

# Towards an automated generator based on OpenLoops + LTD

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based on [ongoing work](#) with

Gloria Bertolotti, Nicolò Giraudo, Florian Herren and Jonas Lindert

see also [talk by Gloria Bertolotti](#) today at 11 AM

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# Loop Tree Duality (LTD)

## Key ideas

- analytic loop-energy integration → 3D phase space for real and virtual d.o.f

$$\int \mathrm{d}q^0 \int \mathrm{d}\mathbf{q}^{D-1} \mathcal{I}_V(q^0, \mathbf{q}) = \int \mathrm{d}\mathbf{q}^{D-1} I_V(\mathbf{q})$$

⇒ local IR cancellations w.o. subtraction terms

⇒ numerical  $N^k$ LO calculations (attractive e.g. for EW multi-loop problems)

## Past and ongoing contributions to LTD

≥ 1999 Seminal work [Soper]

≥ 2008 General formulation [Catani, Rodrigo, Krauss, Gleisberg, Winter, Sborlini, Buchta, Chachamis, Draggiotis, Malamos Driencourt-Mangin, Hernandez-Pinto, ...]

≥ 2019 New groups and directions (e.g. Local Unitarity) [Capatti, Hirschi, Kermanschah, Pelloni, Ruijl, Vicini, Tramontano, Weinzierl, Runkel, Szor, Vesga, Kromin, Schwanemann, Ramirez-Uribe, Renteria-Olivo, Renteria-Estrada, Martinez de Lejarza, Torres Bobadilla, Dhani, Cieri, Aguilera-Verdugo, ...]

Active & promising field. But potential for collider pheno still to be demonstrated.

# OpenLoops+LTD project [Bertolotti, Giraudo, Herren, Lindert, SP]

**Long term goal: NNLO automation** (not discussed in this talk)

Based on “combination” of LTD with

- NLO automation in OpenLoops2 [Buccioni, Maierhöfer, Lang, Lindert, SP, Zhang, Zoller '18]
- OpenLoops automation of 2-loop integrands [SP, Schär, Zoller '22]

**First objective: NLO automation** (first preliminary results today)

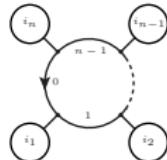
Main features of envisaged tool

- MC generator of real and “virtual” events with local IR cancellations
- flexible predictions for arbitrary observables (e.g. via Rivet)

Key motivation: assess potential of LTD vs established NLO generators

# LTD in a snapshot [Catani, Rodrigo et al.]

## Generic $n$ -point one-loop diagram



$$\mathcal{A} = -i \int D^D q \frac{N(q)}{\prod_{i=0}^{n-1} D_i(q)}$$

$$D^D q = \mu^{2\varepsilon} \frac{d^D q}{(2\pi)^D}$$

$$\begin{aligned} D_i(q) &= (q + p_i)^2 - m_i^2 + i0 \\ &= (q^0 - E_i^+)(q^0 - E_i^-) \end{aligned}$$

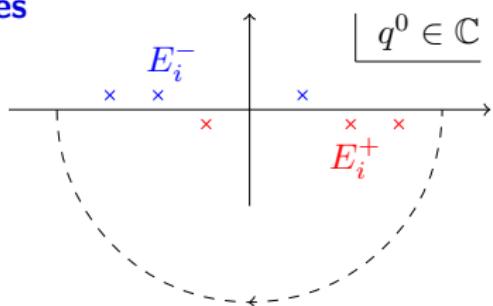
## Positive and negative energy poles in $q^0$ space

$$E_i^\pm(\mathbf{q}) = -p_i^0 \pm \epsilon_i(\mathbf{q}), \quad \epsilon_i(\mathbf{q}) = \sqrt{|\mathbf{q} + \mathbf{p}_i|^2 + m_i^0 - i0}$$

## Analytic $q^0$ integration $\rightarrow$ sum over $n$ residues

$$\mathcal{A} = \int D^{D-1} \mathbf{q} I(\mathbf{q})$$

$$I(\mathbf{q}) = - \sum_{i=0}^{n-1} \frac{1}{2\epsilon_i} \frac{N(q)}{\prod_{j \neq i} D_j(q)} \Big|_{q^0=E_i^+}$$



# Automation of standard LTD integrand in OpenLoops

$$I(\mathbf{q}) = - \int D^{D-1} \mathbf{q} \sum_{i=0}^{n-1} \frac{1}{2\epsilon_i} \frac{N(q)}{\prod_{j \neq i} D_j(q)} \Big|_{q^0 = E_i^+} \quad \mathcal{A} = \int D^{D-1} \mathbf{q} I(\mathbf{q})$$

## OpenLoops implementation of LTD integrand

- similar ingredients as standard 1-loop integrand
- ⇒ automated for any SM processes at NLO QCD+EW

## Polynomial numerator in OpenLoops

$$N(\mathbf{q}) = \sum_{r=0}^R \underbrace{N_{\mu_1 \dots \mu_r}(\{p_i\}, m_i)}_{\text{computed numerically}} q^{\mu_1} \dots q^{\mu_r}$$

- full information about analytic  $q$ -dependence of integrand
- $I(\mathbf{q})$  evaluations for many  $\mathbf{q}$ 's very fast ⇒ speeds up MC integration

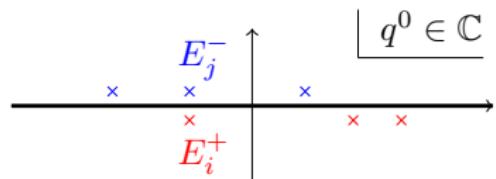
Challenges: UV+threshold+IR cancellation & small  $I(\mathbf{q})$  variance (fast integ.)

# Spurious singularities [Catani, Rodrigo et al.]

$$I(\mathbf{q}) = - \sum_{i=0}^{n-1} \frac{1}{2\epsilon_i} \frac{N(E_i^+, \mathbf{q})}{\prod_{j \neq i} (E_i^+ - E_j^+)(E_i^+ - E_j^-)}$$

## Physical singularities of $I(\mathbf{q})$ (see later)

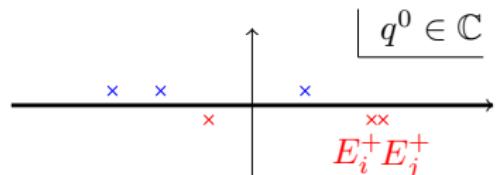
- in  $\mathbf{q}$  regions where  $E_i^+(\mathbf{q}) \rightarrow E_j^-(\mathbf{q})$
- $q^0$ -contour pinched  $\Rightarrow$  threshold+IR sing.



## Spurious singularities of LTD residues

- in  $\mathbf{q}$  regions where  $E_i^+(\mathbf{q}) \rightarrow E_j^+(\mathbf{q})$
- $q^0$  contour not pinched  $\Rightarrow I(\mathbf{q})$  finite ...

... but **dual cancellations** between singularities from  $q^0 = E_i^+, E_j^+$  residues

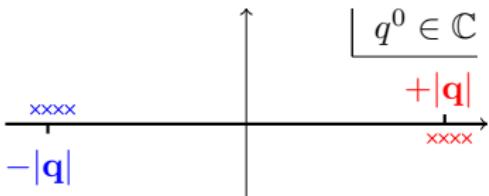


We observe significant numerical instabilities only in the deep UV region ...

# Dual cancellations in the UV region

## UV scaling of LTD on-shell energies

$$E_i^\pm(\mathbf{q}) \xrightarrow[|\mathbf{q}| \rightarrow \infty]{} \pm |\mathbf{q}| + \mathcal{O}(|\mathbf{q}|^0)$$



$$I(\mathbf{q}) = - \sum_{i=0}^{n-1} \frac{1}{2\epsilon_i} \underbrace{\frac{N(E_i^+, \mathbf{q})}{\prod_{j \neq i} (E_i^+ - E_j^+)}}_{\mathcal{O}(|\mathbf{q}|^0)} \underbrace{\frac{(E_i^+ - E_j^-)}{(E_i^+ - E_j^-)}}_{\mathcal{O}(|\mathbf{q}|^1)} \Rightarrow \text{residues} \propto I(\mathbf{q}) \times |\mathbf{q}|^{n-1}$$

Implications for  $\mathbf{q}$ -intergation in deep UV region  $|\mathbf{q}|/Q_{\text{hard}} \geq 10^P$

- contribution of this region is at most  $\mathcal{O}(10^{-P})$  of full integral
  - however dual cancellations jeopardize  $(n-1) \times P$  digits
- $\Rightarrow$  possible fake orders-of-magnitude enhancements

Instabilities can be avoided through systematic expansion in  $1/|\mathbf{q}|$

# Expansion of LTD intergand at $\mathbf{q} \rightarrow \infty$

Expansion of  $D$ -dim integrand for  $q^2 - \mu_{\text{tad}}^2 \gg \Delta_i$  [Chetyrkin, Misiak, Münz]

$$(q + p_i)^2 - m_i^2 = \underbrace{q^2 - \mu_{\text{tad}}^2}_{\mathcal{O}(q^2)} - \underbrace{(m_i^2 - p_i^2 - \mu_{\text{tad}}^2 - 2q \cdot p_i)}_{\Delta_i = \mathcal{O}(q)}$$

$$\mathcal{I}(q) = \frac{N(q)}{\prod_{i=0}^{n-1} D_i(q)} \xrightarrow[q^2 \rightarrow \infty]{} \mathcal{I}_{\text{tad}}(q) = \sum_{k=n}^{n+p(X)} \frac{U_k(q)}{(q^2 - \mu_{\text{tad}}^2)^k} + \mathcal{O}(q^{-X})$$

Expanded LTD integrand  $\equiv$  residues of single poles at  $q_0 = \epsilon_{\text{tad}} = \sqrt{|\mathbf{q}|^2 + \mu_{\text{tad}}^2}$

$$I_{\text{tad}}(\mathbf{q}) = \int dq^0 \mathcal{I}_{\text{tad}}(q) = \underbrace{\sum_{k=n}^{n+p} \frac{1}{(k-1)!} \frac{\partial^{k-1}}{\partial q_0^{k-1}} \frac{U_k(q^0, \mathbf{q})}{(q^0 + \epsilon_{\text{tad}})^k}}_{\text{automated in OL+LTD up to 2nd order in } 1/|\mathbf{q}|} \Big|_{q_0=\epsilon_{\text{tad}}}$$

Similar technique used for UV renormalisation...

# UV renormalisation

Standard renormalisation in  $D$  dimensions with UV and rational CTs

$$\mathcal{A} = -i \int D^D q \mathcal{I}(q) \ni \epsilon_{\text{UV}}^{-1} \implies R\mathcal{A} = \mathcal{A} + \delta Z + \delta R \not\ni \epsilon_{\text{UV}}^{-1}$$

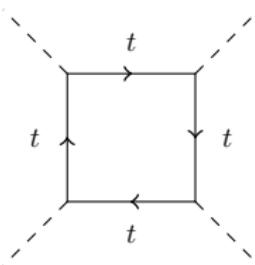
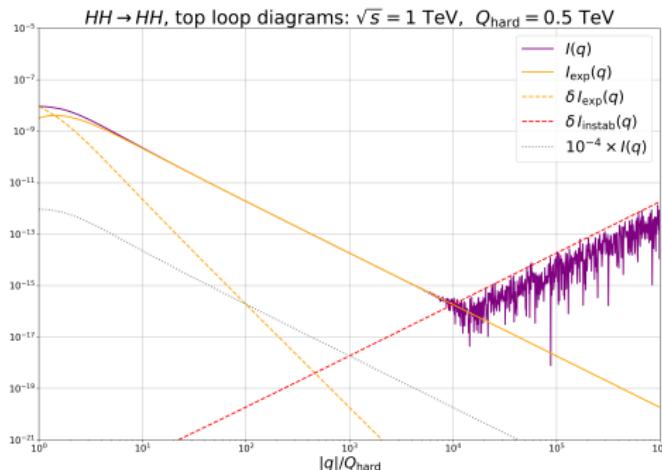
Local UV subtraction using divergent part of UV tadpole expansion

$$\begin{aligned} R\mathcal{A} &= \underbrace{-i \int D^D q [\mathcal{I}(q) - \mathcal{I}_{\text{tad}}^{\text{div}}(q)]}_{\text{LTD}} + \underbrace{\delta Z + \delta R - i \int D^D q \mathcal{I}_{\text{tad}}^{\text{div}}(q)}_{\text{analytic } \epsilon_{\text{UV}}^{-1} \text{ pole cancellation}} \\ &\xrightarrow{\text{LTd}} \int D^3 q [I(\mathbf{q}) - I_{\text{tad}}^{\text{div}}(\mathbf{q})] \end{aligned}$$

- subtracted LTD intergrand UV finite
- matching to correct  $\delta Z$  in dim reg via integrated tadpole integral

Expansion and renormalisation automated at NLO QCD+EW

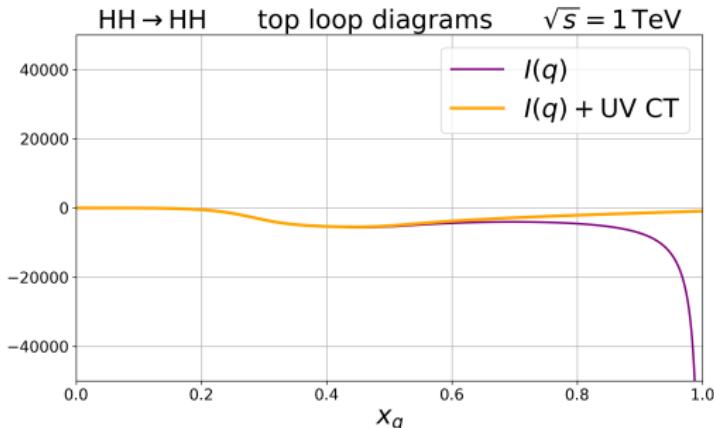
# Example of UV instability & expansion



- UV subtracted LTD integrand features convergent  $d|\mathbf{q}|/|\mathbf{q}|^2$  scaling
- but becomes completely **unstable** at  $|\mathbf{q}|/Q_{\text{hard}} > 10^4$
- expansion  $\Rightarrow$  stability and **better than  $10^{-4}$  accuracy** for  $|\mathbf{q}|/Q_{\text{hard}} > 10^2$

# Convenient parametrisation of $\mathbf{q}$ and UV subtraction

**Tan-parametrisation:**  $|\mathbf{q}| = Q_{\text{hard}} \tan\left(\frac{\pi}{2} x_{\mathbf{q}}\right)$  [Becker et al. '10]

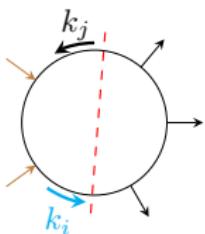


$$\int_0^\infty d|\mathbf{q}| |\mathbf{q}|^2 \longrightarrow \int_0^1 dx_{\mathbf{q}}$$

$$I(\mathbf{q}) \longrightarrow \underbrace{\frac{|\mathbf{q}|^2 d|\mathbf{q}|}{dx_{\mathbf{q}}}}_{\text{Jacobian}} I(\mathbf{q})$$

- ⇒ renormalised integrands  $\propto d|\mathbf{q}|/|\mathbf{q}|^2$  become flat at  $x_{\mathbf{q}} \rightarrow 1$
- ⇒ deep UV region  $|\mathbf{q}|/Q_{\text{hard}} > 10^4 \equiv x_{\mathbf{q}} \in [0.9999, 1]$

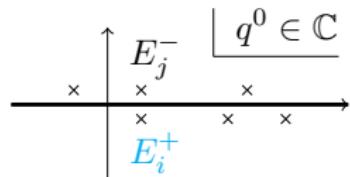
# Threshold singularities from two-particle cuts



$$\begin{array}{ll} -k_j^0 > 0 & k_j^2 = m_j^2 \\ p_{ij}^0 > 0 & \\ p_{ij}^2 \geq (m_i + m_j)^2 & +k_i^0 > 0 \quad k_i^2 = m_i^2 \end{array}$$

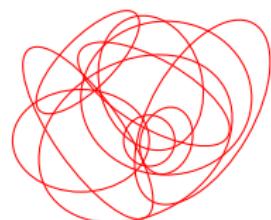
Threshold singularity from  $q^0 = E_i^+$  LTD residue

$$\mathcal{A}_{ij}^{(\text{thr})} = \int \frac{D^{D-1} \mathbf{k}_i}{2\epsilon_i} \frac{g_{ij}(\mathbf{k}_i)}{(E_i^+ - E_j^+) \underbrace{(E_i^+ - E_j^- - i0)}_{\text{threshold sing.}}}$$



Challenges for general solution

- multiple cuts per diagram and residue
- singular surface = multiple overlapping ellipsoids
- $\mathbf{q}$ -contour deformation [Soper, Capatti et al.] challenging



Local subtraction in  $\mathbf{q} \in \mathbb{R}^3$  space much more natural, simple and efficient

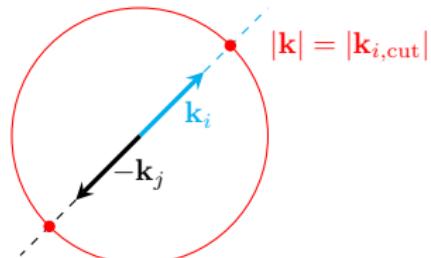
# Local subtraction in cut-CM frame [Kermanschah et al.]

## On-shell back-to-back 2-body decay

$$|\mathbf{k}_i|^2 \rightarrow |\mathbf{k}_{i,\text{cut}}|^2 = \frac{\lambda(m_i^2, m_j^2, p_{ij}^2)}{4p_{ij}^2}$$

$$\epsilon_i^2 \rightarrow \epsilon_{i,\text{cut}}^2 = |\mathbf{k}_{i,\text{cut}}|^2 + m_i^2$$

## Spherical singular surface



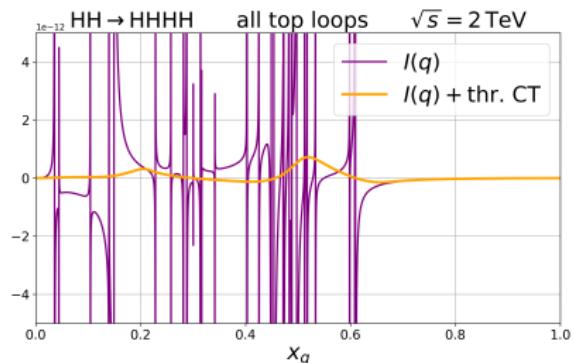
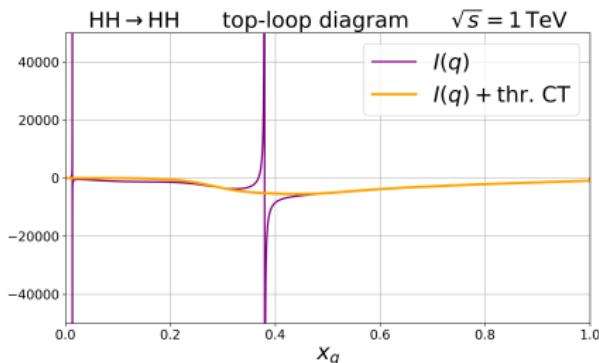
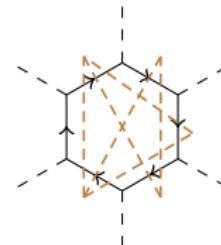
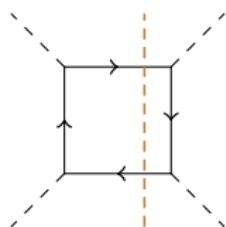
## Threshold singularity and 1-dim local subtraction

$$\mathcal{A}_{ij}^{(\text{thr})} = \int d\Omega_i \int_{m_i}^{\infty} d\epsilon_i \underbrace{\frac{1}{\epsilon_i - \epsilon_{i,\text{cut}} - i0}}_{\text{local subtraction}} \left[ f_{ij}(\epsilon_i, \Omega_i) - \underbrace{f_{ij}(\epsilon_{i,\text{cut}}, \Omega_i)}_{\text{local subtraction}} \right] \\ \text{PV} \left( \frac{1}{\epsilon_i - \epsilon_{i,\text{cut}}} \right) + i\pi \delta(\epsilon_i - \epsilon_{i,\text{cut}})$$

- subtraction defined in CM frame of each cut and “boosted” to LAB
- integrated subtraction terms added back  $\Rightarrow i\pi$  absorbtive parts

Entirely automated for one-loop diagrams with real masses

# LTD integrands with threshold subtractions



Smooth subtracted integrands also for non-trivial multi-cut configurations!

# MC integration & NLO predictions: virtual part

**Integrand with UV+threshold subtractions in  $\Phi_V = (\Phi_B, \mathbf{q})$  space**

$$I_V(\Phi_V) = \sum_{\text{diag/col/hel}} \left[ I_{\text{LTD}}(\Phi_V) - I_{\text{UV}}^{(\text{subt})}(\Phi_V) - I_{\text{thr}}^{(\text{subt})}(\Phi_V) \right]$$

**Integration with  $B \times \frac{V}{B}$  factorisation to suppress variance in  $\mathbf{q}$ -space**

$$\sigma_{\text{NLO}}^{(V)} = \int d\Phi_V I_V(\Phi_V) = \int d\Phi_B I_B(\Phi_B) \int D^3\mathbf{q} \underbrace{r_{V/B}(\Phi_V)}_{I_V(\Phi_V)/I_B(\Phi_B)}$$

**MC integration of  $V/B$  using unweighted Born sample**

$$\sigma_{\text{NLO}}^{(V)} = \frac{1}{N_B} \sum_{i=1}^{N_B} \underbrace{w_{\text{MC}}(\mathbf{q}^{(i)})}_{\equiv D^3\mathbf{q}/d^3x} r_{V/B}(\Phi_V^{(i)}) , \quad \Phi_V^{(i)} = \underbrace{(\Phi_B^{(i)}, \mathbf{q}^{(i)})}_{\text{one random } \mathbf{q}^{(i)} \text{ for each } \Phi_B^{(i)}}$$

**Boosting MC convergence by sampling over multiple  $\mathbf{q}^{(ij)}$  at fixed  $\Phi_B^{(i)}$**

- very fast for  $N_{\mathbf{q}} \leq 10-100$  in OpenLoops
- can reduce statistical uncertainty by up to a factor  $\sqrt{N_{\mathbf{q}}}$

# Integration of Virtual and Real corrections

$$\sigma_{\text{NLO}}^{(\text{B}+\text{V}+\text{R})} = \int d\Phi_B \left\{ I_B(\Phi_B) + I_{\text{CT}}(\Phi_B) + I_{\text{subt}}^{(\text{int})}(\Phi_B) \right. \\ \left. + \int D^3q \left[ I_V(\Phi_V) - I_{\text{subt}}(\Phi_V) + I_R(\Phi_R(\Phi_V)) \right] \right\}_{\Phi_V=(\Phi_B, q)}$$

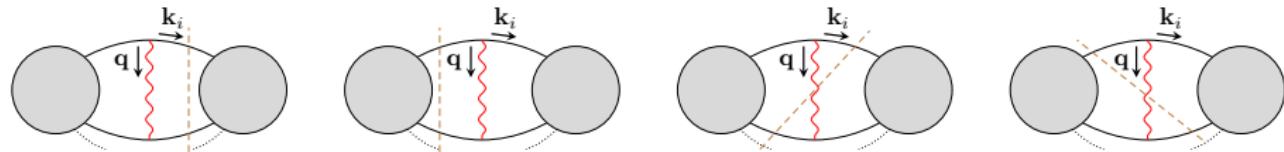
## Ingredients and features of NLO master formula

- $\Phi_B$  space  $\ni$  Born + renormalisation CTs
- $\Phi_{V/B}$  space  $\ni$  local and integrated UV + field-ren. + threshold subtr. terms
- $q^3$  integration of V + R connected through  $\Phi_V \rightarrow \Phi_R(\Phi_V)$  mapping
- $I_R(\Phi_R)$  includes usual  $|\mathcal{A}_{\text{real}}|^2$  and  $d\Phi_R/d\Phi_V$  Jacobian

Each real radiation event accompanied by a “virtual radiation” event

Main task: local cancellation of IR divergences

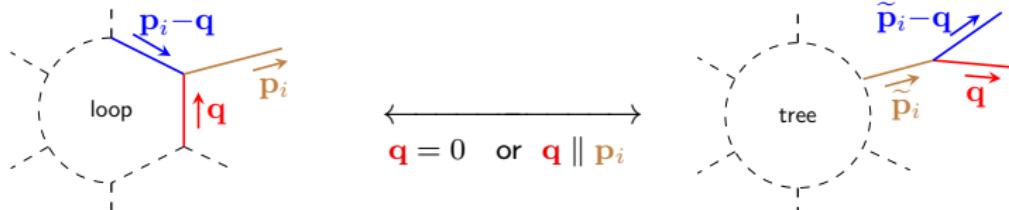
# Matching real and virtual IR singularities



## Cutkosky cuts of 2-loop forward scattering diagrams [Soper]

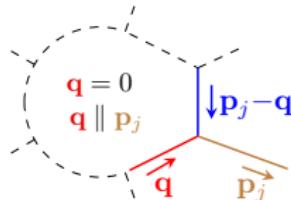
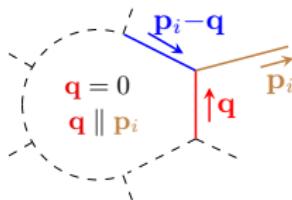
- fixed  $q$  and  $k_i \Rightarrow$  IR finite combination of B-V and R-R interferences
- we use this as guideline to align virtual and real momenta
- but we assign  $q$  in a more flexible way while keeping fixed hard kinematics

## Example of $q$ alignment at “amplitude” level



Same loop diagrams can require different parametrisations in different  $q$  regions!

# Aligning virtual singularities through loop sectors



**Requirement:** all virtual IR singularities should be at  $\mathbf{q} = 0$  and  $\mathbf{q} \parallel \mathbf{p}_k$

- to achieve this we split loop diagrams into sectors with different singularities
- and in each loop sector we apply the required **q-shift and/or flip**

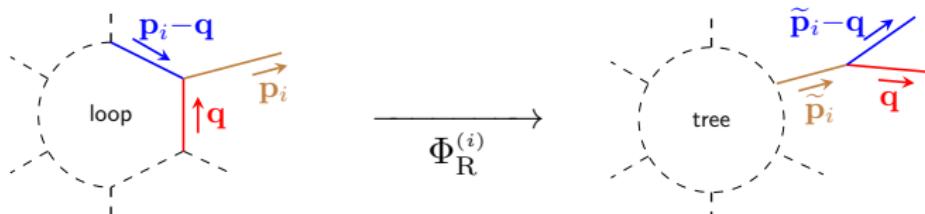
**Projectors to separate the singular sectors of a loop diagram  $\Gamma$**

$$\sum_{\alpha \in \mathcal{S}_{\Gamma}} \epsilon_{\alpha}(\mathbf{q}) = 1, \quad \epsilon_{\alpha}(\mathbf{q}) \in [0, 1], \quad \epsilon_{\alpha}(\mathbf{q}) \xrightarrow[\mathbf{q} \rightarrow \mathbf{q}_{\beta \text{ sing}}]{} \delta_{\alpha\beta}$$

**Alignment via sector-dependent  $\mathbf{q} \rightarrow \sigma_{\alpha}\mathbf{q} + \mathbf{k}_{\alpha}$  shifts and flips** ( $\sigma_{\alpha} = \pm$ )

$$\mathcal{A}_{\Gamma} = \int D^3\mathbf{q} \left( \sum_{\alpha} \epsilon_{\alpha}(\mathbf{q}) \right) I_{\Gamma}(\mathbf{q}) = \sum_{\alpha} \int D^3\mathbf{q} \, \epsilon_{\alpha}(\sigma_{\alpha}\mathbf{q} + \mathbf{k}_{\alpha}) I_{\Gamma}(\sigma_{\alpha}\mathbf{q} + \mathbf{k}_{\alpha})$$

# Matching of R+V singularities through global sectors



Each collinear region requires a different mapping  $(\Phi_B, \mathbf{q}) \rightarrow \Phi_R^{(i)}(\Phi_B, \mathbf{q})$

- we split the  $\Phi_V$  and  $\Phi_R$  spaces into **global collinear sectors**
- we use Catani–Seymour mappings
- we identify the loop momentum  $\mathbf{q}$  with the unresolved real momentum

Master formula for  $V + R$  integration with global sectors

$$\sigma_{\text{NLO}}^{(V+R)} = \int d\Phi_B \sum_\alpha \int D^3 q \left[ \epsilon_\alpha^{(V)}(\Phi_V) I_V^{(\text{subt})}(\Phi_V) + \epsilon_\alpha^{(R)}(\Phi_R) I_R(\Phi_R) \right]_{\Phi_R = \Phi_R^{(i)}(\Phi_V)}$$

⇒ generation of MC events & finite predictions for any IR finite observables

# Automation, implementation and validation

## Status (work in progress)

- Generic algorithm applicable to arbitrary processes without initial-state collinear singularities (next step)
- Currently almost completely automated and validated against Sherpa+OpenLoops for  $e^+e^- \rightarrow t\bar{t} + X$  processes

## Cross section comparisons

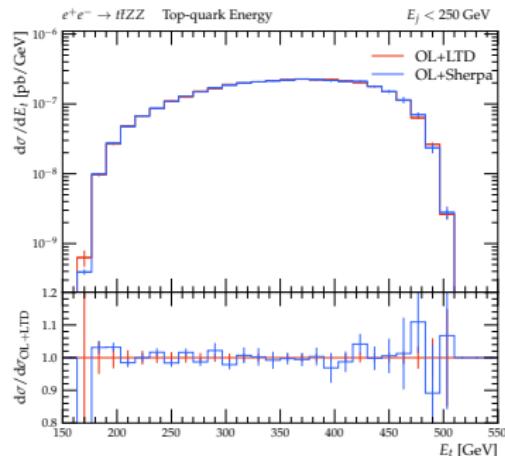
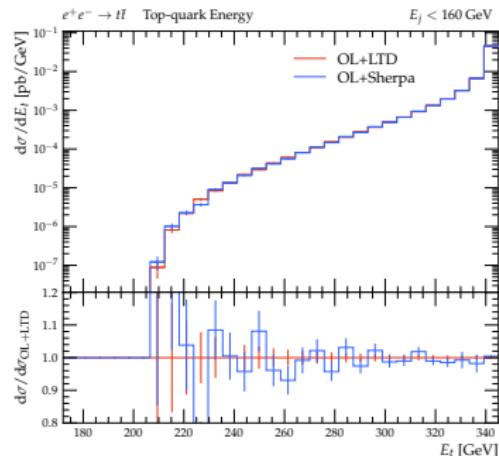
similar moderate stat. (1M evts,  $N_q = 1$ ) & runtimes (on a laptop)

process	OL+Sherpa		$\sigma$	Comparison	
	$\sigma$	$\Delta\sigma/\sigma$		$\frac{\sigma_{\text{Sherpa}} - \sigma_{\text{LTD}}}{\sigma_{\text{Sherpa}}}$	$\frac{\sigma_{\text{Sherpa}} - \sigma_{\text{LTD}}}{\Delta\sigma_{\text{Sherpa}}}$
$e^+e^- \rightarrow t\bar{t}$	359.35	0.11%	359.27	0.02%	0.2 $\sigma$
$e^+e^- \rightarrow t\bar{t}Z$	5.2406	0.11%	5.2366	0.08%	0.7 $\sigma$
$e^+e^- \rightarrow t\bar{t}ZZ$	0.04595	0.12%	0.04591	0.10%	0.9 $\sigma$
$e^+\nu_e \rightarrow t\bar{b}$	742.32	0.11%	3741.19	0.15%	1.4 $\sigma$

$\mathcal{O}(10^{-3})$  agreement & similar or better accuracy than Sherpa+OL

# Differential observables for $e^+e^- \rightarrow t\bar{t}$ and $t\bar{t}ZZ$

Results generated with **OL+LTD & Rivet** (automatically for any observable)



Very good consistency within statistical errors

- 1-2% per bin in the bulk (accuracy in the tails can be easily augmented)
- OL+LTD statistical uncertainties competitive with OL+Sherpa

More details and results in the talk by Gloria Bertolotti

# Summary

## Key features of OpenLoops+LTD at NLO

- local cancellation of threshold and UV singularities
- local IR cancellations via **loop sectors** and **global sectors**
- Automated MC generator based on Born events that emit real and “virtual” radiation

## First results

- performance of first  $e^+e^- \rightarrow t\bar{t} + \text{multi-}Z$  calculations very promising
- performance for more involved applications still to be investigated

## Next steps

- validation for processes with final-state collinear singularities (in progress)
- local cancellation of initial-state collinear singularities

# Backup slides

# Example of local cancellation test

