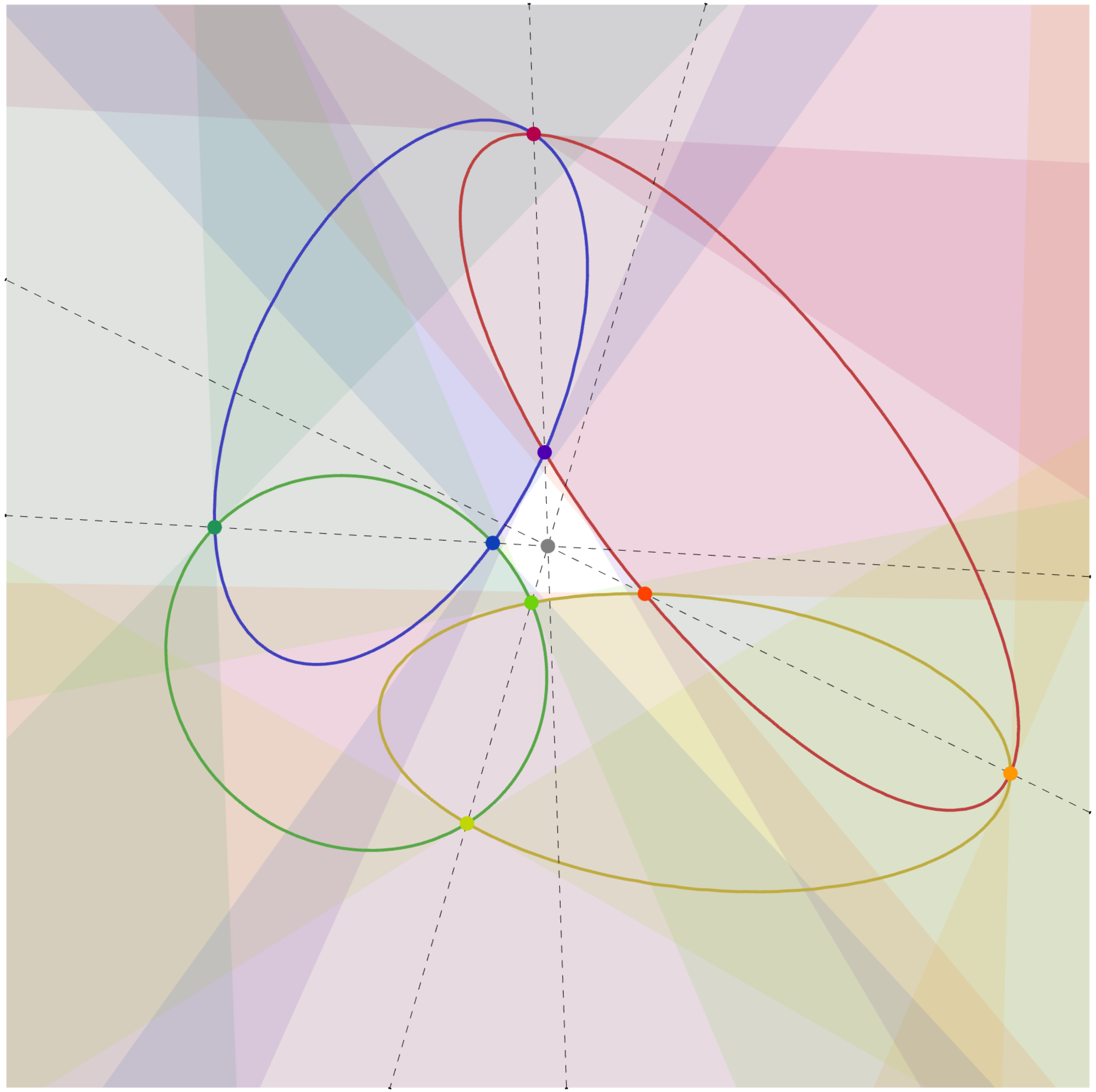
Numerical Integration of Loop Amplitudes in Momentum Space

Dario Kermanschah

Theory Challenges in the Precision Era of the Large Hadron Collider

GGI Workshop, 14.9.23, Florence



GGI TUM ETH zürich

Predictions for hadron collisions

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

numerical

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

numerical!

~~analytical?~~

LO $|\mathscr{A}_n^{(0)}|^2$

NLO $2\,\mathrm{Re}\,\mathscr{A}_n^{(1)}\left(\mathscr{A}_n^{(0)}\right)^* + |\mathscr{A}_{n+1}^{(0)}|^2$

automated

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

two-loop amplitude:

many two-loop integrals

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

→ sidestep using direct numerical integration?

double real-emission:

infrared singularities

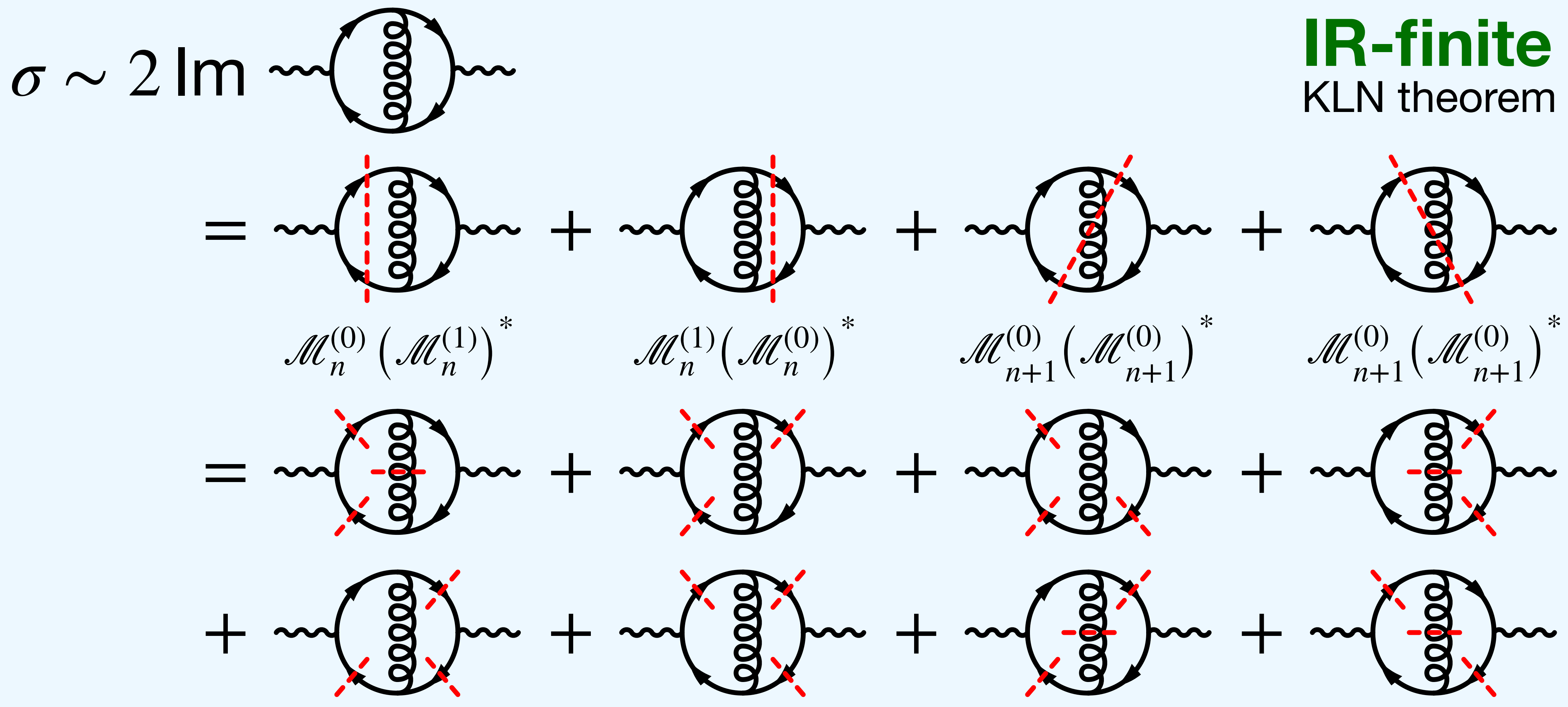
- phase space slicing / subtraction of local counterterms
  ↯ rapidly growing number of soft/collinear limits

→ unify loop & phase space integration?

→ locally IR cancellations between real & virtual?

IR-finite

KLN theorem



Monte Carlo integration of loop integrals in momentum space?

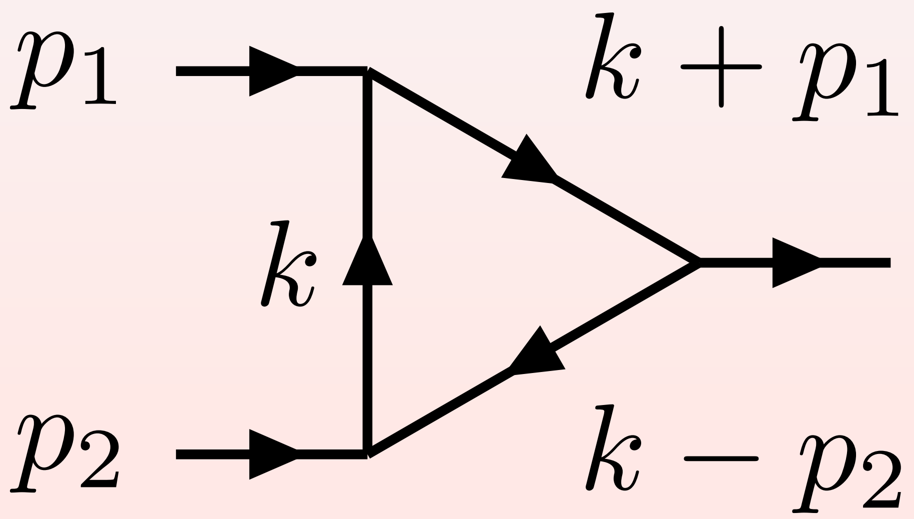
go to $d = 4$ dimensions

⚠️ 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: → Steven's talk



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

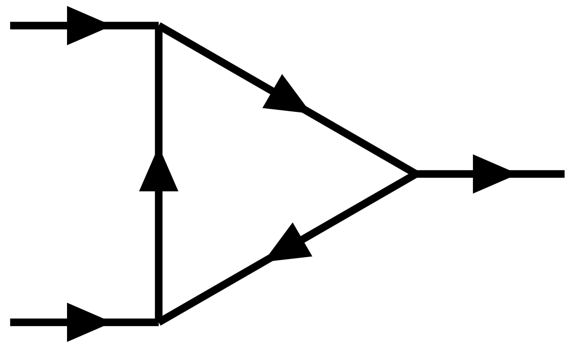
↯ poles in the integration domain

✔ causal prescription

⚠️ implement causal prescription for numerical integration?

Loop-Tree Duality (residue theorem for loop energies)

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



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

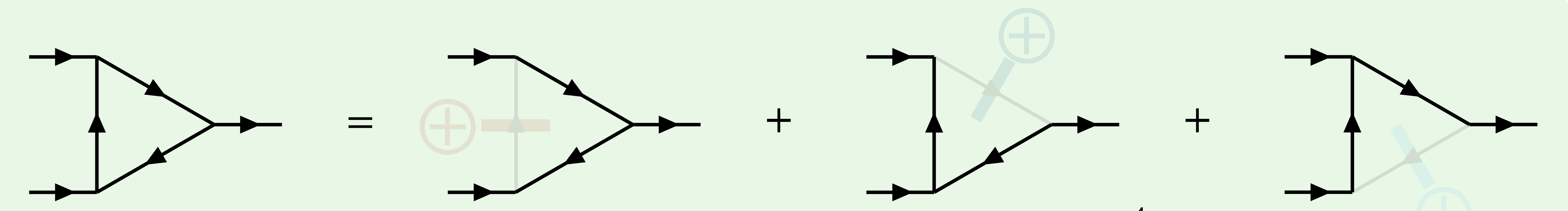
$$= \lim_{\epsilon\to 0}\int \frac{\mathrm{d}^3\vec{k}}{(2\pi)^3}\int\frac{\mathrm{d}k^0}{(2\pi)}\,\frac{1}{k^0-E_3}\,\frac{1}{k^0+E_3}\,\frac{1}{(k^0+p_1^0)-E_1}\,\frac{1}{(k^0+p_1^0)+E_1}\,\frac{1}{(k^0-p_2^0)-E_2}\,\frac{1}{(k^0-p_2^0)+E_2}$$

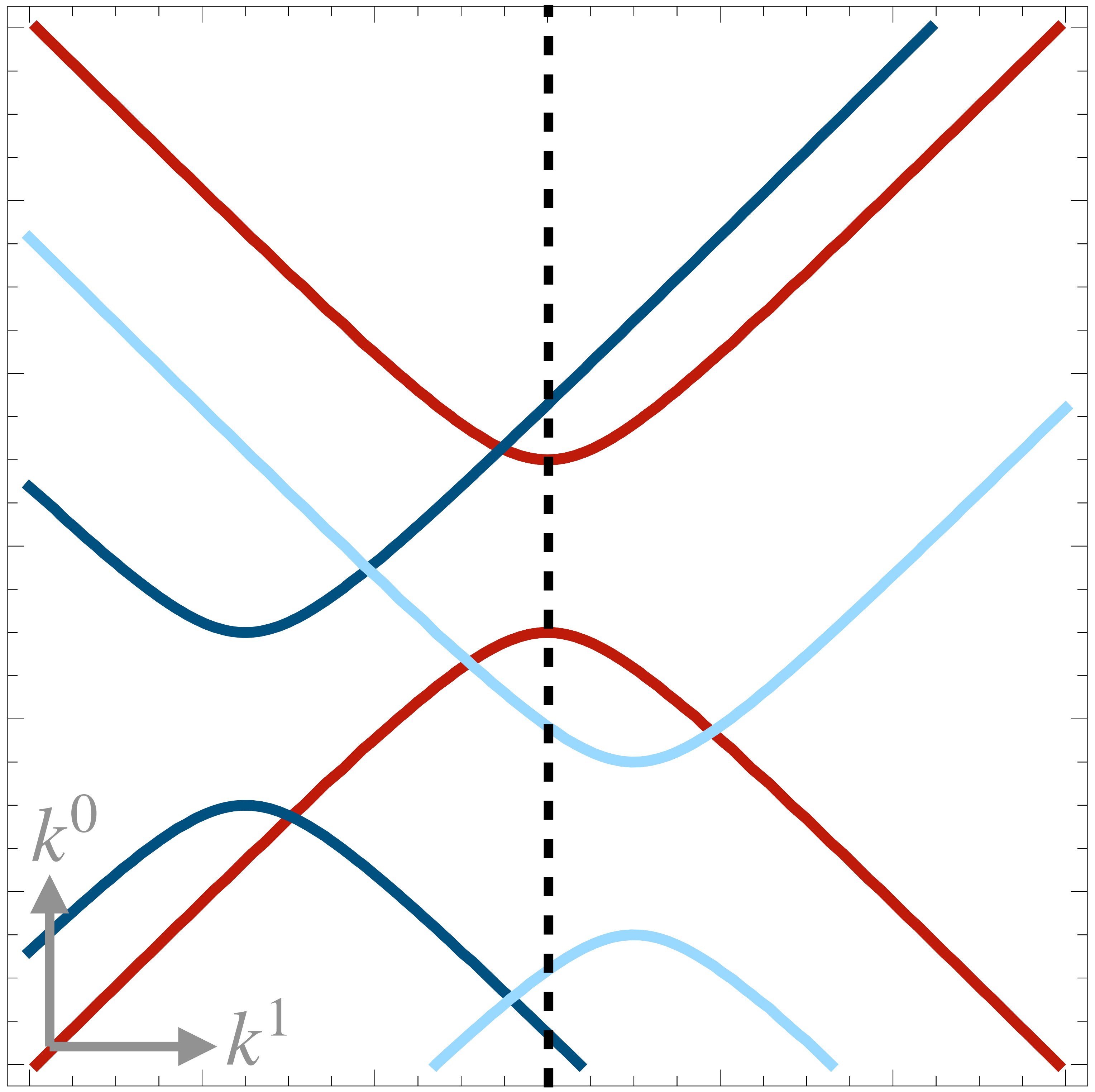
$$= -\,\mathrm{i}\lim_{\epsilon\to 0}\int \frac{\mathrm{d}^3\vec{k}}{(2\pi)^3}\Bigg[\frac{1}{2E_3}\,\frac{1}{(E_3+p_1^0)^2-E_1^2}\,\frac{1}{(E_3-p_2^0)^2-E_2^2}$$
$$+\frac{1}{(E_1-p_1)^2-E_3^2}\,\frac{1}{2E_1}\,\frac{1}{(E_1-p_1-p_2^0)^2-E_2^2}$$
$$+\frac{1}{(E_2+p_2^0)^2-E_3^2}\,\frac{1}{(E_2+p_2^0+p_1^0)^2-E_1^2}\,\frac{1}{2E_2}\Bigg]$$

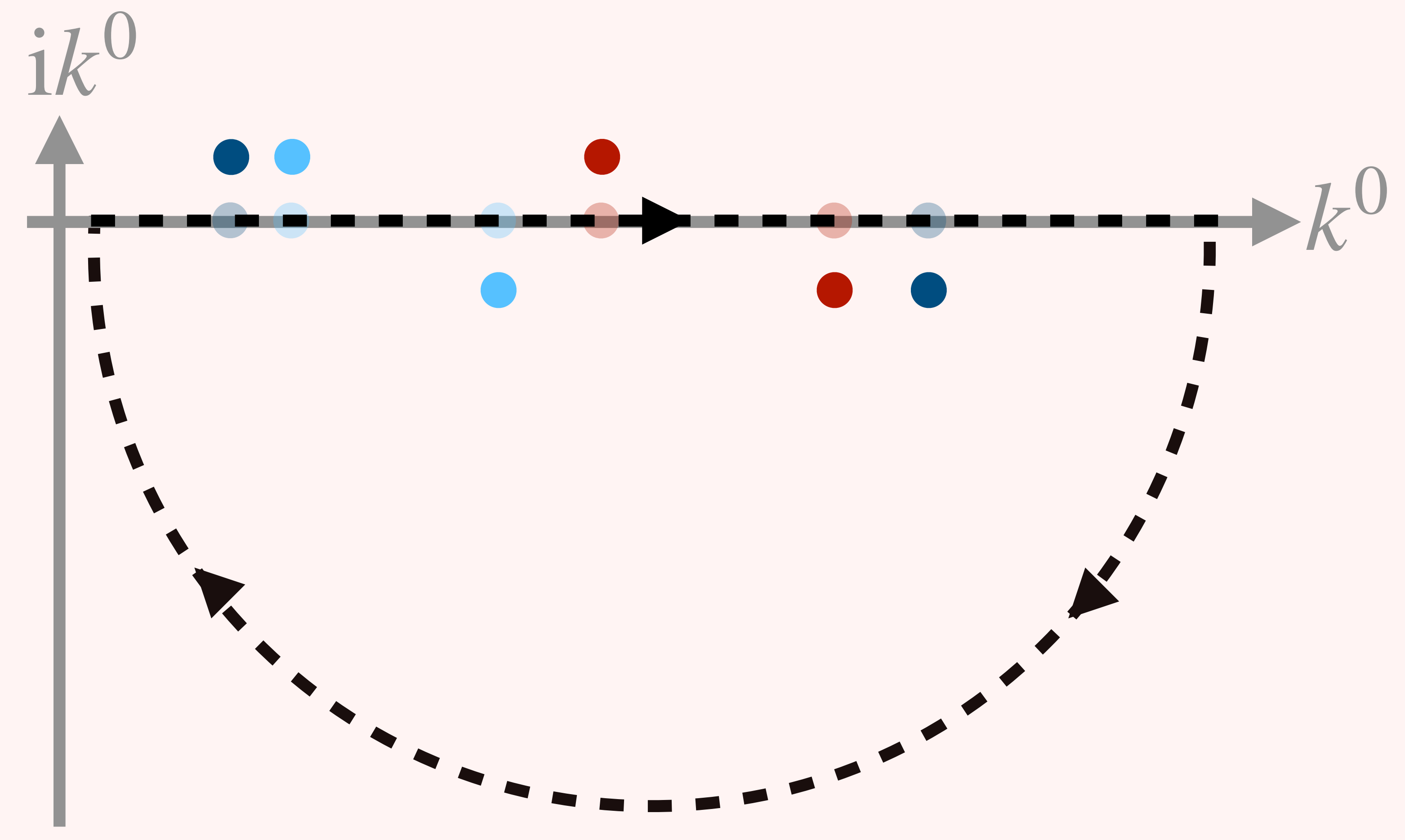
$$E_1=\sqrt{\left(\vec{k}+\vec{p}_1\right)^2+m^2-\mathrm{i}\epsilon}$$

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

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







Loop-Tree Duality beyond one loop

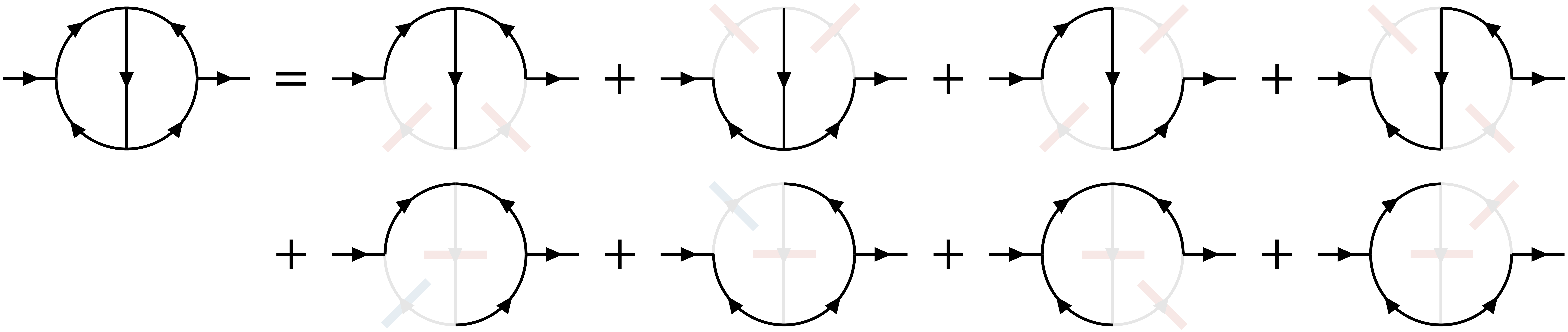
[Capatti, Hirschi, **DK**, Ruijl: 1906.06138]

[Runkel, Szor, Vesga, Weinzierl: 1902.02135]

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

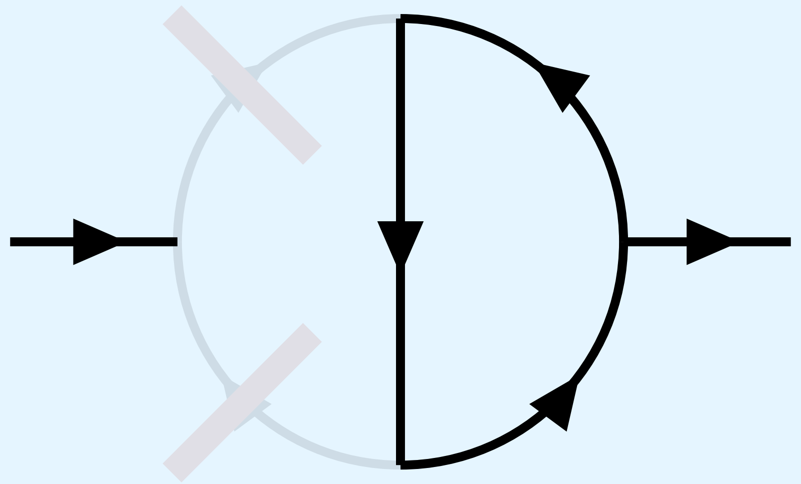
positive OS energy

negative OS energy

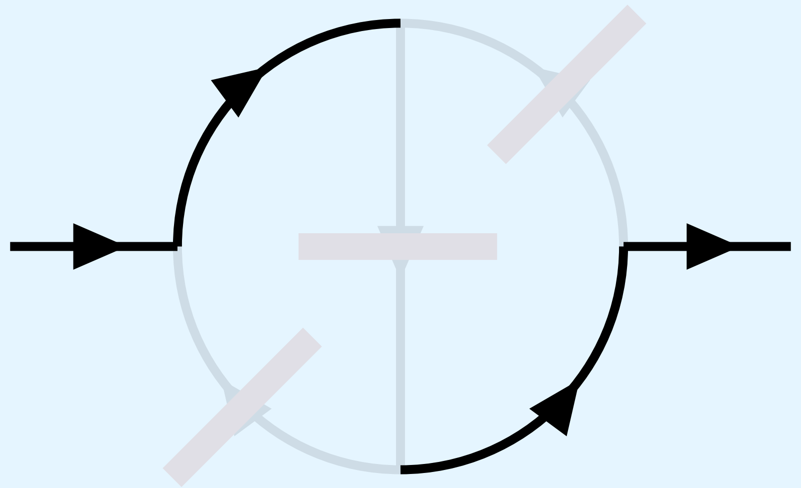


cut into a **single tree**

⚠ no loops ⚠



⚠ no forest ⚠



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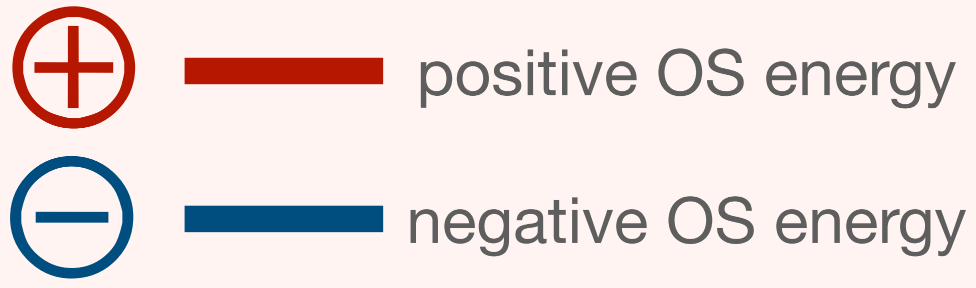

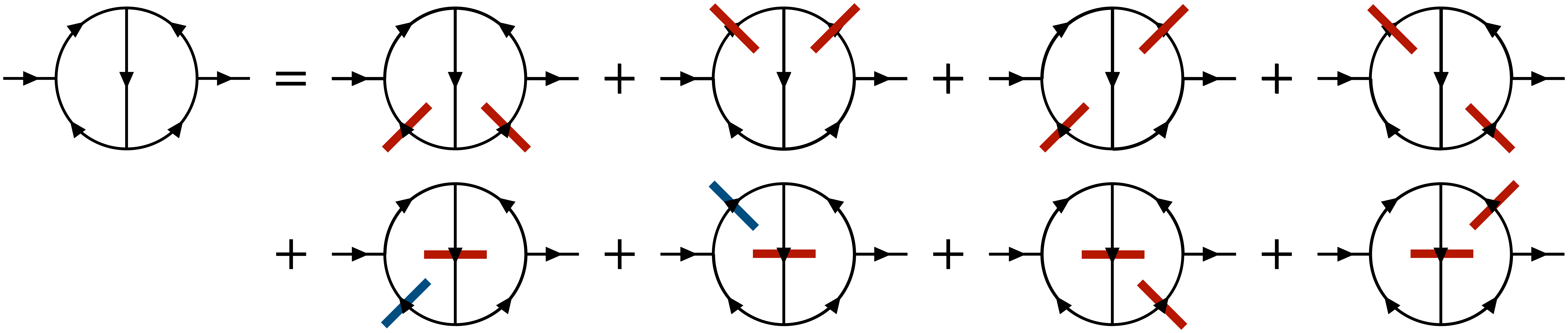

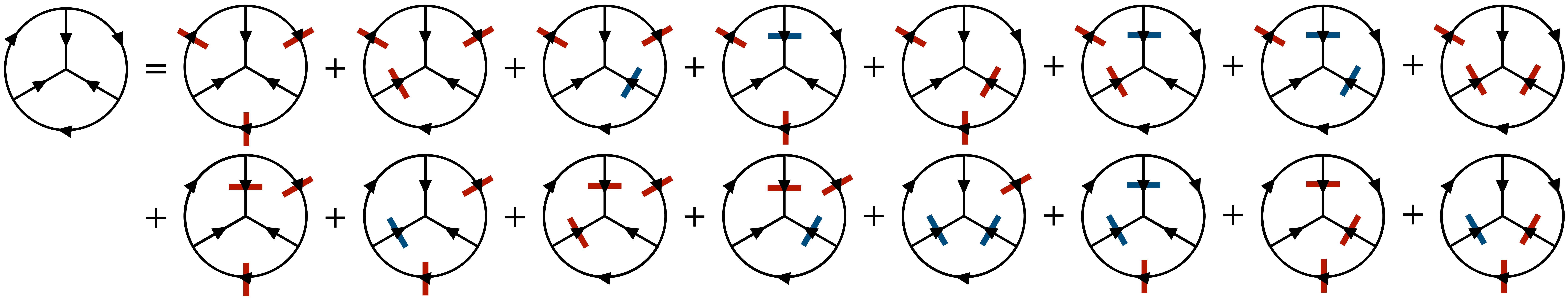

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⊕ positive OS energy

⊖ negative OS energy

Loop integral

$$I = \int \prod_{j=1}^{n} \frac{\mathrm{d}^d k_j}{(2\pi)^d} \frac{N}{\prod_{i\in\mathbf{e}} D_i}$$

Feynman propagator

$$D_i = q_i^2 - m_i^2 + \mathrm{i}\epsilon$$

causal prescription

LTD

$$I = (-\mathrm{i})^n \int \prod_{j=1}^{n} \frac{\mathrm{d}^{d-1}\vec{k}_j}{(2\pi)^{d-1}} \sum_{\mathbf{b}\in\mathscr{B}} \mathrm{Res}_{\mathbf{b}}[\mathscr{I}]$$

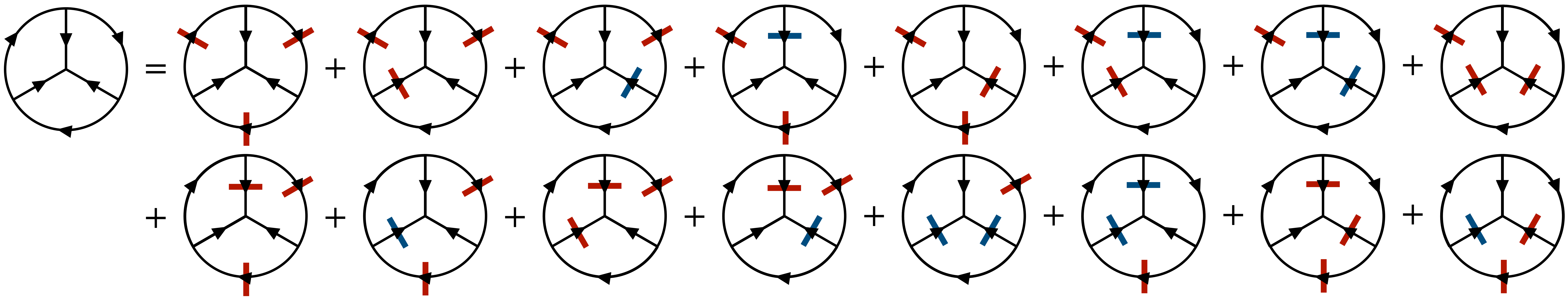
loop momentum basis

Dual integrand (residue)

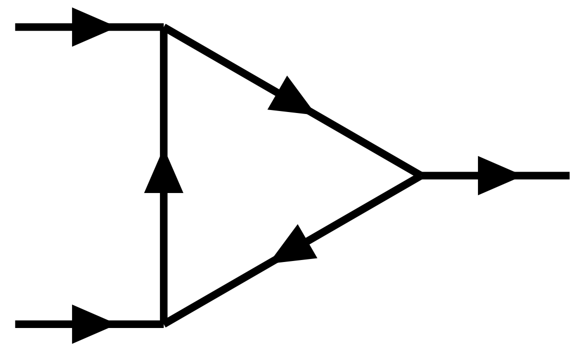
$$\mathrm{Res}_{\mathbf{b}}[\mathscr{I}] = \frac{1}{\prod_{i\in\mathbf{b}} 2E_i} \frac{N}{\prod_{i\in\mathbf{e}\setminus\mathbf{b}} D_i}\Bigg|_{\{q_j^0=\sigma_j^{\mathbf{b}}E_j\}_{j\in\mathbf{b}}}$$

sign of on-shell energy (cut structure)

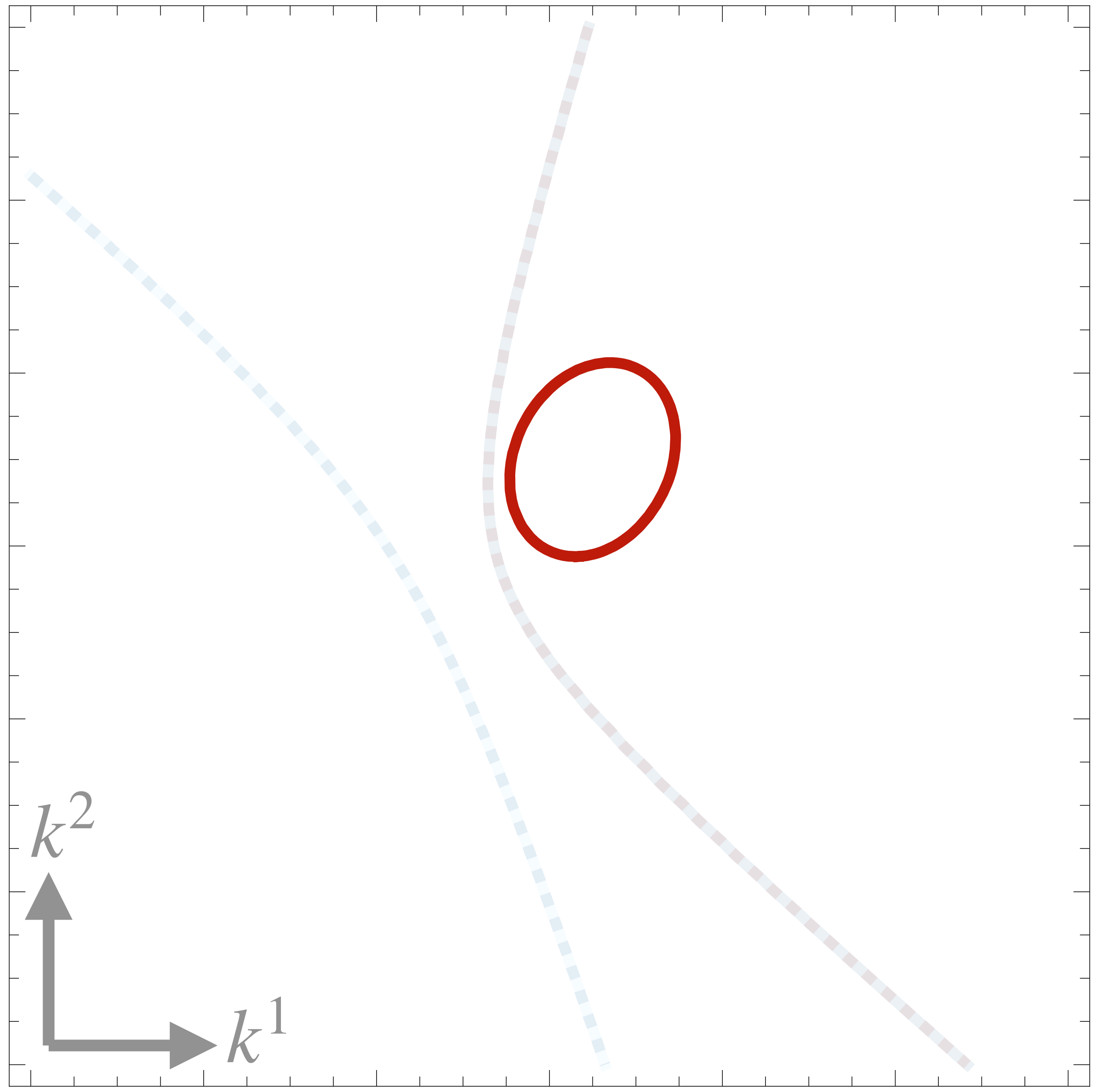
Dual integrands depend on **integration order, contour closure, momentum routing** but their sum (i.e. the LTD expression) is independent



Monte Carlo integration of LTD? ⚠️ Remaining singularities!



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



Hyperboloid

spurious singularities

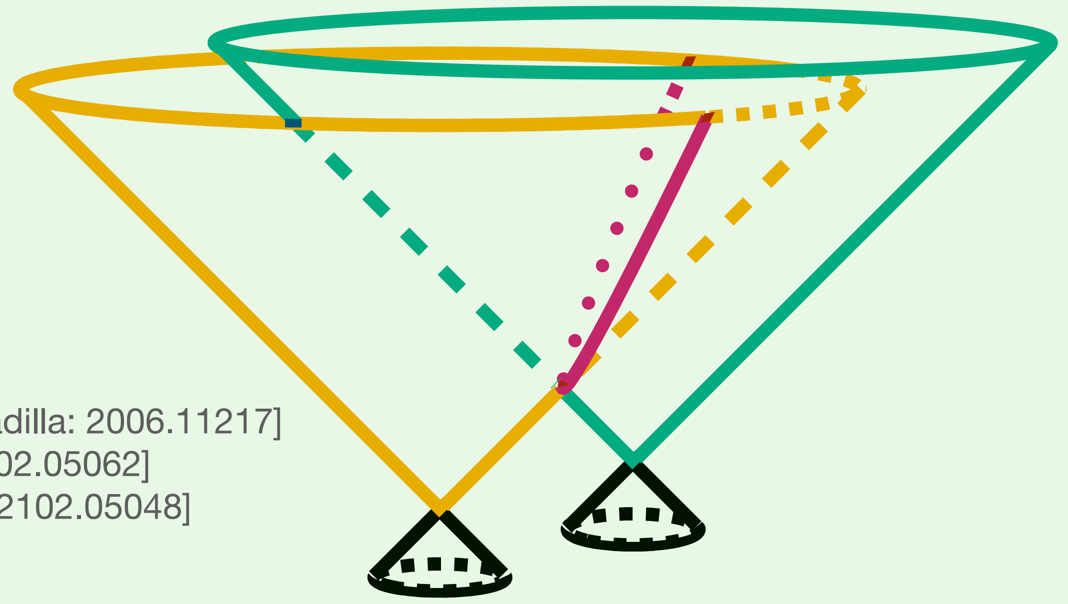
cause numerical instabilities

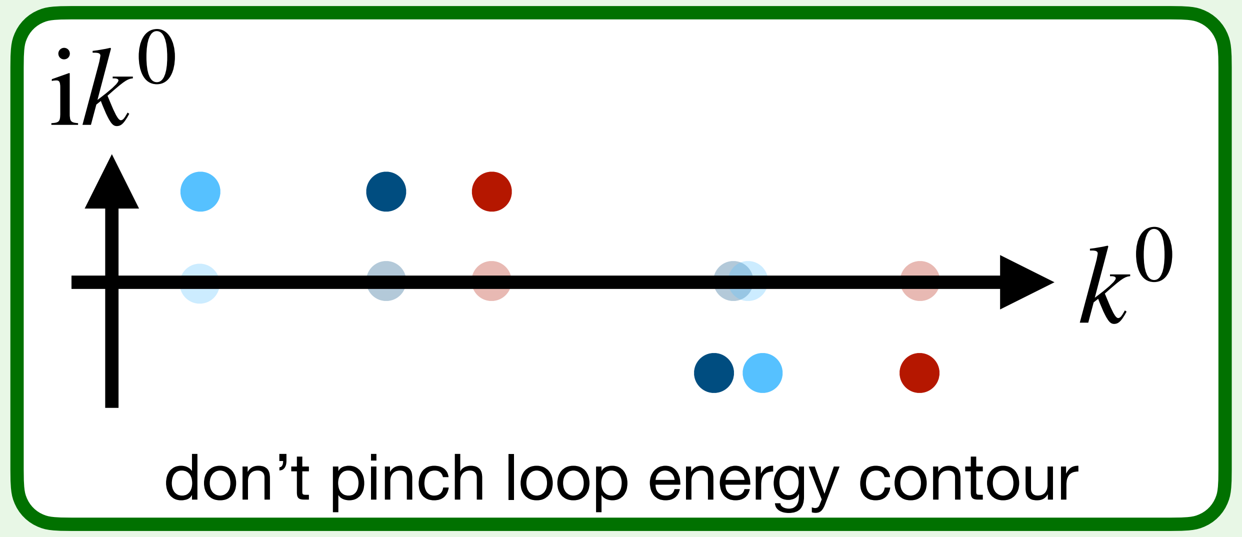
→ remove with

causal LTD [Aguilera-Verdugo, Hernandez-Pinto, Rodrigo, Sborlini, Bobadilla: 2006.11217] [Capatti, Hirschi, **DK**, Pelloni, Ruijl: 2009.05509] [Sborlini: 2102.05062] [Benincasa, Bobadilla: 2112.09028] [Bobadilla: 2103.09237, 2102.05048] [Kromin, Schwanemann, Weinzierl: 2208.01060]

TOPT

CFF [Capatti: 2211.09653]



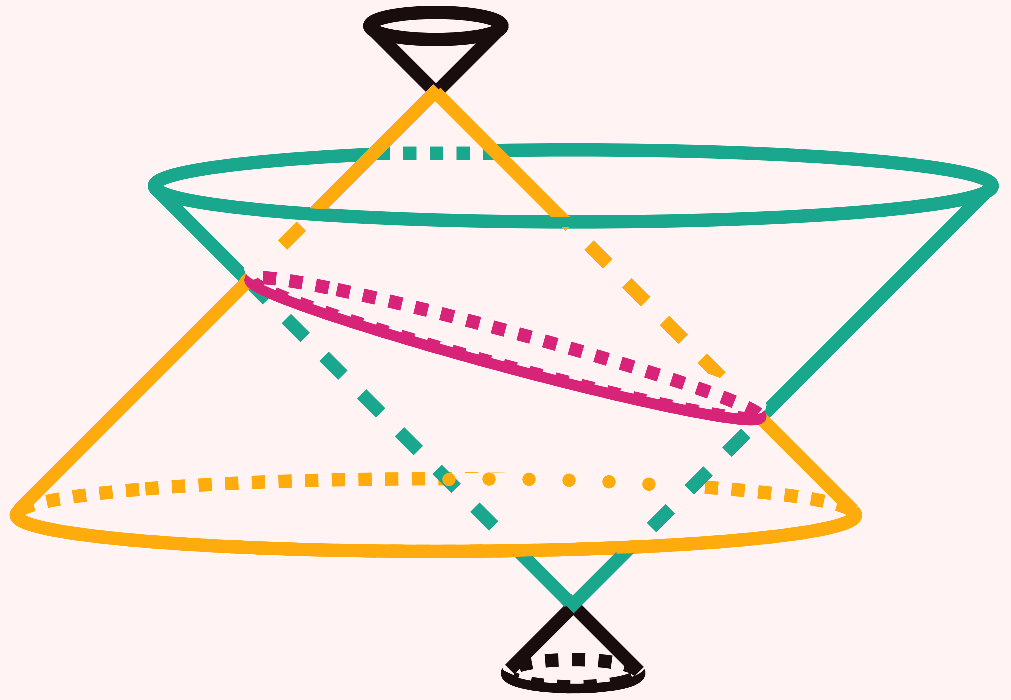


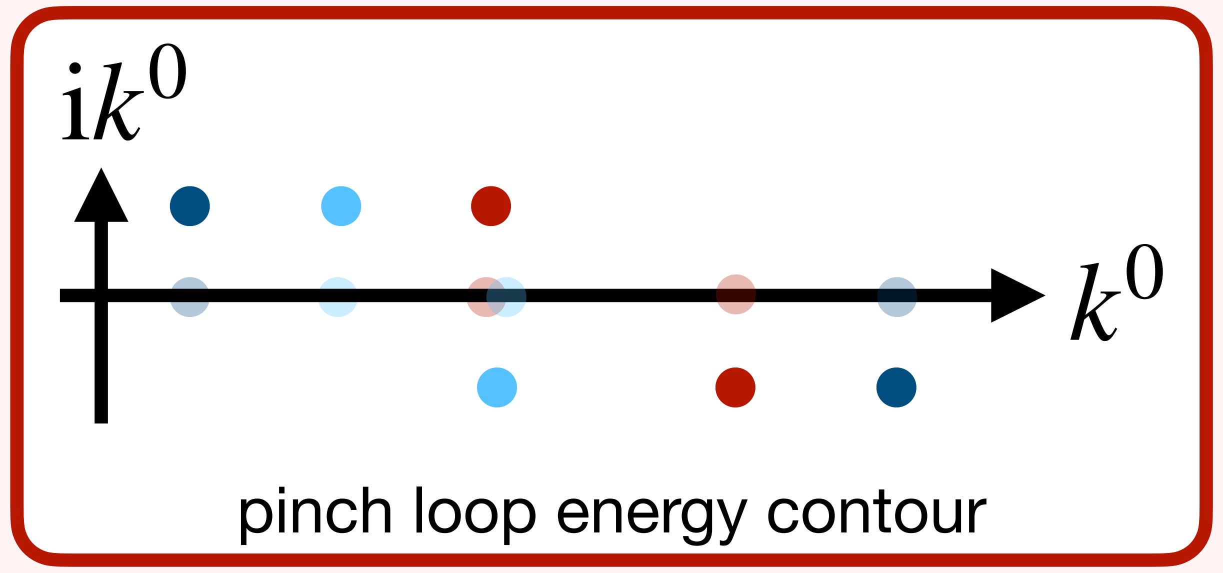
Ellipsoid

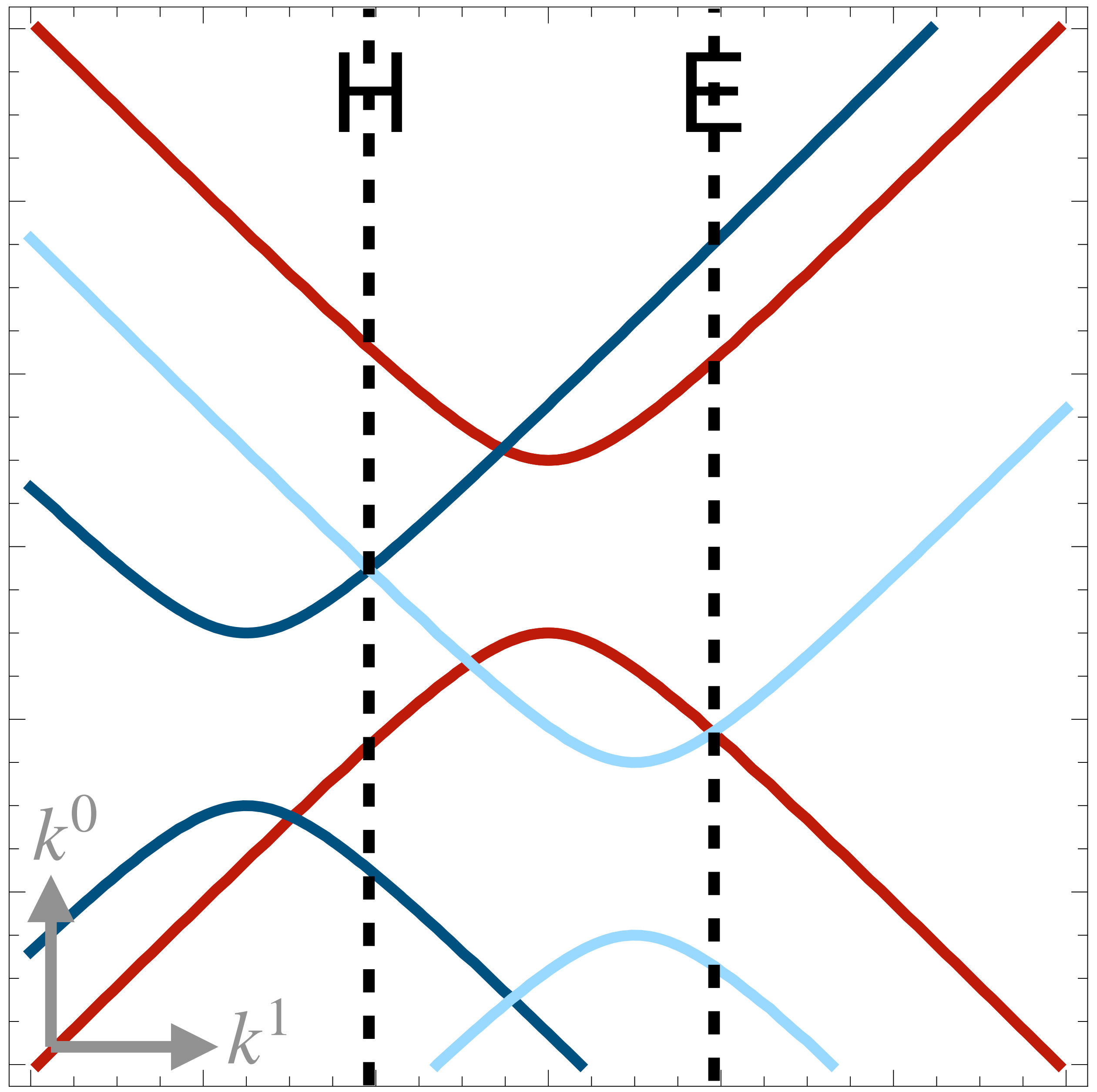
threshold singularities

treated before numerical integration

→ contour deformation or subtraction





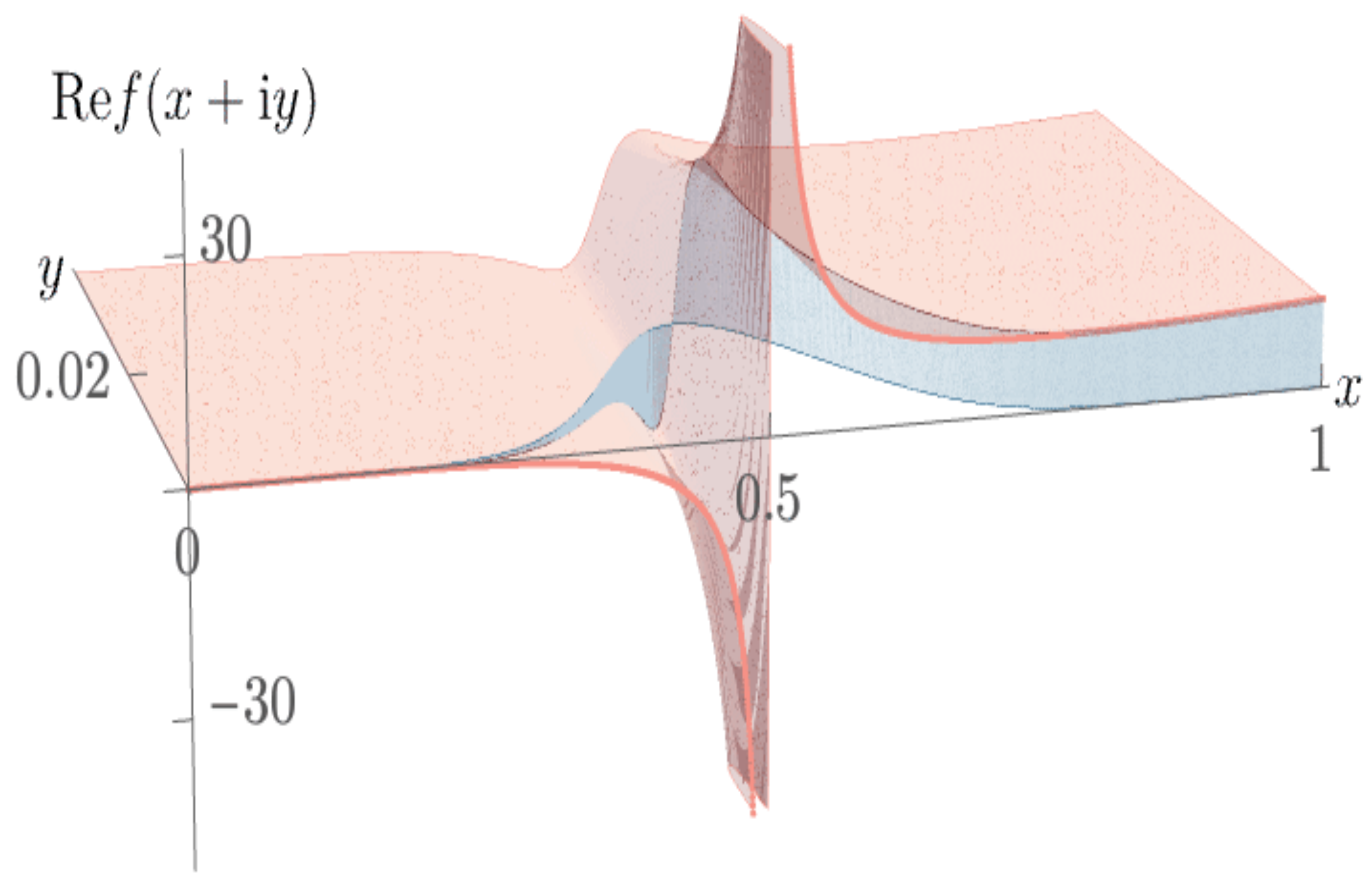


Monte Carlo numerical integration with poles

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

contour deformation

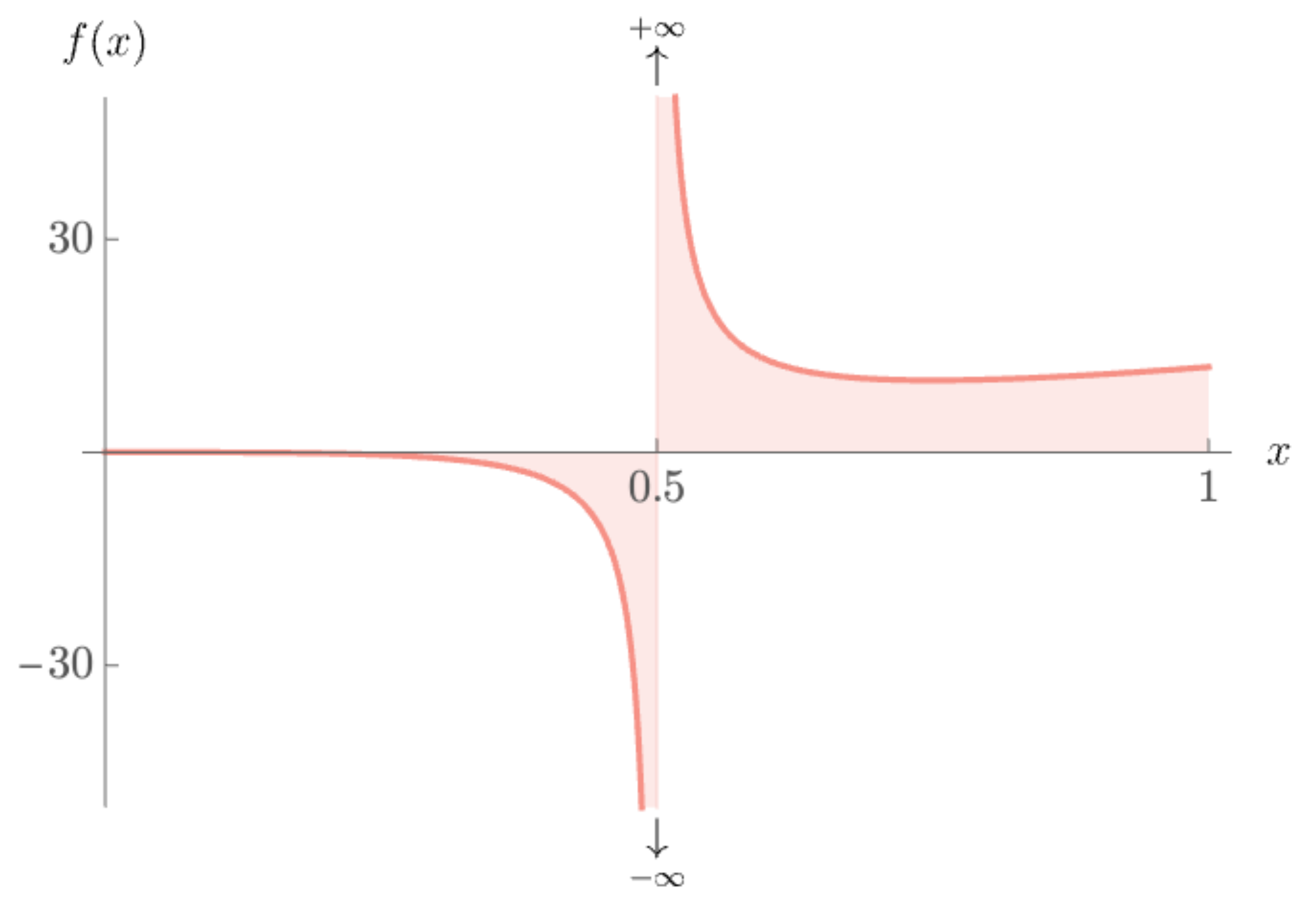
$\mathbb{R} \to \mathbb{C}$



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

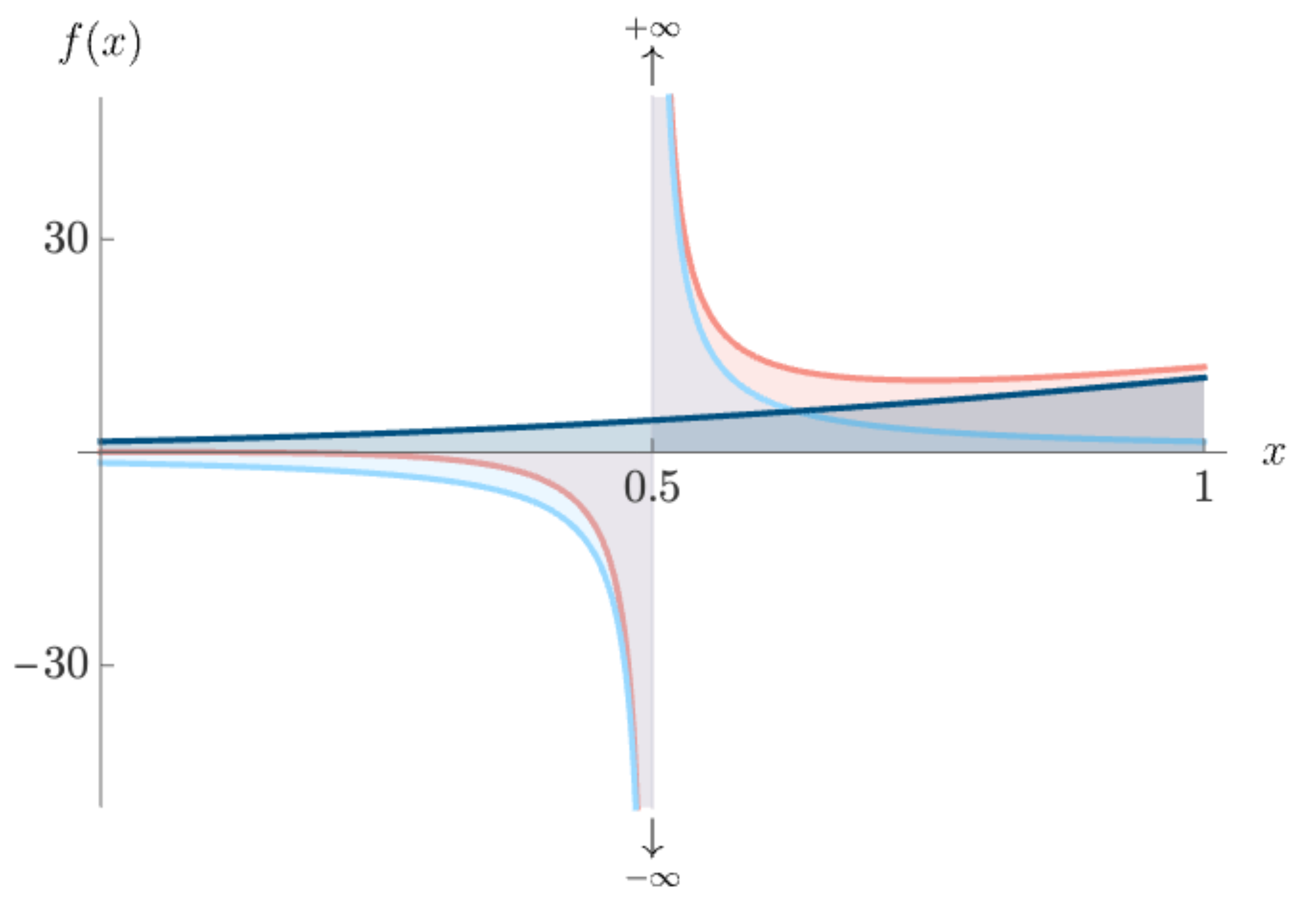
infinities cancel



subtraction

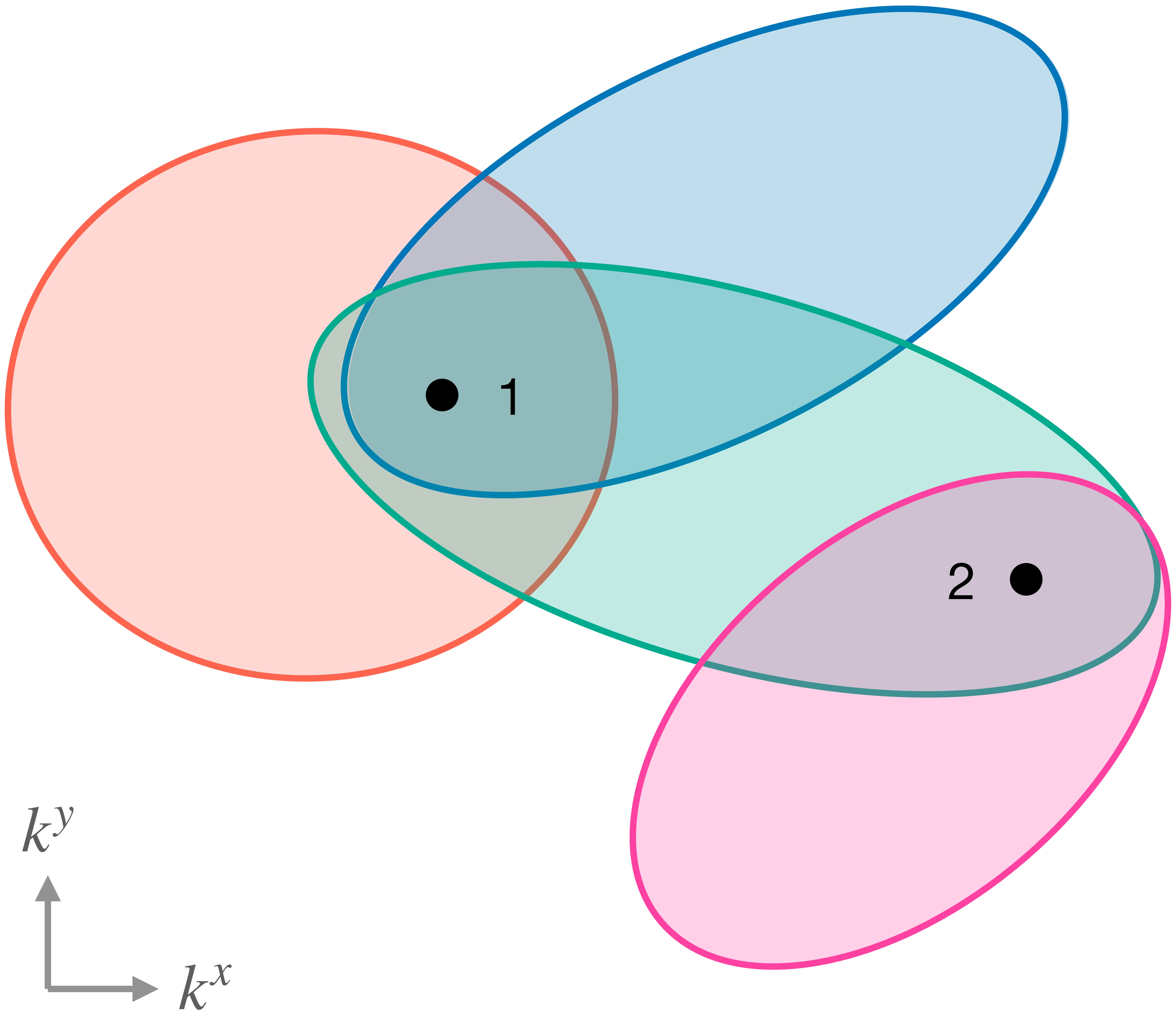
$f_{\mathrm{ct}}(x) = \frac{3}{4}\frac{1}{x-\frac{1}{2}}$ $\quad$ $\mathrm{PV}\int_0^1 f_{\mathrm{ct}}(x)\,\mathrm{d}x = 0$

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



Contour deformation in the spatial momenta

in 4 dim: one loop: [Gong, Nagy, Soper: 0812.3686]
multi-loop: [Becker, Weinzierl: 1211.0509]
in 3 dim: one loop: [Buchta, Chachamis, Draggiotis, Rodrigo: 1510.00187]
[Kromin, Schwanemann, Weinzierl: 2208.01060]
multi-loop: [Capatti, Hirschi, **DK**, Pelloni, Ruijl: 1912.09291]



$$\mathcal{E}_i - \mathrm{i}\epsilon \quad \text{where} \quad \epsilon > 0$$

$$\vec{k} \to \vec{k} - \mathrm{i}\vec{\kappa}(\vec{k}) \quad \text{where} \quad \vec{\kappa}(\vec{k}) \cdot \vec{\nabla}\mathcal{E}_i > 0$$

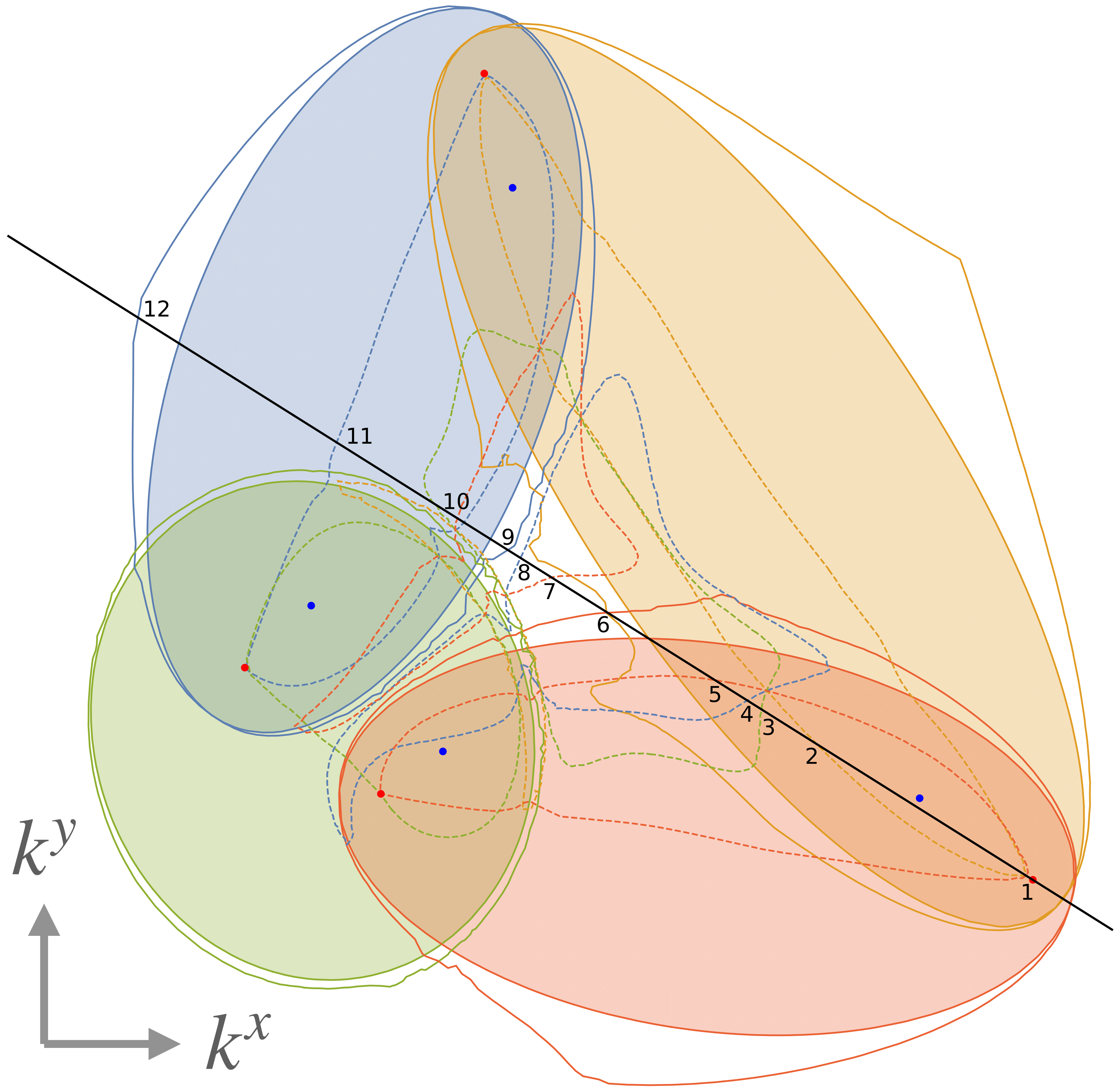
$$\vec{\kappa} = \lambda(\vec{k})\Big((\vec{k} - \vec{s}_1)\; T(\mathcal{E}_4) + (\vec{k} - \vec{s}_2)\; T(\mathcal{E}_1)T(\mathcal{E}_2) \Big)$$

$\lambda(\vec{k})$ such that deformation does not cross
- ✗ branch cuts (from square roots)
- ✗ other poles in the complex plane

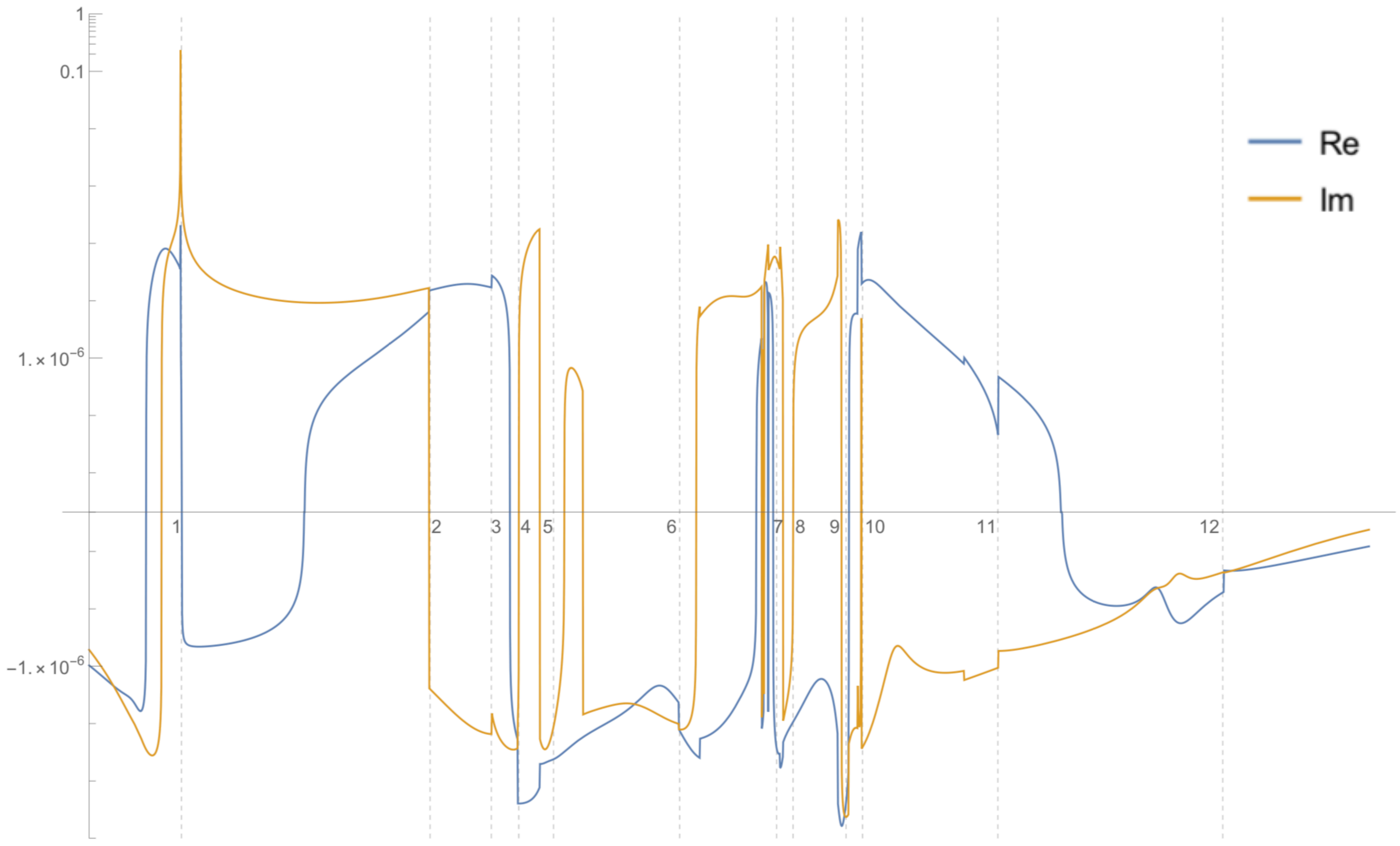
- solution relies on identification of **all overlaps** of ellipsoids
  → computationally expensive, efficiency depends on PS point
- generalised to arbitrary multi-loop configurations
- difficult to determine **optimal** direction and magnitude

Integrand along deformed contour

[Capatti, Hirschi, **DK**, Pelloni, Ruijl: 1912.09291]



threshold singularities of a box diagram



integrand along line segment using contour deformation

Subtraction of threshold singularities

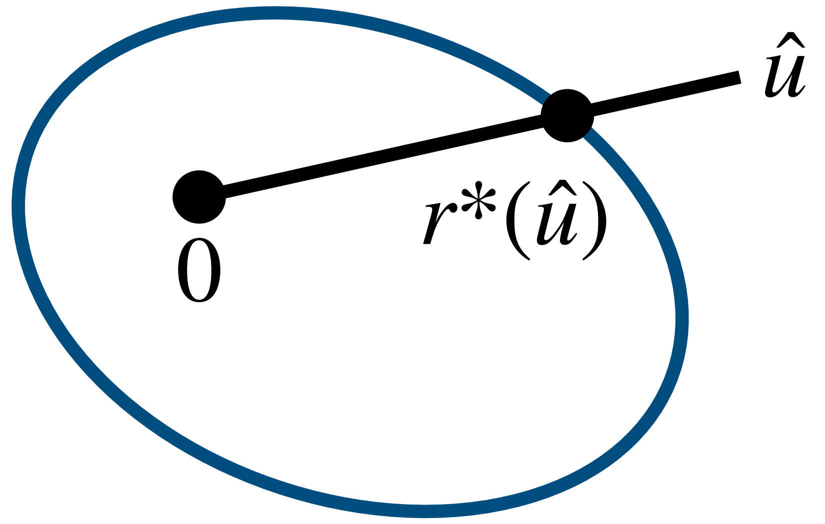
[**DK**: 2110.06869]

Idea

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

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

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



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

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

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

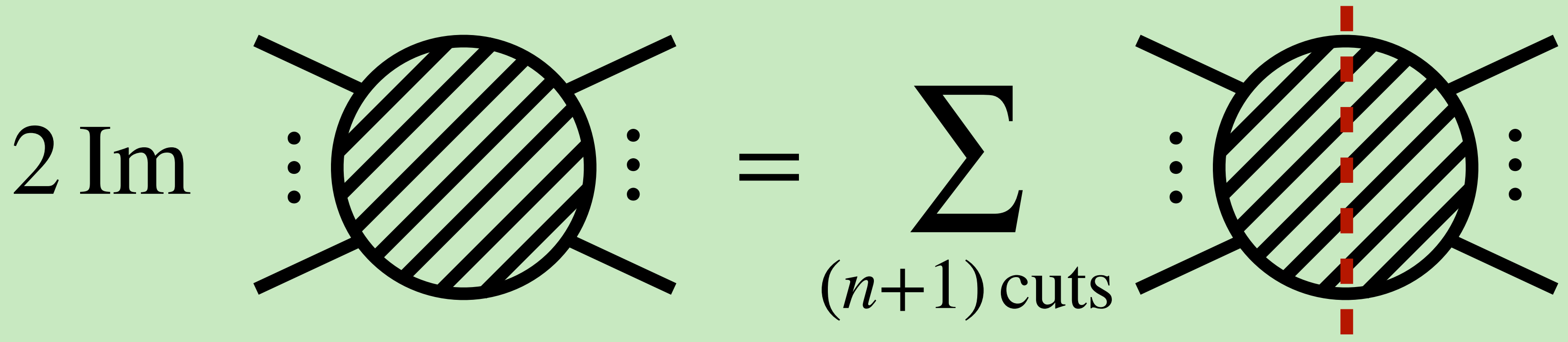
$$2\,\mathrm{Im}\, A(i \to f) = \sum_x \int \mathrm{d}\Pi_x\, A(i \to x)\, A^*(f \to x)$$

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]

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

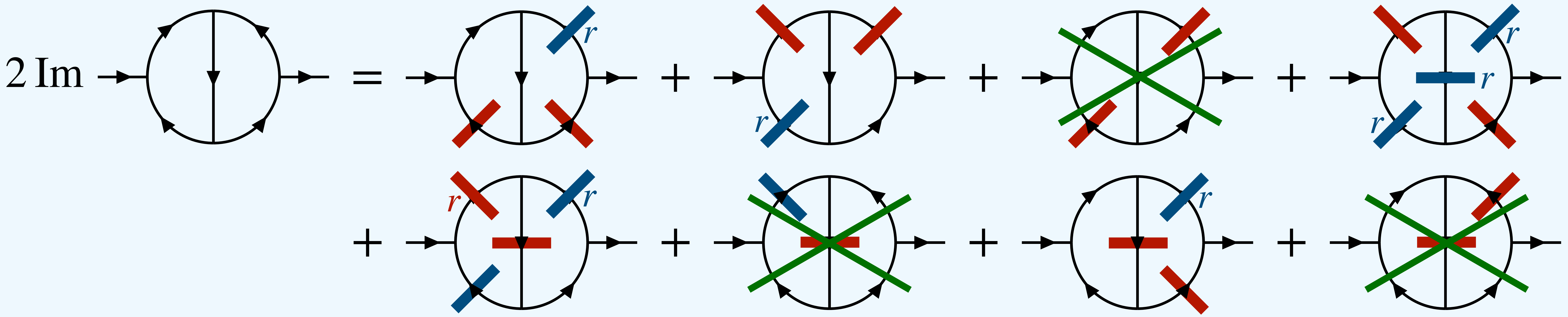
⚠️ residue ⇔ cut propagator



Subtraction of threshold singularities

[**DK**: 2110.06869]

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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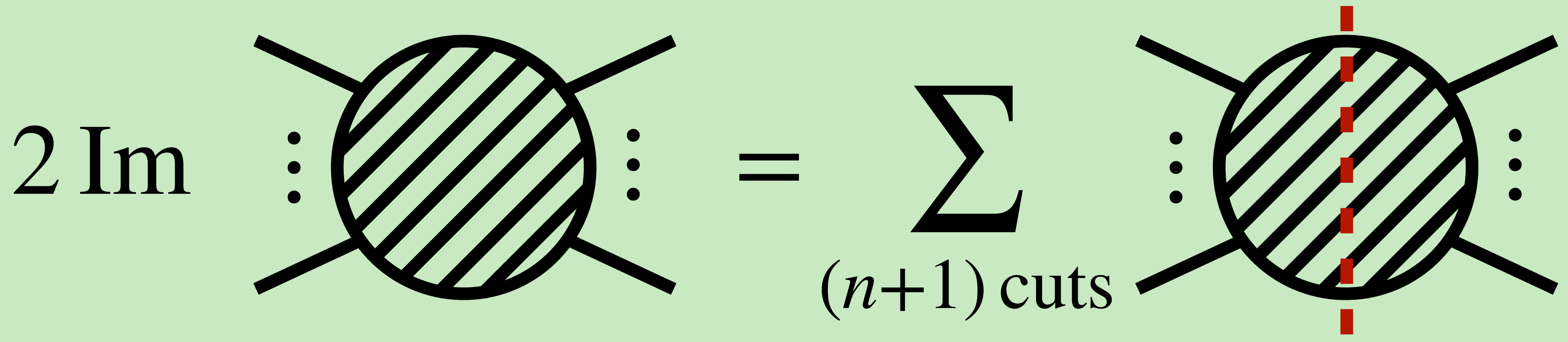
⚠ residue ⇔ cut propagator



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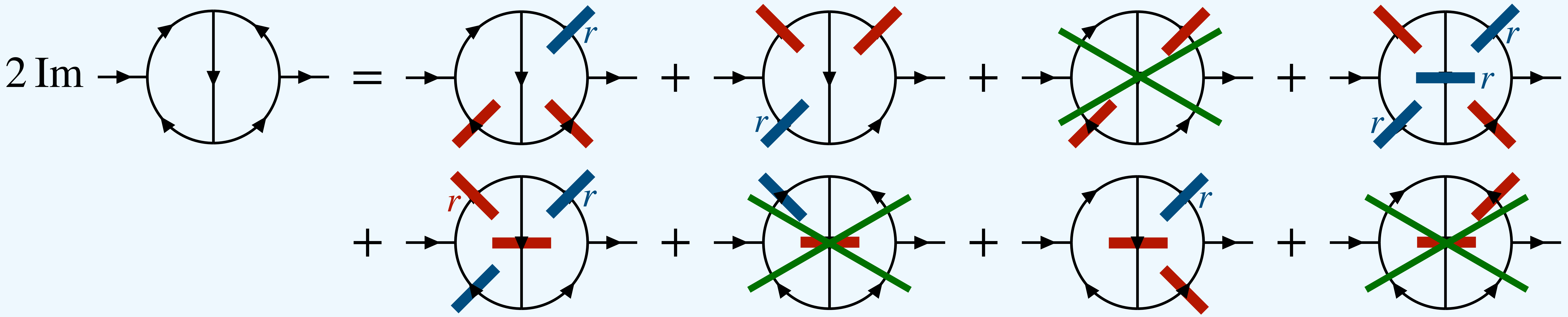

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*

representation depends on parameterisation

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

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

*

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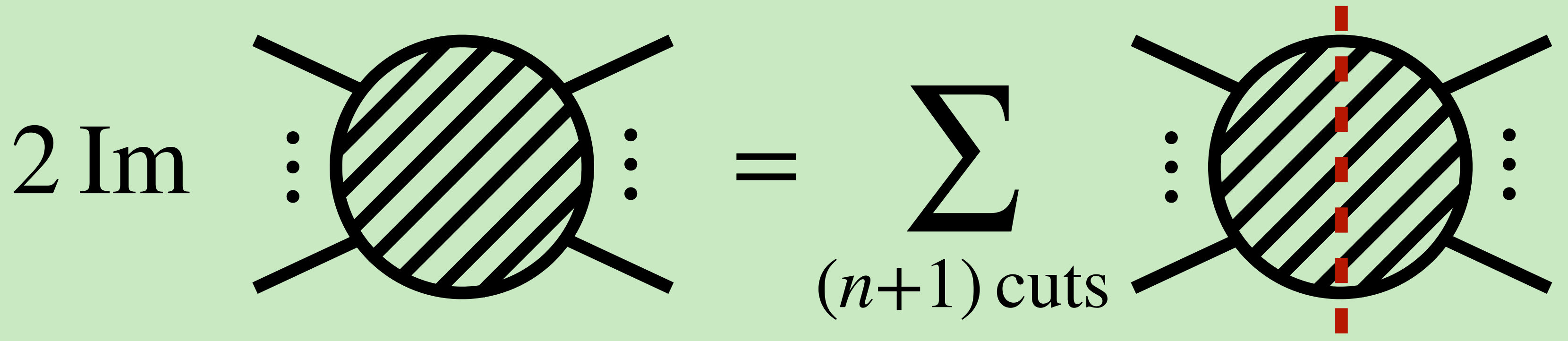
[Soper: hep-ph/9804454, hep-ph/9910292]
Local Unitarity [Capatti, Hirschi, Pelloni, Ruijl: 2010.01068]

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

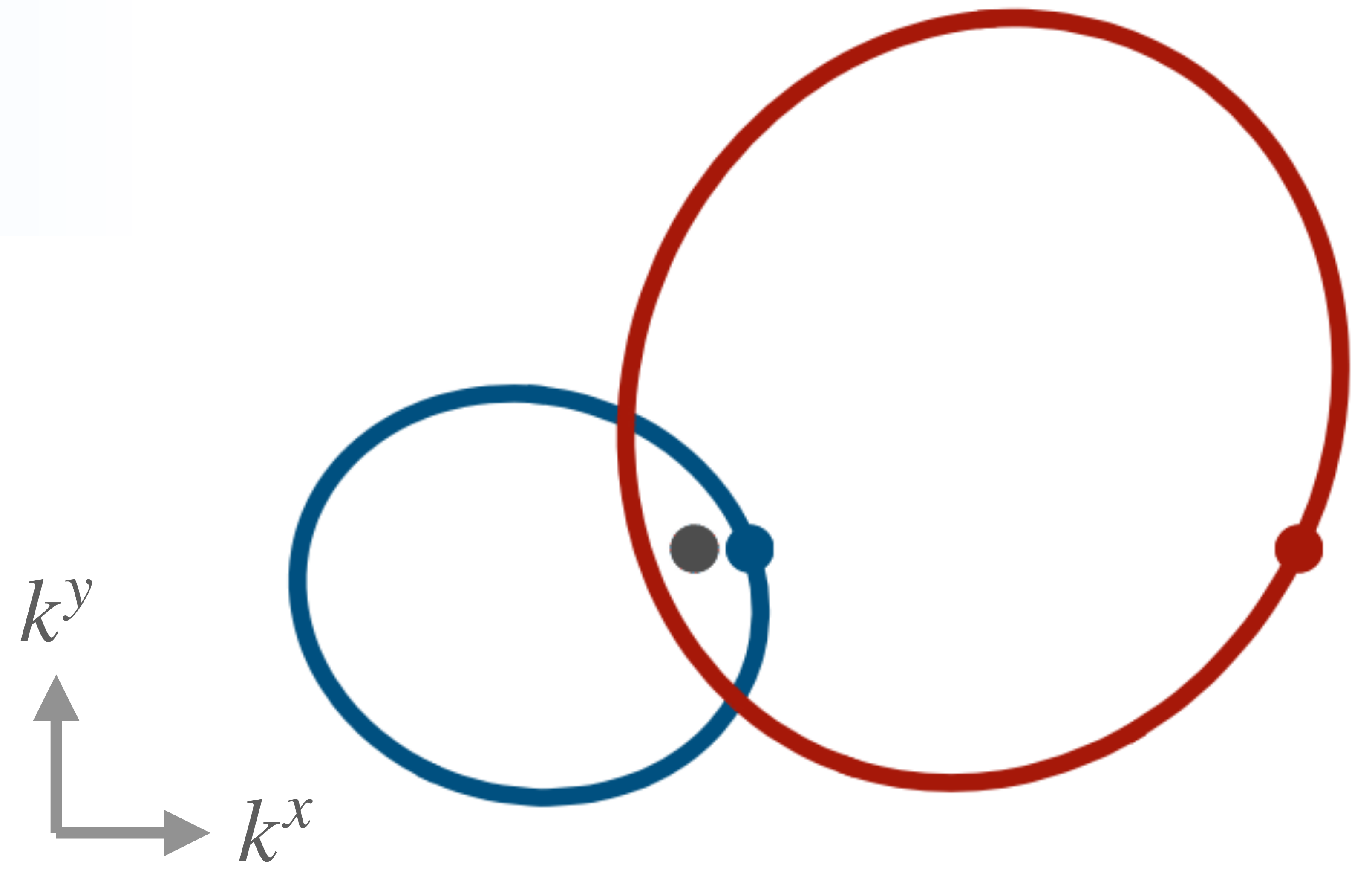
⚠️ residue ⇔ cut propagator



Overlaps of threshold singularities

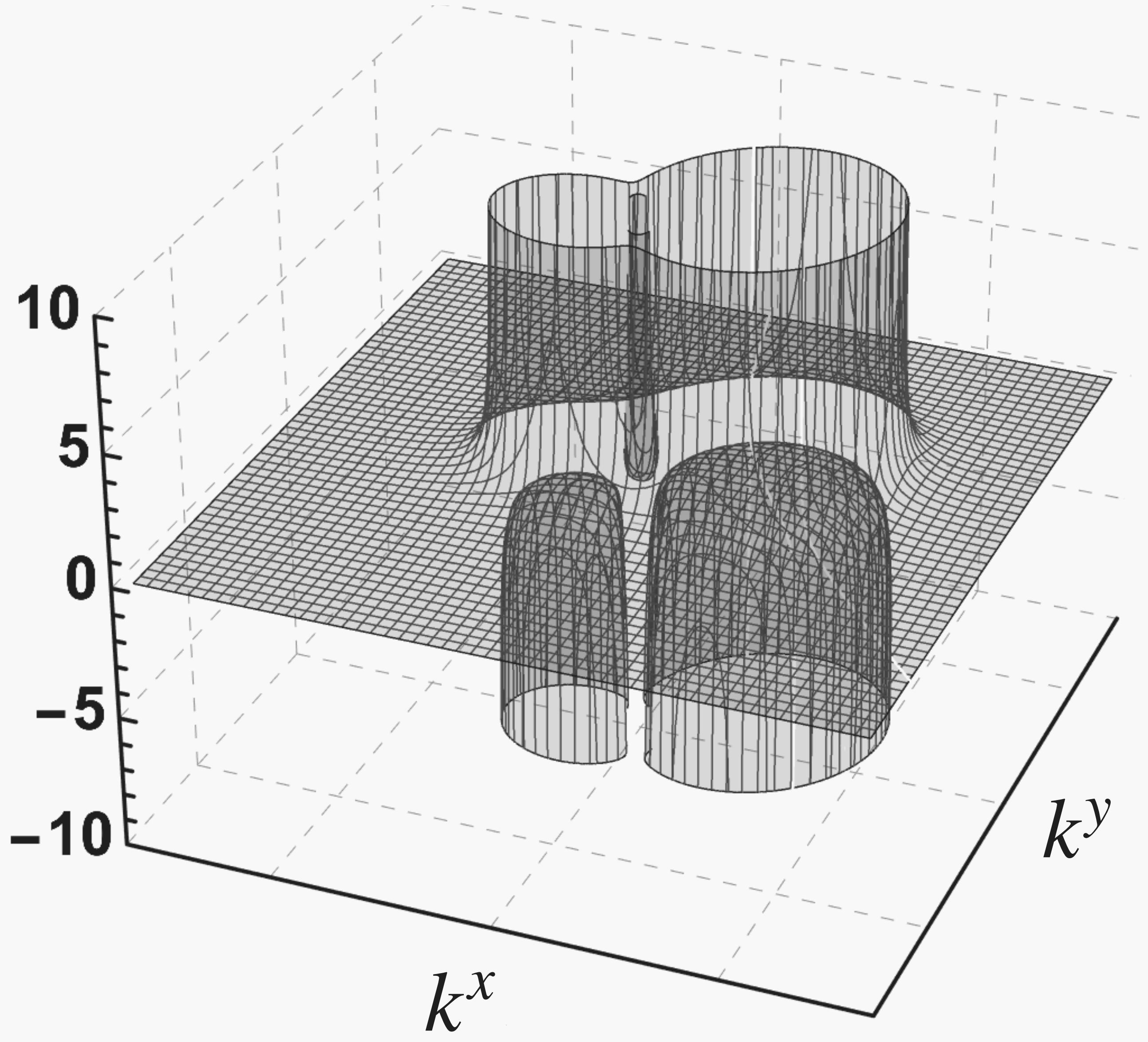
Construct a counterterm for each threshold

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

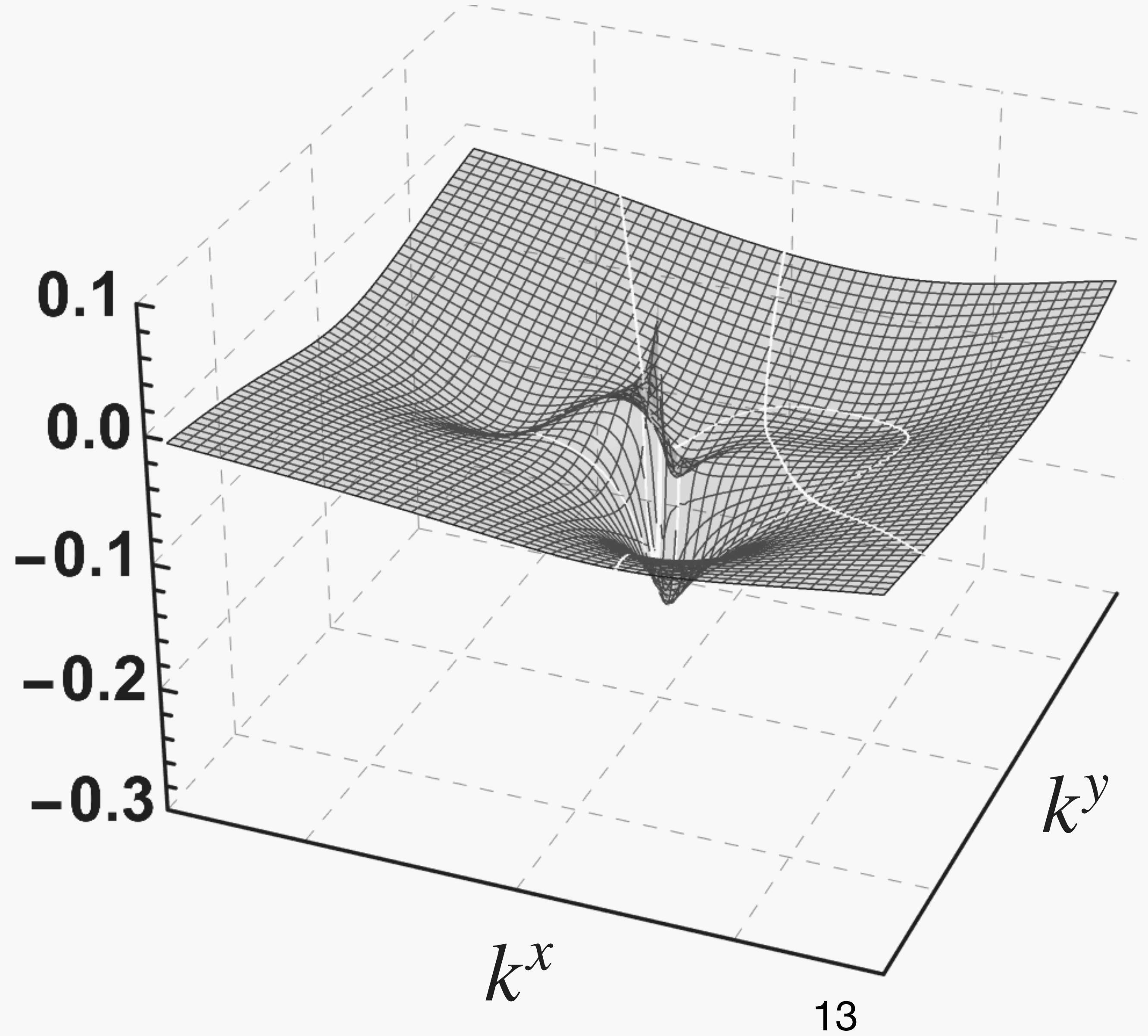


Real Part (Cauchy Principal Value)

$\mathcal{I}$

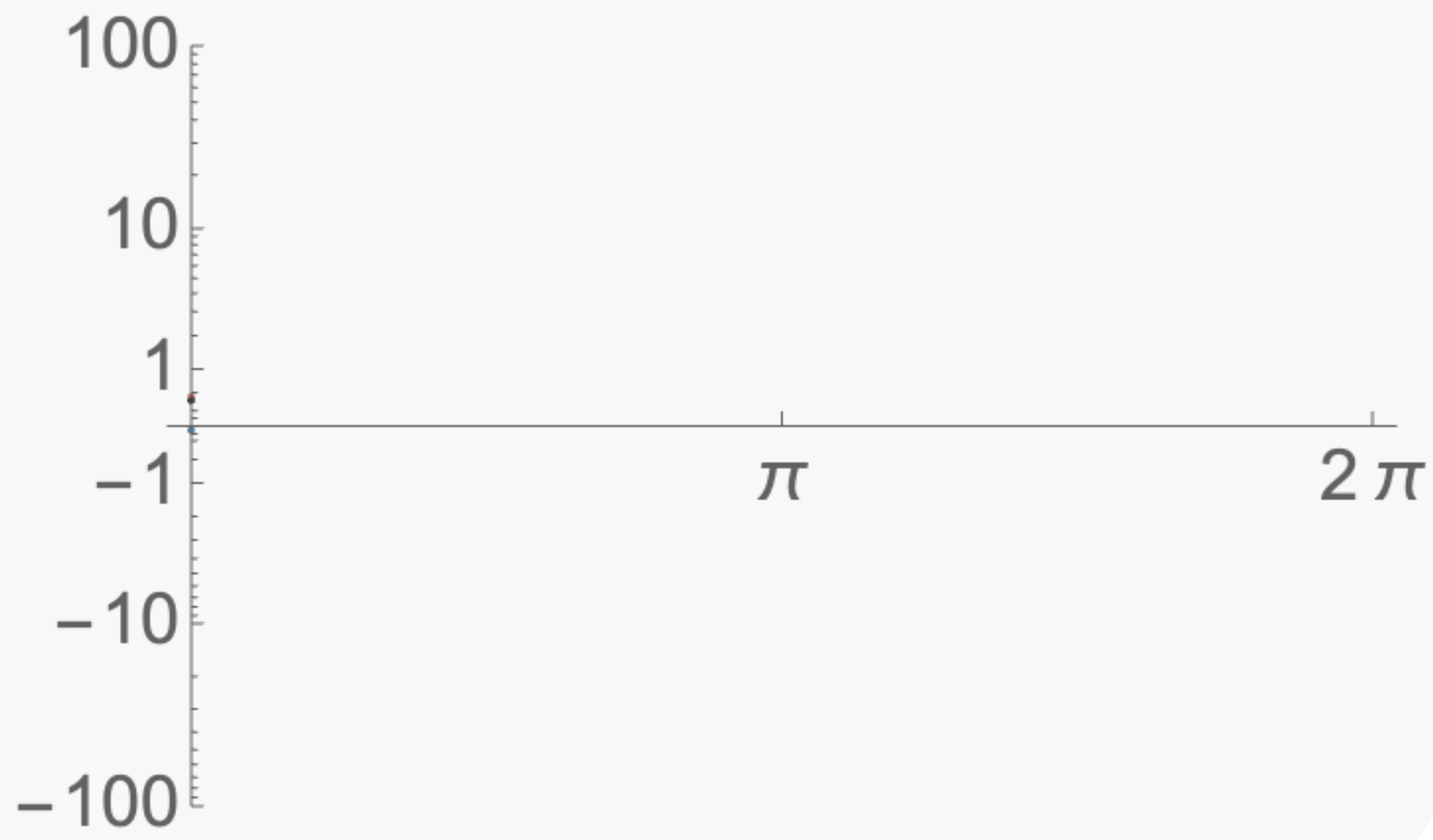


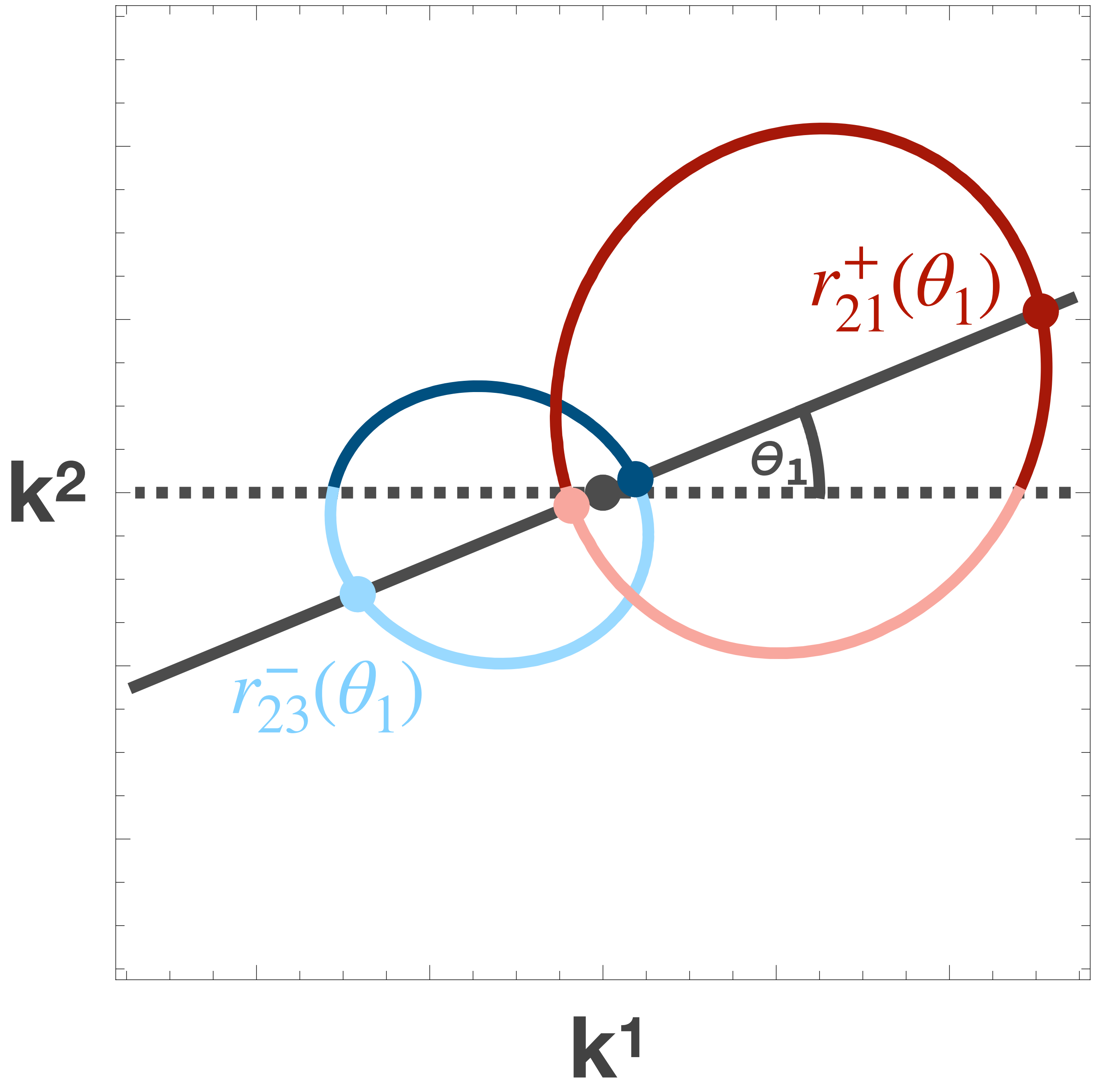
$\mathcal{I} - \mathrm{CT}_{\bigcirc} - \mathrm{CT}_{\circ}$



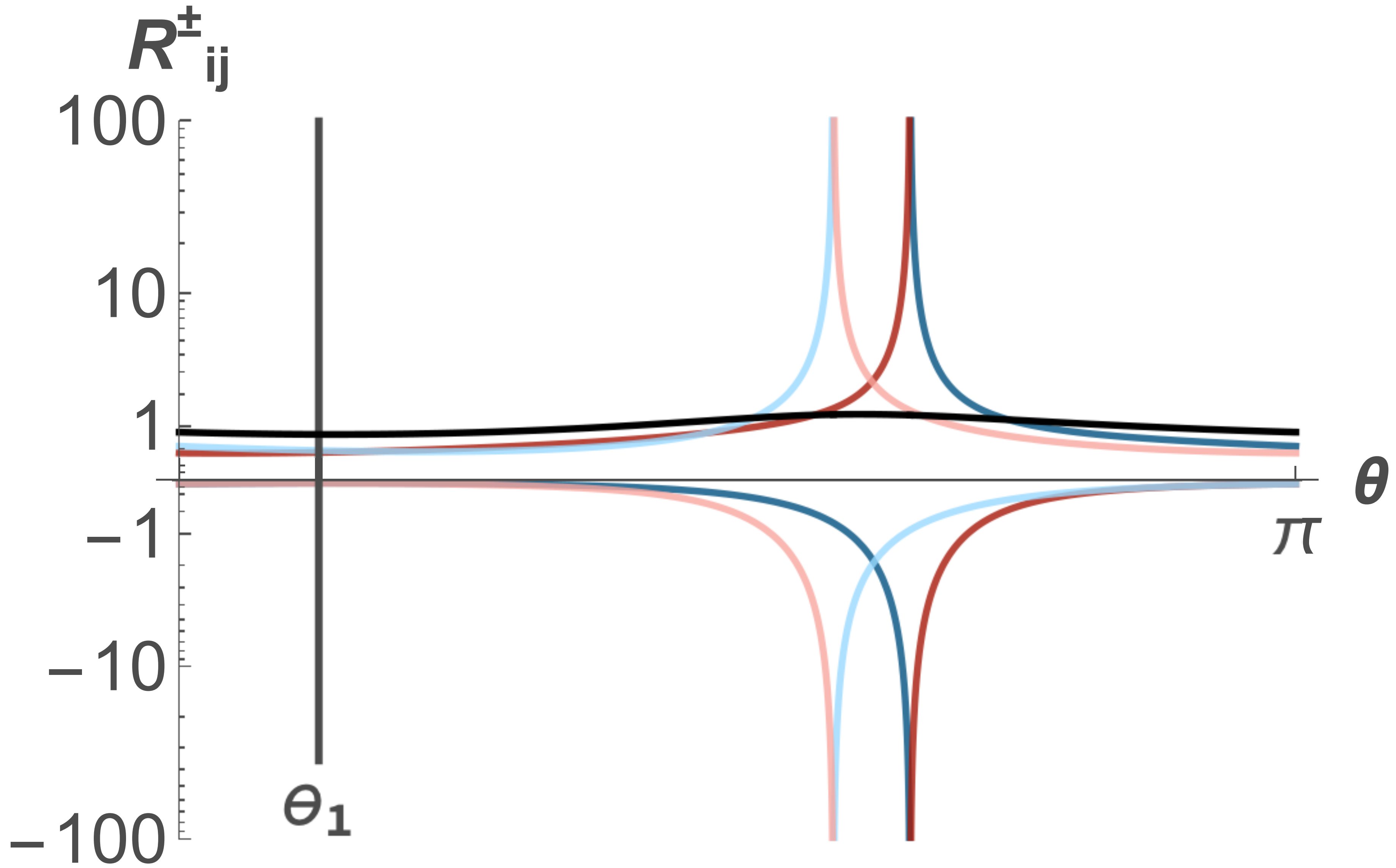
Imaginary Part (integrated couterterms)

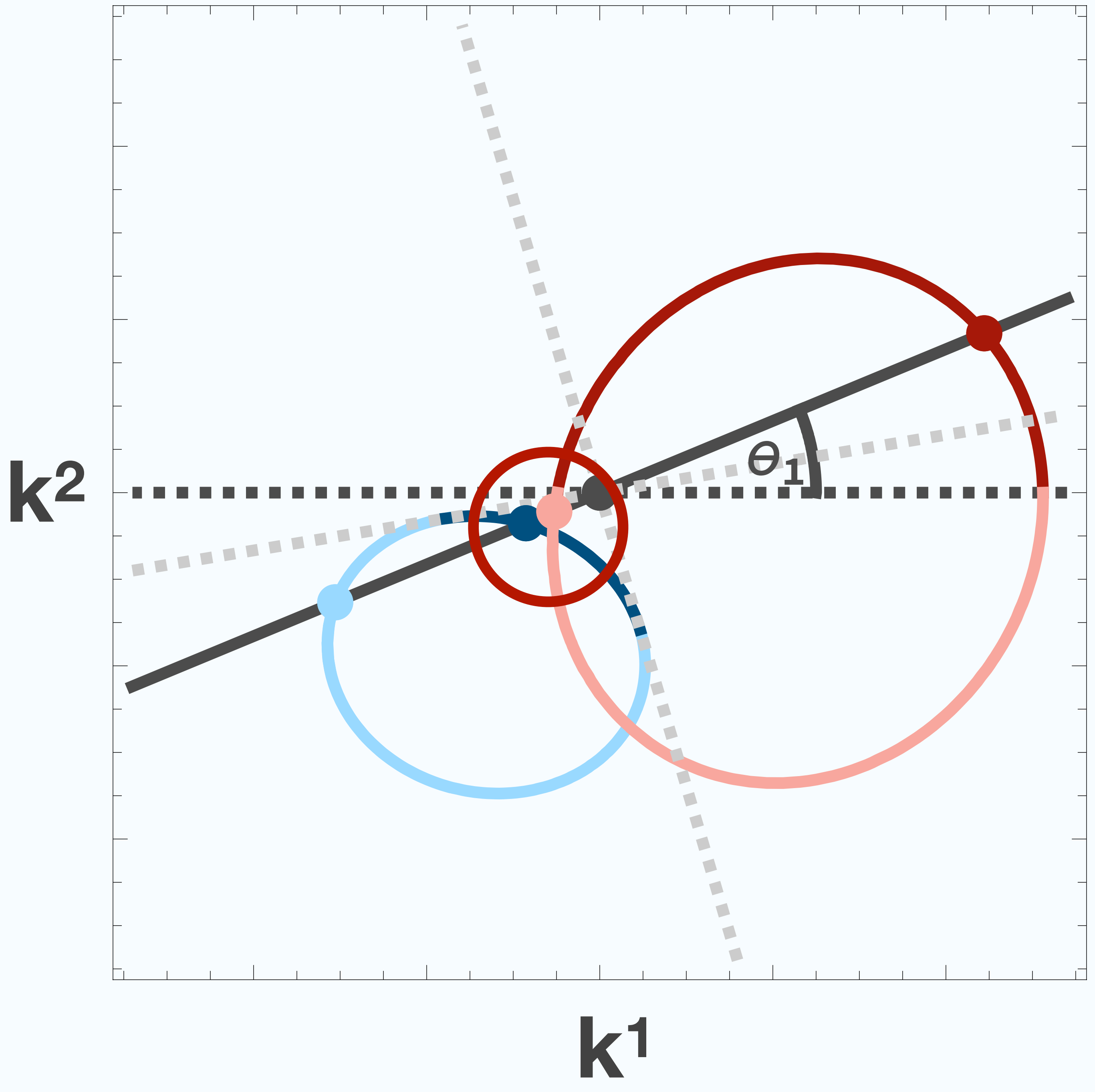
$\mathrm{Res}_{\bigcirc}[\mathcal{I}] + \mathrm{Res}_{\circ}[\mathcal{I}]$



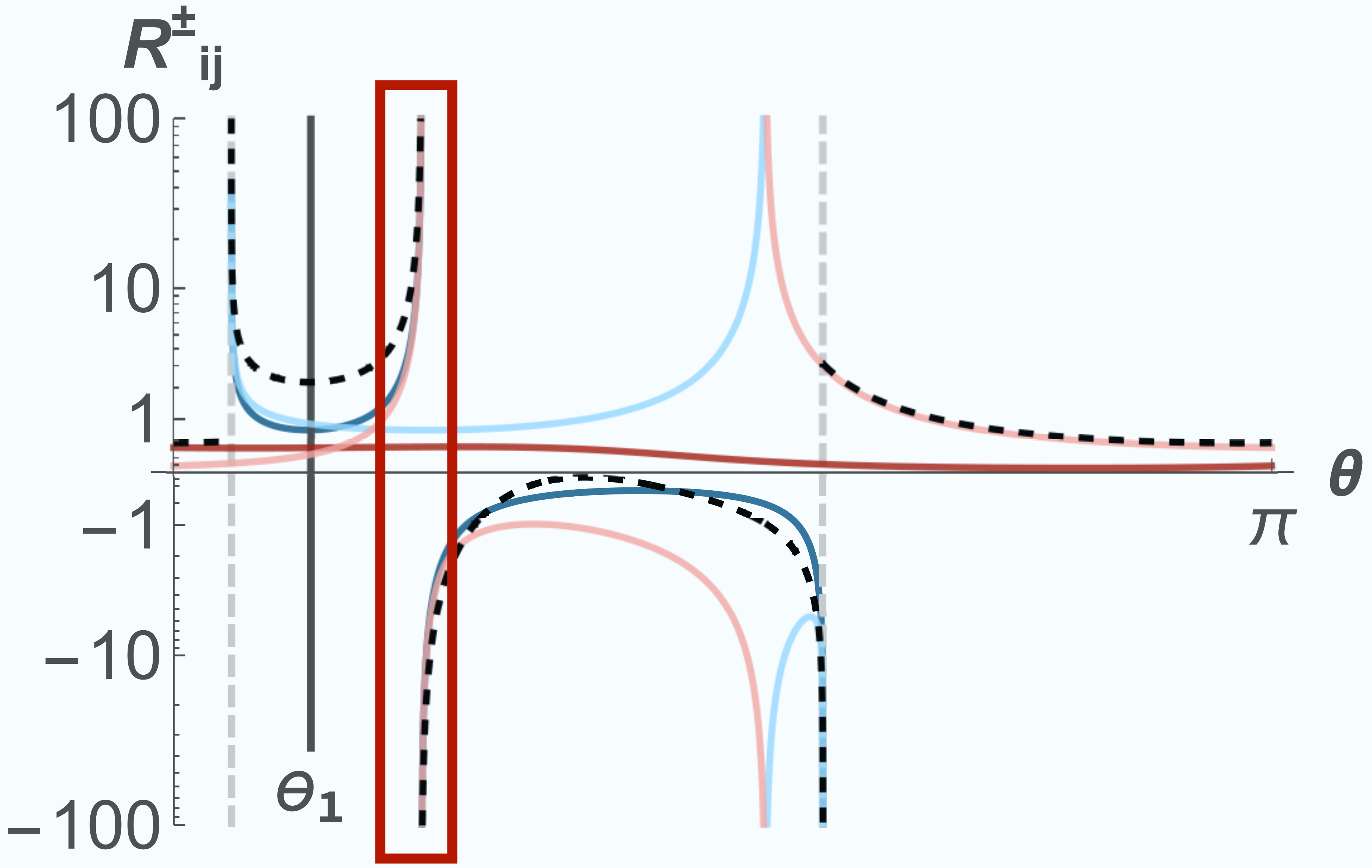


no locally pinched poles





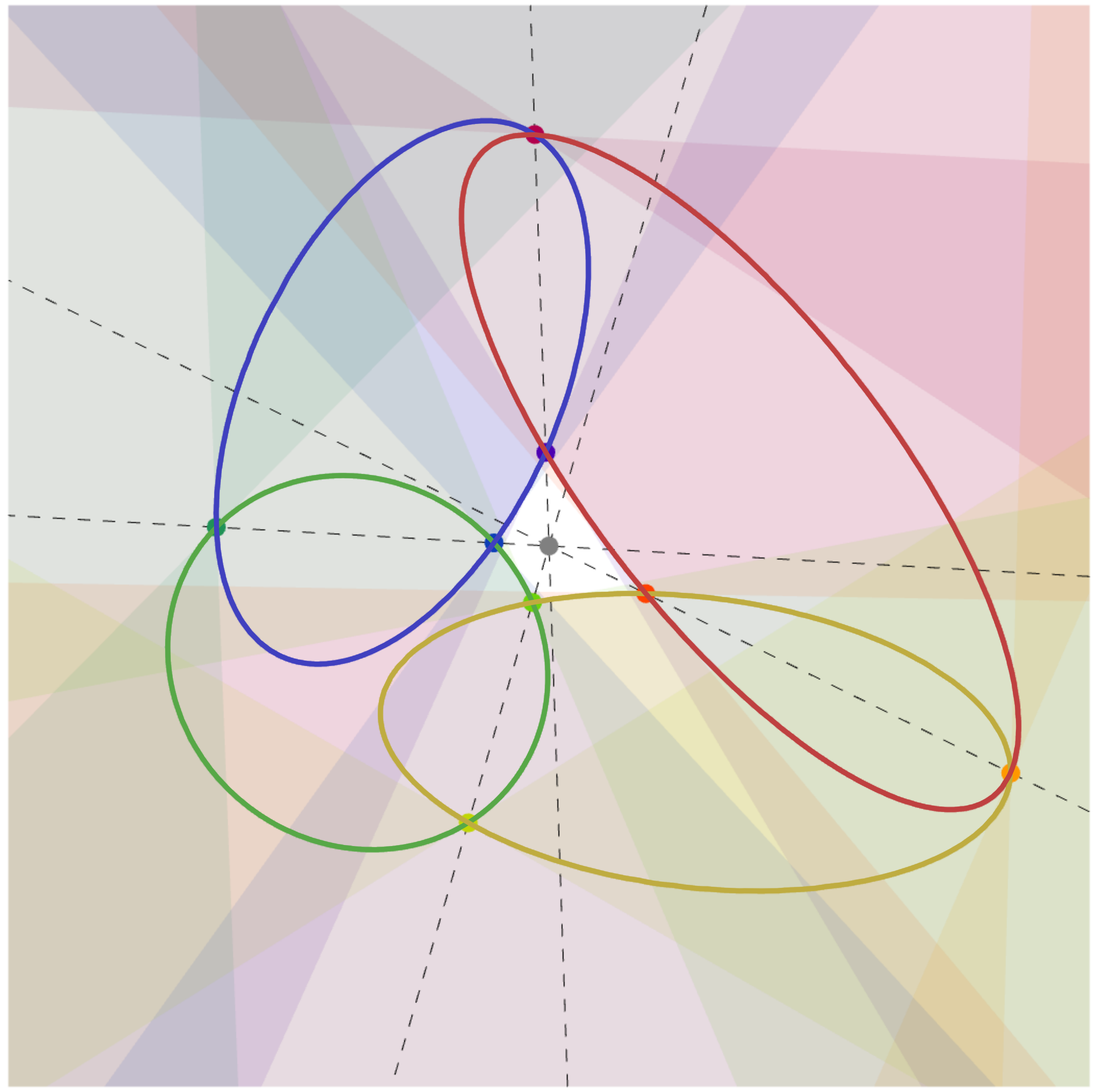
locally pinched poles



What to do if there is no single overlap?

centre outside overlap ⇏ pinched poles

⚠️ but inconvenient integrable singularities



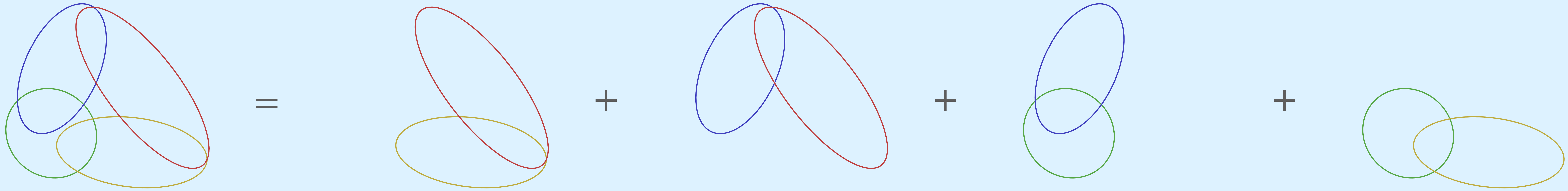
Observations

- 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

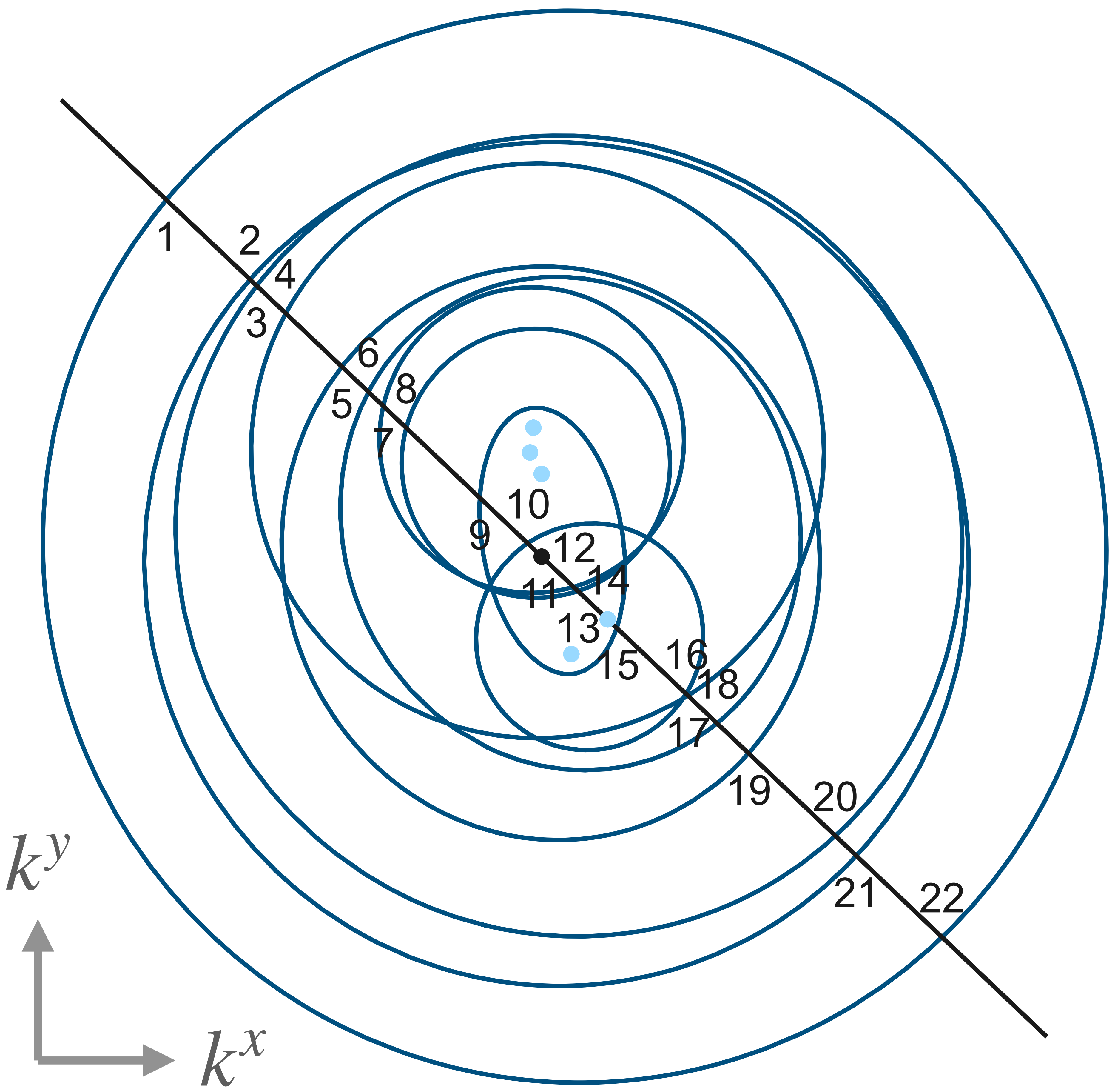
build a channel for each overlap

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

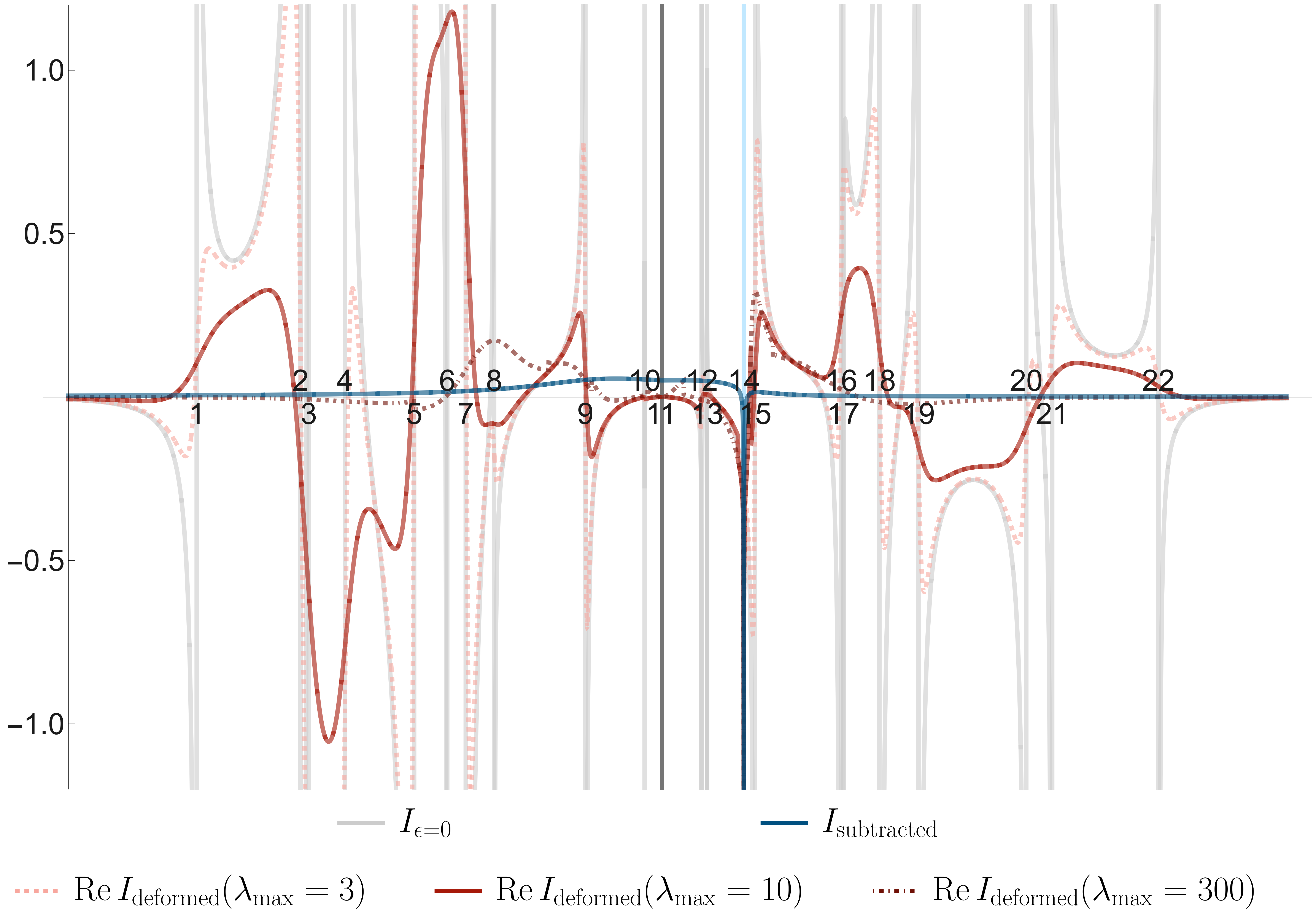


$$\mathscr{I} = \frac{(\mathscr{E}_1\mathscr{E}_2)^2}{(\mathscr{E}_1\mathscr{E}_2)^2 + (\mathscr{E}_2\mathscr{E}_3)^2 + (\mathscr{E}_3\mathscr{E}_4)^2 + (\mathscr{E}_4\mathscr{E}_1)^2}\mathscr{I} + \frac{(\mathscr{E}_2\mathscr{E}_3)^2}{(\mathscr{E}_1\mathscr{E}_2)^2 + (\mathscr{E}_2\mathscr{E}_3)^2 +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

Comparison of threshold subtraction & contour deformation



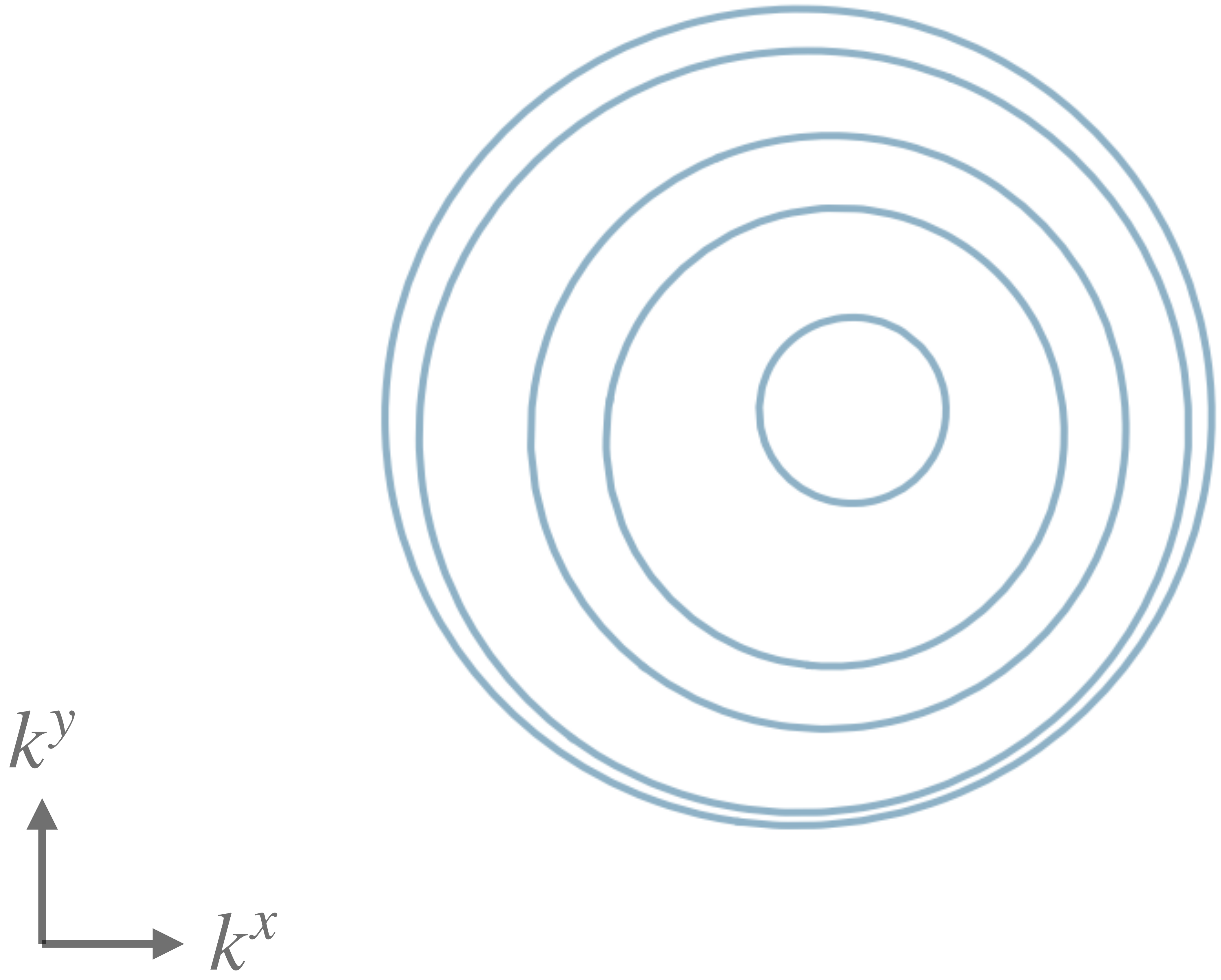
threshold singularities of a pentagon

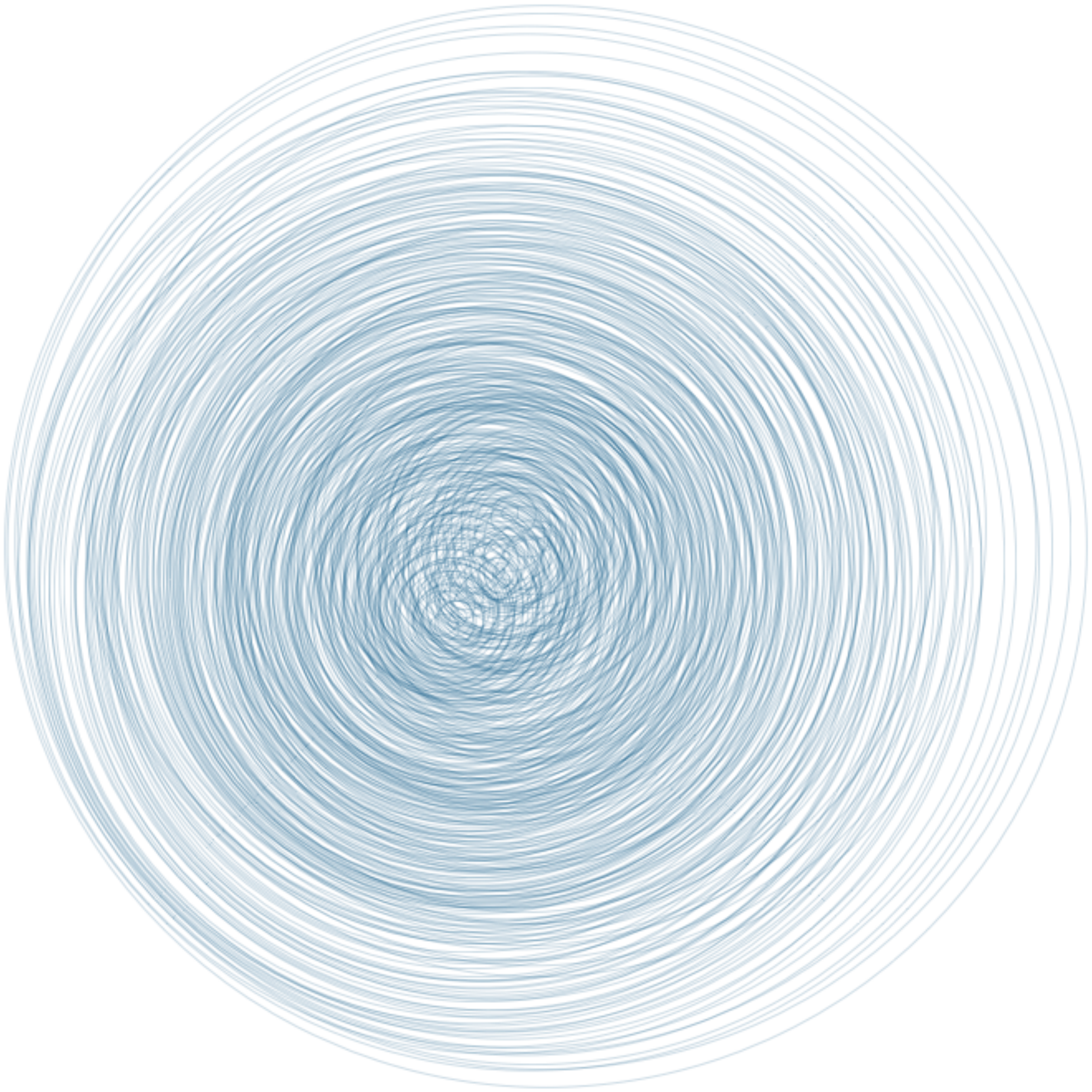


integrand of real part along line segment obtained using **threshold subtraction** or **contour deformation** with different maximal deformation magnitude

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		





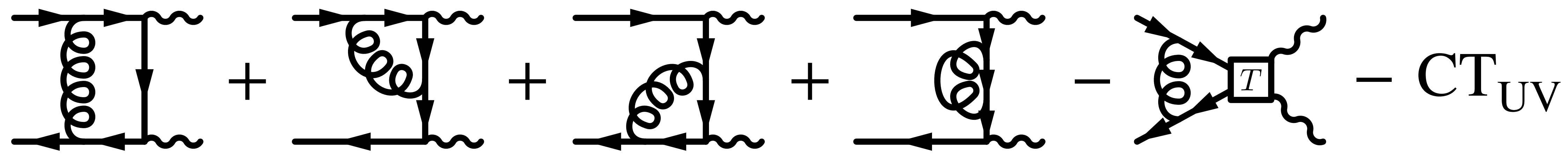
Numerical integration of scattering amplitudes

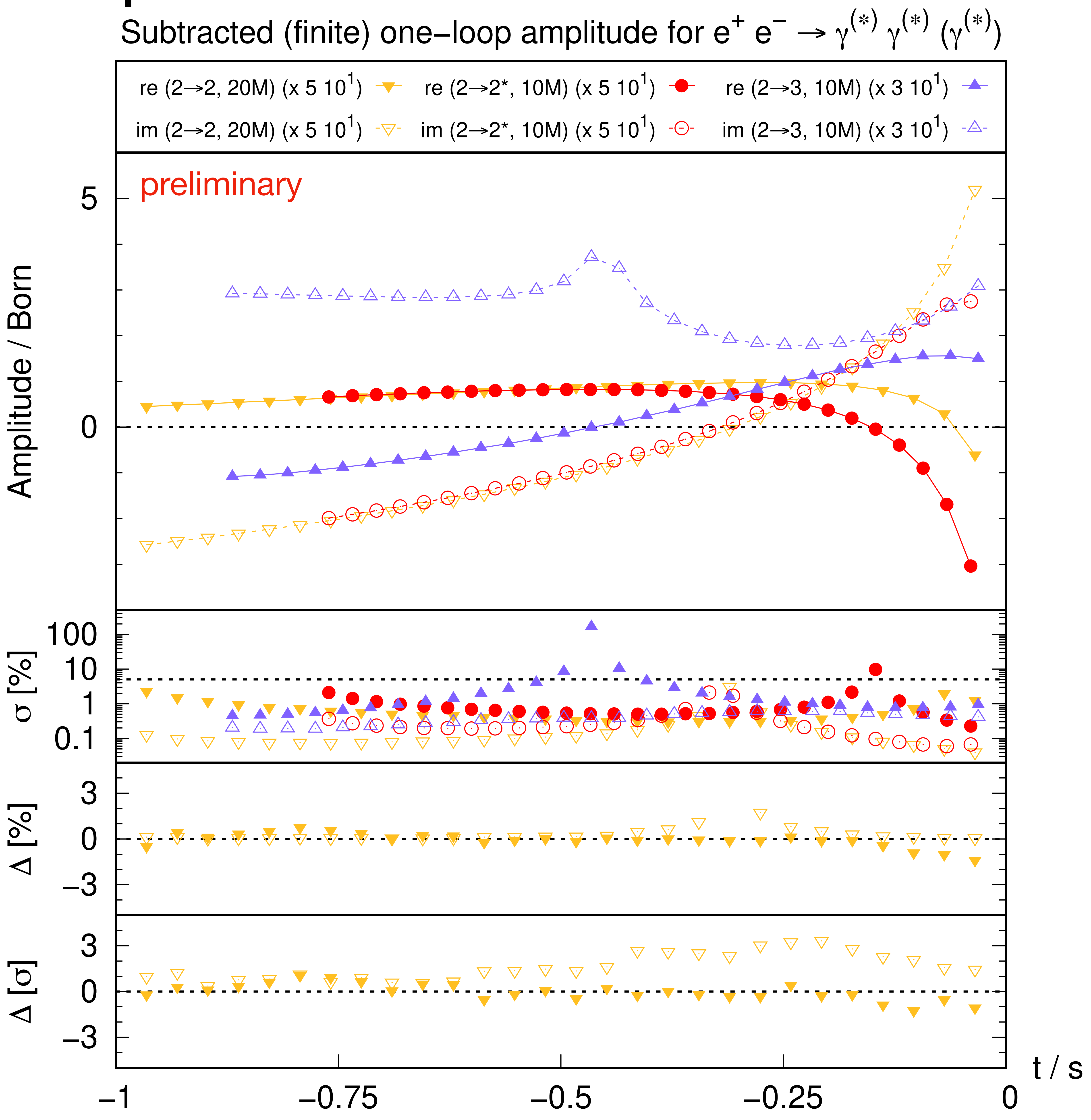
Numerical integration of finite amplitudes in $D = 4$

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

One loop





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

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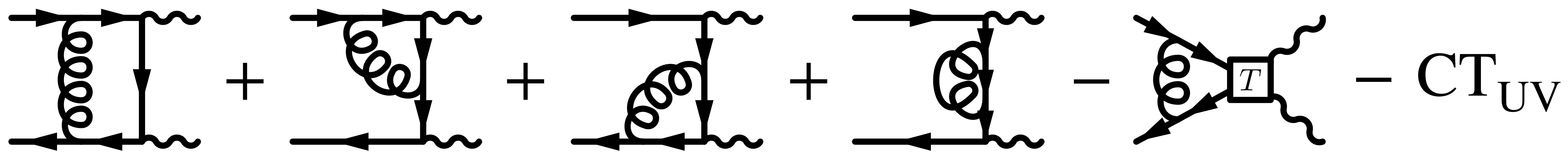
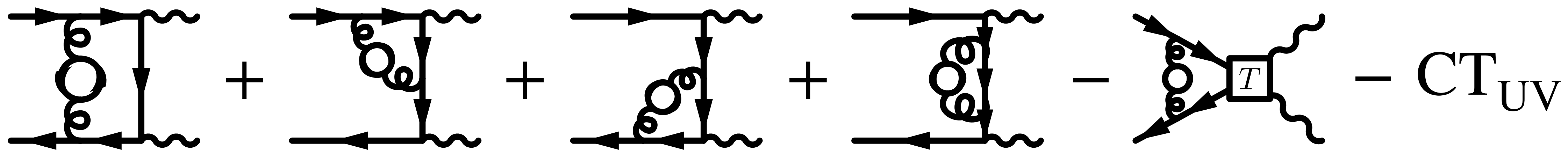
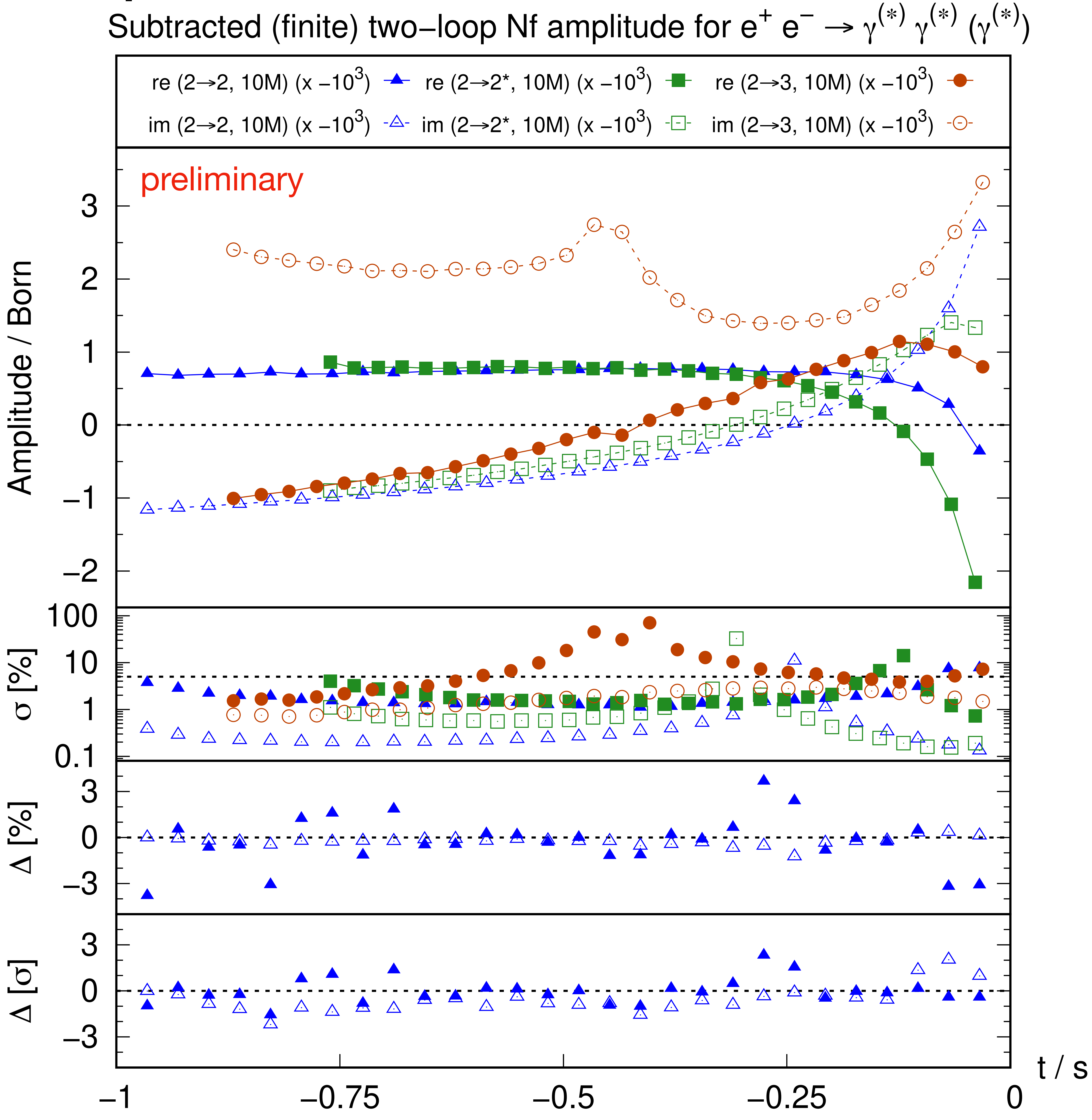


Two loop N_f





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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

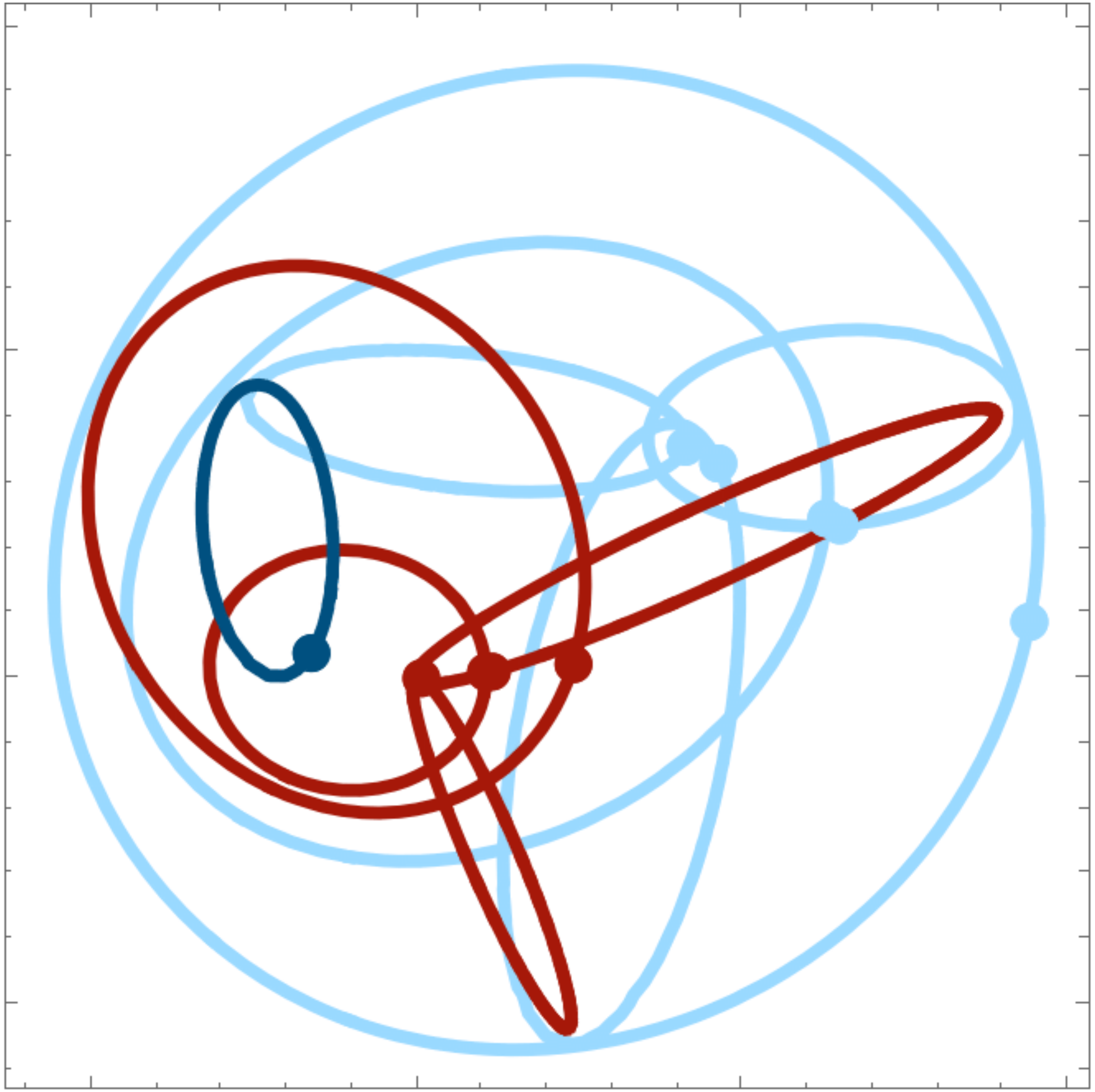
- Threshold subtraction

  → 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!