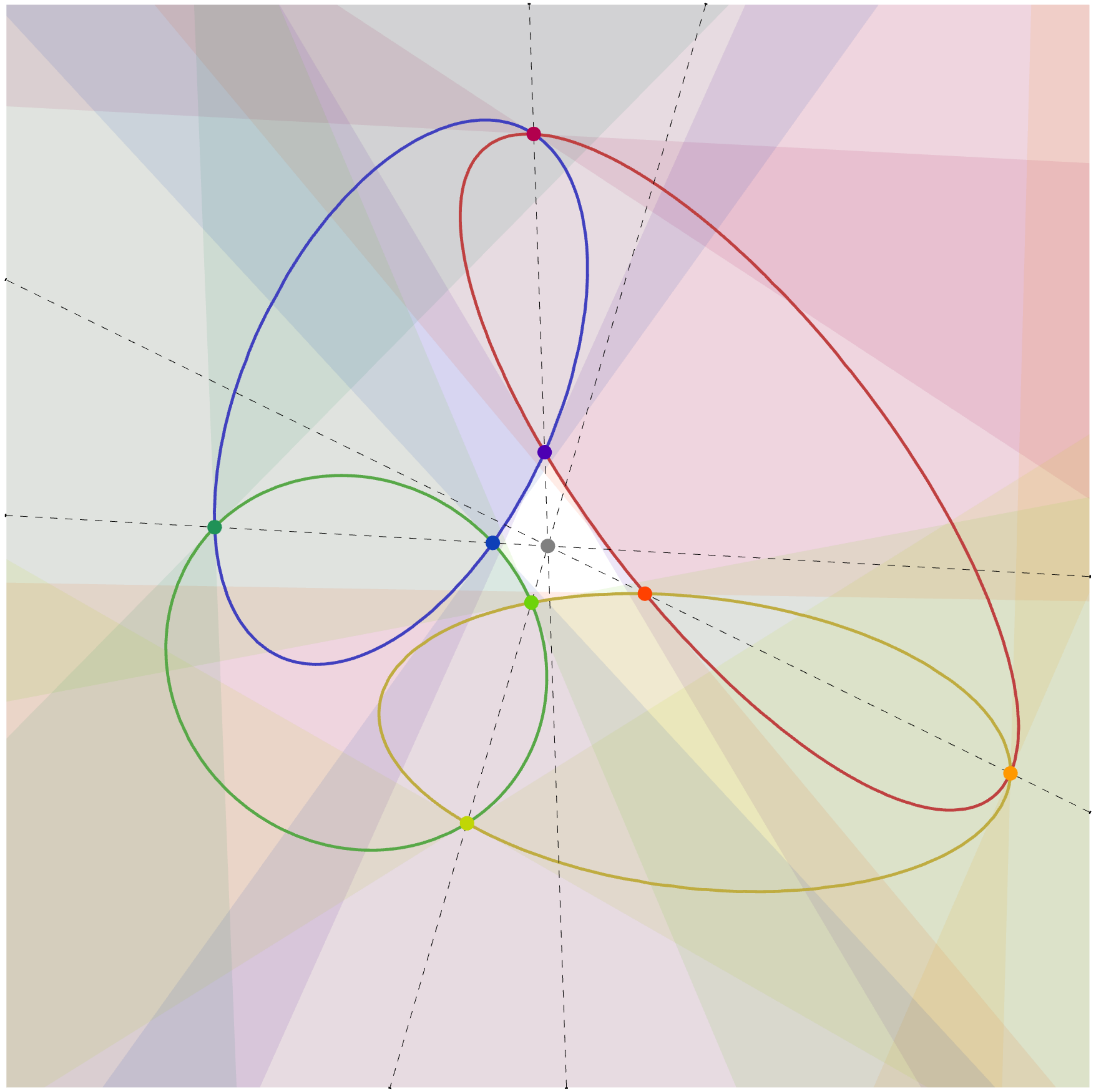
Numerical Integration of Loop Integrals in Momentum Space using Threshold Subtraction

Dario Kermanschah

LoopFest XXI



28 June 2023

Predictions for hadron collisions

$$\sigma \sim \sum_{ab} \int \mathrm{d}x_1\, \mathrm{d}x_2\, f_a(x_1) f_b(x_2)\, \mathrm{d}\Pi\, O(\Pi)\, |\mathscr{A}|^2$$

numerical

$$\mathscr{A}^{(l)} \sim \int \mathrm{d}k_1 \dots \mathrm{d}k_l\, \mathscr{I}^{(l)}$$

numerical!

~~analytical?~~

LO	$\lvert\mathscr{A}_n^{(0)}\rvert^2$	automated
NLO	$2\,\mathrm{Re}\,\mathscr{A}_n^{(1)}\left(\mathscr{A}_n^{(0)}\right)^* + \lvert\mathscr{A}_{n+1}^{(0)}\rvert^2$	
NNLO	$2\,\mathrm{Re}\,\mathscr{A}_n^{(2)}\left(\mathscr{A}_n^{(0)}\right)^* + \lvert\mathscr{A}_n^{(1)}\rvert^2 + 2\,\mathrm{Re}\,\mathscr{A}_{n+1}^{(1)}\left(\mathscr{M}_{n+1}^{(0)}\right)^* + \lvert\mathscr{A}_{n+2}^{(0)}\rvert^2$	

two-loop amplitude:

many two-loop integrals

- IBP reduction to master integrals
  ↯ large systems of equations
- solve master integrals (in dimensional regularisation) using differential equations
  - analytically: using knowledge about function space class of multiple polylogs (MPLs)
    ↯ new (elliptic) classes at two loops
  - numerically: power series ↯ automatable / efficient enough?

→ sidestep using direct numerical integration?

double real-emission:

infrared singularities

- phase space slicing / subtraction of local counterterms
  ↯ rapidly growing number of soft/collinear limits

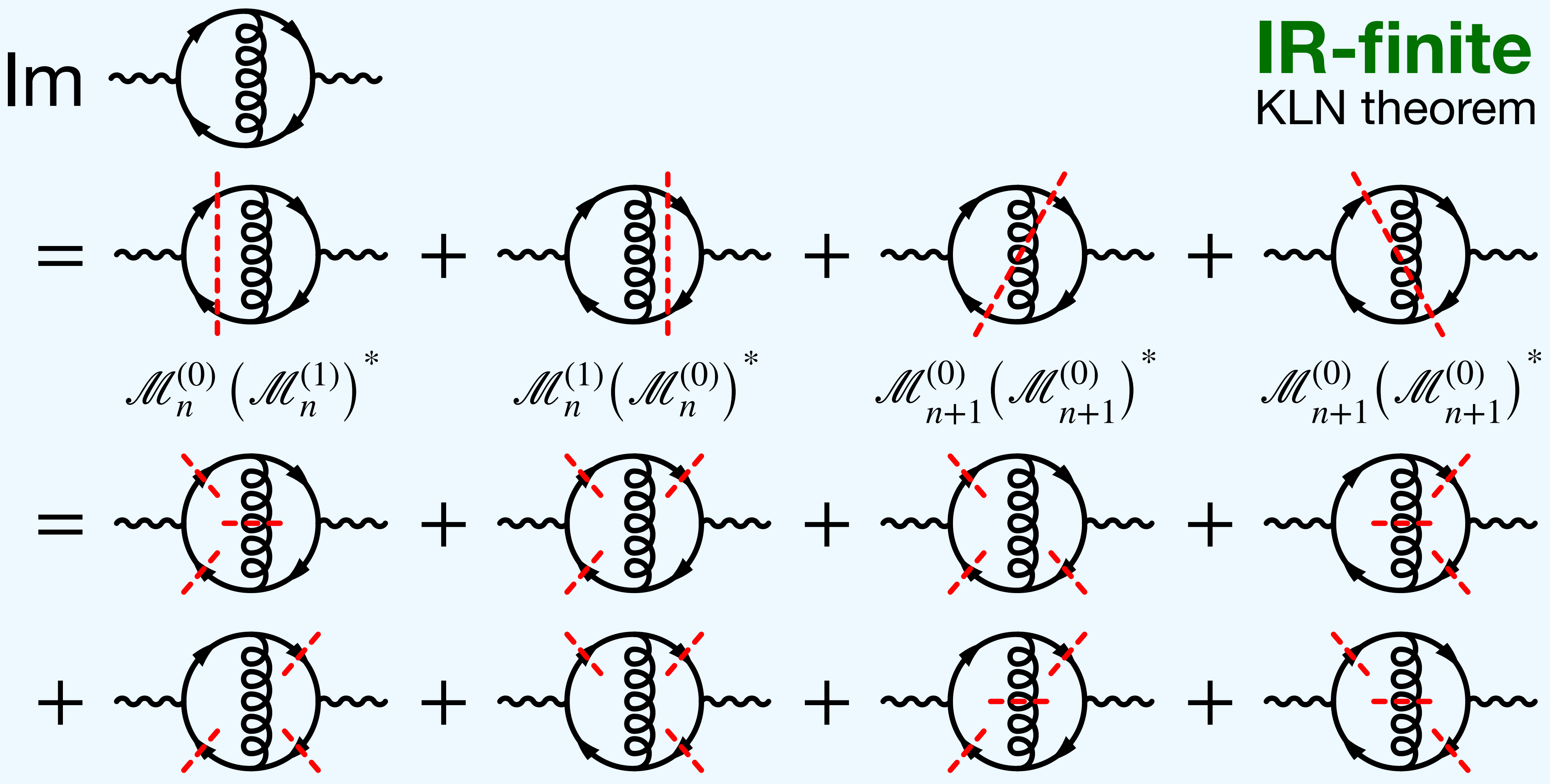
→ unify loop & phase space integration?

→ locally IR cancellations between real & virtual?

IR-finite

KLN theorem

$\sigma \sim 2\,\mathrm{Im}$



$\mathscr{M}_n^{(0)}\left(\mathscr{M}_n^{(1)}\right)^*$ $\quad \mathscr{M}_n^{(1)}\left(\mathscr{M}_n^{(0)}\right)^*$ $\quad \mathscr{M}_{n+1}^{(0)}\left(\mathscr{M}_{n+1}^{(0)}\right)^*$ $\quad \mathscr{M}_{n+1}^{(0)}\left(\mathscr{M}_{n+1}^{(0)}\right)^*$

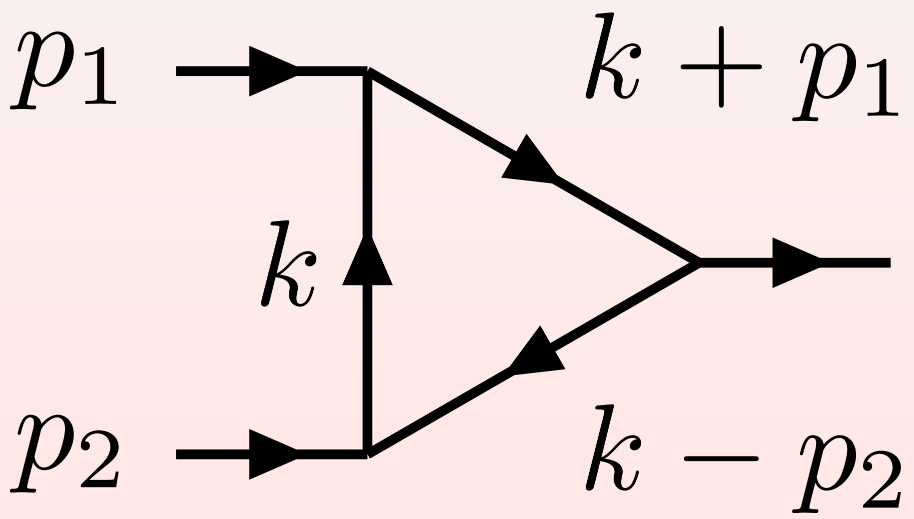
Monte Carlo integration of loop integrals in momentum space?

go to $d = 4$ dimensions

⚠️ remove UV and IR singularities

Momentum space:	local UV counterterms:		[Bogoliubov, Parasiuk, Hepp, Zimmermann] [Chetyrkin, Tkachov, Smirnov] [Herzog, Ruijl: 1703.03776]
	local IR counterterms:	one loop:	[Nagy, Soper: hep-ph/0308127] [Assadsolimani, Becker, Weinzierl: 0912.1680]
		two loop:	[Anastasiou, Haindl, Sterman, Yang, Zeng: 2008.12293] [Anastasiou, Sterman: 2212.12162]
	local IR cancellations between real & virtual:		[Soper: hep-ph/9804454, hep-ph/9910292] [Capatti, Hirschi, Pelloni, Ruijl: 2010.01068]

Feynman parameters:	Sector Decomposition:	[Binoth, Heinrich: hep-ph/0004013] [Carter, Heinrich: 1011.5493] [Smirnov, Tentyukov: 0807.4129]



$$p_3 = p_1 + p_2 = \lim_{\epsilon \to 0} \int \frac{\mathrm{d}^4 k}{(2\pi)^4} \frac{1}{k^2 - m^2 + \mathrm{i}\epsilon} \frac{1}{(k+p_1)^2 - m^2 + \mathrm{i}\epsilon} \frac{1}{(k-p_2)^2 - m^2 + \mathrm{i}\epsilon}$$

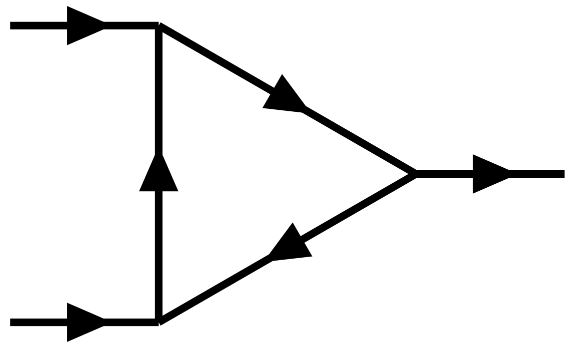
↯ poles in the integration domain

✔ causal prescription

⚠️ implement causal prescription for numerical integration?

Loop-Tree Duality (residue theorem for loop energies)

[Catani, Gleisberg, Krauss, Rodrigo, Winter: 0804.3170]



$$= \lim_{\epsilon\to 0}\int \frac{d^4k}{(2\pi)^4}\frac{1}{k^2-m^2+i\epsilon}\,\frac{1}{(k+p_1)^2-m^2+i\epsilon}\,\frac{1}{(k-p_2)^2-m^2+i\epsilon}$$

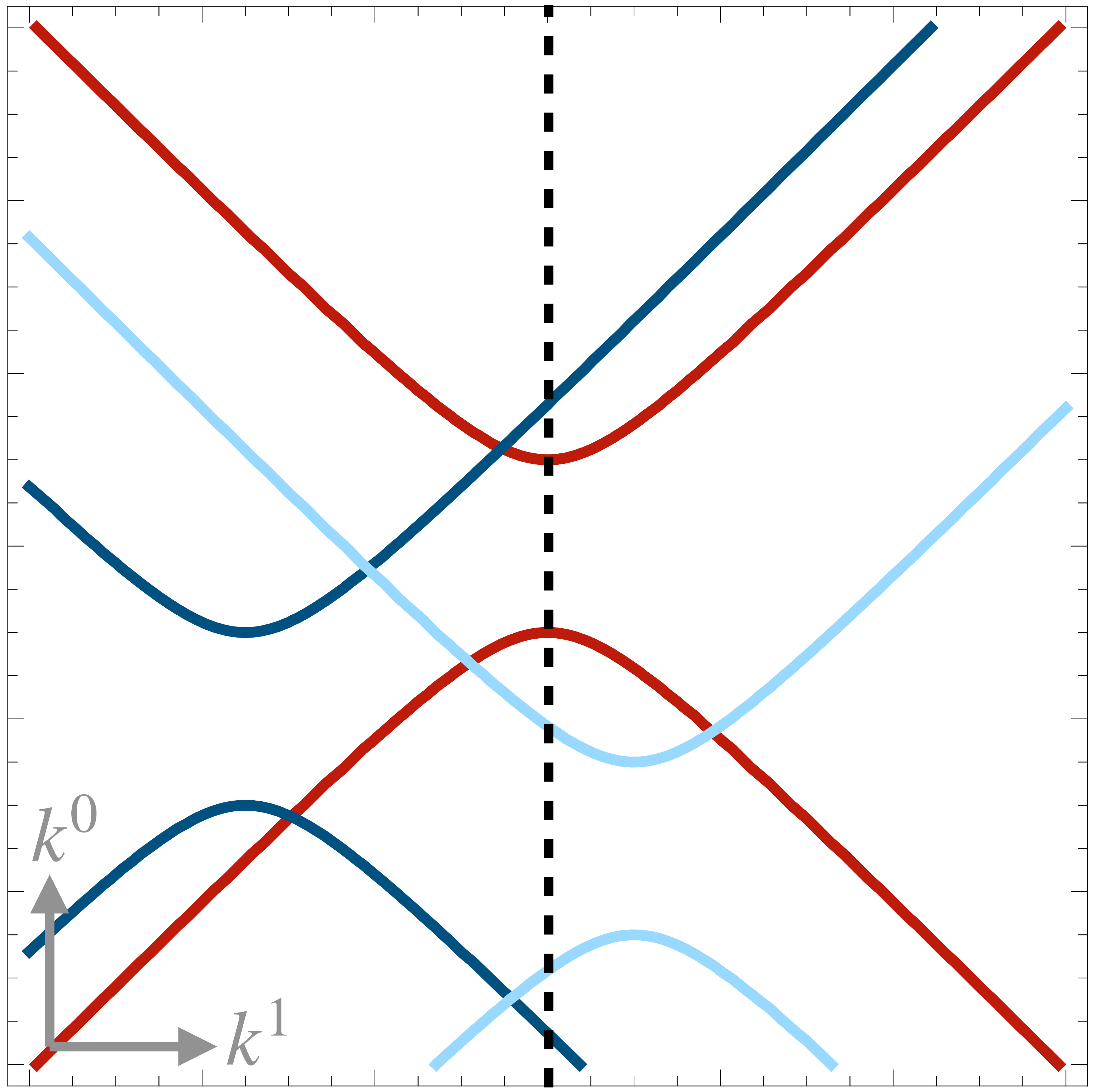
$$= \lim_{\epsilon\to 0}\int \frac{d^3\vec{k}}{(2\pi)^3}\int\frac{dk^0}{(2\pi)}\,\frac{1}{k^0-E_3}\,\frac{1}{k^0+E_3}\,\frac{1}{(k^0+p_1^0)-E_1}\,\frac{1}{(k^0+p_1^0)+E_1}\,\frac{1}{(k^0-p_2^0)-E_2}\,\frac{1}{(k^0-p_2^0)+E_2}$$

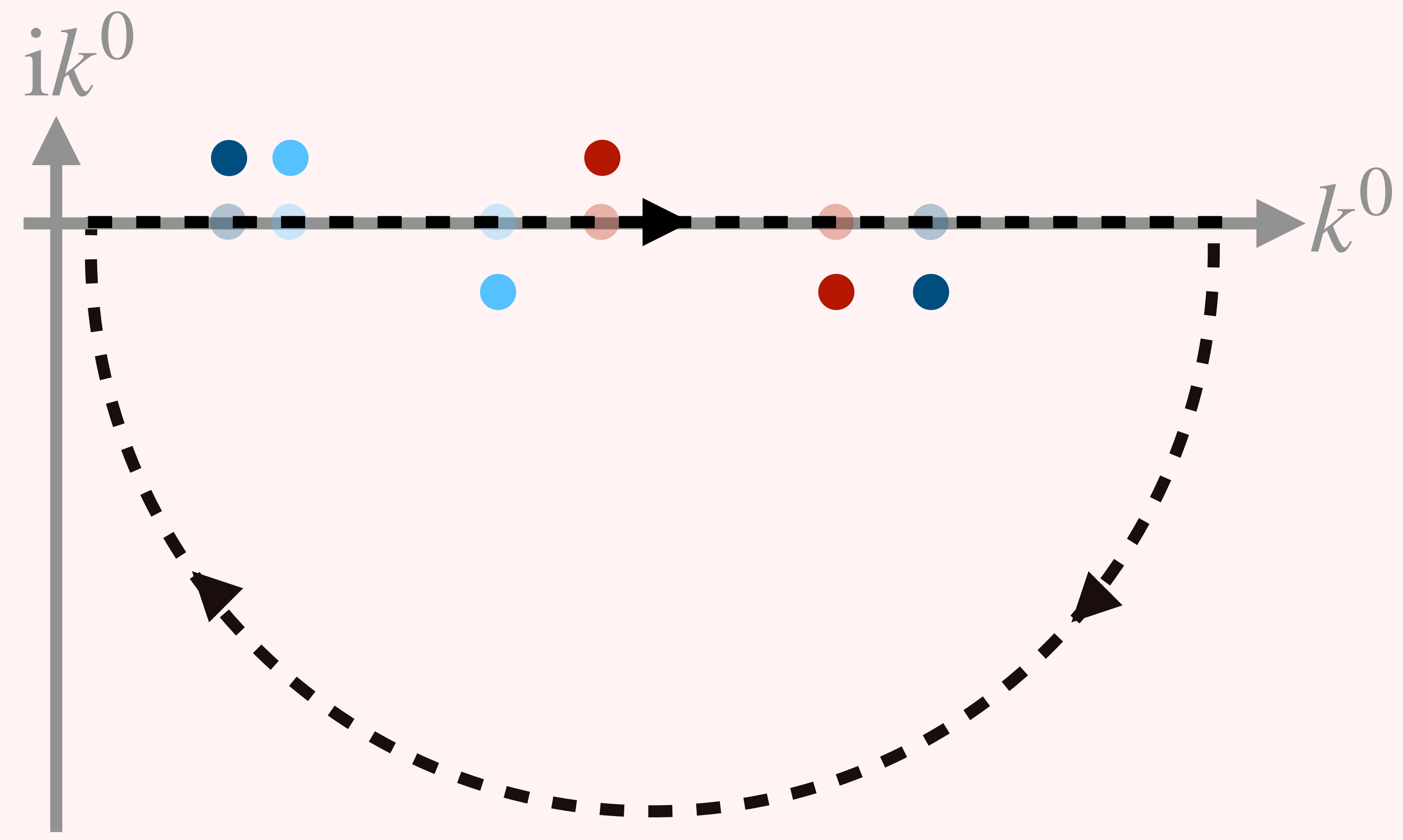
$$= -i\lim_{\epsilon\to 0}\int \frac{d^3\vec{k}}{(2\pi)^3}\Bigg[\frac{1}{2E_3}\,\frac{1}{(E_3+p_1^0)^2-E_1^2}\,\frac{1}{(E_3-p_2^0)^2-E_2^2}$$
$$+\frac{1}{(E_1-p_1)^2-E_3^2}\,\frac{1}{2E_1}\,\frac{1}{(E_1-p_1-p_2^0)^2-E_2^2}$$
$$+\frac{1}{(E_2+p_2^0)^2-E_3^2}\,\frac{1}{(E_2+p_2^0+p_1^0)^2-E_1^2}\,\frac{1}{2E_2}\Bigg]$$

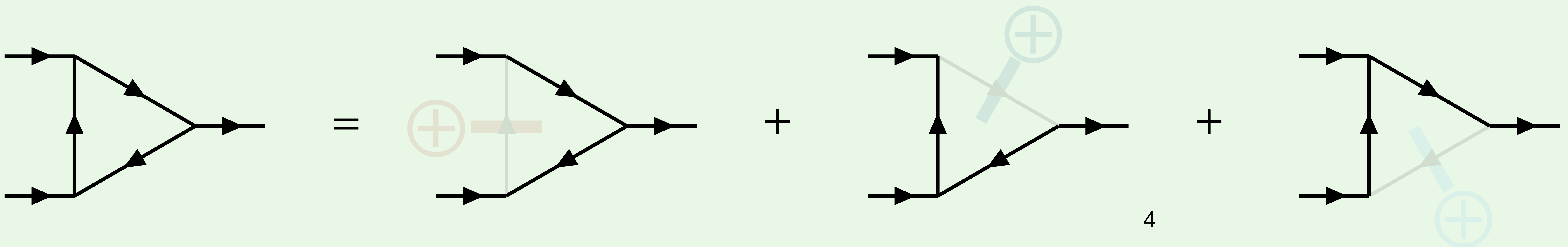
$$E_1 = \sqrt{\left(\vec{k}+\vec{p}_1\right)^2+m^2-i\epsilon}$$

$$E_2 = \sqrt{\left(\vec{k}-\vec{p}_2\right)^2+m^2-i\epsilon}$$

$$E_3 = \sqrt{\vec{k}^2+m^2-i\epsilon}$$







Loop-Tree Duality beyond one loop

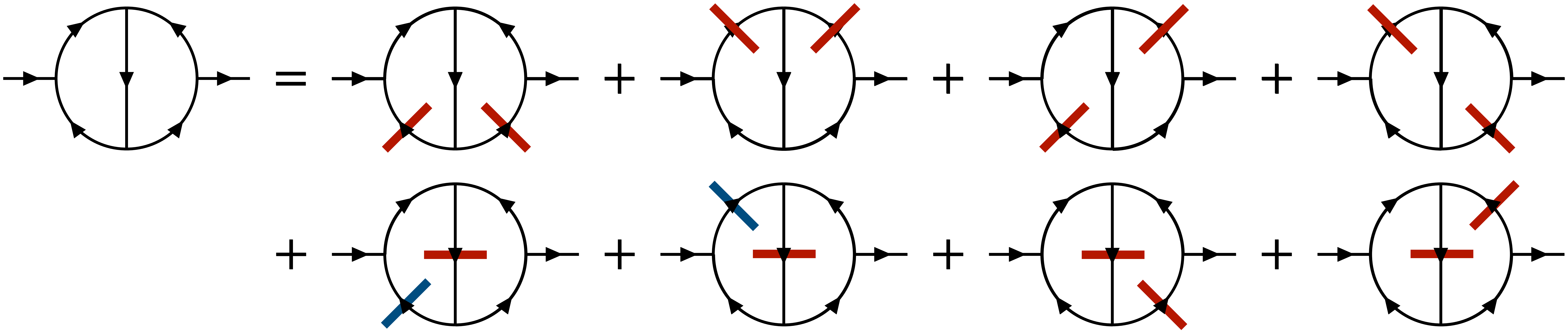
[Capatti, Hirschi, **DK**, Ruijl: 1906.06138]

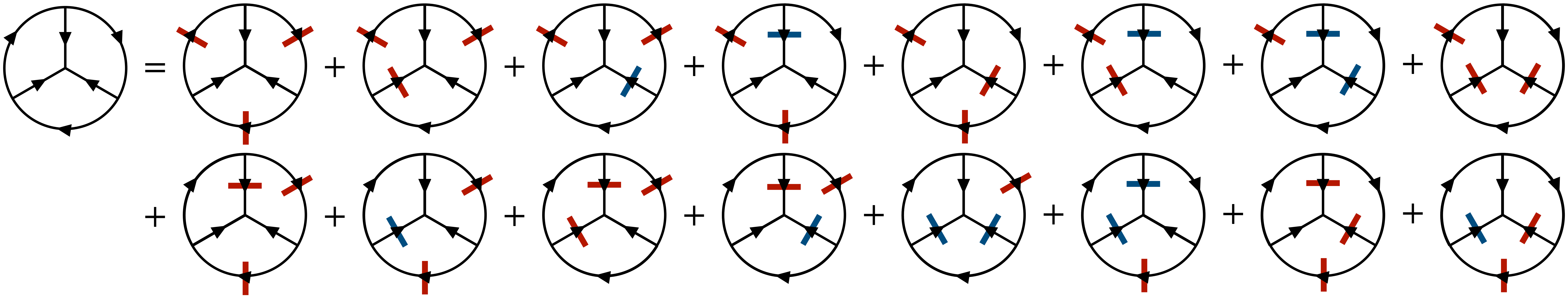
[Runkel, Szor, Vesga, Weinzierl: 1902.02135]

[Aguilera-Verdugo, Driencourt-Mangin, Hernandez-Pinto, Plenter, Ramirez-Uribe, Renteria-Olivo, Rodrigo, Sborlini, Bobadilla, Tracz: 2001.03564]

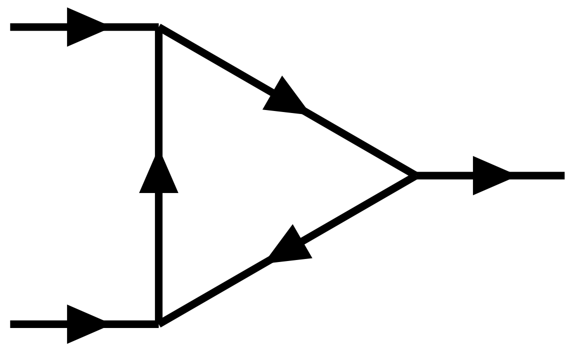
⊕ positive OS energy

⊖ negative OS energy





Monte Carlo integration of LTD? ⚠️ Remaining singularities!



$$= -\mathrm{i}\lim_{\epsilon\to 0}\int\frac{\mathrm{d}^3\vec{k}}{(2\pi)^3}\left[\frac{1}{2E_3}\frac{1}{E_3-E_1+p_1^0}\frac{1}{E_3+E_1+p_1^0}\frac{1}{E_3-E_2-p_2^0}\frac{1}{E_3+E_2-p_2^0}\right.$$
$$+\frac{1}{E_1-E_3-p_1}\frac{1}{E_1+E_3-p_1}\frac{1}{2E_1}\frac{1}{E_1-E_2-p_1-p_2^0}\frac{1}{E_1+E_2-p_1-p_2^0}$$
$$\left.+\frac{1}{E_2-E_3+p_2^0}\frac{1}{E_2+E_3+p_2^0}\frac{1}{E_2-E_1+p_2^0+p_1^0}\frac{1}{E_2+E_1+p_2^0+p_1^0}\frac{1}{2E_2}\right]$$

Hyperboloid

spurious singularities

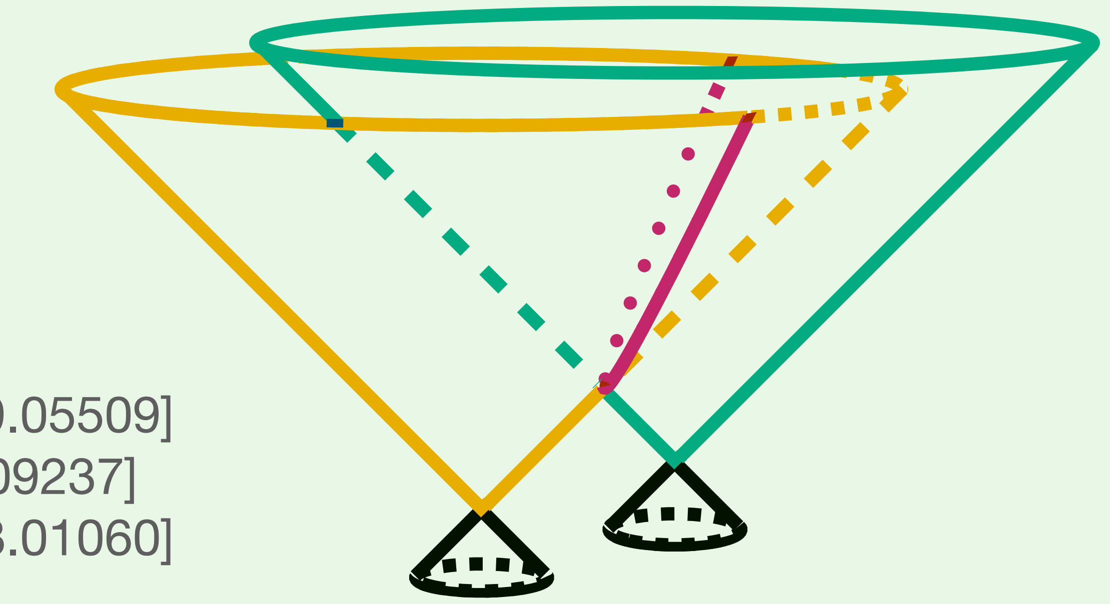
cause numerical instabilities

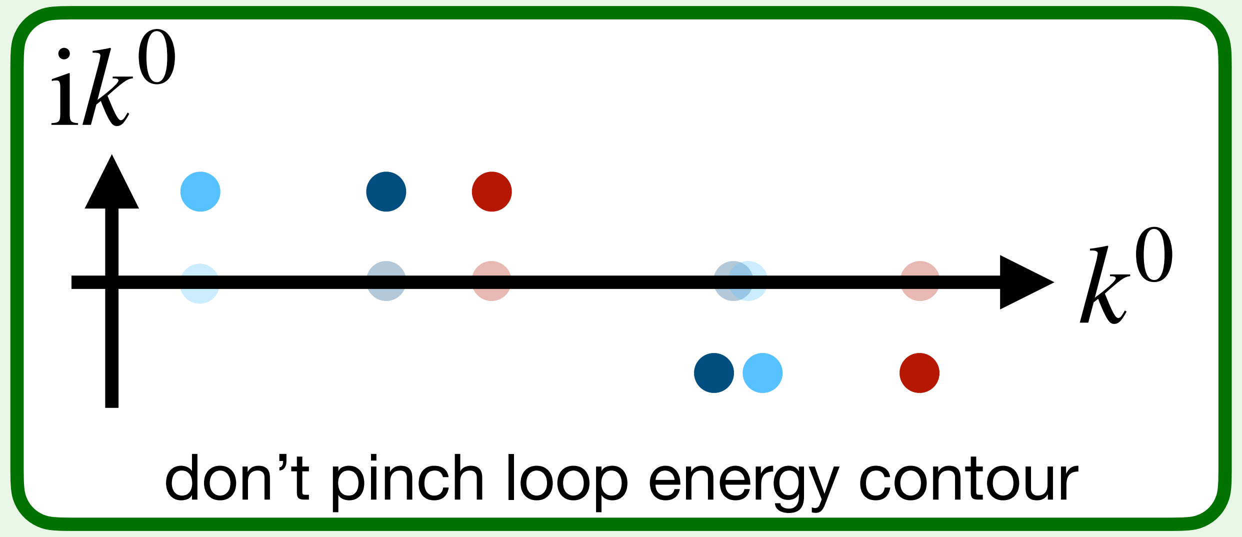
→ remove with

causal LTD [Capatti, Hirschi, **DK**, Pelloni, Ruijl: 2009.05509]

TOPT [Sborlini: 2102.05062] [Bobadilla: 2103.09237] [Kromin, Schwanemann, Weinzierl: 2208.01060]

CFF [Capatti: 2211.09653]



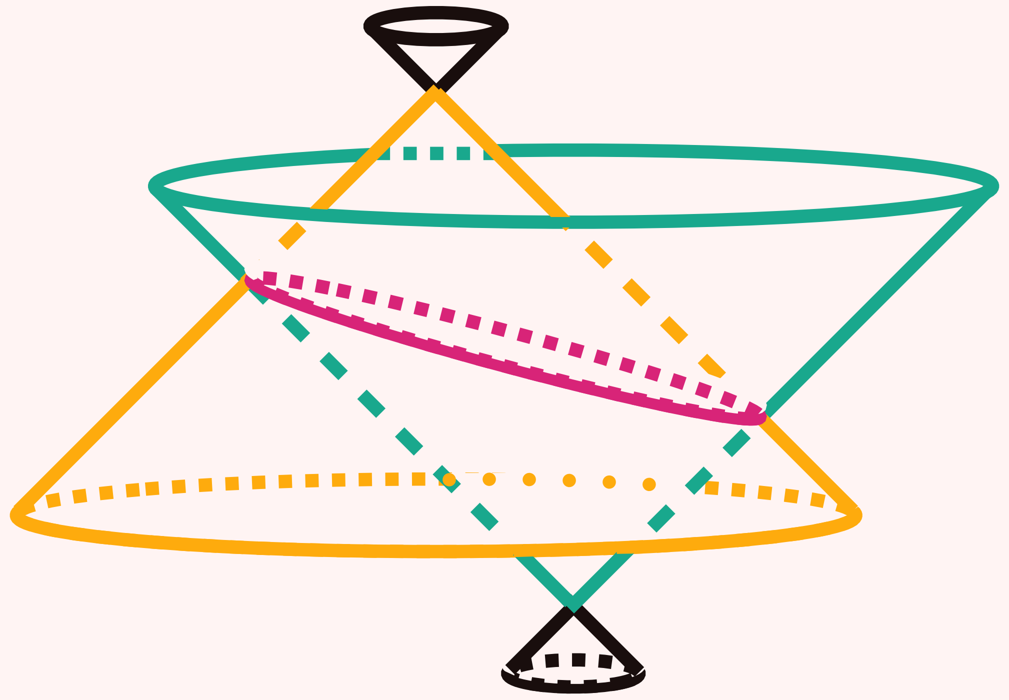


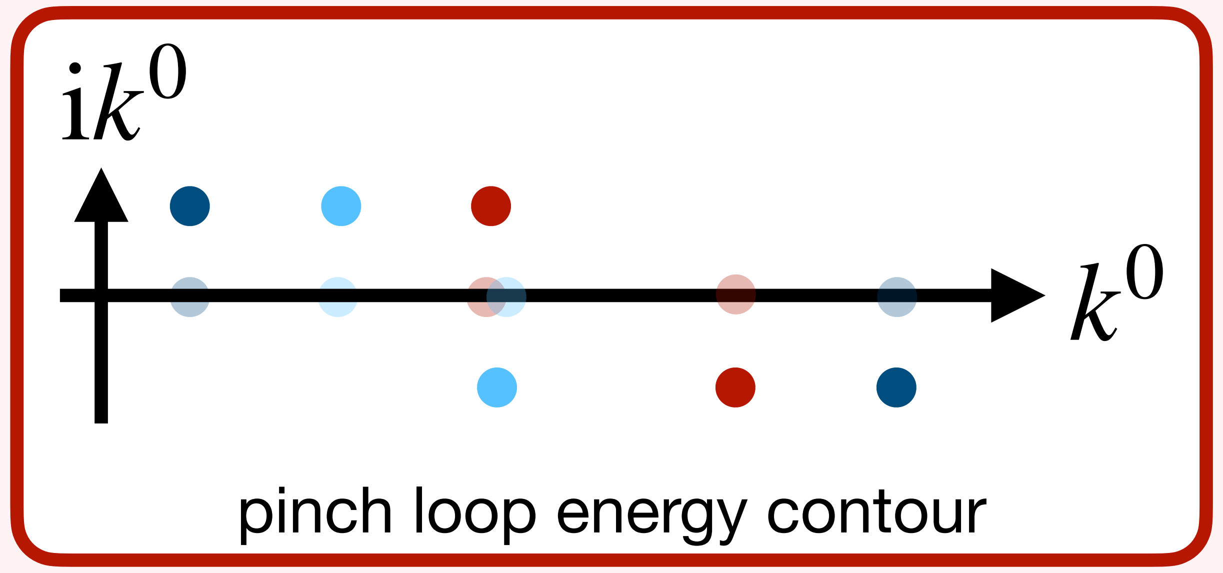
Ellipsoid

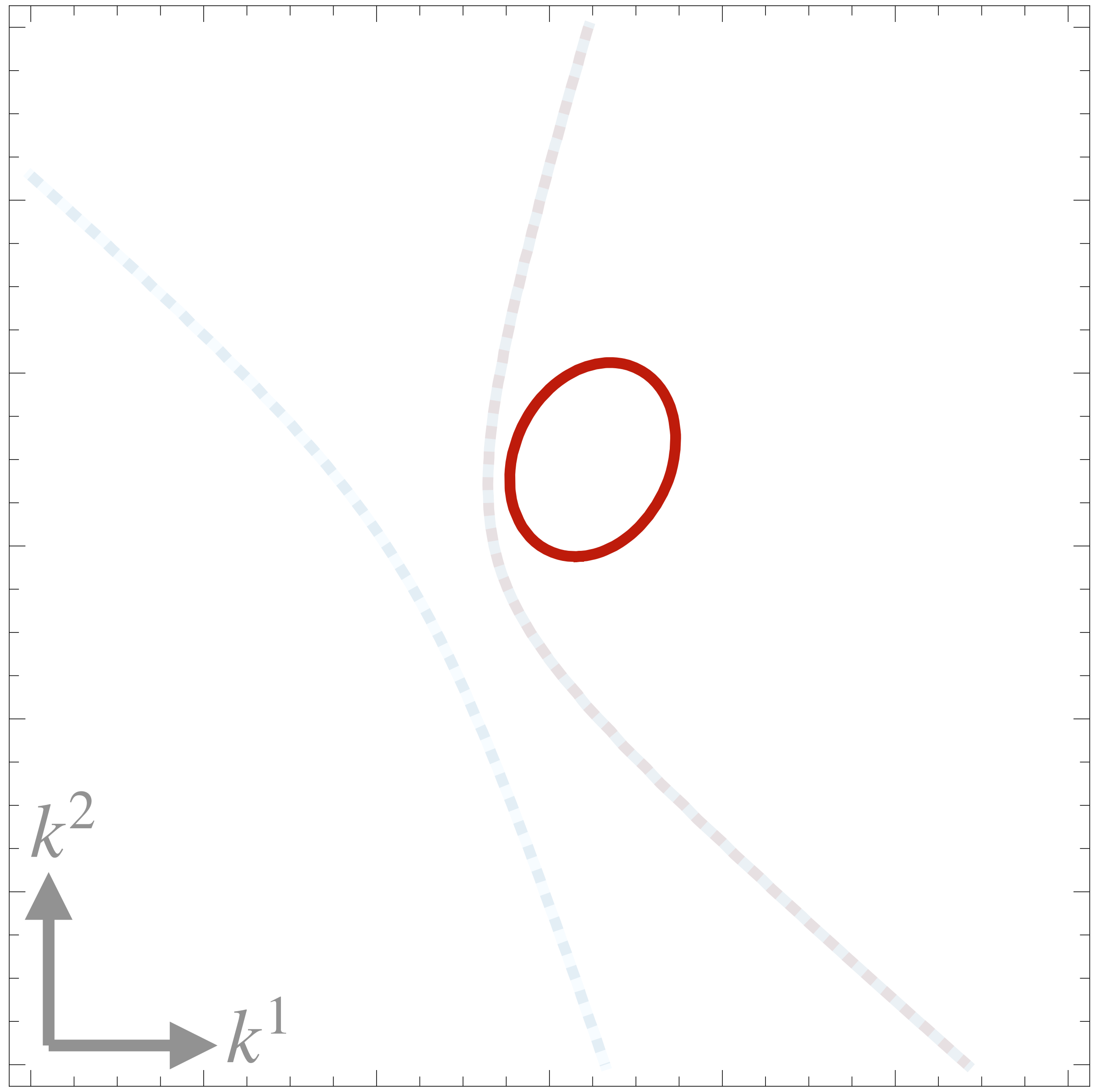
threshold singularities

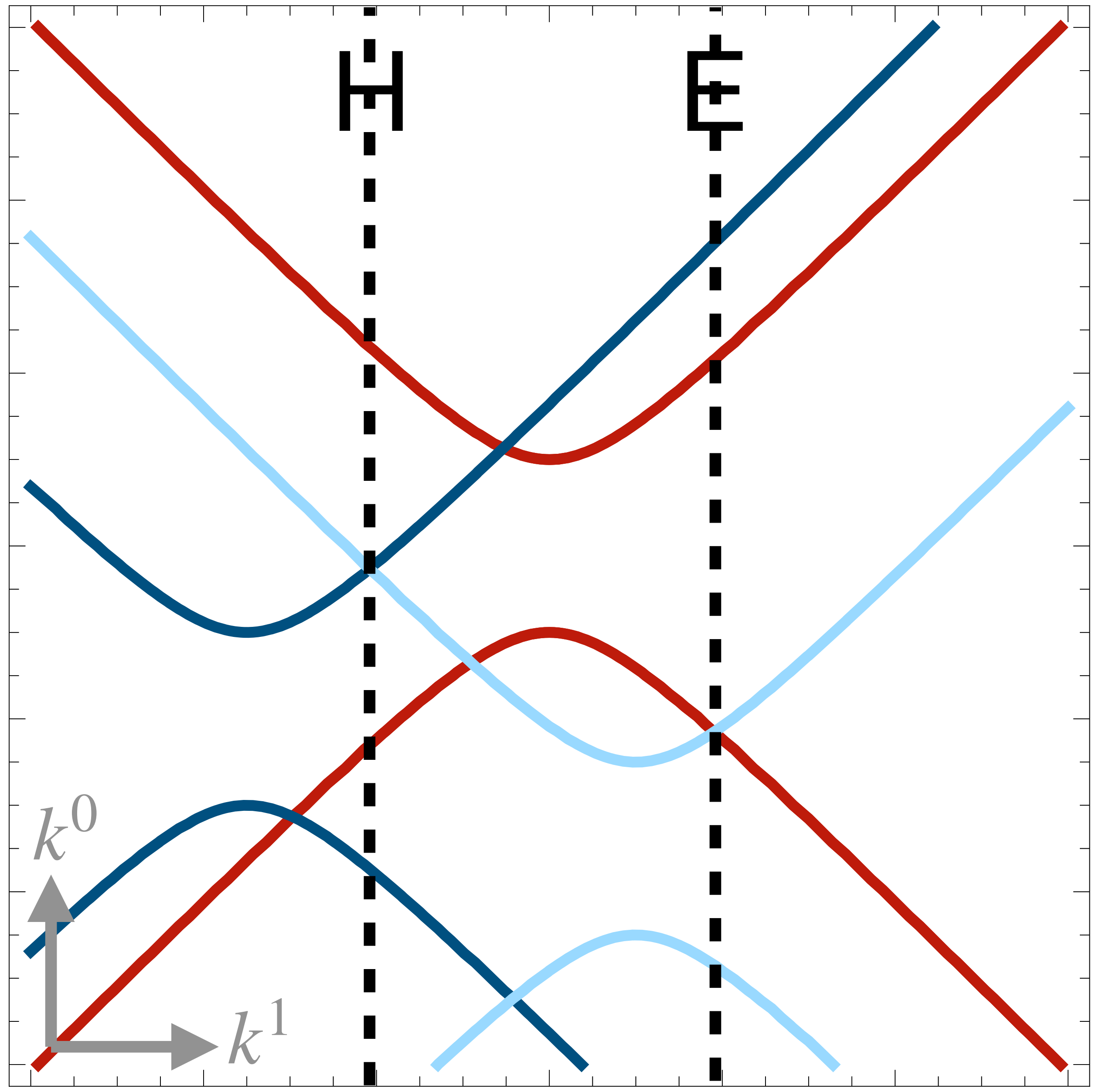
treated before numerical integration

→ contour deformation or subtraction







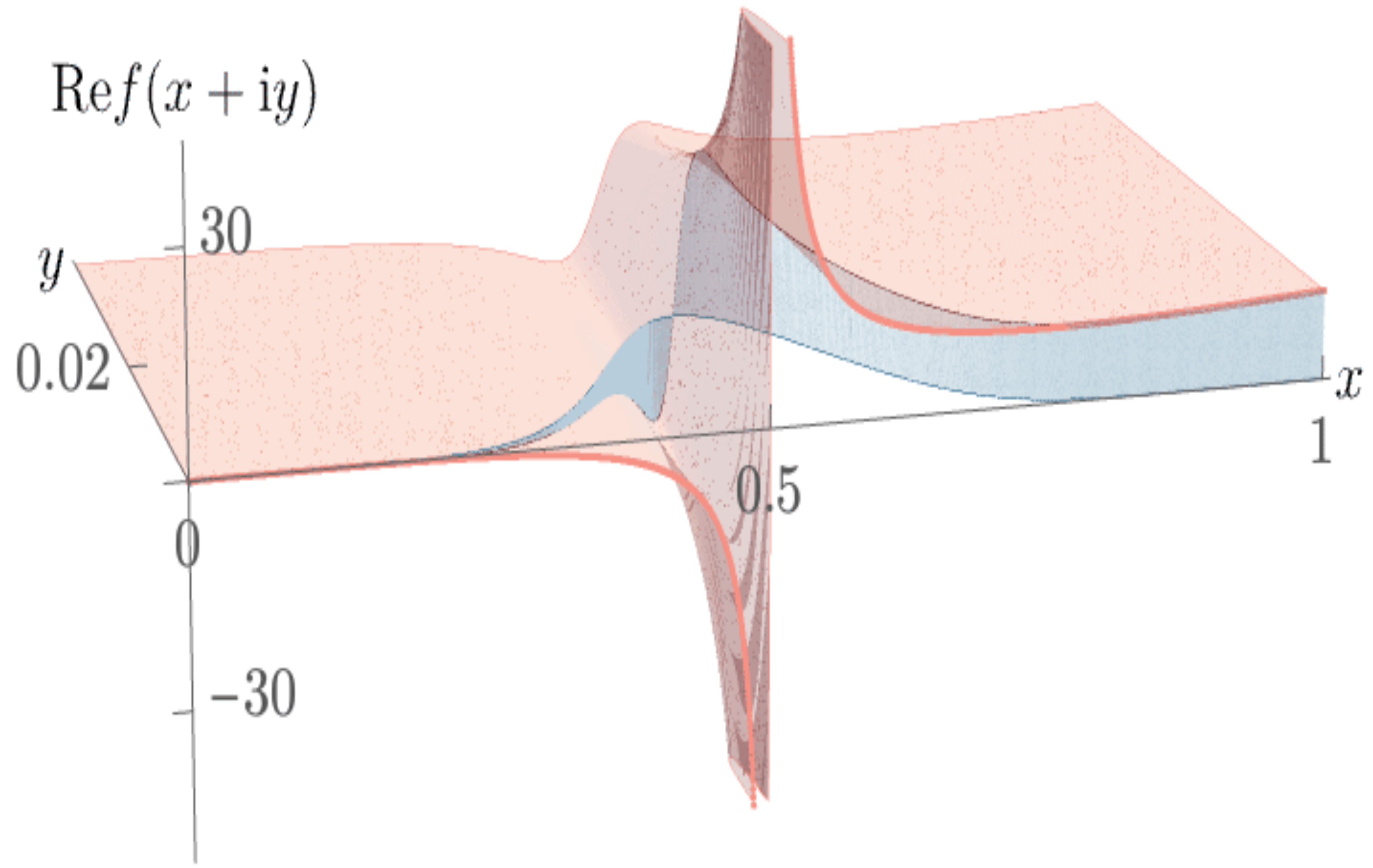


Monte Carlo numerical integration with poles

$$\lim_{\epsilon \to 0} \int_0^1 \frac{6x^3 \mathrm{d}x}{x - \frac{1}{2} + \mathrm{i}\epsilon} = 5 - \frac{3}{4}\mathrm{i}\pi$$

contour deformation

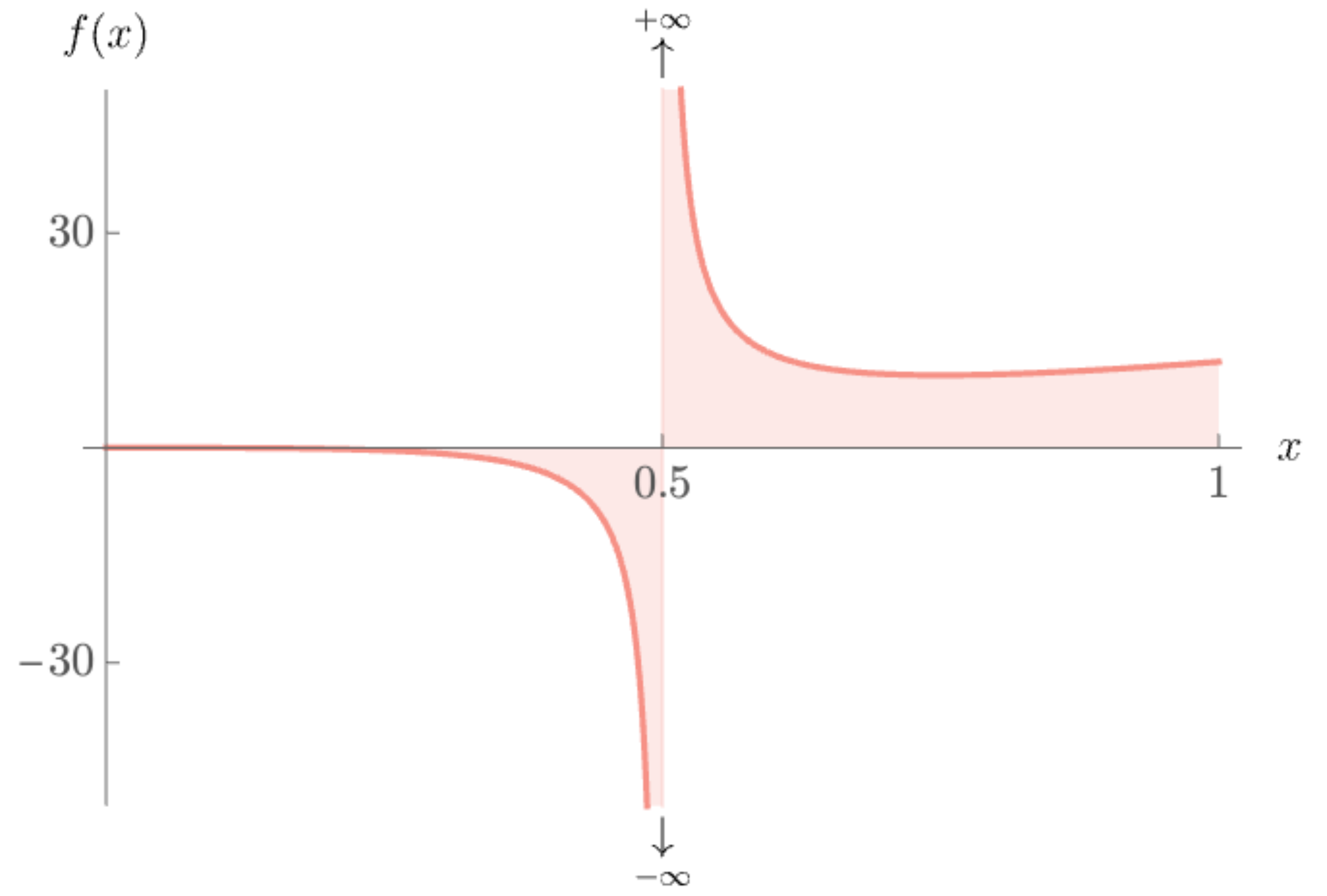
$\mathbb{R} \to \mathbb{C}$



use $\frac{1}{x - x_0 + \mathrm{i}\epsilon} = \mathrm{PV}\frac{1}{x - x_0} - \mathrm{i}\pi\delta(x_0)$ **& evaluate Cauchy Principal Value**

symmetric evaluation

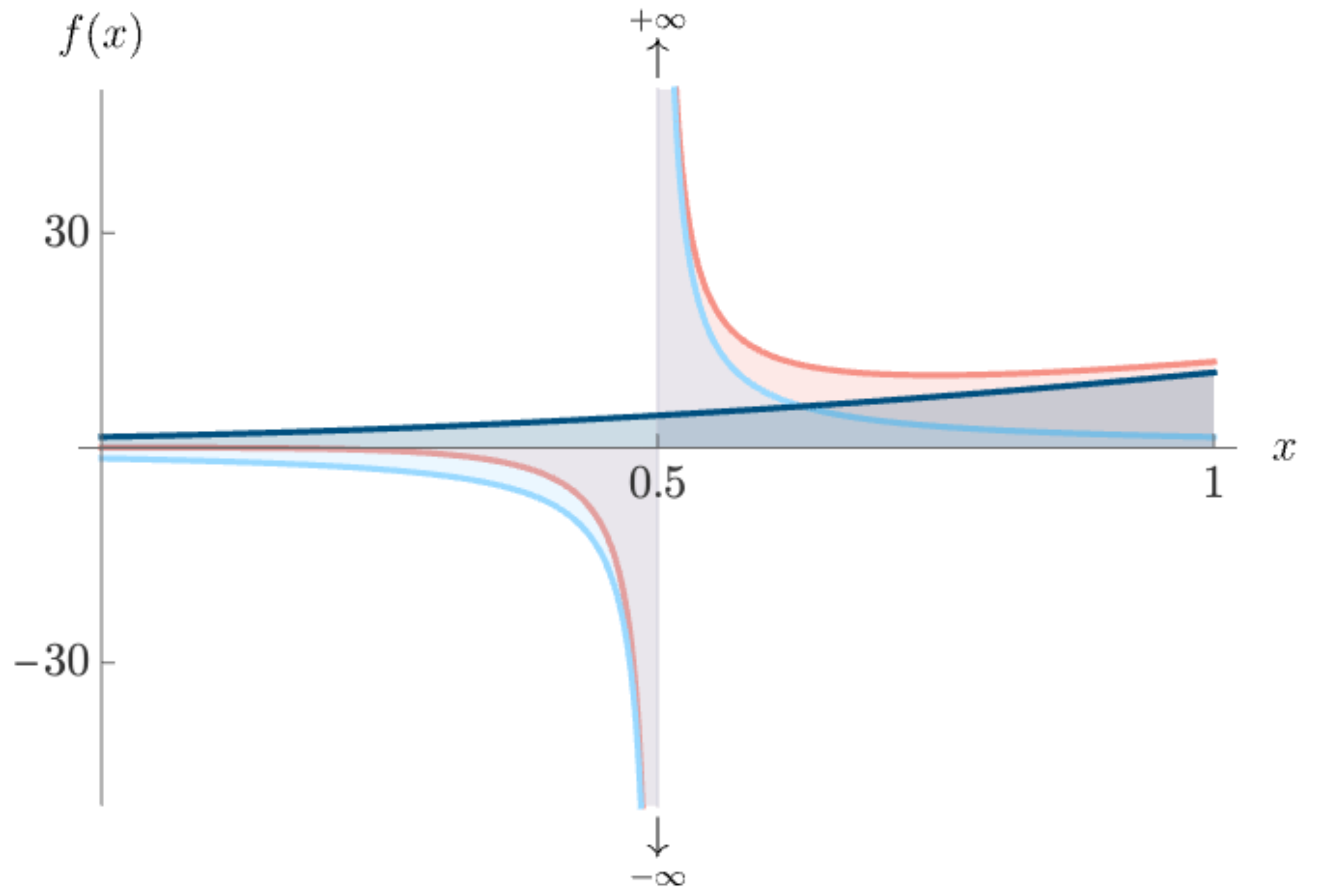
infinities cancel



subtraction

$f_{\mathrm{ct}}(x) = \frac{3}{4}\frac{1}{x - \frac{1}{2}}$ $\quad \mathrm{PV}\int_0^1 f_{\mathrm{ct}}(x)\,\mathrm{d}x = 0$

$f(x) - f_{\mathrm{ct}}(x) =$ function without poles



Subtraction of threshold singularities

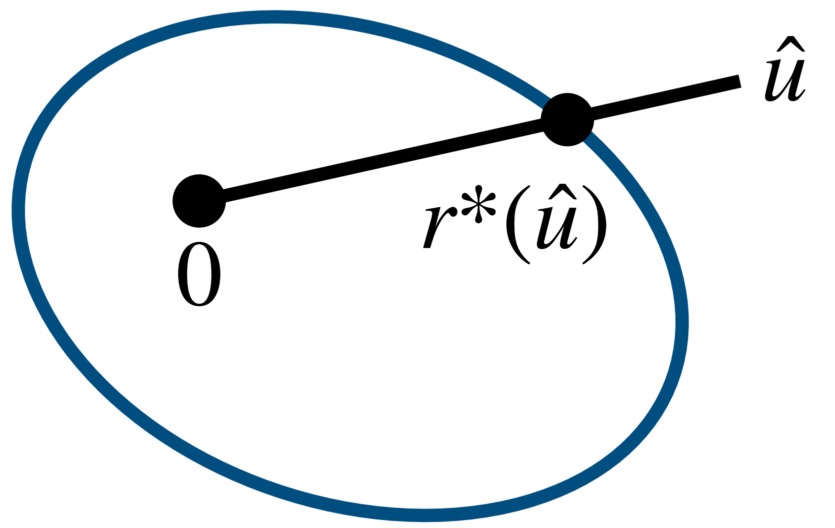
[Kilian, Kleinschmidt: 0912.3495]
[**DK**: 2110.06869]

Idea

$$\mathcal{I}_{\text{LTD}}(\vec{k}) = \frac{F(\vec{k})}{\mathscr{E}} \qquad \vec{k} = r\hat{u}$$

$$r^2 \mathcal{I}_{\text{LTD}}(r\hat{u}) = \underbrace{\frac{\overset{\text{residue}}{R_{\mathscr{E}}(\hat{u})}}{r - r^*(\hat{u})}}_{\sim \text{CT}_{\mathscr{E}}(r,\hat{u})} + \mathcal{O}\left((r - r^*(\hat{u}))^0\right)$$

$$\mathscr{E} \equiv E_i + E_j - p_i^0 + p_j^0 = 0$$



$$\frac{1}{x - x_0 + \text{i}\epsilon} = \text{PV}\frac{1}{x - x_0} - \text{i}\pi\delta(x_0) \quad \Rightarrow \quad \int \text{d}r\, \text{CT}_{\mathscr{E}}(r, \hat{u}) = -\,\text{i}\pi\, R_{\mathscr{E}}(\hat{u})$$

solve for $r^*(\hat{u})$
analytically (one loop)
or numerically (multi-loop)

$$\text{Re}\, I = -\int_{S^{3n-1}} \frac{\text{d}^{3n-1}\hat{u}}{(2\pi)^{3n}} \int_0^\infty \text{d}r \left(r^2 \mathcal{I}_{\text{LTD}}(r\hat{u}) - \sum_{\mathscr{E}\in E_O} \text{CT}_{\mathscr{E}}(r, \hat{u}) \right)$$

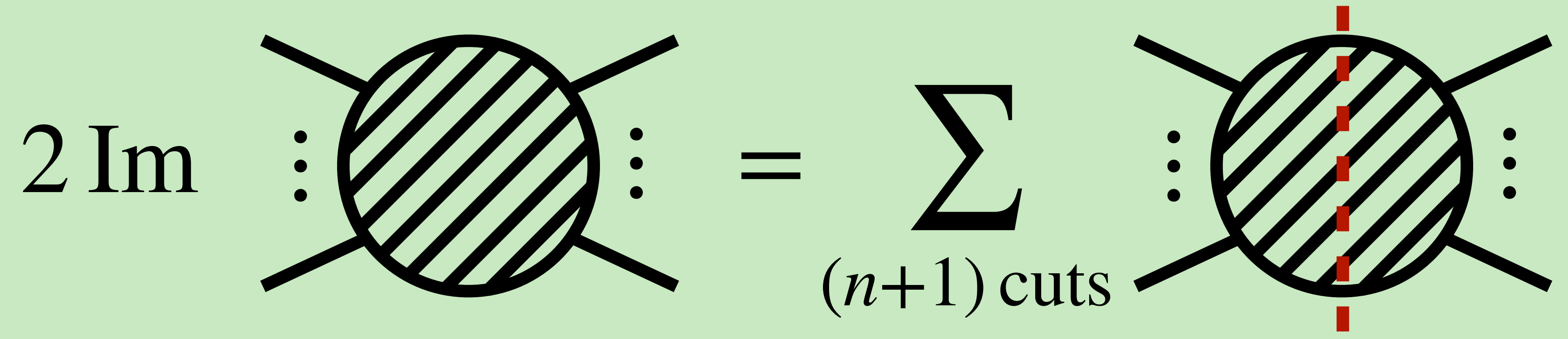
$$2\,\text{Im}\, A(i \to f) = \sum_x \int \text{d}\Pi_x\, A(i \to x)\, A^*(f \to x)$$

locally finite representation of generalised optical theorem (including local IR cancellations)

similar to:
[Soper: hep-ph/9804454, hep-ph/9910292]
Local Unitarity [Capatti, Hirschi, Pelloni, Ruijl: 2010.01068]

$$\text{Im}\, I = -\frac{1}{2}\int_{S^{3n-1}} \frac{\text{d}^{3n-1}\hat{u}}{(2\pi)^{3n-1}} \sum_{\mathscr{E}\in E_O} R_{\mathscr{E}}(\hat{u})$$

⚠️ residue ⇔ cut propagator



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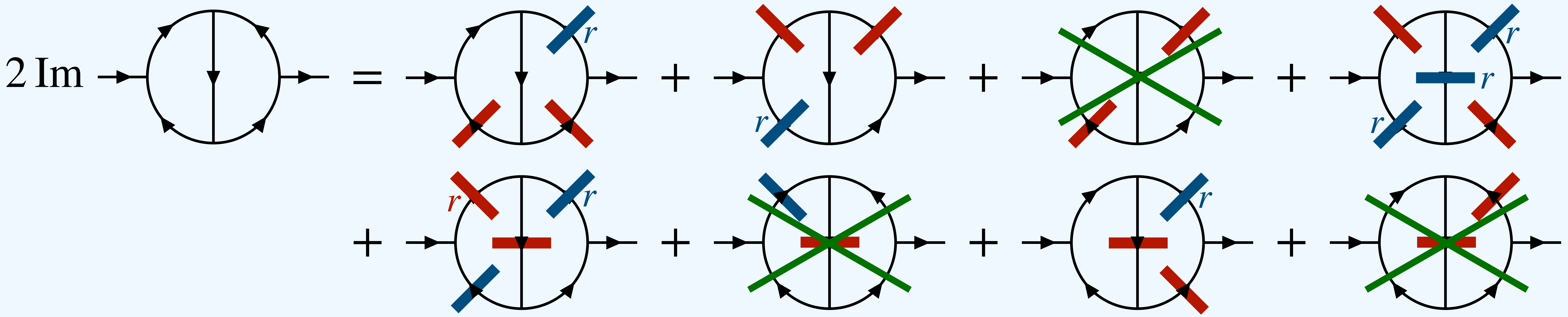
Local alignment of singularities: Identify all thresholds for $p^0 > 0$ and parameterise in r



→ Optical theorem but IR- and threshold singularities cancel *locally* among the summands!

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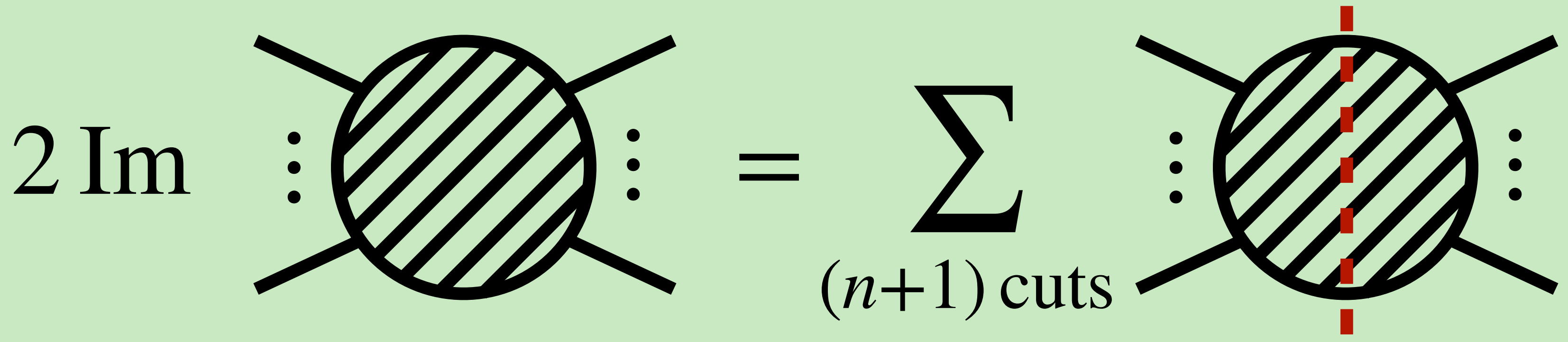

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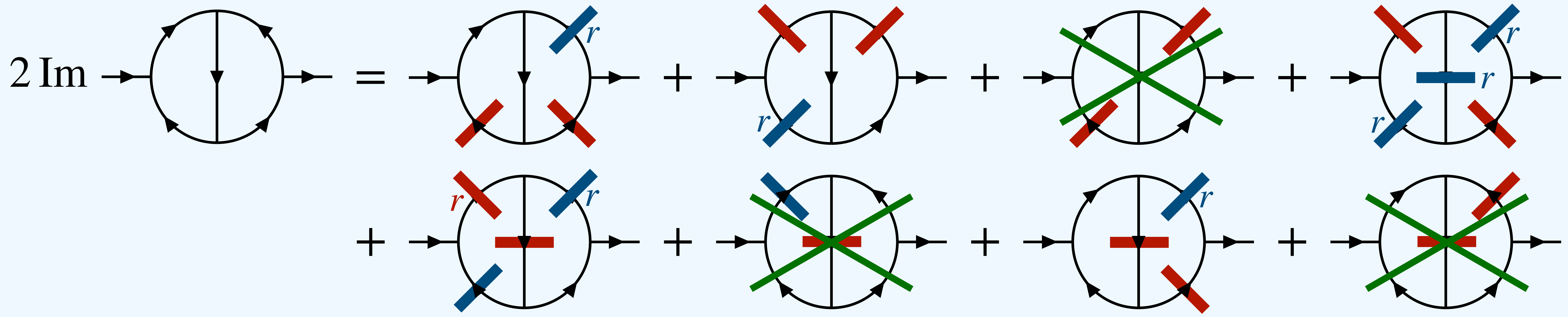

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*

representation depends on parameterisation

only valid if poles **never pinch** the r-contour

in particular if origin of spherical coordinates **inside all ellipsoids**

*

$$\mathrm{Re}\, I = -\int_{S^{3n-1}} \frac{\mathrm{d}^{3n-1}\hat{u}}{(2\pi)^{3n}} \int_0^\infty \mathrm{d}r \left(r^2 \mathcal{I}_{\mathrm{LTD}}(r\hat{u}) - \sum_{\mathscr{E}\in E_O} \mathrm{CT}_{\mathscr{E}}(r,\hat{u}) \right)$$

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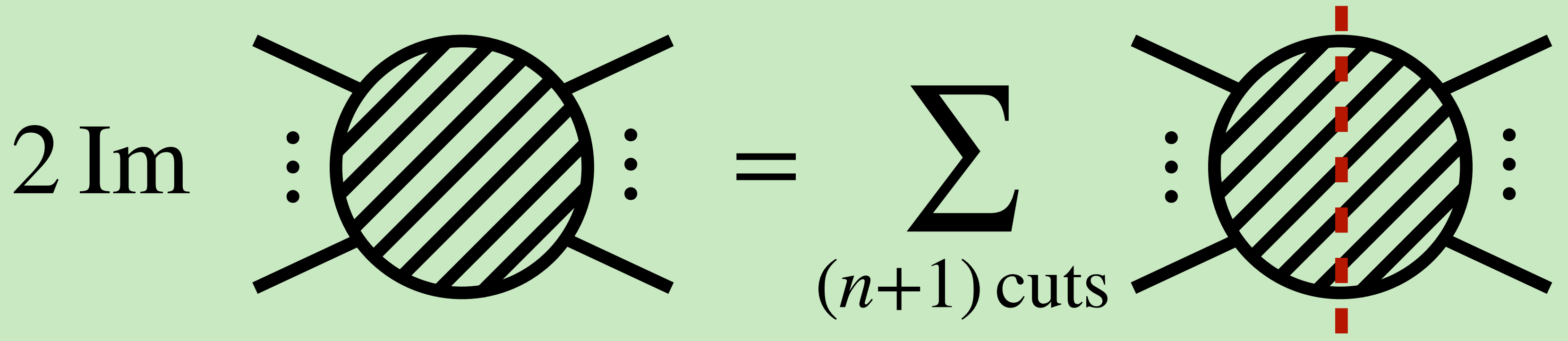
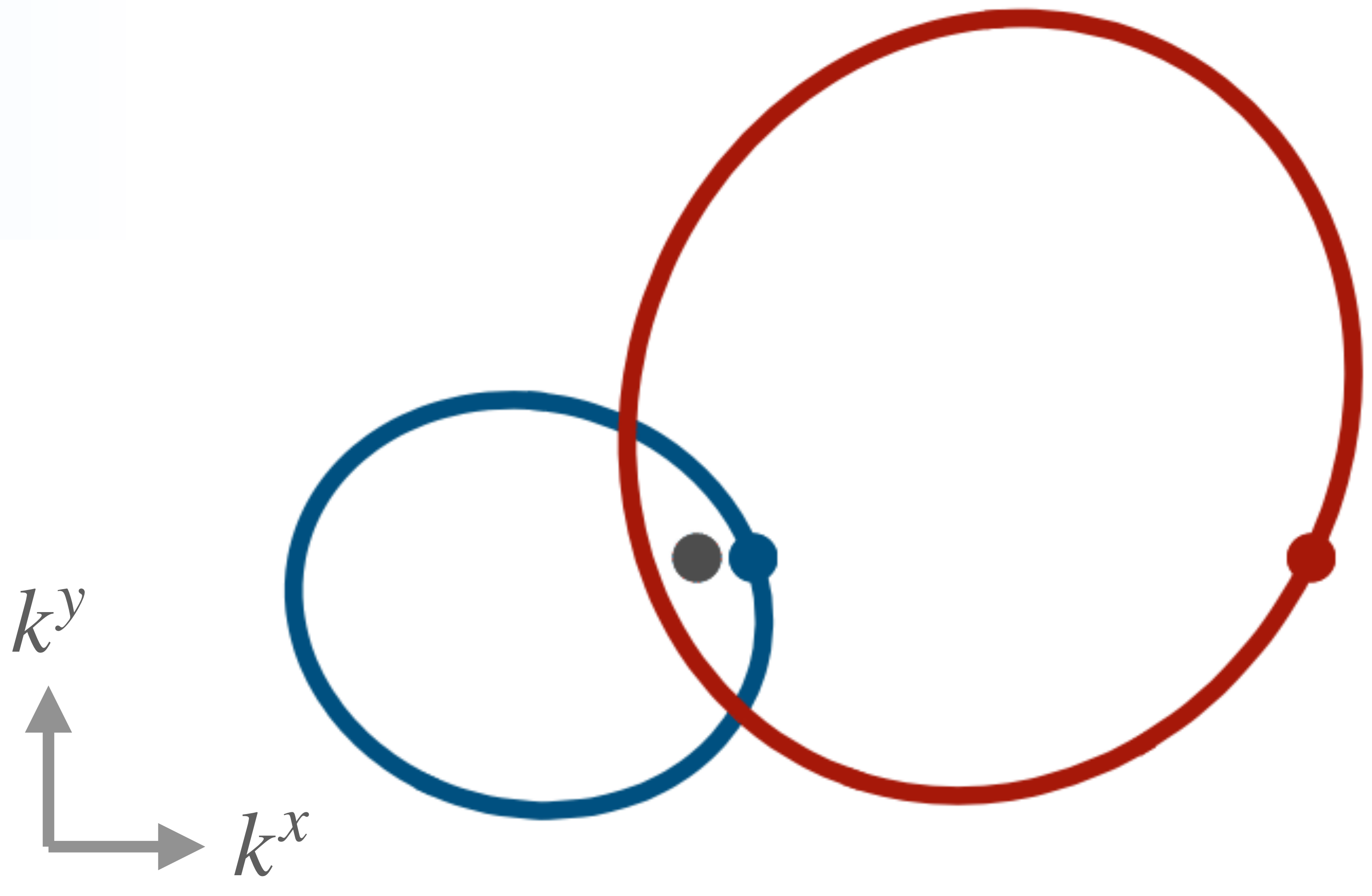
⚠ residue ⇔ cut propagator



Overlaps of threshold singularities

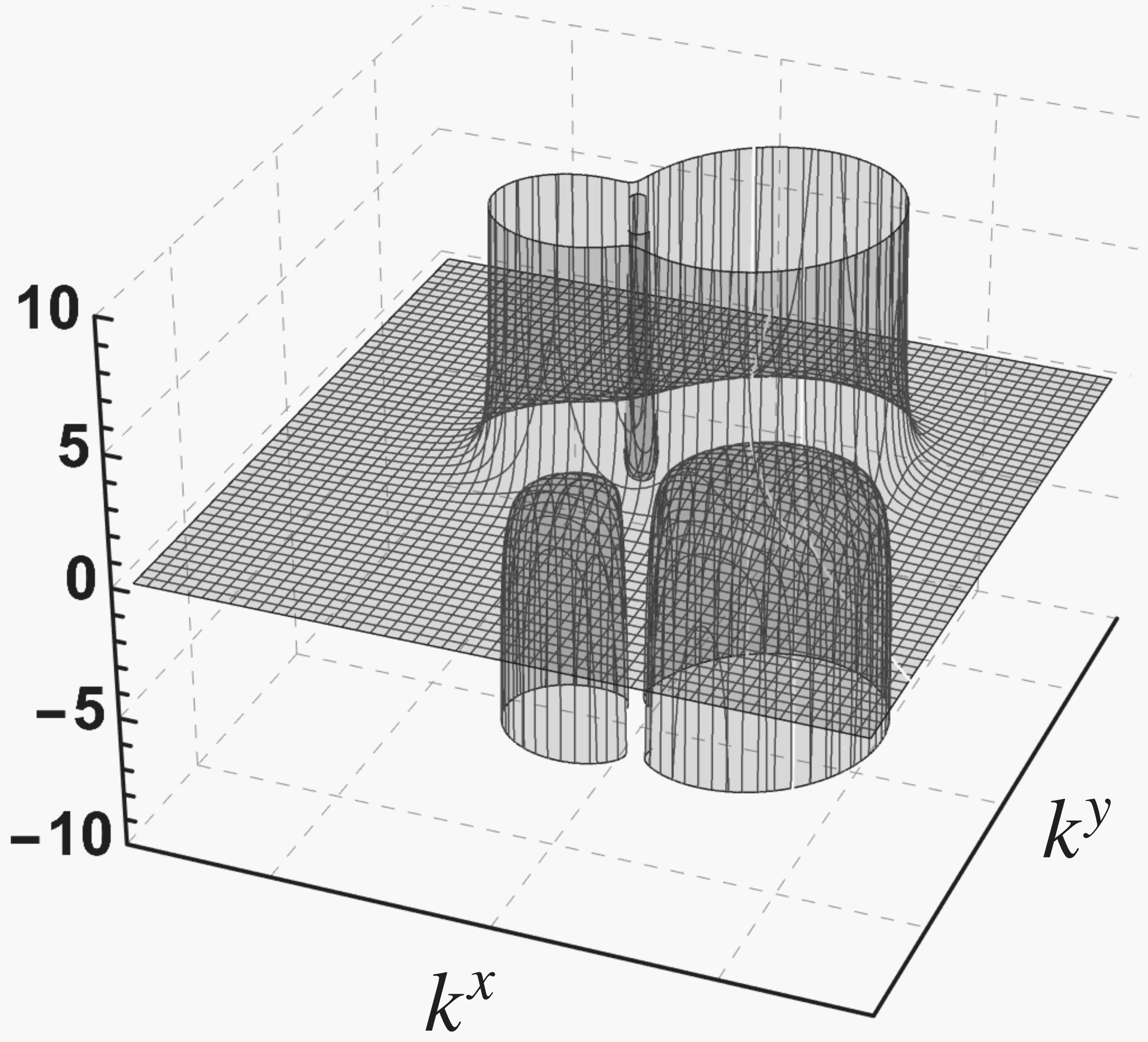
Construct a counterterm for each threshold

$$\mathrm{CT}_{\color{red}\bigcirc} \propto \frac{\mathrm{Res}_{\color{red}\bigcirc}[\mathcal{I}]}{r - r^*_{\color{red}\bigcirc}} \qquad \mathrm{CT}_{\color{blue}\circ} \propto \frac{\mathrm{Res}_{\color{blue}\circ}[\mathcal{I}]}{r - r^*_{\color{blue}\circ}}$$

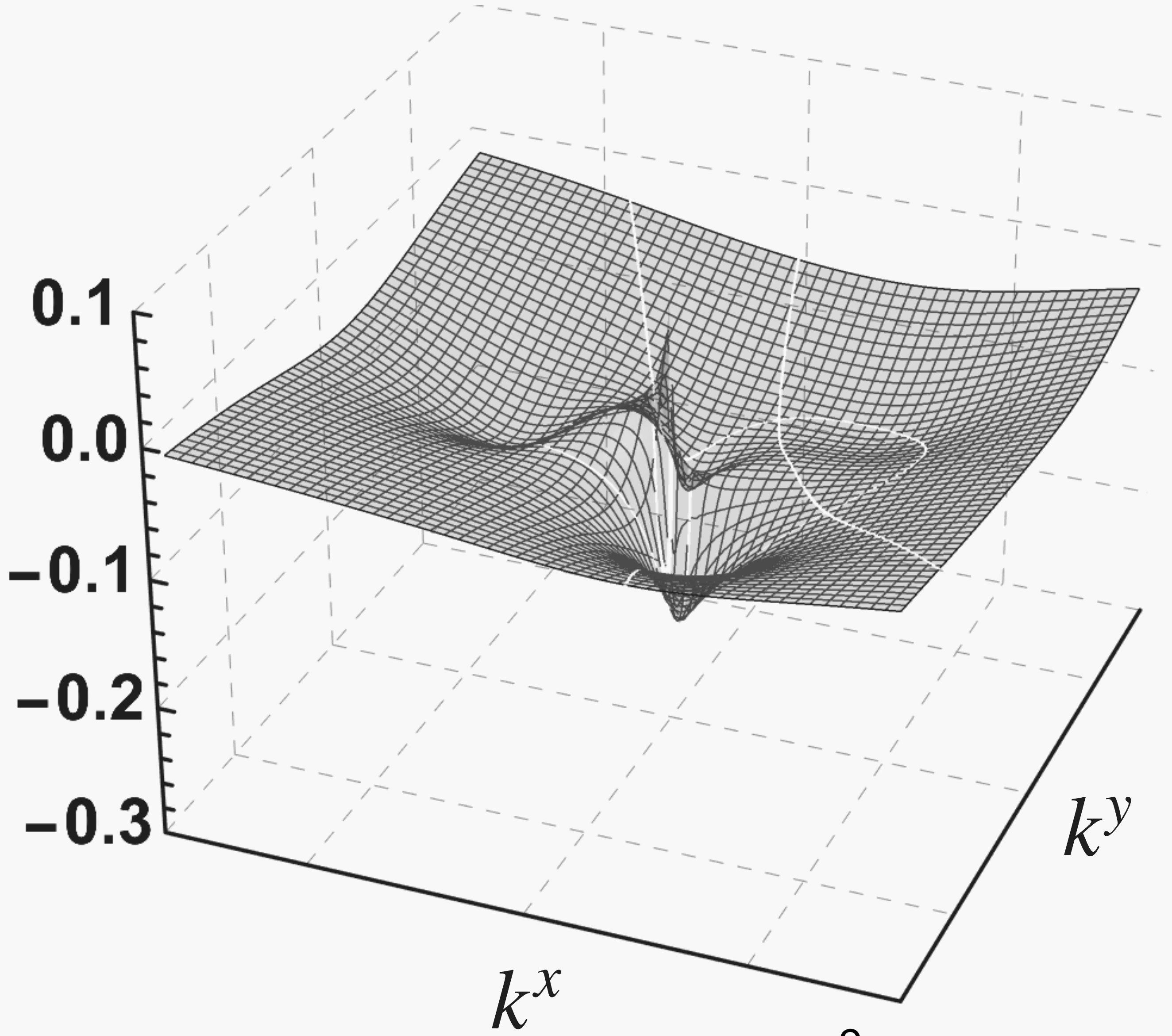


Real Part (Cauchy Principal Value)

$\mathcal{I}$

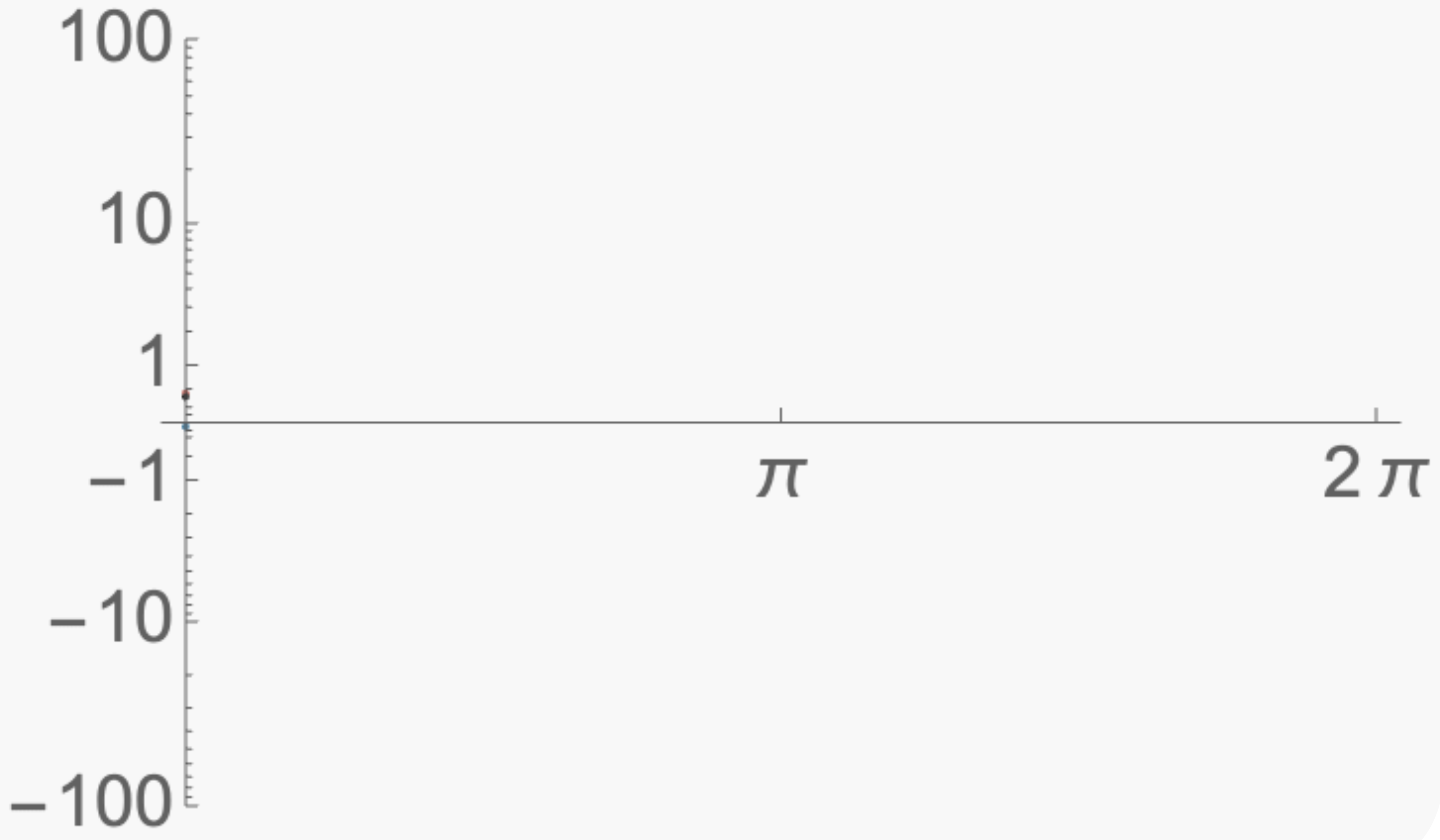


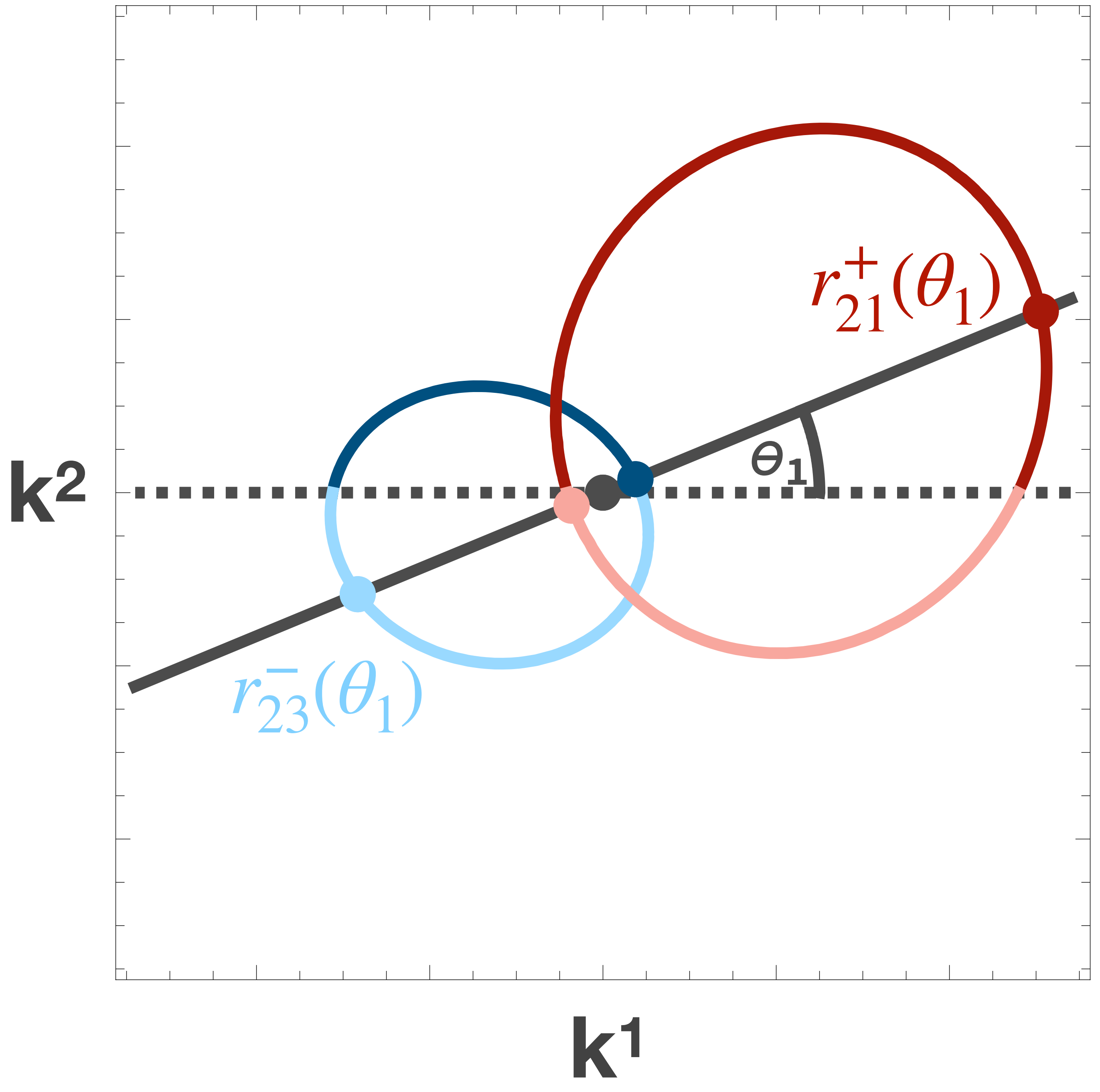
$\mathcal{I} - \mathrm{CT}_{\color{red}\bigcirc} - \mathrm{CT}_{\color{blue}\circ}$



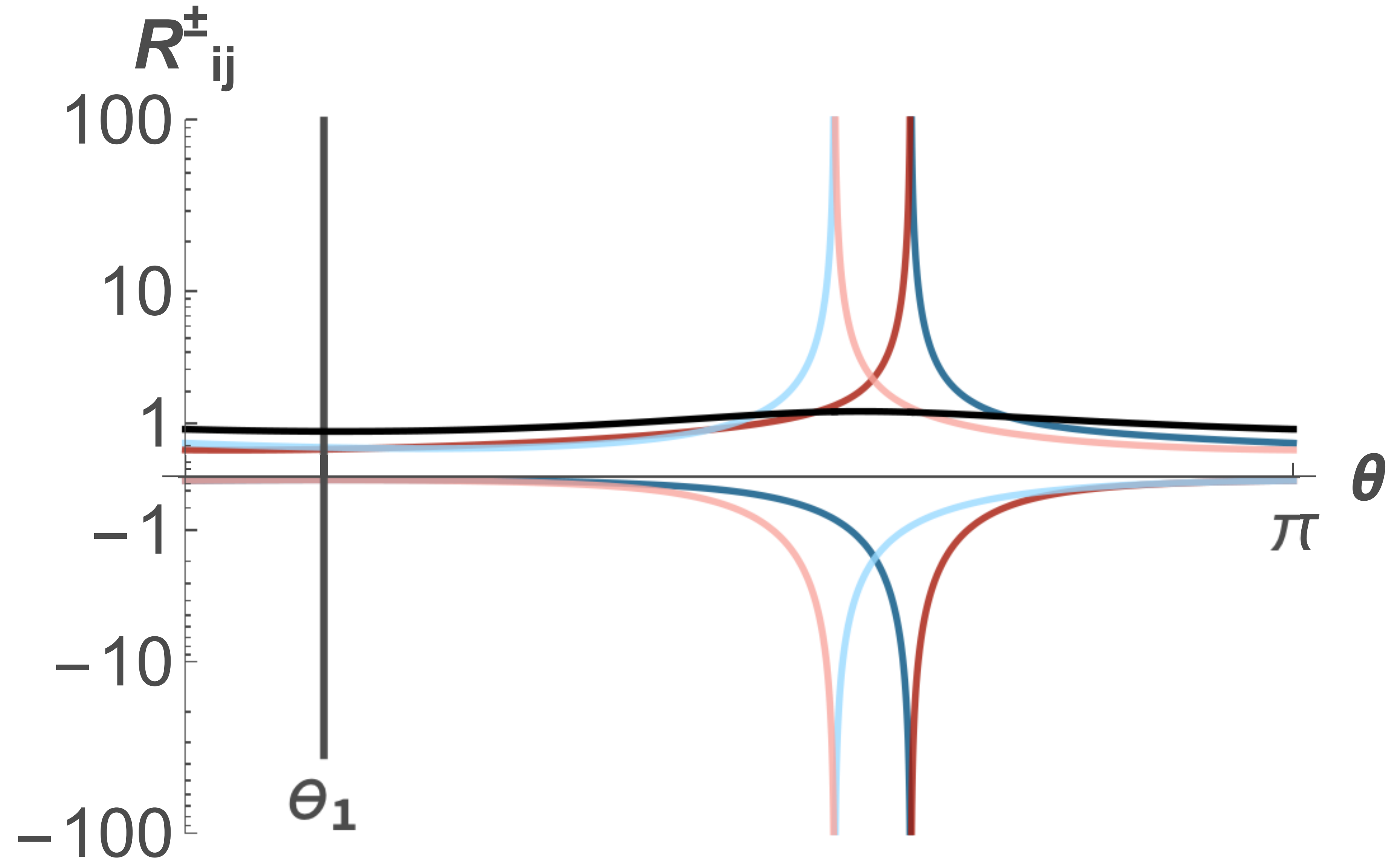
Imaginary Part (integrated couterterms)

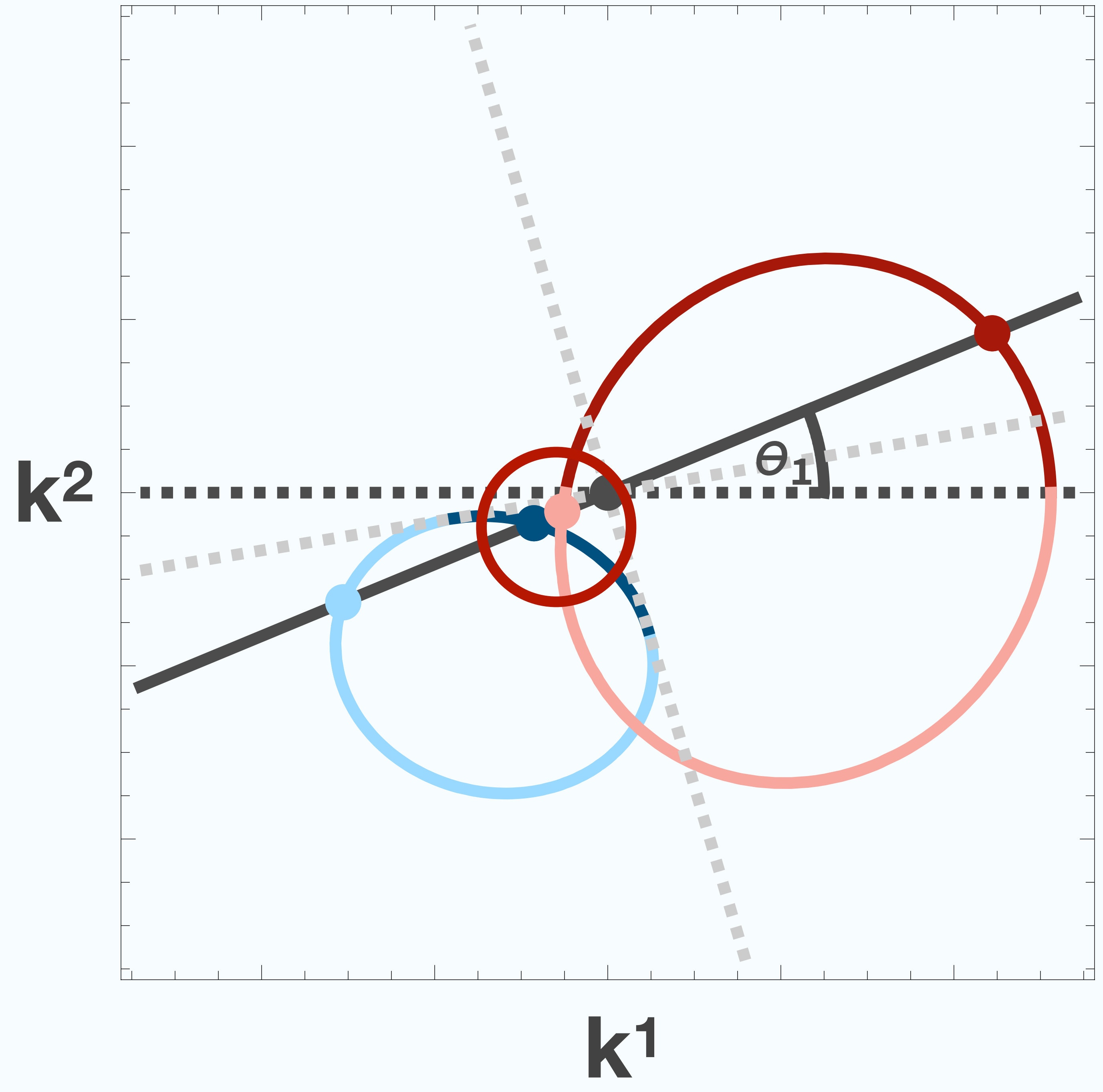
$\mathrm{Res}_{\color{red}\bigcirc}[\mathcal{I}] + \mathrm{Res}_{\color{blue}\circ}[\mathcal{I}]$



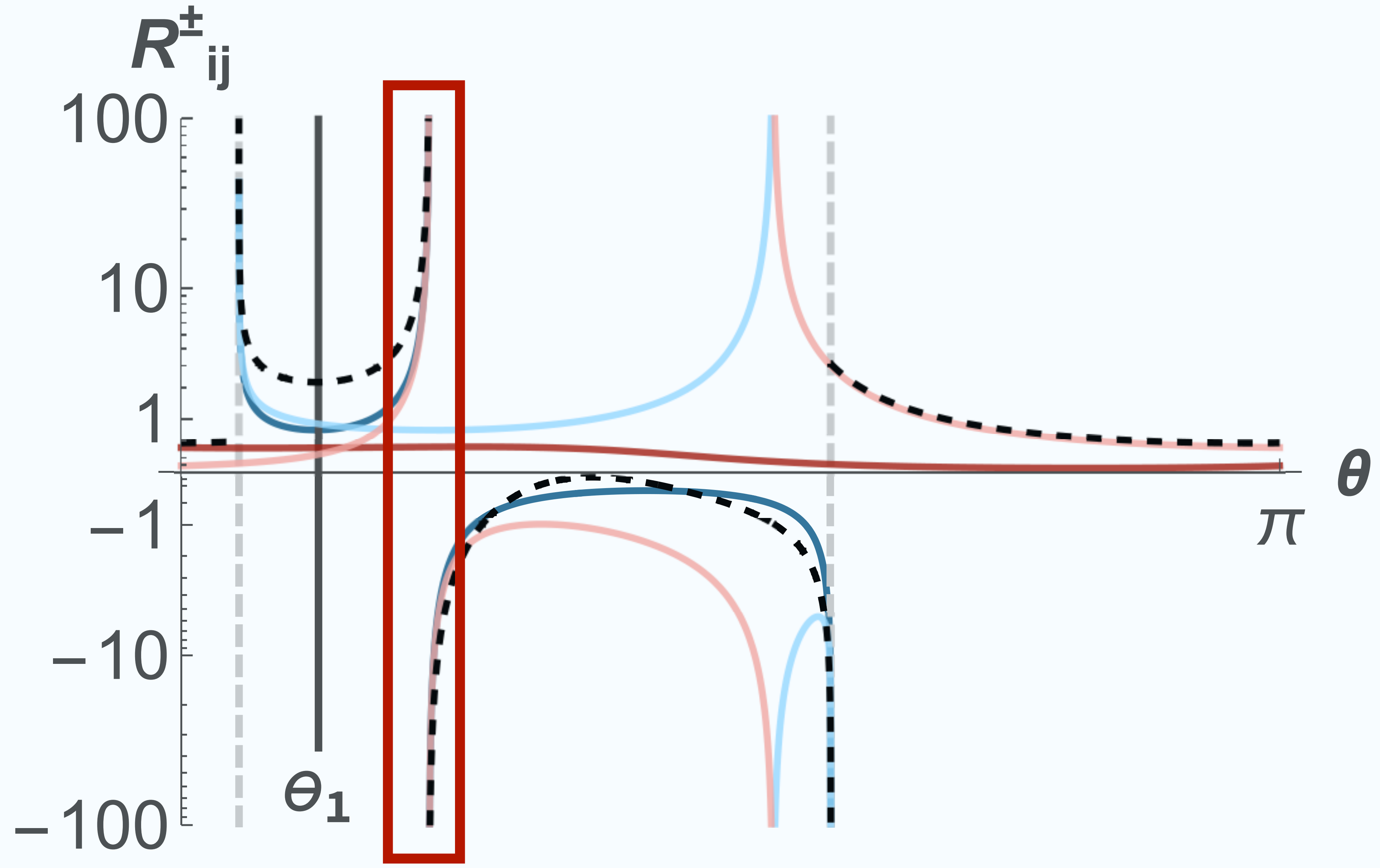


no locally pinched poles





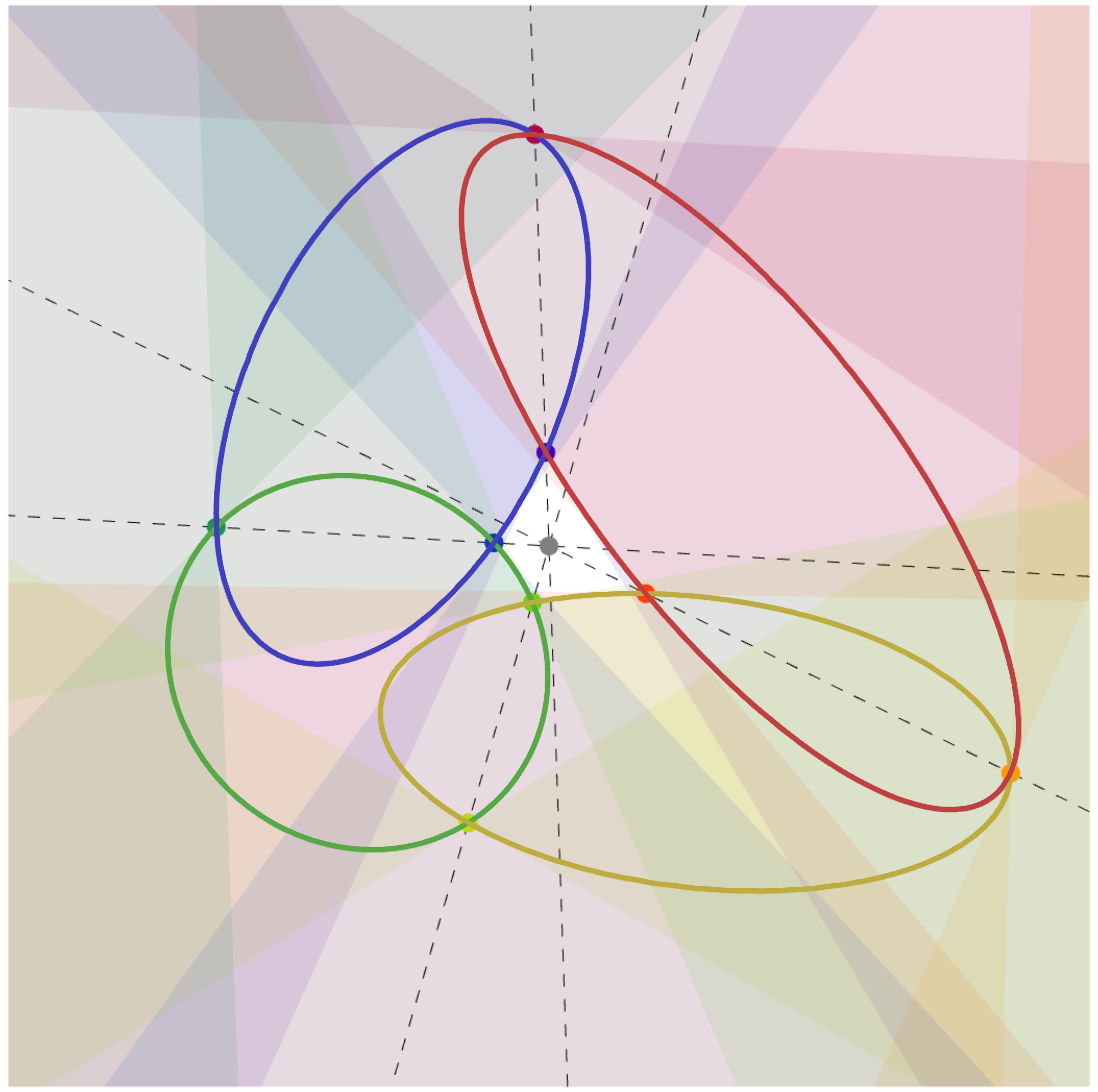
locally pinched poles



What to do if there is no single overlap?

centre outside overlap $\not\Rightarrow$ pinched poles

⚠️ but inconvenient integrable singularities



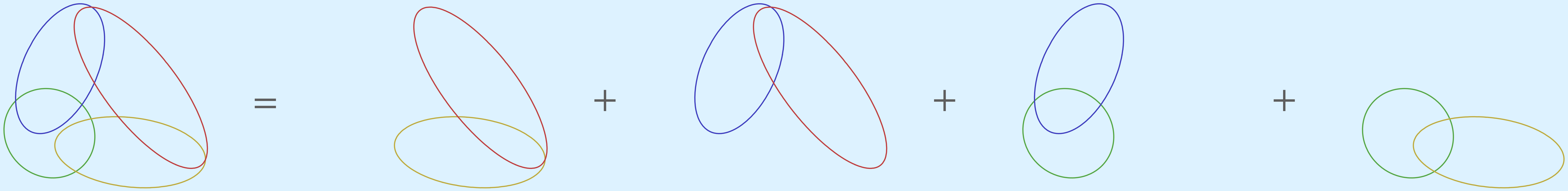
General observations

- not all intersections are double poles
  → group thresholds accordingly (only E-surfaces that share a LMB)
- using partial fractioning, TOPT, CFF to separate groups

Multi-channelling

build a channel for each overlap

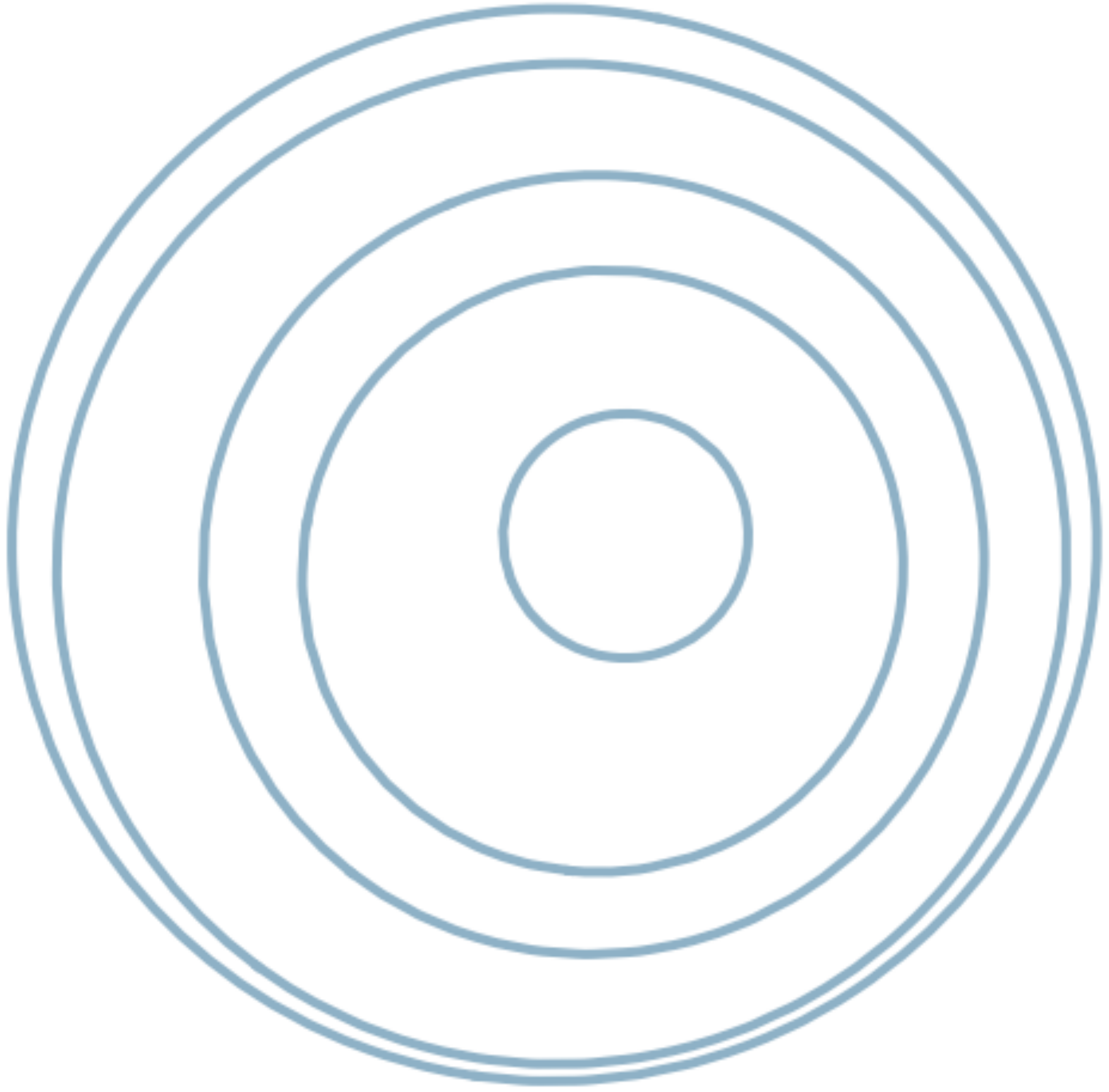
e.g. multiply with $1 = \frac{(\mathcal{E}_1\mathcal{E}_2)^2 + (\mathcal{E}_2\mathcal{E}_3)^2 + (\mathcal{E}_3\mathcal{E}_4)^2 + (\mathcal{E}_4\mathcal{E}_1)^2}{(\mathcal{E}_1\mathcal{E}_2)^2 + (\mathcal{E}_2\mathcal{E}_3)^2 + (\mathcal{E}_3\mathcal{E}_4)^2 + (\mathcal{E}_4\mathcal{E}_1)^2}$

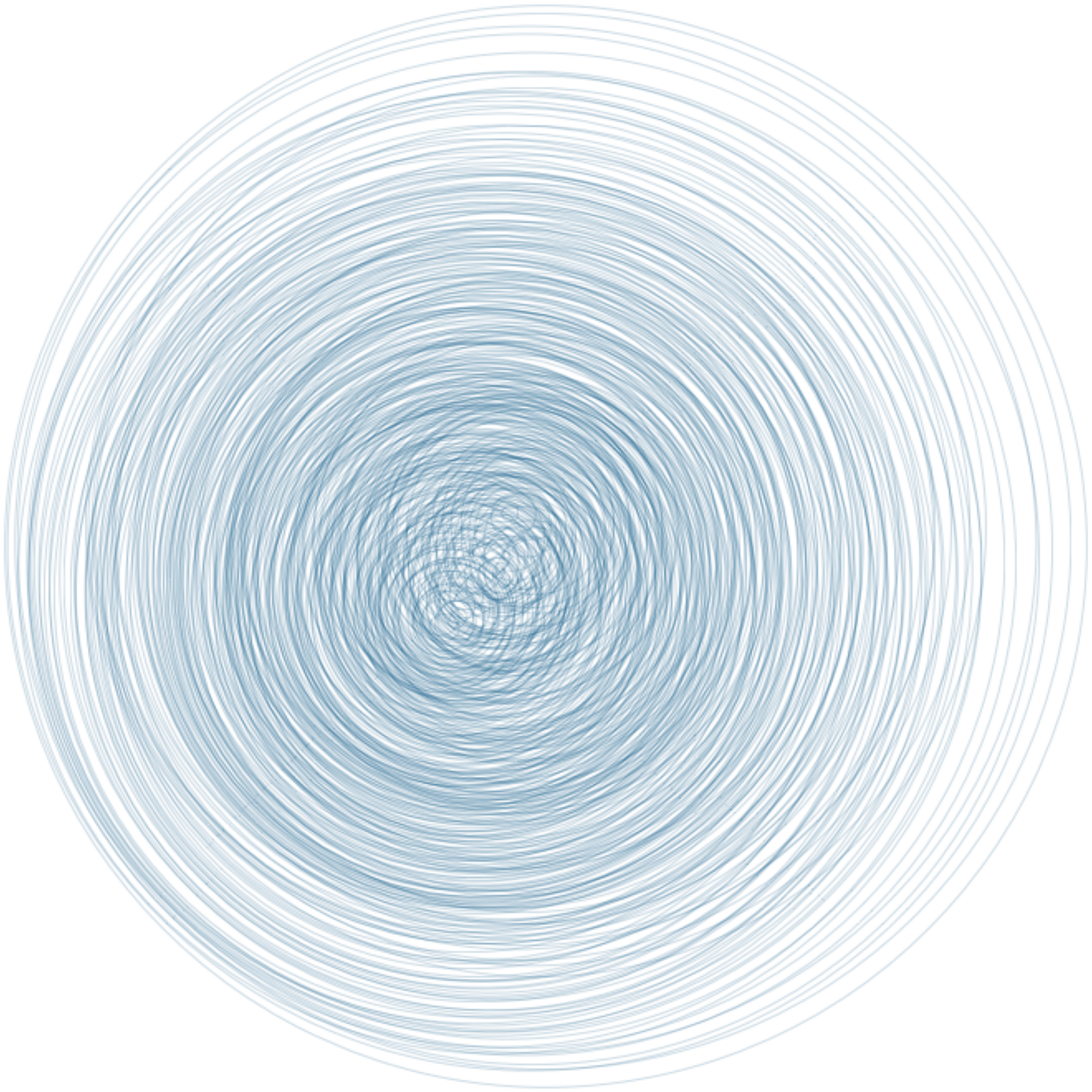


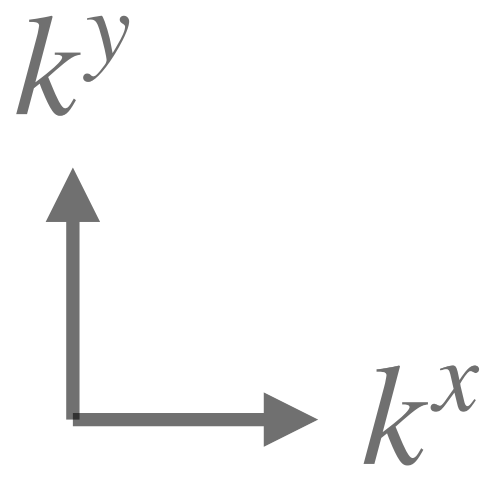
$$\mathcal{I} = \frac{(\mathcal{E}_1\mathcal{E}_2)^2}{(\mathcal{E}_1\mathcal{E}_2)^2 + (\mathcal{E}_2\mathcal{E}_3)^2 + (\mathcal{E}_3\mathcal{E}_4)^2 + (\mathcal{E}_4\mathcal{E}_1)^2}\mathcal{I} + \frac{(\mathcal{E}_2\mathcal{E}_3)^2}{(\mathcal{E}_1\mathcal{E}_2)^2 + (\mathcal{E}_2\mathcal{E}_3)^2 + (\mathcal{E}_3\mathcal{E}_4)^2 + (\mathcal{E}_4\mathcal{E}_1)^2}\mathcal{I} + \frac{(\mathcal{E}_3\mathcal{E}_4)^2}{(\mathcal{E}_1\mathcal{E}_2)^2 + (\mathcal{E}_2\mathcal{E}_3)^2 + (\mathcal{E}_3\mathcal{E}_4)^2 + (\mathcal{E}_4\mathcal{E}_1)^2}\mathcal{I} + \frac{(\mathcal{E}_4\mathcal{E}_1)^2}{(\mathcal{E}_1\mathcal{E}_2)^2 + (\mathcal{E}_2\mathcal{E}_3)^2 + (\mathcal{E}_3\mathcal{E}_4)^2 + (\mathcal{E}_4\mathcal{E}_1)^2}\mathcal{I}$$

Threshold subtraction is stable for high multiplicities of external legs

Topology	Kin.	N_E	N_G	N_G^{max}	N_P	Phase	Exp.	Reference	Numerical	Δ [σ]	Δ [%]	Δ [%]|·|
 Triacontagon	1L30P.I	5	1	1	10^9	Re	-02	-1.007398	-1.007449 +/- 0.001467	0.035	0.005	0.002
					10^9	Im		3.175180	3.175183 +/- 0.000085	0.030	8e-05	
	1L30P.II	6	1	1	10^9	Re	-12	-4.166377	-4.165527 +/- 0.006697	0.127	0.020	0.016
					10^9	Im		3.413930	3.413917 +/- 0.000075	0.182	4e-04	
	1L30P.III	408	15	354	10^9	Re	-09	-2.991654	-2.984733 +/- 0.026977	0.257	0.231	0.231
					10^9	Im		-0.000000	-0.000001 +/- 0.003831	3e-04		
	1L30P.IV	408	15	354	10^9	Re	-07	-1.757748	-1.757913 +/- 0.002169	0.076	0.009	0.009
					10^9	Im		-0.000000	0.000001 +/- 0.000199	0.007		







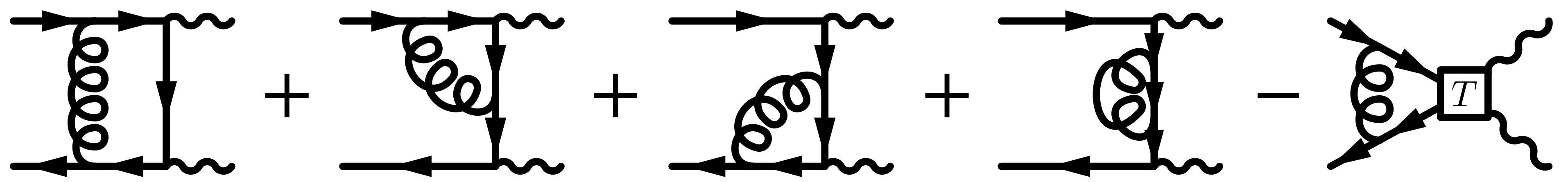
Numerical integration of scattering amplitudes

Numerical integration of finite amplitudes in $D = 4$

- Exploit local factorisation of IR singularities
  [Anastasiou, Haindl, Sterman, Yang, Zeng: 2008.12293]
  [Anastasiou, Sterman: 2212.12162]
- Local UV counterterms with BPHZ / R* operation
  [Bogoliubov, Parasiuk, Hepp, Zimmermann]
  [Chetyrkin, Tkachov, Smirnov]
  [Herzog, Ruijl: 1703.03776]

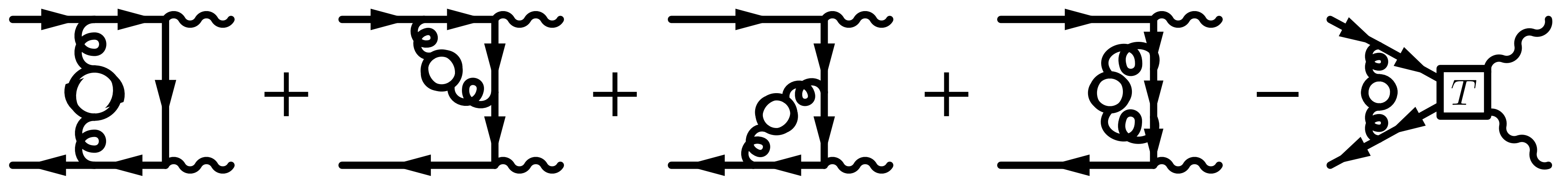
Example: $e^+ e^- \to \gamma^{(*)}\, \gamma^{(*)}$
[Anastasiou, Haindl, Sterman, Yang, Zeng: 2008.12293]

One loop



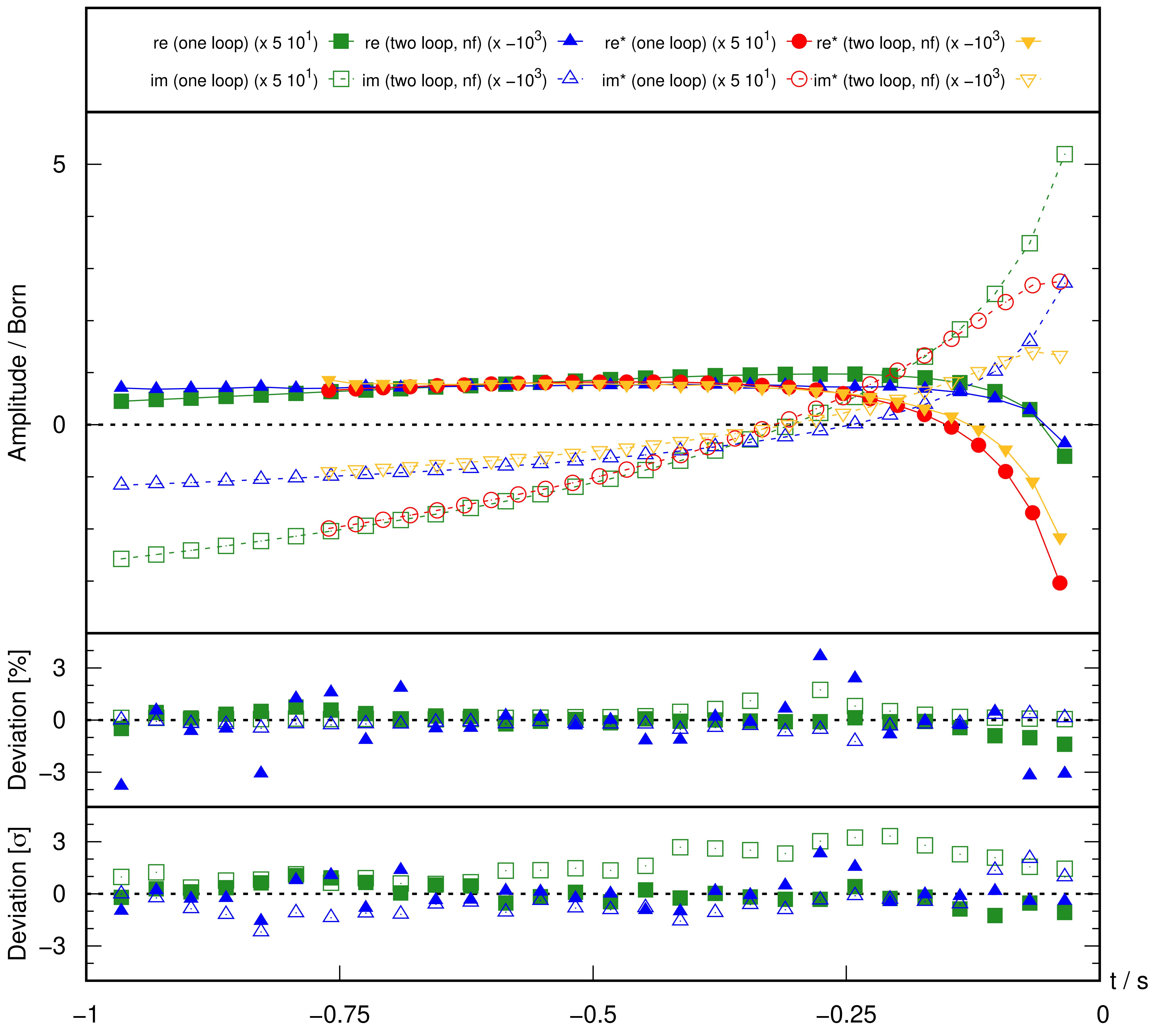
$- \mathrm{CT}_{\mathrm{UV}}$

Two loop n_f



$- \mathrm{CT}_{\mathrm{UV}}$

Subtracted (finite) amplitude for $e^+ e^- \to \gamma^{(*)} \gamma^{(*)}$



thanks to C. Anastasiou, J. Karlen, A. Lazopoulos, M. Vicini

Conclusion

Gained understanding of threshold singularity structure and cancellation mechanisms in loop integrals at $\mathscr{A}-$level *and* cross sections at $|\mathscr{A}|^2-$level

Presented tools to tackle challenging multi-loop integrals, amplitudes (and fully inclusive cross sections) with Monte Carlo numerical integration

- (causal) Loop-Tree Duality, TOPT, CFF

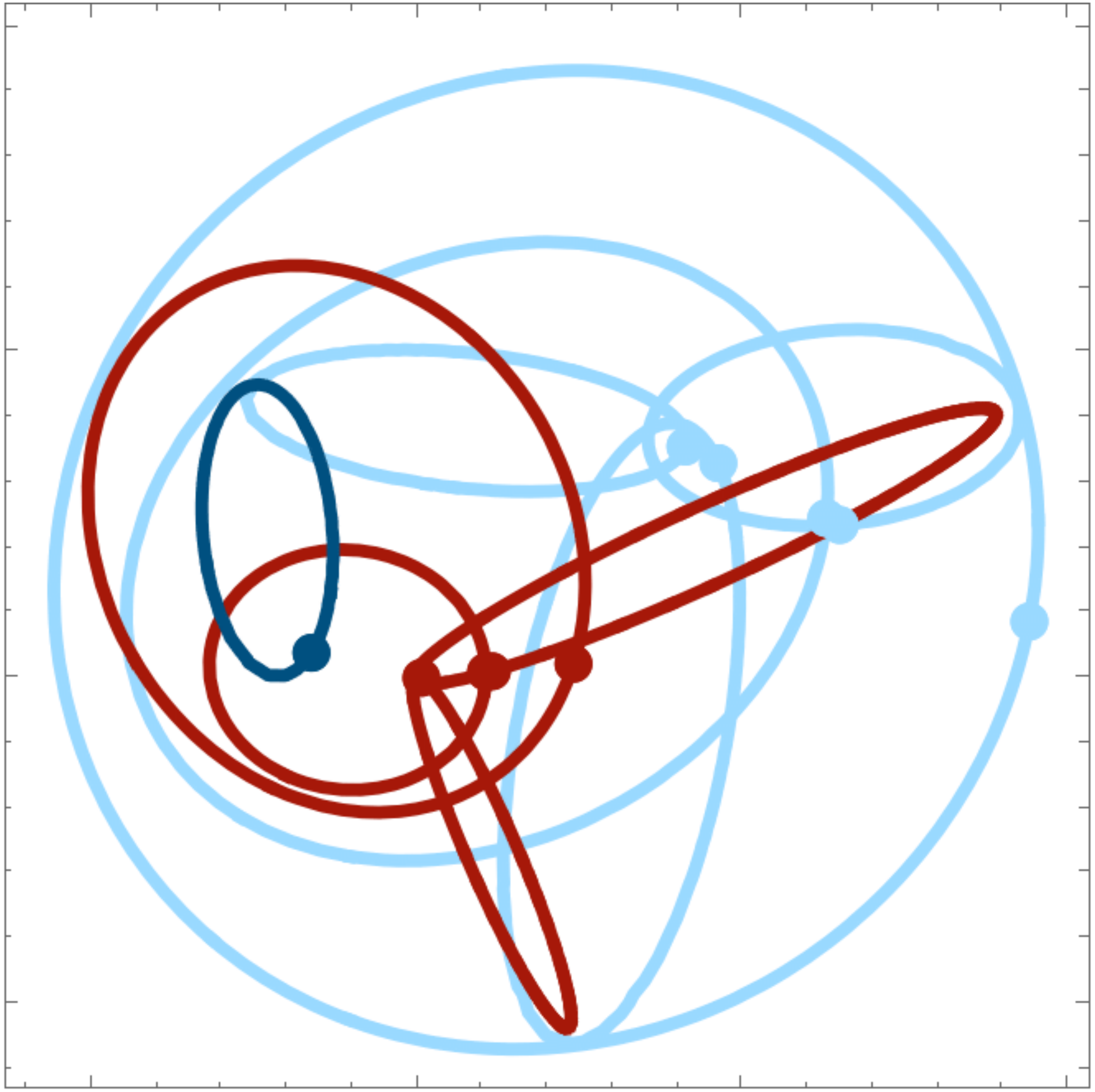
  → convenient threshold structure
- Threshold subtraction

  → flat integrand and efficient integration

  → locally finite optical theorem (access to direct numerical integration of cross sections)

→ improvements & extensions necessary for differential cross sections

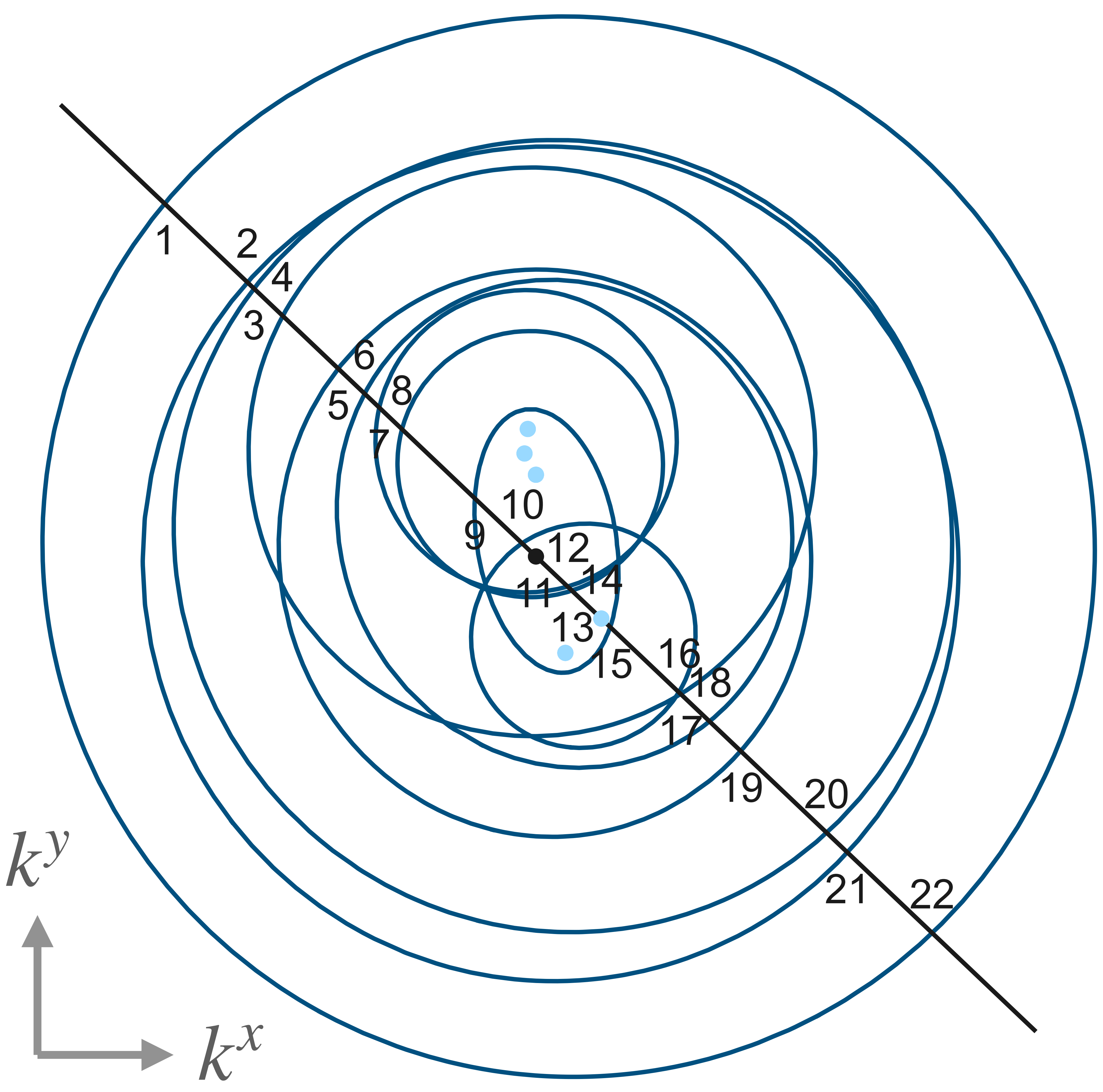
→ ready for uncharted territory of two-loop amplitudes



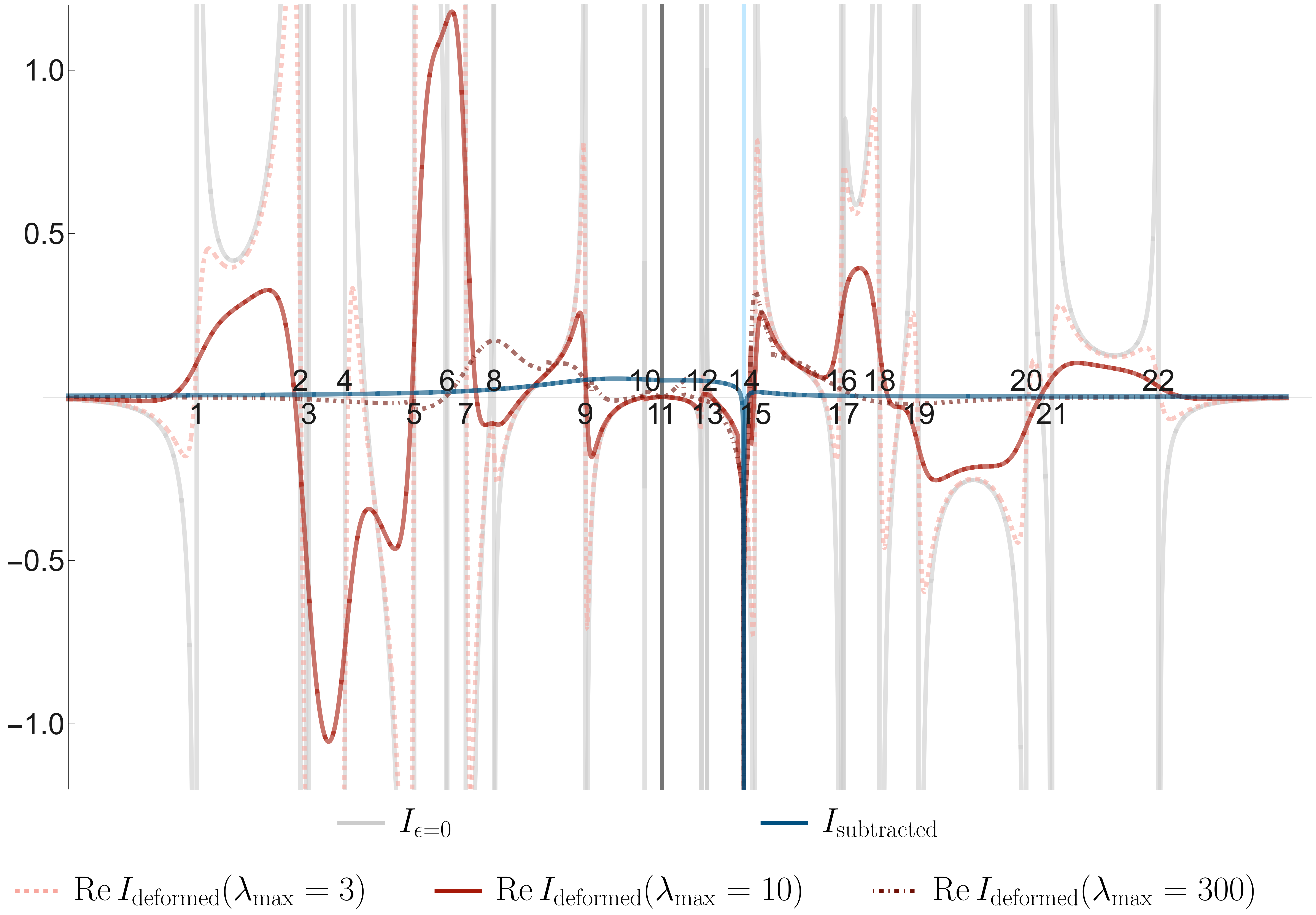
Thank you!

Backup

Comparison of threshold subtraction & contour deformation



threshold singularities of a pentagon



integrand of real part along line segment obtained using **threshold subtraction** or **contour deformation** with different maximal deformation magnitude