





# Local Analytic Sector Subtraction at NNLO

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in collaboration with:

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based on [Magnea et al., arXiv:1806.09570, arXiv:1809.05444]

# Motivation

- The Standard Model (SM) is not the end of the story: new physics under investigation at high-energy colliders.
- No spectacular discoveries at the LHC: search for small effects. Very precise knowledge of the SM required.
- QCD predictions more stable when including higher-order corrections.

Needed theoretical predictions with the highest possible precision, in order to compare them with experimental data.

# Strong efforts in calculations at next-to-next-to-leading order in $\alpha_S$ (NNLO QCD).

Many schemes available for NNLO subtraction:

→ N-jettiness, qT-subtraction, Antenna, Sector Improved, Nested Soft-Collinear, Colorful, Projection to Born, Sector Decomposition,  $\varepsilon$ -prescription, Geometric, Unsubtraction

### Anatomy of subtractions at NLO

Massless, partons in the final state only: NLO contribution

$$\frac{d\sigma_{\rm NLO}}{dX} = \int d\Phi_n \, V \, \delta_n + \int d\Phi_{n+1} \, R \, \delta_{n+1} \, . \tag{1}$$

where  $R = \left| \mathcal{A}_{n+1}^{(0)} \right|^2$ ,  $V = 2 \operatorname{Re} \left[ \mathcal{A}_n^{(0)*} \mathcal{A}_n^{(1)} \right]$ , and  $X = \operatorname{IRC}$  safe obs.,  $X_i = \operatorname{computed}$  with  $i^{\text{th}}$ -body kinematics,  $\delta_i = \delta(X - X_i)$ .

In  $d = 4 - 2\epsilon$ , phase-space integration of R results in explicit infrared (IR) poles in  $\epsilon$ , which cancel those of V, if X infrared safe, ensuring the cross section is finite (KLN). **Subtraction procedure**: avoiding analytic integration of the full R amplitudes by adding and subtracting to Eq. (1) a counterterm

$$\frac{d\sigma_{\rm NLO}}{dX}\Big|_{\rm ct} = \int d\Phi_{n+1} \,\overline{K} \,\delta_n \,, \qquad I = \int d\Phi_{\rm rad} \,\overline{K} \,, \tag{2}$$

 $d\Phi_{n+1}\overline{K}$  has the same singular limits of  $d\Phi_{n+1}R$  and must be simple to be analytically integrated in *d* dim.

$$\frac{d\sigma_{\mathsf{NLO}}}{dX} = \int d\Phi_n \left( V + I \right) \delta_n + \int d\Phi_{n+1} \left( R \,\delta_{n+1} - \overline{K} \,\delta_{n+1} \right) \tag{3}$$

First and the second terms separately finite in d = 4: efficient numerical integration.

Two main subtraction schemes at NLO:

Frixione-Kunst-Signer procedure [Frixione, Kunst, Signer, hep-ph/9512328]

- Partition of the radiative phase-space with sector functions
- Different parameterization for each sector
- Analytical integration, after eliminating sector functions (sum rules): can be not trivial, due to non optimal parameterization

Catani-Seymour procedure [Catani, Seymour, hep-ph/9605323]

- A counterterm reproduces the IR singularities related to a parton pair in all of phase-space: complicated structure
- Sum of counterterms, each reparameterized with a specific kinematic mapping
- Analytical integration of each term: can be non trivial, as counterterms have a complicated structure

#### How much can we simplify the NLO subtraction procedure? Our strategy:

Frixione-Kunst-Signer procedure [Frixione, Kunst, Signer, hep-ph/9512328]

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Partition of the radiative phase-space  $\Phi_{n+1}$  with sector functions  $W_{ij}$  (i, j = 1, ..., n+1 final-state partons)

- minimal singularity structure: R W<sub>ij</sub> is singular only in one soft (S<sub>i</sub>) and one collinear (C<sub>ij</sub>) configuration
- normalization and sum rules:

$$\sum_{i,\,j\neq i} \mathcal{W}_{ij} = 1, \qquad \mathsf{S}_i \sum_{j\neq i} \mathcal{W}_{ij} = 1, \qquad \mathsf{C}_{ij} \sum_{ab \,\in\, \mathsf{perm}(ij)} \mathcal{W}_{ab} = 1\,,$$

- Summing over sectors sharing a singularity, and taking the singular limit on the sum, the W's disappear: simplified analytic integration of the counterterm.
- Choice of sector functions very similar to FKS  $(s_{qi} = 2 q_{cm} \cdot k_i, s_{ij} = 2 k_i \cdot k_j)$ :

$$\mathcal{W}_{ij} = rac{\sigma_{ij}}{\sum\limits\limits_{k,\ l 
eq k} \sigma_{kl}} \,, \quad ext{with} \quad \sigma_{ij} = rac{1}{e_i \, w_{ij}} \,, \ e_i = rac{s_{qi}}{s} \,, \ w_{ij} = rac{s \, s_{ij}}{s_{qi} \, s_{qj}} \,.$$

# A minimal scheme at NLO (2)

Singular structure of *R* in sector *ij* in terms of dot products  $\{s_{ab} = 2p_a \cdot p_b\}$ : **S**<sub>*i*</sub> *R* = leading term in *R*  $(k_{\perp}^{\mu} \rightarrow 0)$ , **C**<sub>*ij*</sub> *R* = leading term in *R*  $(k_{\perp}^{\mu} \rightarrow 0)$ .

$$\mathbf{S}_{i} R(\{k\}) = -\mathcal{N}_{1} \sum_{l, m} \underbrace{\delta_{f,g} \frac{s_{lm}}{s_{il} s_{im}}}_{\text{Eikonal kernel}} B_{lm}(\{k\}_{f})$$

$$\mathbf{C}_{ij} R(\{k\}) = \frac{\mathcal{N}_{1}}{s_{ij}} \underbrace{P_{ij}^{\mu\nu}(s_{ir}, s_{jr})}_{\text{Altarelli-Parisi split. f.}} B_{\mu\nu}(\{k\}_{fj}, k)$$

$$\mathbf{S}_{i} \mathbf{C}_{ij} R(\{k\}) = 2\mathcal{N}_{1} C_{fj} \delta_{f,ig} \frac{s_{jr}}{s_{ij} s_{ir}} B(\{k\}_{f})$$

- Candidate counterterm in sector ij:  $K_{ij} = (\mathbf{S}_i + \mathbf{C}_{ij} \mathbf{S}_i \mathbf{C}_{ij})R \mathcal{W}_{ij}$
- Minimal structure as FKS, but no parametrisation yet: freedom to be exploited to simplify analytic integration.

# A minimal scheme at NLO (3)

Need a momentum mapping  $\{k_1, ..., k_{n+1}\} \rightarrow \{\bar{k}_1, ..., \bar{k}_n\}$  to factorize radiation  $d\Phi_{rad}$  from Born phase-space  $d\Phi_n$ , and integrate counterterm  $\rightarrow$  Catani-Seymour mappings

Mapping {k} → {k̄}<sup>(abc)</sup>: freedom to choose a, b, c as we want. Optimal choice: adapt to invariants appearing in the kernels.

$$\begin{split} \overline{\mathbf{S}}_{i} R\left(\{k\}\right) &= -\mathcal{N}_{1} \sum_{l, m} \delta_{f_{i}g} \frac{s_{lm}}{s_{il} s_{im}} B_{lm}\left(\{\overline{k}\}^{(ilm)}\right) \\ \overline{\mathbf{C}}_{ij} R\left(\{k\}\right) &= \frac{\mathcal{N}_{1}}{s_{ij}} P_{ij}^{\mu\nu}(s_{ir}, s_{jr}) B_{\mu\nu}\left(\{\overline{k}\}^{(ijr)}\right) \\ \overline{\mathbf{S}}_{i} \overline{\mathbf{C}}_{ij} R\left(\{k\}\right) &= 2\mathcal{N}_{1} C_{f_{j}} \delta_{f_{i}g} \frac{s_{jr}}{s_{ij} s_{ir}} B\left(\{\overline{k}\}^{(ijr)}\right) \end{split}$$

Definition for the local counterterm (barred limits on W's act as unbarred):

$$\overline{K}_{ij} \equiv \left(\overline{\mathbf{S}}_{i} + \overline{\mathbf{C}}_{ij} - \overline{\mathbf{S}}_{i} \overline{\mathbf{C}}_{ij}\right) R \mathcal{W}_{ij}, \qquad \overline{K} = \sum_{i,i \neq i} \overline{K}_{ij}, \qquad (4)$$

# A minimal scheme at NLO (4)

Getting rid of sector functions in  $\overline{K}$ :

$$\overline{K} = \sum_{i,j\neq i} \overline{K}_{ij} = \sum_{i} (\overline{\mathbf{S}}_{i}R) [\underline{\mathbf{S}}_{i} \sum_{j\neq i} \mathcal{W}_{ij}] + \sum_{i,j>i} (\overline{\mathbf{C}}_{ij}R) [\underline{\mathbf{C}}_{ij}(\mathcal{W}_{ij} + \mathcal{W}_{ji})] - \sum_{i,j\neq i} \overline{\mathbf{S}}_{i} \overline{\mathbf{C}}_{ij}R$$

$$= \sum_{i} \overline{\mathbf{S}}_{i}R + \sum_{i,j>i} \overline{\mathbf{C}}_{ij} \left(1 - \overline{\mathbf{S}}_{i} - \overline{\mathbf{S}}_{j}\right) R.$$
(5)

Recall: 
$$\frac{d\sigma_{\text{NLO}}}{dX} = \int d\Phi_n \left( V + I \right) \delta_n + \int d\Phi_{n+1} \left( R \,\delta_{n+1} - \overline{K} \,\delta_{n+1} \right)$$

Final result for the integrated counterterm (over  $d\Phi_{rad}$ ):

$$I(\{\bar{k}\}) = -\mathcal{N}_{1} \sum_{l, m \neq l} \frac{(4\pi)^{\epsilon-2}}{\bar{s}_{lm}^{\epsilon}} \frac{\Gamma(1-\epsilon)\Gamma(2-\epsilon)}{\epsilon^{2}\Gamma(2-3\epsilon)} B_{lm}(\{\bar{k}\})$$
$$-\mathcal{N}_{1} \sum_{p} \frac{(4\pi)^{\epsilon-2}}{\bar{s}_{pr}^{\epsilon}} \frac{\Gamma(1-\epsilon)\Gamma(2-\epsilon)}{\epsilon\Gamma(2-3\epsilon)} \left(\frac{C_{A}+4T_{R}N_{f}}{2(3-2\epsilon)} \delta_{f_{pg}} + \frac{C_{F}}{2} \delta_{f_{p}\{q,\bar{q}\}}\right) B(\{\bar{k}\}).$$
(6)

exact in  $\epsilon$ , virtual poles analytically reproduced, finite parts checked for a variety of differential distributions (against MadGraph\_MC@NLO).

NLO: bridge between FKS (minimality and phase space sectoring) and CS (Lorentz invariance and kinematics mappings)  $\rightarrow$  Simplified analytic cterm integration

These nice properties can be exported to NNLO

$$\frac{d\sigma_{\text{NNLO}}}{dX} = \int d\Phi_n \, VV \, \delta_n + \int d\Phi_{n+1} \, RV \, \delta_{n+1} + \int d\Phi_{n+2} \, RR \, \delta_{n+2}. \tag{7}$$

Add and subtract local counterterms:

$$\int d\Phi_{n+2} \,\overline{K}^{(1)} \,\delta_{n+1} \,, \qquad \int d\Phi_{n+2} \,(\overline{K}^{(2)} + \overline{K}^{(12)}) \,\delta_n \,, \qquad \int d\Phi_{n+1} \,\overline{K}^{(\mathsf{RV})} \,\delta_n \,. \tag{8}$$

 $\overline{K}^{(1)}$ : same single-unresolved singularities as RR $(\overline{K}^{(2)} + \overline{K}^{(12)})$ : same double-unresolved singularities as RR, the first features double-unres. limits (pure), the second single-unres. limits of double-unres. ones (mixed)  $\overline{K}^{(RV)}$ : same single-unresolved singularities as RV

Integrated counterterms (in *d*-dimensions):

$$I^{(i)} = \int d\Phi_{\mathrm{rad},i} \,\overline{K}^{(i)} \,, \quad I^{(12)} = \int d\Phi_{\mathrm{rad},1} \,\overline{K}^{(12)} \,, \quad I^{(\mathrm{RV})} = \int d\Phi_{\mathrm{rad}} \,\overline{K}^{(\mathrm{RV})} \,,$$

#### Subtracted NNLO

$$\frac{d\sigma_{\text{NNLO}}}{dX} = \int d\Phi_n \underbrace{\left(VV + I^{(2)} + I^{(\text{RV})}\right)}_{\text{finite in d=4 and in } \Phi_n} \delta_n \\
+ \int d\Phi_{n+1} \left[ \underbrace{\left(RV + I^{(1)}\right)}_{\text{finite in d=4, singular in } \Phi_{n+1}} \delta_{n+1} - \underbrace{\left(\overline{K}^{(\text{RV})} - I^{(12)}\right)}_{\text{finite in d=4, singular in } \Phi_{n+1}} \delta_n \right] \\
+ \int d\Phi_{n+2} \underbrace{\left[RR \, \delta_{n+2} - \overline{K}^{(1)} \, \delta_{n+1} - \left(\overline{K}^{(2)} + \overline{K}^{(12)}\right) \, \delta_n\right]}_{\text{finite in d=4 and in } \Phi_{n+2}}.$$
(9)

## Sector functions at NNLO (1)

Partition of  $\Phi_{n+2}$  with sector functions  $\mathcal{W}_{ijkl}$ ,  $(\sum_{ijkl} \mathcal{W}_{ijkl} = 1)$ . Our choice:

$$\mathcal{W}_{ijkl} = \frac{\sigma_{ijkl}}{\sum\limits_{a, b \neq a} \sum\limits_{\substack{c \neq a \\ d \neq a, c}} \sigma_{abcd}}, \qquad \sigma_{ijkl} = \frac{1}{e_i^{\alpha} w_{ij}^{\beta}} \frac{1}{(e_k + \delta_{kj} e_i) w_{kl}}, \qquad \alpha > \beta > 1.$$

*RR* W<sub>abcd</sub> is singular only in few configurations
 (S<sub>ab</sub> = a b uniformly soft, C<sub>ijk</sub> = j k uniformly collinear to i, SC<sub>ijk</sub> = i soft and j, k collinear, CS<sub>ijk</sub> = i, j collinear and k soft)

Sum rules in double-unresolved limits: summing over sectors sharing the same singularity, and taking that singular limit on the sum, W functions disappear. In the single-unresolved limits, NNLO sector functions factorise NLO sector functions. For example

$$\mathbf{C}_{ij} \, \mathcal{W}_{ijkl} = \mathcal{W}_{kl} \, \mathbf{C}_{ij} \, \mathcal{W}_{ij}^{(\alpha\beta)} \,, \qquad \qquad \mathbf{S}_i \, \mathcal{W}_{ijkl} = \mathcal{W}_{kl} \, \mathbf{S}_i \, \mathcal{W}_{ij}^{(\alpha\beta)} \,,$$

where

$$\mathcal{W}_{ij}^{(\alpha\beta)} = rac{\sigma_{ij}^{(lphaeta)}}{\sum\limits_{a, b \neq a} \sigma_{ab}^{(lphaeta)}}, \qquad \sigma_{ab}^{(lphaeta)} = rac{1}{(e_a)^{lpha}(w_{ab})^{eta}}$$

with the same properties of NLO sector functions.

Allows  $(RV + I^{(1)})$  and  $(K^{(RV)} - I^{(12)})$  to be finite in d = 4 NLO sector by NLO sector.

# Counterterms at NNLO (1): sector $W_{ijkj}$

 Candidate (not remapped) counterterms built collecting singular limits of RRW, written in terms of dot products.

Ex. sector W<sub>ijkj</sub> (nonzero limits: S<sub>i</sub>, C<sub>ij</sub>, S<sub>ik</sub>, C<sub>ijk</sub>, SC<sub>ijk</sub>, CS<sub>ijk</sub>):

$$\begin{split} \mathcal{K}_{ijkj}^{(1)} &= \left[ \mathbf{S}_{i} + \mathbf{C}_{ij}(1 - \mathbf{S}_{i}) \right] RR \, \mathcal{W}_{ijkj}, \\ \mathcal{K}_{ijkj}^{(2)} &= \left[ \mathbf{S}_{ik} + \mathbf{C}_{ijk}(1 - \mathbf{S}_{ik}) + \mathbf{SC}_{ijk}(1 - \mathbf{S}_{ik})(1 - \mathbf{C}_{ijk}) \right. \\ &+ \mathbf{CS}_{ijk}(1 - \mathbf{SC}_{ijk})(1 - \mathbf{S}_{ik})(1 - \mathbf{C}_{ijk}) \right] RR \, \mathcal{W}_{ijkj}, \\ \mathcal{K}_{ijkj}^{(12)} &= - \left[ \mathbf{S}_{i} + \mathbf{C}_{ij}(1 - \mathbf{S}_{i}) \right] \left[ \mathbf{S}_{ik} + \mathbf{C}_{ijk}(1 - \mathbf{S}_{ik}) + \mathbf{SC}_{ijk}(1 - \mathbf{S}_{ik})(1 - \mathbf{C}_{ijk}) \right. \\ &+ \left. \mathbf{CS}_{ijk}(1 - \mathbf{SC}_{ijk})(1 - \mathbf{S}_{ik})(1 - \mathbf{C}_{ijk}) \right] RR \, \mathcal{W}_{ijkj}, \end{split}$$

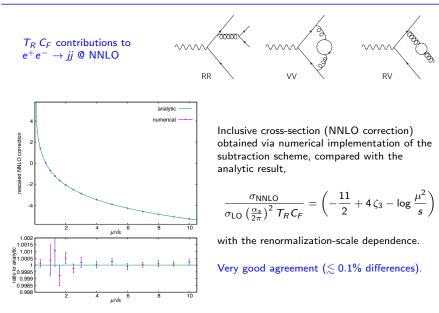
S<sub>ij</sub> RR, C<sub>ikj</sub> RR, SC<sub>ijk</sub> RR: universal kernels [Catani, Grazzini, hep-ph/9908523].

- Simplifications possible  $\rightarrow$  SC<sub>*ijk*</sub>, CS<sub>*ijk*</sub> cancel in the sum  $K^{(2)} + K^{(12)}$ .
- Limits on RR and on W functions commute.

Different kernels / different terms in the same kernel are parametrized with different NNLO mappings, to simplify integration.

- $\overline{K}^{(1)}$  to be integrated over  $d\Phi_{n+1}$ , thanks to the factorization properties of  $W_{abcd}$ and the sum rules of  $W_{ab}^{(\alpha\beta)}$  (same integral as at NLO,  $I^{(1)}$ ) –  $I^{(1)}$  has the same  $1/\epsilon$  structure as RV, NLO sector by NLO sector.
- $\overline{K}^{(12)}$  to be integrated over  $d\Phi_{n+1}$ , thanks to the factorization properties of  $W_{abcd}$ and the sum rules of  $W^{(\alpha\beta)}_{ab}$ –  $I^{(12)}$  has the same  $1/\epsilon$  structure as  $\overline{K}^{(RV)}$ , NLO sector by NLO sector.
- $\overline{K}^{(2)}$  to be integrated over  $d\Phi_{n+2}$ ,  $\mathcal{W}$  functions disappear from  $\overline{K}^{(2)}$  as well as from  $I^{(2)}$  thanks to sum rules analytic integration of NNLO kernels × Born matrix-elements, without  $\mathcal{W}$  functions.

## Proof-of-concept



A subtraction procedure at NNLO: local, analytic, general, efficient.

Present procedure is designed for final-state QCD radiation and massless partons.

Status and wishlist:

- implementation in a differential numerical code is in progress,
- analytic integration of part of the double-unresolved and real-virtual counterterms is ongoing,
- we are planning to exted such a procedure to initial state radiation (conceptually straightforward), and to massive partons (more involved)

# Backup slides

### Mapping from NLO to Born kinematics

• Catani-Seymour massless final-state mapping  $\{k\} \rightarrow \{\bar{k}\}^{(abc)}$ :

$$\bar{k}_{i}^{(abc)} = k_{i}, \text{ if } i \neq a, b, c, \quad \bar{k}_{b}^{(abc)} = k_{a} + k_{b} - \frac{s_{ab}}{s_{ac} + s_{bc}} k_{c}, \quad \bar{k}_{c}^{(abc)} = \frac{s_{abc}}{s_{ac} + s_{bc}} k_{c}$$

with  $s_{abc} = s_{ab} + s_{ac} + s_{bc}$ , and  $\bar{k}_b^{(abc)} + \bar{k}_c^{(abc)} = k_a + k_b + k_c$ .

• Catani-Seymour variables  $y, z \in [0, 1]$  for mapping  $\{k\} \rightarrow \{\bar{k}\}^{(abc)}$ :

$$s_{ab} = y \, s_{abc} \,, \qquad s_{ac} = z(1-y) \, s_{abc} \,, \qquad s_{bc} = (1-z)(1-y) \, s_{abc}$$

Phase-space factorization:

$$\begin{split} d\Phi_{n+1} &= d\Phi_n^{(abc)} d\Phi_{rad}^{(abc)}, \qquad d\Phi_{rad}^{(abc)} \equiv d\Phi_{rad} \left( \bar{s}_{bc}^{(abc)}; y, z, \phi \right) \\ \int d\Phi_{rad} \left( s; y, z, \phi \right) &\equiv N(\epsilon) \, s^{1-\epsilon} \int_0^{\pi} d\phi \, \sin^{-2\epsilon} \phi \int_0^1 dy \int_0^1 dz \left[ y(1-y)^2 \, z(1-z) \right]^{-\epsilon} (1-y), \\ N(\epsilon) &\equiv \frac{(4\pi)^{\epsilon-2}}{\sqrt{\pi} \, \Gamma(1/2-\epsilon)}, \qquad \bar{s}_{bc}^{(abc)} \equiv 2 \, \bar{k}_b^{(abc)} \cdot \bar{k}_c^{(abc)} = s_{abc} \, . \end{split}$$

•  $\phi = \text{azimuth between } \vec{k}_a \text{ and an reference three-momentum } (\neq \vec{k}_b, \vec{k}_c).$ 

Sum rules in double-unresolved limits: summing over sectors sharing the same singularity, and taking that singular limit on the sum, W functions disappear.

$$\begin{split} \mathbf{S}_{ik} \left( \sum_{b \neq i} \sum_{d \neq i, k} \mathcal{W}_{ibkd} + \sum_{b \neq k} \sum_{d \neq k, i} \mathcal{W}_{kbid} \right) &= 1, \\ \mathbf{C}_{ijk} \sum_{abc \in \text{perm}(ijk)} \left( \mathcal{W}_{abbc} + \mathcal{W}_{abcb} \right) &= 1, \\ \mathbf{S}_{ijk} \sum_{abc \in \text{perm}(kl)} \left( \mathcal{W}_{abbc} + \mathcal{W}_{abcb} \right) &= 1, \\ \mathbf{S}_{ikl} \sum_{b \neq i} \left( \mathcal{W}_{ibkl} + \mathcal{W}_{iblk} \right) &= 1, \\ \mathbf{S}_{ikl} \sum_{b \neq i} \left( \mathcal{W}_{ibkl} + \mathcal{W}_{iblk} \right) &= 1, \\ \mathbf{S}_{ikl} \sum_{b \neq i} \left( \mathcal{W}_{ibkl} + \mathcal{W}_{iblk} \right) &= 1, \\ \mathbf{S}_{ikl} \sum_{b \neq i} \left( \mathcal{W}_{ibkl} + \mathcal{W}_{iblk} \right) &= 1. \end{split}$$

Simplifications possible, thanks to idempotency relations

 $(1 - \mathbf{S}_i) \, \mathbf{S}_{icd} \, RR \, \mathcal{W}_{ibcd} = 0 \,, \qquad (1 - \mathbf{C}_{ij}) \, \mathbf{C}_{ijk} \, RR \, \mathcal{W}_{ijkd} = 0 \,.$ 

• Limits SC, CS: disappear from  $K^{(2)} + K^{(12)}$ :

$$\mathcal{K}_{ijkj}^{(2)} + \mathcal{K}_{ijkj}^{(12)} = (1 - \mathbf{S}_i)(1 - \mathbf{C}_{ij}) \Big[ \mathbf{S}_{ik} + \mathbf{C}_{ijk}(1 - \mathbf{S}_{ik}) \Big] RR \mathcal{W}_{ijkj},$$

very simple structure!

Still, since integrated I<sup>(12)</sup> and I<sup>(2)</sup> enter separately, they receive contributions from SC and CS (which however cancel in the sum).

# Counterterms at NNLO: $\overline{K}^{(2)}$

Remapped pure double-unresolved counterterm, to be integrated over  $d\Phi_{n+2}$ :

$$\begin{split} \overline{\mathcal{K}}^{(2)} &= \sum_{i} \left\{ \sum_{j>i} \overline{\mathbf{S}}_{ij} + \sum_{j>i} \sum_{k>j} \overline{\mathbf{C}}_{ijk} \left( 1 - \overline{\mathbf{S}}_{ij} - \overline{\mathbf{S}}_{ik} - \overline{\mathbf{S}}_{jk} \right) \right. \\ &+ \sum_{j>i} \sum_{\substack{k>i \ k\neq j}} \sum_{\substack{l>k \ k\neq j}} \overline{\mathbf{C}}_{ijkl} \left( 1 - \overline{\mathbf{S}}_{ik} - \overline{\mathbf{S}}_{jk} - \overline{\mathbf{S}}_{jl} - \overline{\mathbf{S}}_{jl} \right) \\ &+ \sum_{j\neq i} \sum_{\substack{k\neq i \ k\neq j}} \overline{\mathbf{S}} \overline{\mathbf{C}}_{ijk} \left( 1 - \overline{\mathbf{S}}_{ij} - \overline{\mathbf{S}}_{ik} \right) \left( 1 - \overline{\mathbf{C}}_{ijk} - \sum_{l\neq i,j,k} \overline{\mathbf{C}}_{iljk} \right) \\ &+ \sum_{j>i} \sum_{\substack{k\neq i \ k\neq j}} \overline{\mathbf{C}} \overline{\mathbf{S}}_{ijk} \left( 1 - \overline{\mathbf{S}}_{ik} - \overline{\mathbf{S}}_{jk} \right) \left( 1 - \overline{\mathbf{C}}_{ijk} - \sum_{l\neq i,j,k} \overline{\mathbf{C}}_{iljk} \right) \\ &+ \sum_{j>i} \sum_{\substack{k\neq i,j}} \overline{\mathbf{C}} \overline{\mathbf{S}}_{ijk} \left( 1 - \overline{\mathbf{S}}_{ik} - \overline{\mathbf{S}}_{jk} \right) \left( 1 - \overline{\mathbf{C}}_{ijk} - \sum_{l\neq i,j,k} \overline{\mathbf{C}}_{ijkl} \right) \right\} RR \,, \end{split}$$