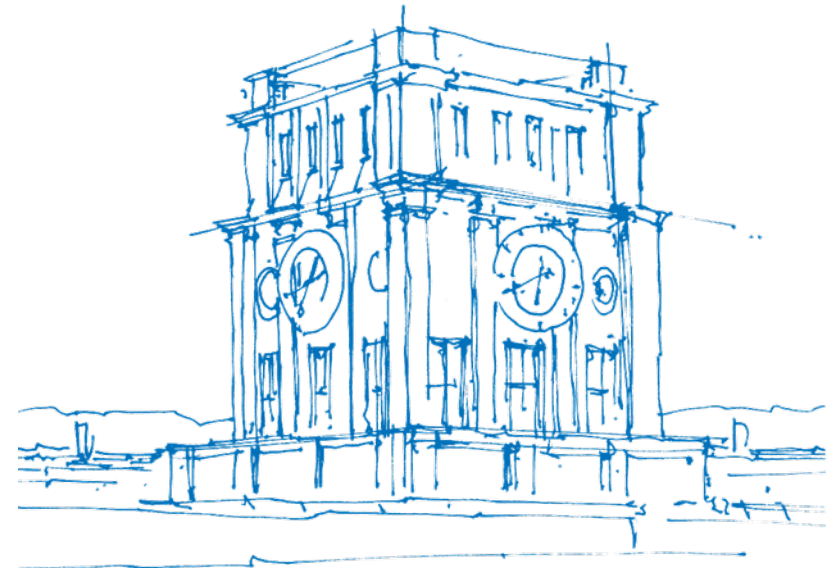
In collaboration with: D. Baranowski, K. Melnikov, and C.-Y. Wang

Based on: 2111.13594 and 2204.094559

Maximilian Delto

CERN QCD seminar

10th of June 2022



TUM Uhrenturm

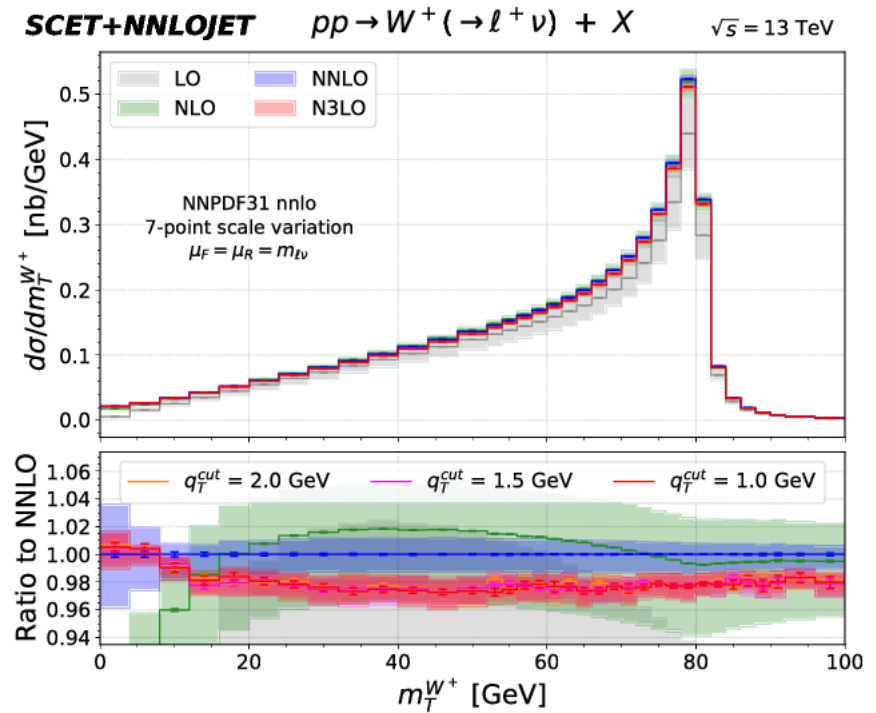
Motivation

Fully-differential description of LHC cross sections have recently reached N3LO in perturbative QCD.

⇒ Higgs production [Chen et al. '21]

⇒ Drell-Yan [Chen et al. '22]

These computations are vital for precise studies at the LHC.



[Chen et al. '22]

Infrared divergences

$$\left. \frac{d\sigma}{d\mathbf{O}} \right|_{\alpha_s} = 2\Re \left[\underbrace{\left[\text{loop diagram} \right]}_{\sim 1/\epsilon^2} \times \left[\text{tree diagram} \right] \right] \mathcal{F}_0 d\Phi_X + \left| \text{tree diagrams with } k_4 \right|^2 \mathcal{F}_0^{(1)} d\Phi_{X+g} + d\sigma^{gq} + d\sigma^{\text{pdf}}$$

$\frac{1}{p_1 \cdot k_4} \sim \frac{1}{E_1 E_4 (1 - \cos \theta_{14})}$

- soft and collinear divergences arise from
 - **loop integrals** in virtual corrections
 - **phase-space integration** over on-shell momenta of final-state partons in real-emission corrections

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- need to be regulated, extracted and cancelled
- only then can the limit $\epsilon \rightarrow 0$ be taken prior to numerical simulation

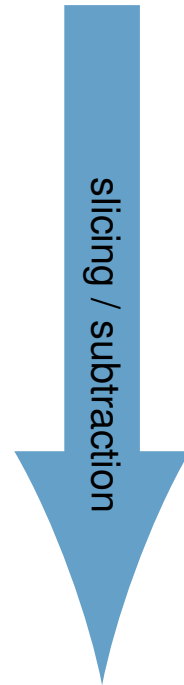
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⇒ *slicing* and *subtraction* schemes are used to define contributions that are individually finite



$$d\sigma \Big|_{\alpha_s} = d\sigma_{X+1} + d\sigma_X$$

$$\mathcal{I} = \int_0^1 \frac{dx}{x^{1-n\epsilon}} f(x)$$

Subtraction schemes

⇒ subtract and add back a term that approximates the divergent behavior

$$\mathcal{I} = \frac{f(0)}{n\epsilon} + \int_0^1 dx \frac{f(x) - f(0)}{x} + \mathcal{O}(\epsilon)$$

- ☺ local regularisation of divergences
- ☺ numerically stable
- ☹ complex construction, tedious to implement

for example

- CoLoRFull [Somogyi et al. '05]
- Antenna [Gehrmann-De Ridder et al. '05]
- STRIPPER [Czakon '10]
- Nested soft-collinear subtraction [Caola et al. '17]
- Local Analytic Sector Subtraction [Magnea et al. '18]

Slicing schemes

⇒ slice phase space into divergent and finite region

$$\mathcal{I} = \left[\frac{1}{n\epsilon} + \ln(\delta_{\text{cut}}) \right] f(0) + \int_{\delta_{\text{cut}}}^1 \frac{dx}{x} f(x) + \mathcal{O}(\delta, \epsilon)$$

- ☹ small cut-off leads to large numerical cancellations and requires precise control of f
- ☺ achievable at N3LO

for example

- q_T -slicing [Catani et al. ']
- N -jettiness slicing [Boughezal et al. '15]

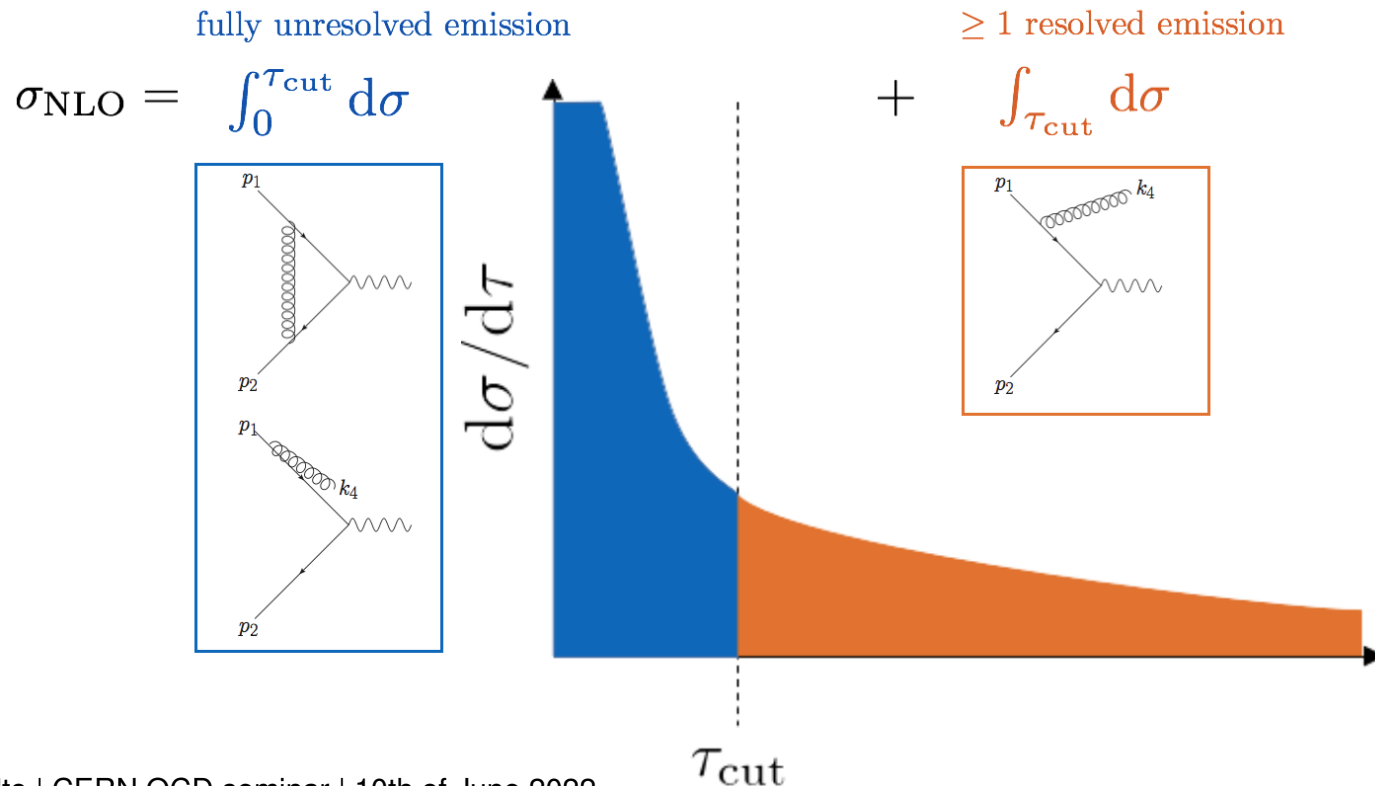
Other schemes

- projection-to-Born [Cacciari et al. '15]
- ...

Zero-jettiness slicing

$$\tau = \sum_j \min_{q \in \{n, \bar{n}\}} \{q \cdot k_j\}$$

- $q \cdot k_j = k_j^0 (1 \mp \cos \theta_j)$ for $q = n, \bar{n}$
- τ vanishes if *all* emitted partons become unresolved (soft / collinear to incoming partons)



Zero-jettiness factorisation

in SCET, the following factorisation formula can be derived [Stewart et al. '09]

$$d\sigma = B \otimes B \otimes S \otimes H \otimes d\sigma_{\text{Born}} + \mathcal{O}(\tau)$$

where the various ingredients are

Beam function

- collinear emission off incoming partons
- process-independent
- known through N3LO
[Ebert et al. '20]
(partial results in
[Behring et al '19])

Soft function

- soft, non-collinear emission
- process-independent
- known through N2LO
[Kelley et al. '11]
[Monni et al. '11]

Hard function

- virtual corrections
- process-dependent

⇒ factorisation allows for explicit cancellation of IR poles

⇒ computation of $\mathcal{O}(\epsilon^0)$ -contribution to cross section in $\tau \leq \tau_{\text{cut}}$ region

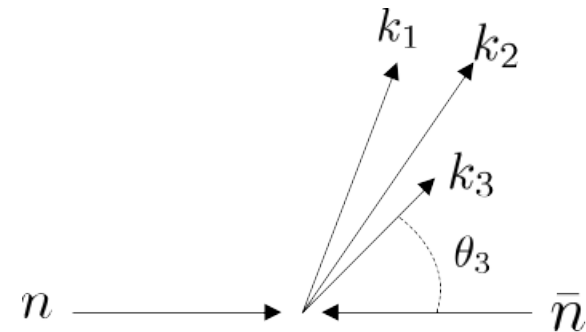
Three-gluon-emission contribution

$$S^{ggg} \Big|_{C_A C_A^2} = 2 \int d\Phi_{\theta\theta\theta}^{nnn} |\mathbf{J}(k_1, k_2, k_3)|^2 + 6 \int d\Phi_{\theta\theta\theta}^{nn\bar{n}} |\mathbf{J}(k_1, k_2, k_3)|^2$$

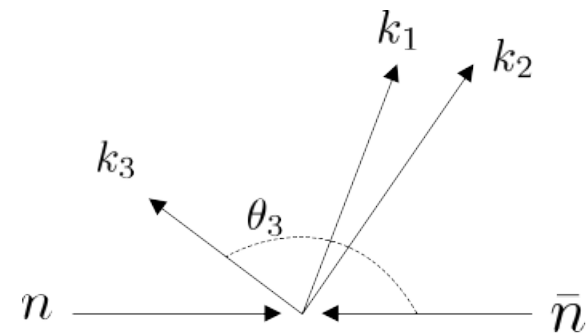
- triple-soft eikonal function $|\mathbf{J}|^2$ [Catani et al. '19] contains $\{q \cdot k_i, q \cdot k_{ij}, q \cdot k_{123}, k_i \cdot k_j, k_{123}^2\}$, $q = n, \bar{n}$

two distinguishable configurations

$$1) d\Phi_{\theta\theta\theta}^{nnn} = \widetilde{[dk]} \delta[\tau - k_{123} \cdot n] \prod_{i=1}^3 \theta[k_i \cdot \bar{n} - k_i \cdot n]$$



$$2) d\Phi_{\theta\theta\theta}^{nn\bar{n}} = \widetilde{[dk]} \delta[\tau - k_{12} \cdot n - k_3 \cdot \bar{n}] \prod_{i=1}^2 \theta[k_i \cdot \bar{n} - k_i \cdot n] f_3(k_3 \cdot n - k_3 \cdot \bar{n})$$



where $\widetilde{[dk]} = \prod_{i=1}^3 d^d k_i \delta[k_i^2]$

Integration-by-parts relations

$$0 = \int \prod_{l=1}^L d^d k_l \frac{\partial}{\partial k_i^\mu} \left[q^\mu \prod_{n=1}^N D_n^{-\alpha_n} \right], \quad q \in \{k_1, \dots, k_L, p_1, \dots, p_E\}, \quad \alpha_n \in \mathbb{Z}, \text{ [Chetyrkin, Tkachov '81]}$$

- set of linearly independent propagators $\{D_n\}$ defines a topology
 - IBP relations relate different integrals within a given topology
- ⇒ reduce given problem to minimal set of “master integrals” [AIR, FIRE, Reduze, LiteRed, Kira,..]
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1. δ -function: reverse unitarity [Anastasiou, Melnikov '02]

$$(-2\pi i) \delta[q^2 - m^2] = \lim_{\sigma \rightarrow 0^+} \left[\frac{1}{q^2 - m^2 + i\sigma} - \frac{1}{q^2 - m^2 - i\sigma} \right] = \frac{1}{[q^2 - m^2]_c}$$

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2. θ -function:

Parametric representation

[Caola et al. '18] [Angeles-Martinez et al. '18]

[Bizon et al. '20] [Baranowski '20]

$$\theta[b - a] = \int_0^1 dz \delta[z \cdot b - a] \quad b, a, b > 0$$

[Chen '20]

$$(2\pi i) \theta[D] = \int_{-\infty}^{+\infty} dx \frac{e^{ixD}}{x + i0^+}$$

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Extended notion of IBPs

[Baranowski et al. '21]

$$\frac{\partial}{\partial k} \{g(k) \theta[f(k)]\} = \overbrace{g' \theta}^{\text{hom}} + \overbrace{g \delta f'}^{\text{inhom}}$$

- ☹ proliferation of topologies
- ☹ manual generation of IBP identities
- ☹ no auxiliary integration

(see also [Luo et al. '19])

Integration-by-parts - example @ NNLO

$$\int \frac{d\Phi_{\theta\theta}^{nn}}{(k_2n)(k_1\bar{n})(k_{12}\bar{n})}, \quad d\Phi_{\theta\theta}^{nn} = [\widetilde{dk}] \delta[\tau - k_{12}n] \theta[k_1\bar{n} - k_1n] \theta[k_2\bar{n} - k_2n]$$

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- “conventional” IBP relation

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- additional inhomogeneous term that requires **partial fraction decomposition**

Integration-by-parts - example @ NNLO

$$\underbrace{\mathcal{T}_{1,1,1,0,1,1,1}^{\text{ex}} = \int \frac{d\Phi_{\theta\theta}^{nn}}{(k_2 n)(k_1 \bar{n})(k_{12} \bar{n})}}_{\text{topology with 2}\theta\text{-functions}}, \quad d\Phi_{f_1 f_2}^{nn} = \widetilde{[dk]} \delta[\tau - k_{12} n] f_1[k_1 \bar{n} - k_1 n] f_2[k_2 \bar{n} - k_2 n]$$

$$0 = [(d-4) - \mathbf{7}^+ \mathbf{6}^- - \mathbf{3}^+ \mathbf{5}^- + \mathbf{3}^+] \mathcal{T}_{1,1,1,0,1,1,1}^{\text{ex}}$$

$$0 = n\bar{n} [\mathbf{7}^+ - \mathbf{6}^+ + \mathbf{1}^+ \mathbf{6}^- - \mathbf{1}^+] \mathcal{T}_{1,1,1,0,1,1,1}^{\text{ex}} + \underbrace{\int \frac{d\Phi_{\delta\theta}^{nn}}{(k_{12} \bar{n})} \left[\frac{1}{(k_1 n)} + \frac{1}{(k_2 n)} \right]}_{\text{topology with 1}\theta\text{-function}}$$

- because of inhomogeneous terms ($\sim \partial_k \theta$), we need new type of topologies:
 - come from all possible ways of replacing $\theta \rightarrow \delta$
 - fall into a hierarchical structure: $\{\theta\theta\} \xrightarrow{\partial_k \theta} \{\delta\theta, \theta\delta\} \xrightarrow{\partial_k \theta} \{\delta\delta\}$
 - relations for $\delta\delta$ topologies have no inhomogeneous terms

Computational setup

Mathematica

- derive symmetry relations

$$\int \frac{d\Phi_{\theta\delta}^{nn}}{(k_1 k_2) (k_2 \bar{n})} \stackrel{k_1 \leftrightarrow k_2}{=} \int \frac{d\Phi_{\delta\theta}^{nn}}{(k_1 k_2) (k_1 \bar{n})}$$

- define list of “seed integrals” for independent sectors
- create IBP relations for seed integrals
- define ordering of integrals that appear in relations
- parse relations to Kira’s “user-defined system of equations” syntax

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Kira⊕FireFly [Maierhöfer et al. '17][Klappert et al. '19]

- find MIs
 - consider all topologies ($\theta\theta, \delta\theta, \theta\delta, \delta\delta$)
 - disregard θ -functions
 - run reduction using “vanilla” Kira
 - corresponds to setting inhomogeneous terms in IBP to zero
- solve “user-defined system of equations”

$$S^{gg} \Big|_{C_A C_A^2} = c_1 I_{1,\delta\delta}^{nn} + \sum_{i=2}^4 c_i I_{i,\delta\theta}^{nn} + \sum_{i=5}^7 c_i I_{i,\theta\theta}^{n\bar{n}}$$

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Reduction ✓

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- expand with HypExp [\[Huber et al. '05\]](#) & integrate with HyperInt [\[Panzer '14\]](#)

$$I_{4,\delta\theta}^{nn} \Big|_{\tau \rightarrow 1} = \frac{2}{\varepsilon^2} + \frac{\pi^2}{3} - \frac{17\pi^4 \varepsilon^2}{90} + \varepsilon^3 [-6\pi^2 \zeta_3 - 26\zeta_5] - \varepsilon^4 \left[\frac{193\pi^6}{810} + 64\zeta_3^2 \right] + \mathcal{O}(\varepsilon^5)$$

Complications for three-gluon emission

Note: $nn\bar{n}$ configuration still work in progress

General complexity

- more “level”: $\theta\theta\theta$, $\delta\theta\theta$, $\theta\delta\theta$, $\theta\theta\delta$, ...
- $\mathcal{O}(400)$ topologies
- integral relations

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Rapidity divergences

- appear for certain observables (e.g. q_T) in the limit of large rapidity and only cancel in *soft+collinear*
- obey a rapidity renormalisation-group formalism [\[Chiu et al.\]](#)
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⇒ require analytic regulator

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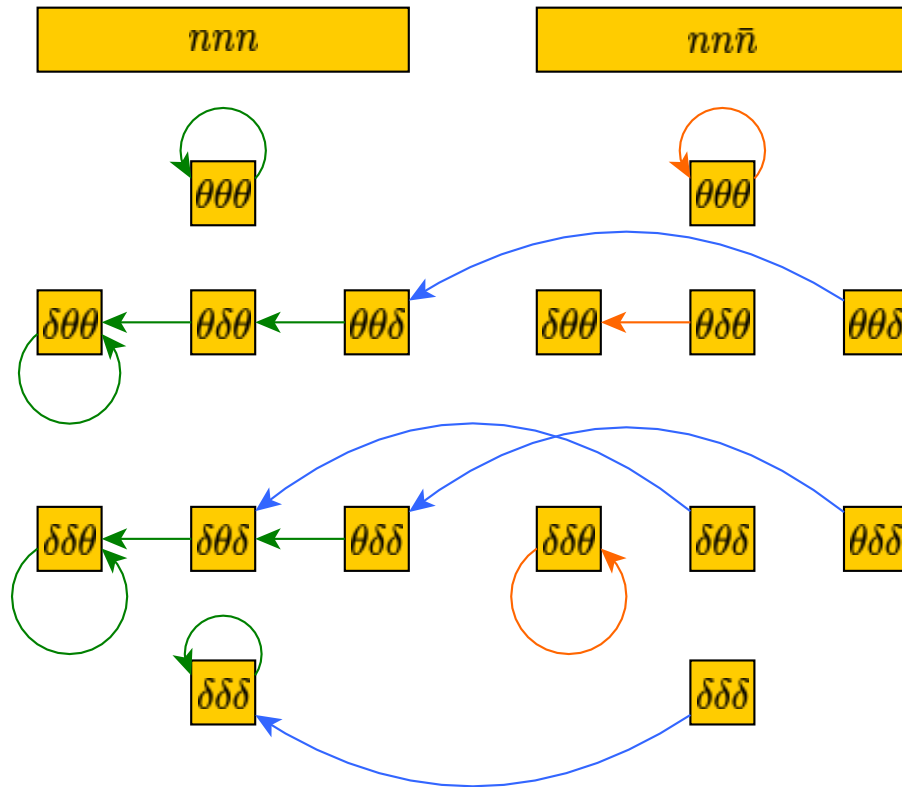
Master integrals

- more complicated master integrals
 \Rightarrow resort to numerical calculation and PSLQ reconstruction

Integral relations at N3LO

$$d\Phi_{f_1 f_2 f_3}^{nnn} \sim \delta[\tau - k_1 \cdot n - k_2 \cdot n - k_3 \cdot n] f_1(k_1 \cdot \bar{n} - k_1 \cdot n) f_2(k_2 \cdot \bar{n} - k_2 \cdot n) f_3(k_3 \cdot \bar{n} - k_3 \cdot n)$$

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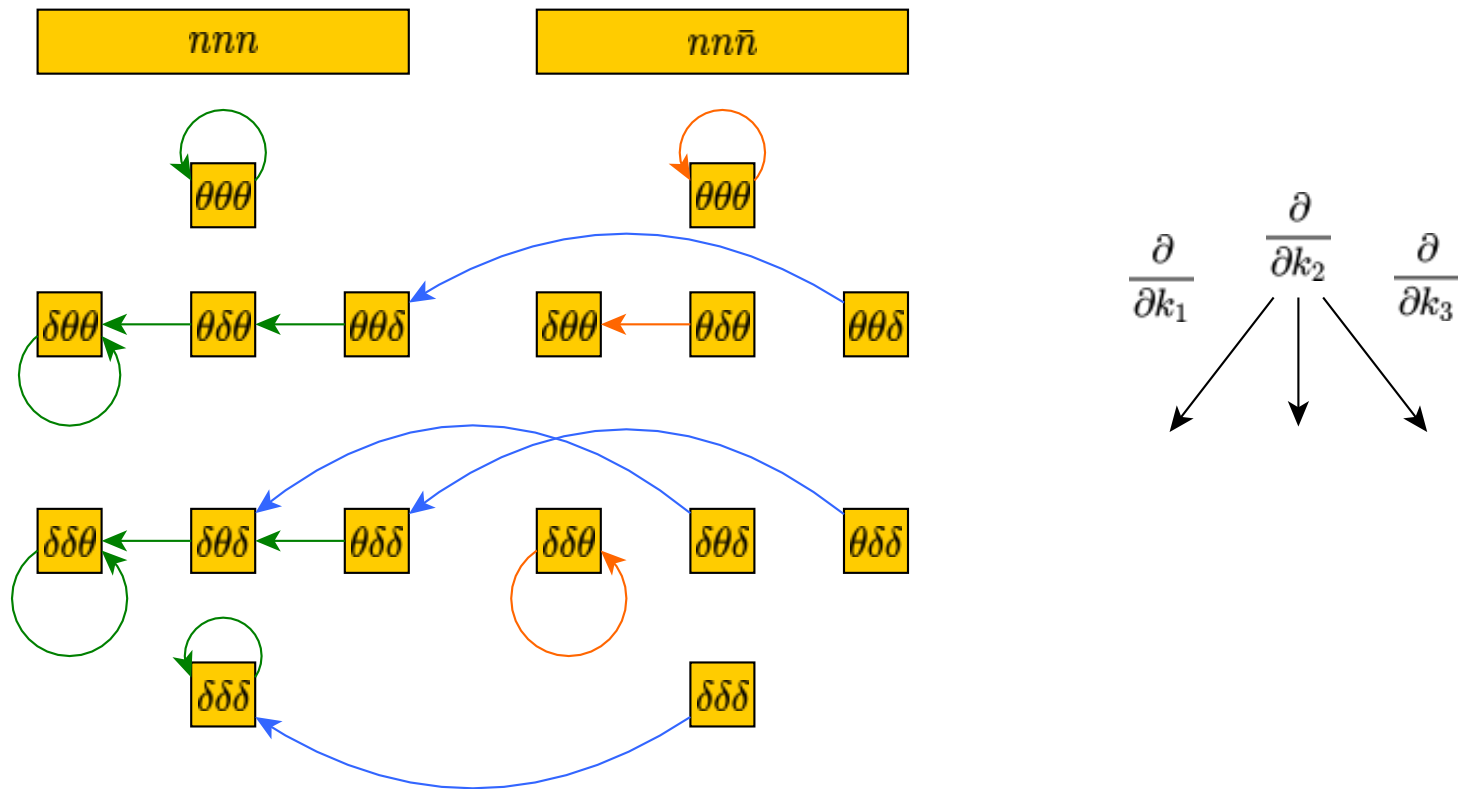


$$\frac{\partial}{\partial k_1} \quad \frac{\partial}{\partial k_2} \quad \frac{\partial}{\partial k_3}$$

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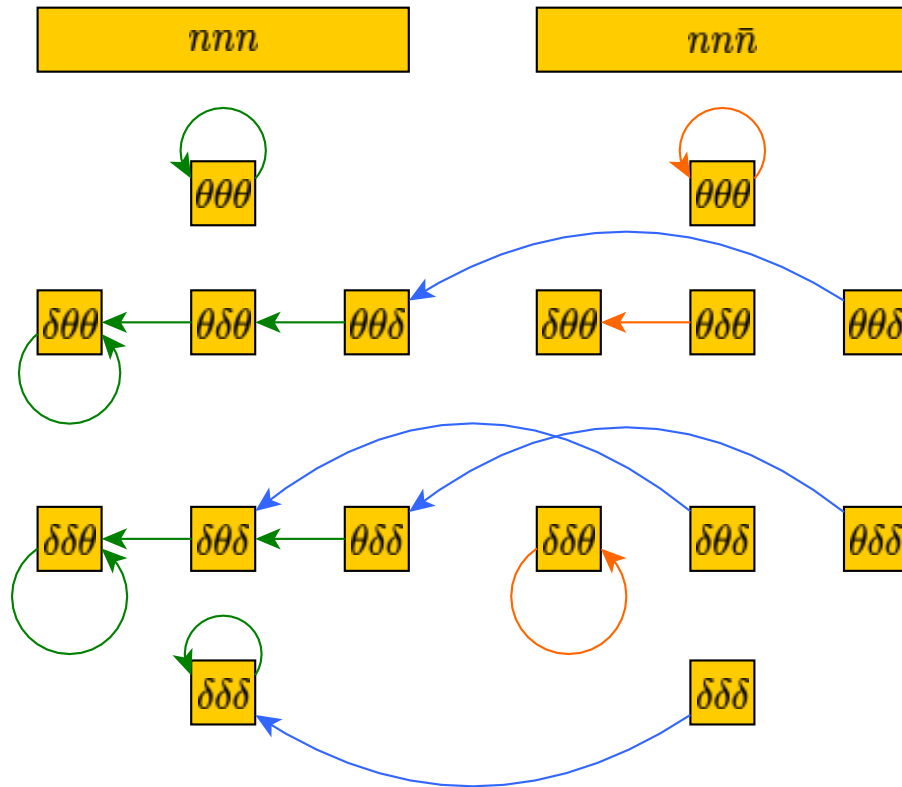
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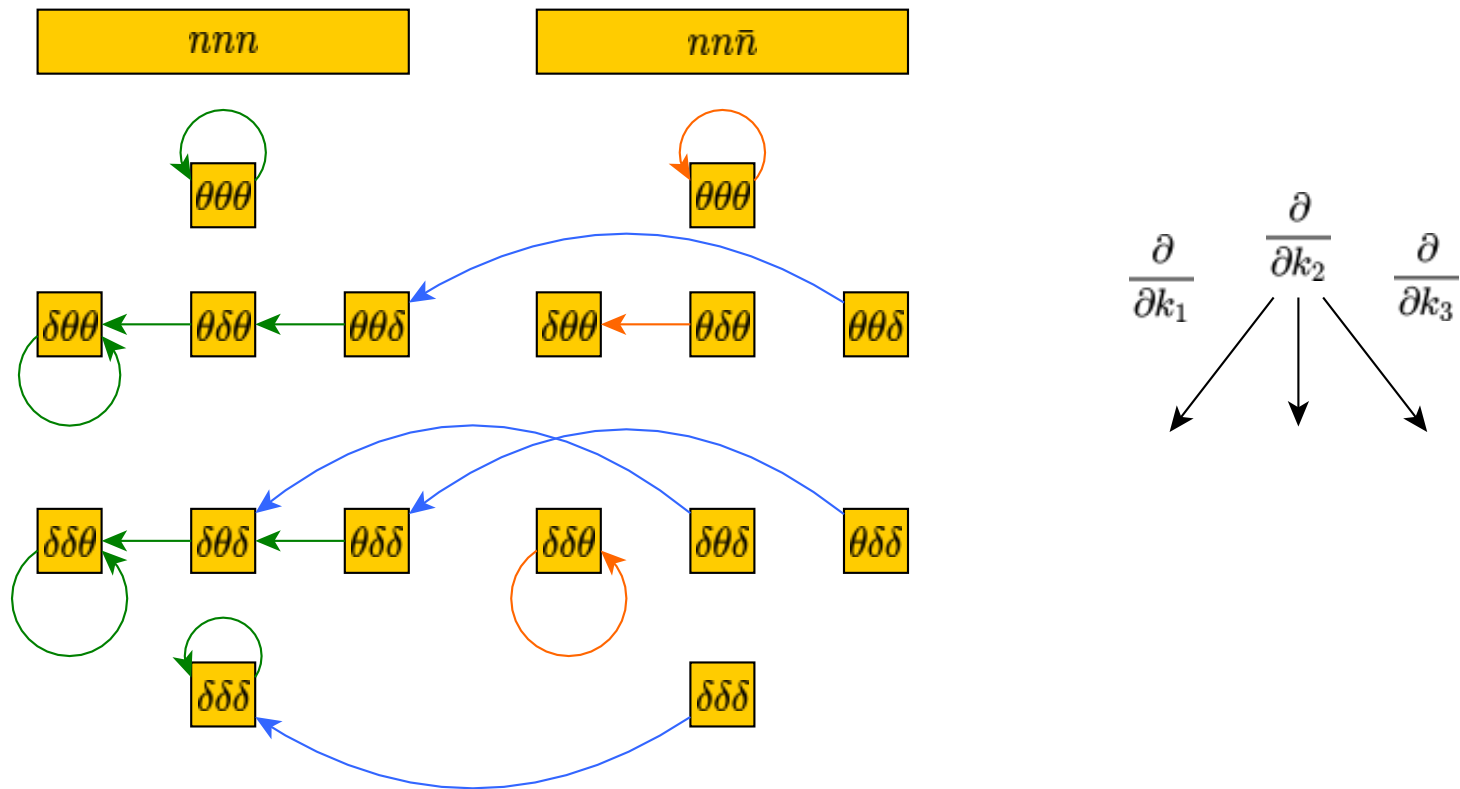


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- arise, when $k_i \cdot n \gg k_i \cdot \bar{n}$ or $k_i \cdot n \gg k_i \cdot \bar{n}$
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$$\frac{\partial}{\partial k_1^\mu} : \quad 0 = I' \theta_1 + I(\bar{n} - n)^\mu \delta_1 \quad \longrightarrow \quad 0 = \left[I' \theta_1 + I(\bar{n} - n)^\mu \delta_1 + \nu n^\mu \frac{I \theta_1}{k_1 \cdot n} \right] (\dots)^\nu$$

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“ $\nu = 0$ ”-reduction
 $\sim 1/\nu$

Rapidity divergences at N3LO

Example

- consider the following master integral

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⇒ $1/\nu$ -pole gets multiplied with reduction coefficient $c \sim \nu$

Master integrals at N3LO

- fall into two categories: with and without the propagator $k_{123}^2 = 2[k_1k_2 + k_1k_3 + k_2k_3]$
 - without k_{123}^2 : compute along the lines discussed for NNLO

$$\sim \int \frac{1}{(k_1k_2)(k_1k_3) \dots}$$
 - with k_{123}^2 : difficult to compute analytically

Numerical computation of MI (see also [\[Liu et al. '17\]](#))

- add parameter m^2 to propagator

$$I = \int \frac{d\Phi_{f_1f_2f_3}^{nnn,v}}{[k_{123}^2] \dots} \longrightarrow J = \int \frac{d\Phi_{f_1f_2f_3}^{nnn,v}}{[k_{123}^2 + m^2] \dots}$$

- using the IBP technology for θ -functions, derive differential equation

$$\partial_{m^2} \mathbf{J} = \hat{K} \mathbf{J}$$

- compute boundary conditions in $m^2 \rightarrow \infty$, where the “bad” propagator simplifies
- solve differential equation numerically, compute the limit $m \rightarrow 0$, and recover I from Taylor-branch in

$$J = \sum c_{n_1 n_2 n_3} (m^2)^{n_1 + n_2 \epsilon} \ln^{n_3}(m^2)$$

- result with 2000 digits, allows to reconstruct analytic expression with PSLQ

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$$\int \frac{(\alpha_i \beta_i)^{-\varepsilon} \delta[\tau - \beta_{123}] \delta[\alpha_1 - \beta_1] \delta[\alpha_2 - \beta_2] \delta[\alpha_3 - \beta_3]}{\left[m^2 + \alpha_1 \beta_2 + \alpha_2 \beta_1 - \sqrt{\alpha_1 \beta_1 \alpha_2 \beta_2} \cos \phi_{12} + 2 \leftrightarrow 3 + 1 \leftrightarrow 3 \right]} \sim [m^2]^{-1}$$

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- no MIs with three θ -functions (zero δ functions)

Result for same-hemisphere contribution

$$\begin{aligned}
 S_3^{mm} = & \frac{24}{\varepsilon^5} + \frac{308}{3\varepsilon^4} + \frac{1}{\varepsilon^3} \left(-12\pi^2 + \frac{3380}{9} \right) + \frac{1}{\varepsilon^2} \left(-1000\zeta_3 + \frac{440\pi^2}{9} + \frac{10048}{9} \right) \\
 & + \frac{1}{\varepsilon} \left(-\frac{2377\pi^4}{45} + \frac{440\zeta_3}{3} + \frac{7192\pi^2}{27} + \frac{253252}{81} \right) \\
 & + \left(-28064\zeta_5 + \frac{1972\zeta_3\pi^2}{3} - \frac{638\pi^4}{15} + 4224\text{Li}_4\left(\frac{1}{2}\right) + 3696\zeta_3 \ln(2) - 176\pi^2 \ln^2(2) + 176\ln^4(2) \right. \\
 & + \frac{13208\zeta_3}{3} + \frac{78848\pi^2}{81} + 96\ln(2) + \frac{1925074}{243} \left. \right) \\
 & + \varepsilon \left(2304 \zeta_{-5,-1} - 4464\zeta_5 \ln(2) + 25784\zeta_3^2 - \frac{67351\pi^6}{567} - 6336G_R(0,0,r_2,1,-1) \right. \\
 & - 6336G_R(0,0,1,r_2,-1) - 3168G_R(0,0,1,r_2,r_4) - 6336G_R(0,0,r_2,-1) \ln(2) + \frac{268895\zeta_5}{3} \\
 & - 45056\text{Li}_5\left(\frac{1}{2}\right) - 45056\text{Li}_4\left(\frac{1}{2}\right) \ln(2) + 176\text{Cl}_4\left(\frac{\pi}{3}\right) \pi - 1056\zeta_3 \text{Li}_2\left(\frac{1}{4}\right) - 3982\zeta_3\pi^2 \\
 & - 21824\zeta_3 \ln^2(2) + 2112\zeta_3 \ln(2) \ln(3) - 1584\text{Cl}_2^2\left(\frac{\pi}{3}\right) \ln(3) - \frac{4400\text{Cl}_2\left(\frac{\pi}{3}\right) \pi^3}{27} + \frac{88\pi^4 \ln(2)}{45} \\
 & - \frac{616\pi^4 \ln(3)}{27} + \frac{11264\pi^2 \ln^3(2)}{9} - \frac{22528\ln^5(2)}{15} + 8576\text{Li}_4\left(\frac{1}{2}\right) + 7504\zeta_3 \ln(2) + \frac{4174\pi^4}{27} \\
 & - \frac{1072\pi^2 \ln^2(2)}{3} + \frac{1072\ln^4(2)}{3} + \frac{554032\zeta_3}{27} - 32\pi^2 \ln(2) + \frac{730378\pi^2}{243} - 384\ln^2(2) + 832\ln(2) \\
 & \left. + \frac{1408681}{81} + \sqrt{3} \left(192\Im \left\{ \text{Li}_3 \left(\frac{\exp(i\pi/3)}{2} \right) \right\} + 160\text{Cl}_2\left(\frac{\pi}{3}\right) \ln(2) - 16\pi \ln^2(2) - \frac{560\pi^3}{81} \right) \right) + \mathcal{O}(\varepsilon^2)
 \end{aligned}$$

- up to $\mathcal{O}(\varepsilon^0)$ only zeta values and $\text{Li}_4\left(\frac{1}{2}\right)$
- at $\mathcal{O}(\varepsilon)$, we find multiple zeta value $\zeta_{-5,-1}$, GPLs with sixth root of unity, ...

Conclusion

- extended notion of IBP relations & reverse unitarity enables us to reduce phase-space integrals that contain Heaviside functions
- the method also provides the means to derive differential equations
- with this, we computed the same-hemisphere configuration of the three-gluon-emission contribution to the zero jettiness function

Outlook

- computation of second configuration ($nn\bar{n}$) currently underway
- remaining contributions are
 - RRR: $gq\bar{q}$ -emission
 - RRV: one-loop corrections to gg - and $q\bar{q}$ -emission
 - RVV: two-loop correction to g -emission
- other observables, e.g. 1-jettiness
- other objects containing Heaviside functions, e.g. soft contributions in subtraction schemes