Numerical threshold subtraction in physical amplitudes

Matilde Vicini
ETH Zurich

Loops & Legs 2024 @ Wittenberg
18th April 2024

collaboration with Dario Kermanschah

N_f virtual corrections to vector boson production at NNLO

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Virtual corrections to vector boson production

1. Why numerical methods are needed at NNLO
2. IR/UV singularities
3. Threshold singularities
4. Results
5. Conclusion

Phenomenological importance of vector boson production

- **Vector boson production: irreducible backgrounds to many new physics searches.**
- **Recent experimental measurements for vector-boson production that use the full Run-2 data are available.**
- **Theoretical computation for colour singlet production in NNLO pQCD up to two bosons is now standard.**
- **The production of three vector bosons remains a challenge in analytical computations.**
  - $q\bar{q} \to \gamma\gamma\gamma$ **recently calculated analytically at NNLO**

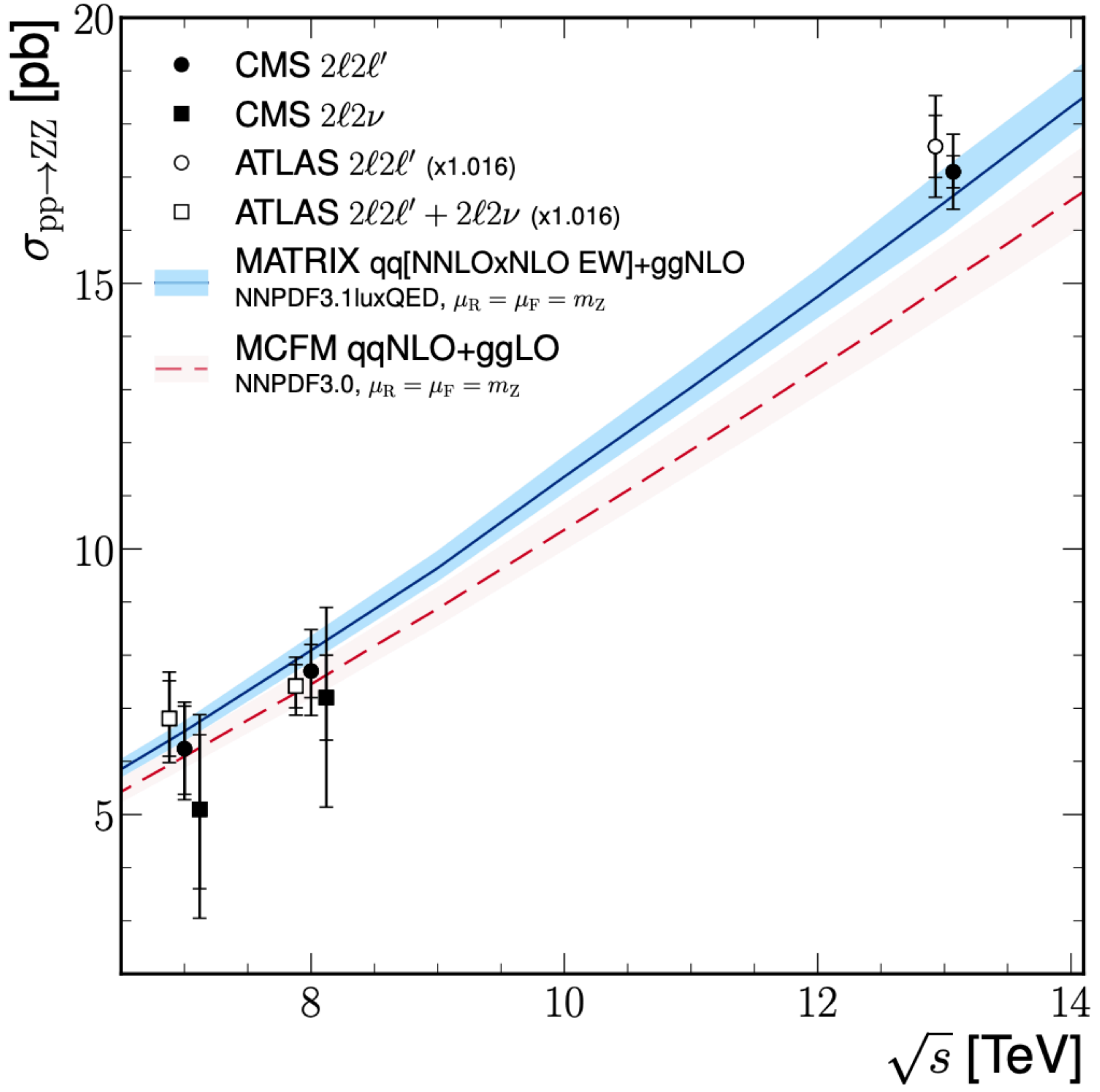
    2010.04681, Kallweit, Sotnikov, Wiesemann

    2010.15834, Abreu, Page, Pascual, Sotnikov

    2012.13553, Chawdhry, Czakon, Mitov, Poncelet

    …
  - **five-point two-loop one-mass scattering**

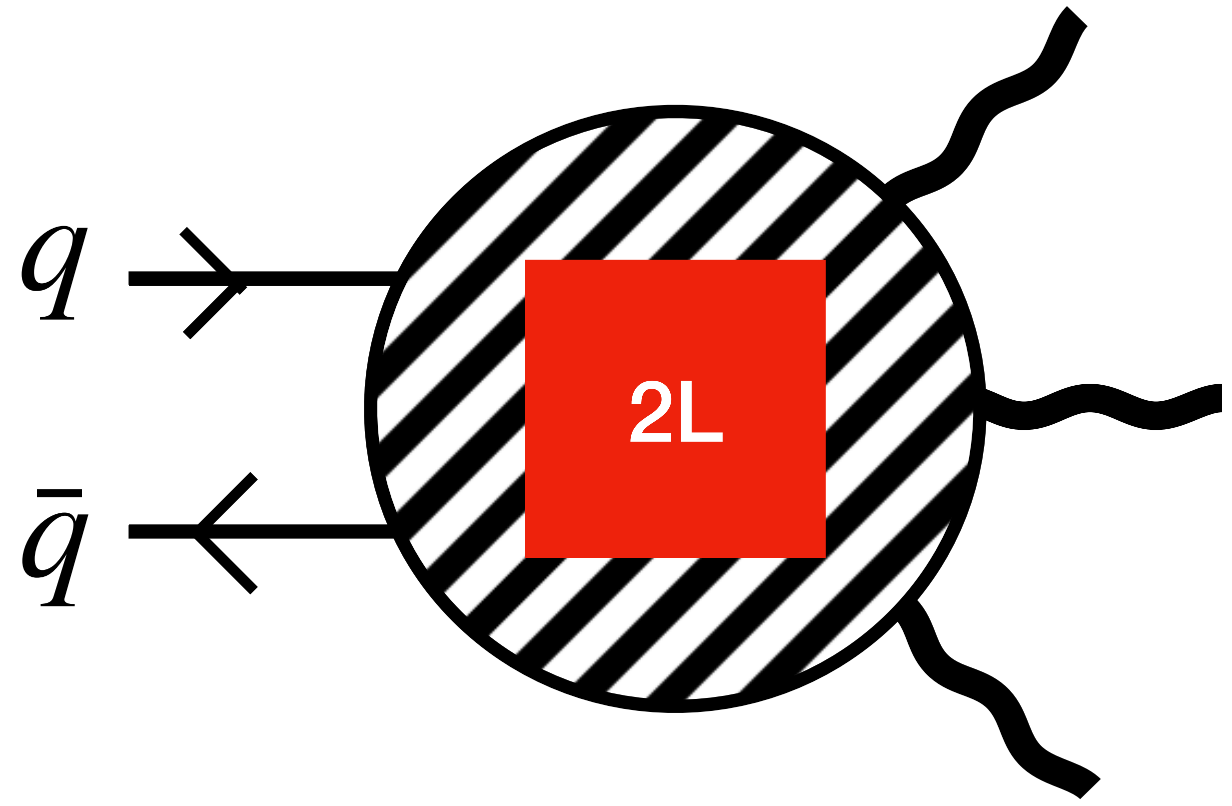
    2306.15431, Abreu, Chicherin, Ita, Page, Sotnikov, Tschernow, Zoia
  - **see more details on status in G. De Laurentis' talk**



Measurements of $\mathrm{pp} \to ZZ$ *production cross-sections and constraints on anomalous triple gauge couplings at* $\sqrt{s} = 13$ *TeV*, **CMS collaboration (2020)**

Why numerical methods are needed at NNLO

- The analytical computation of the two-loop integral is challenging

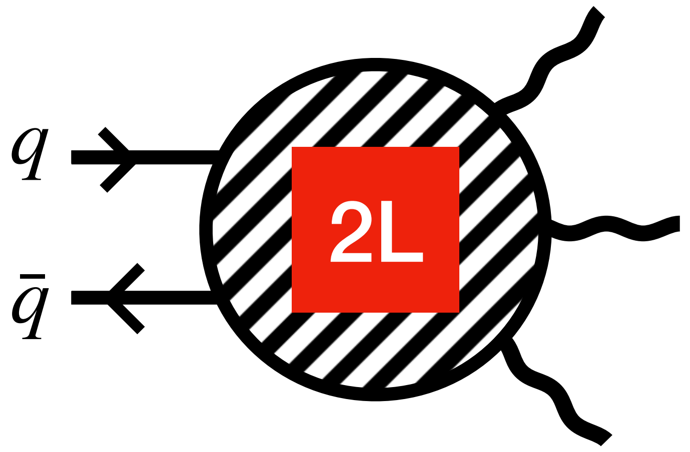


3 external massive vector boson

- High multiplicity in the external legs + many kinematical scales

It is worthwhile to attempt the computation with methods different from the analytical ones!

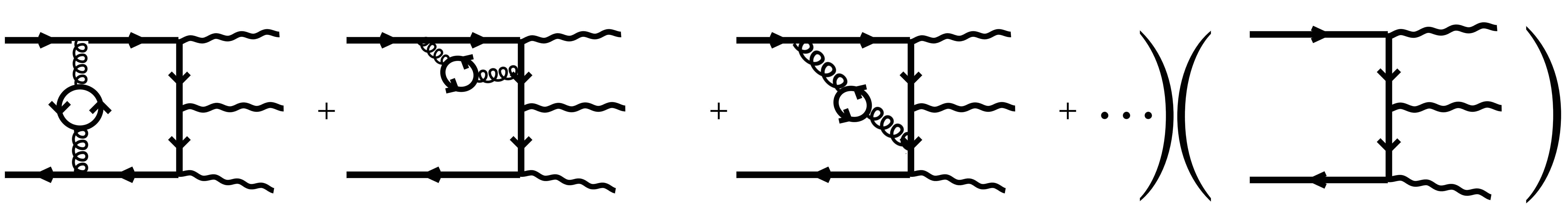
In this talk...



3 external massive vector boson

- **We tackled its first ingredient numerically, i.e. the N_f contribution:**

$$\sigma_{\text{virt}}^{(2,N_f)} \sim \int \mathbf{d}\Phi_3 \frac{1}{F} 2\,\mathrm{Re}\left[\sum_h \left(\cdots + \cdots + \cdots + \ldots \right)\left(\cdots \right)^* \right]$$

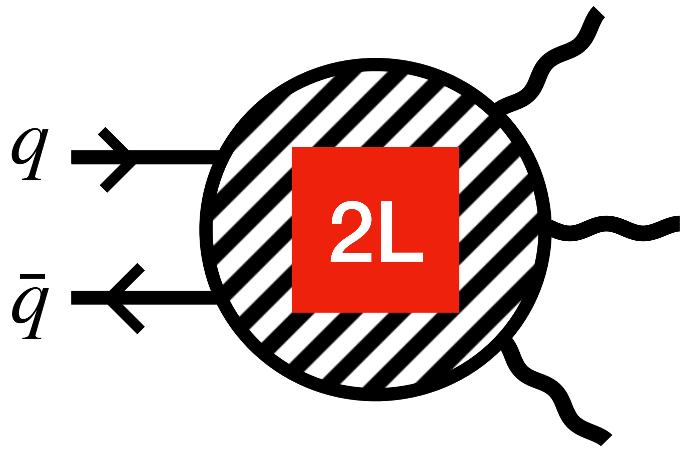


- **To integrate numerically, we need to**

  - **remove infrared (IR) singularities**
  - **remove ultraviolet (UV) singularities**
  - **remove threshold singularities**

before integrating with Monte-Carlo methods

In this talk…



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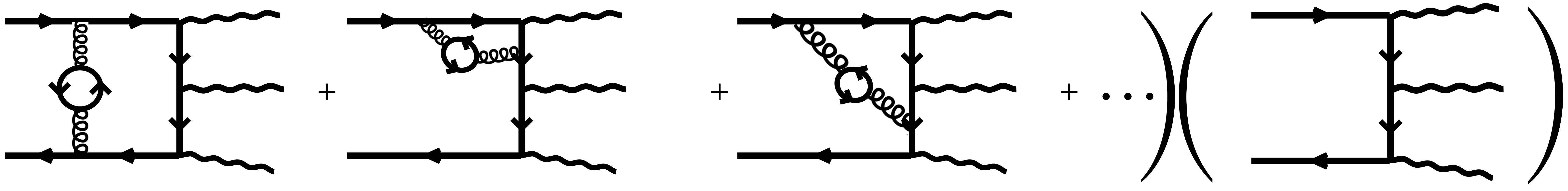

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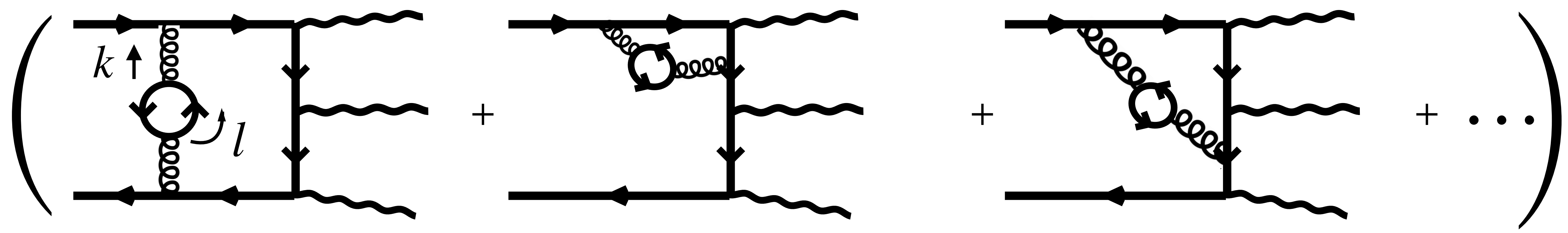
Strategy:

we will subtract local counterterms which we eventually add back integrated

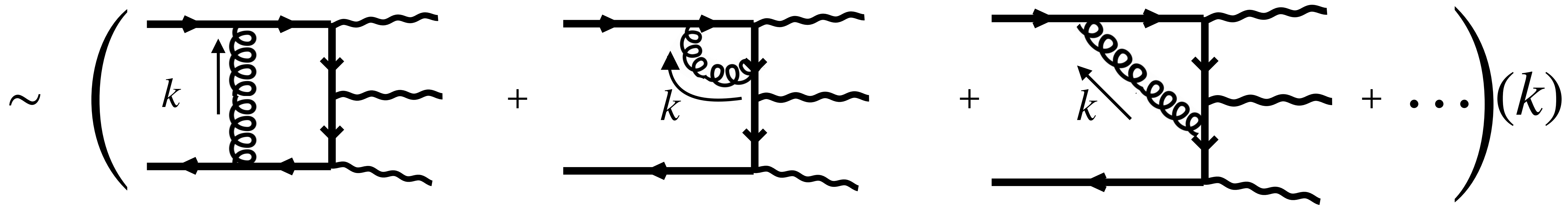
IR divergences

2008.12293, Anastasiou, Haindl, Sterman, Yang, Zeng



has power-like IR singularities

We modify the integrand, performing an initial tensor reduction on the loop momentum l. This leads to



$$\sim \left(\cdots \right)(k)\ \frac{1}{l^2(l+k)^2}$$

Which now has same IR divergences as the one-loop amplitude.

Choice of an alternative integrand as starting point for local subtraction of IR singularities.

IR divergences

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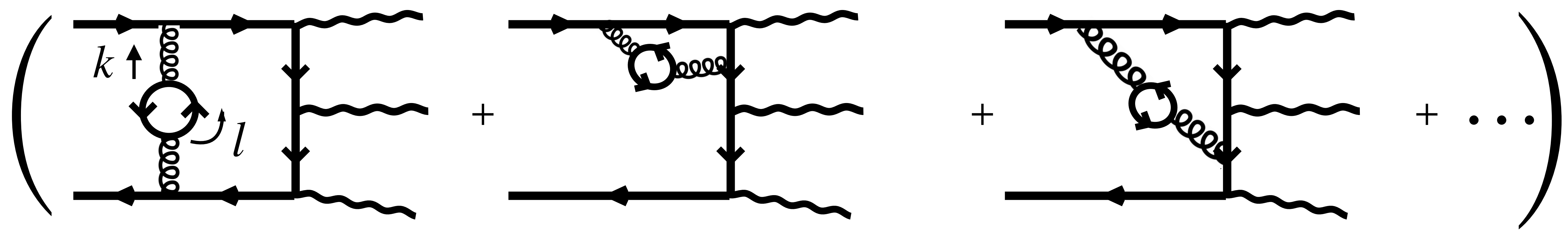

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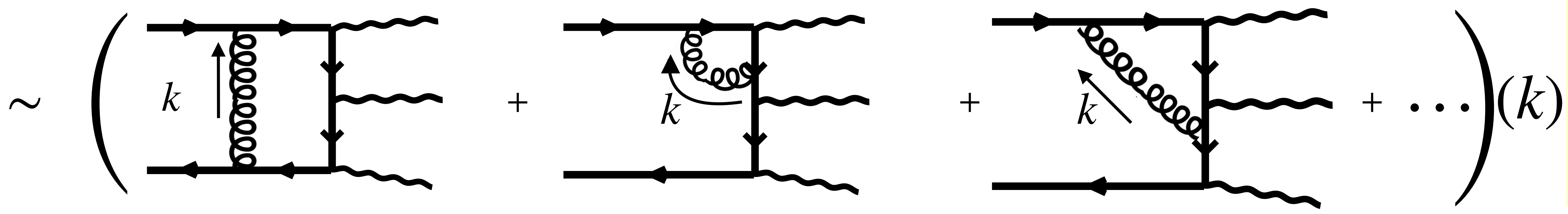

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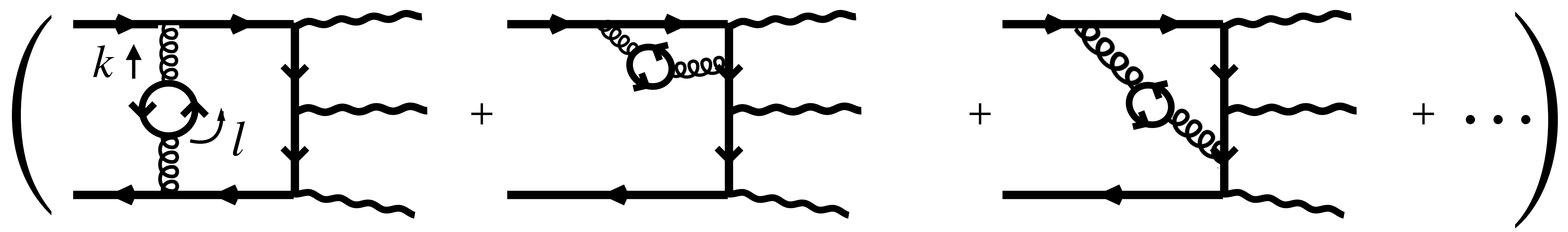

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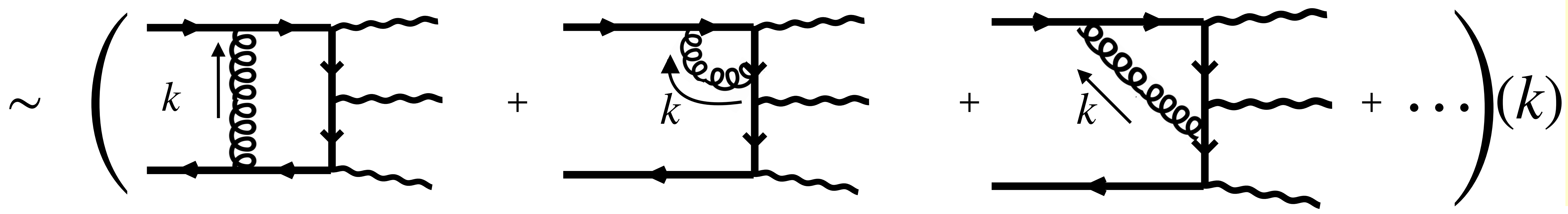


$$\frac{1}{l^2(l+k)^2}$$

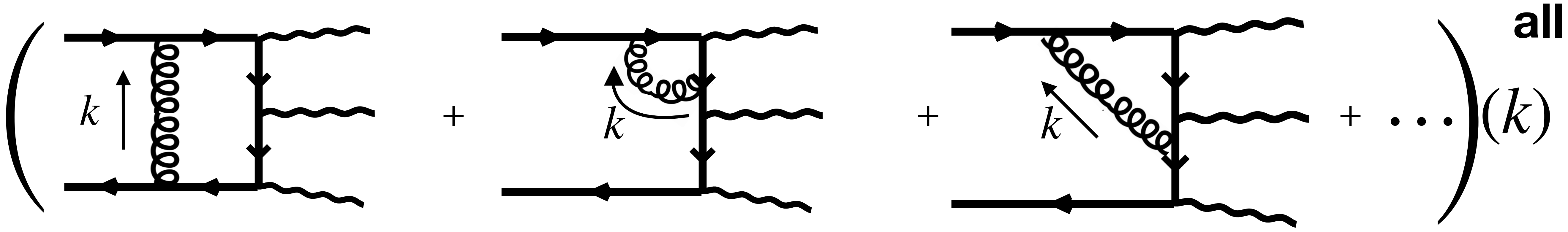
just UV divergent when $l \to \infty$

Which now has same IR divergences as the one-loop amplitude.

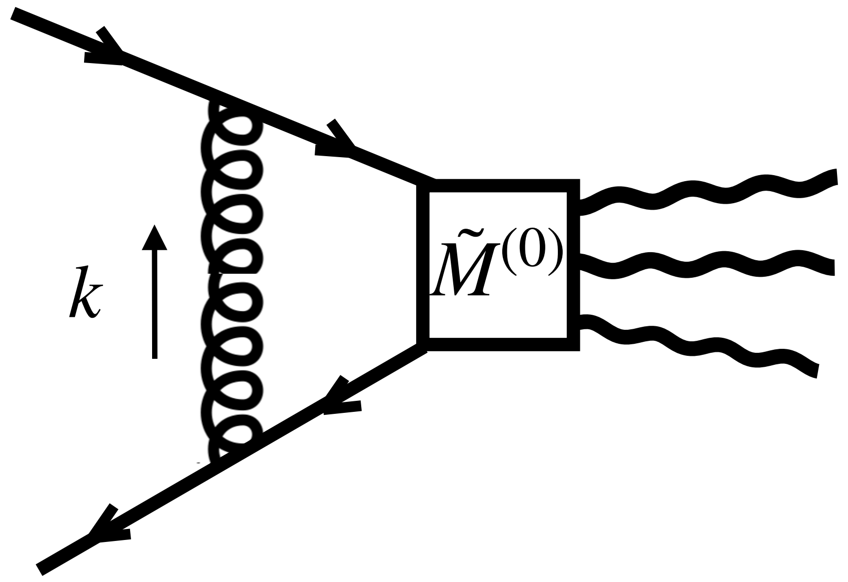
Choice of an alternative integrand as starting point for local subtraction of IR singularities.

The IR counterterm

2008.12293, Anastasiou, Haindl, Sterman, Yang, Zeng



all IR limits →

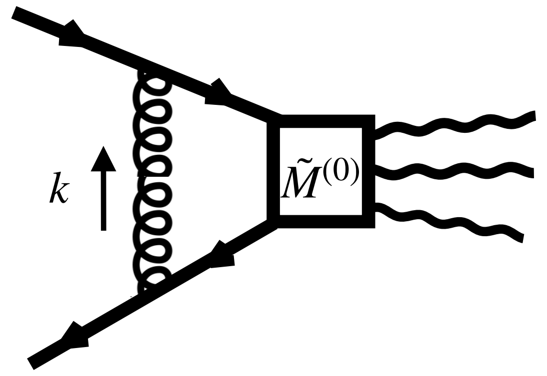


$$= -ig_s^2 C_F \frac{\bar{v}(p_2)\gamma^\mu(\not{k} - \not{p}_2)\left[\widetilde{\mathcal{M}}^{(0)}\right](\not{p}_1 + \not{k})\gamma_\mu u(p_1)}{k^2(k+p_1)^2(k-p_2)^2}$$

The IR form-factor counterterm expresses at the integrand level the integrated Catani-Seymour factorisation of IR divergences:

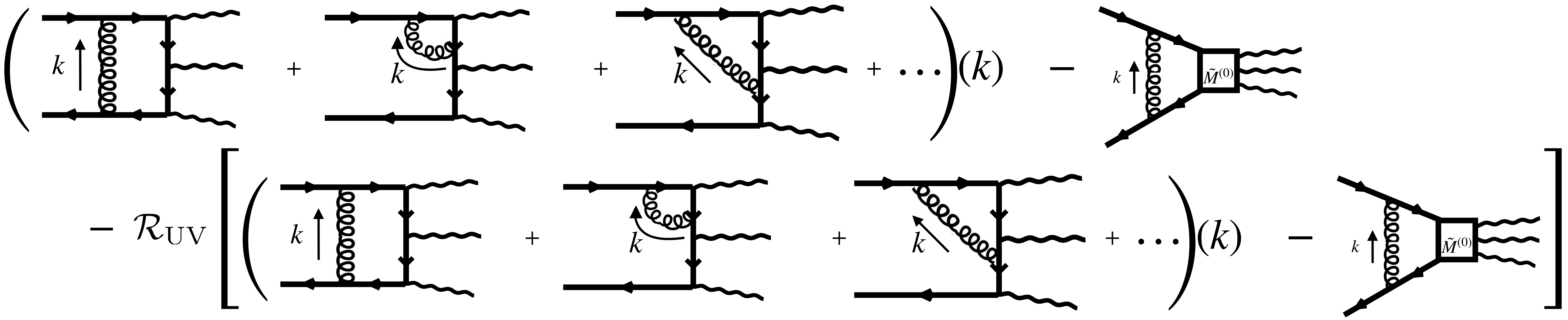
$$M^{(1)} - I^{(1)}M^{(0)} = \text{finite}$$

To get rid of UV divergences at the local level, we also introduce UV counterterms, one for each UV singular diagram, e.g.:

$\mathcal{R}_{\rm UV}\Big($  $\Big)$

$$= -ig_s^2 C_F \frac{\bar{v}(p_2)\gamma^\mu \not{k}\left[\widetilde{\mathcal{M}}^{(0)}\right]\not{k}\gamma_\mu u(p_1)}{(k^2 - M_{\rm UV}^2)^3}$$

Subtracted amplitude in D=4



$=: \mathscr{M}^{(1)}_{\rm finite}(k)$

locally finite in D=4

For the $(2,N_f)$ case:

$$\mathscr{M}^{(2,N_f)}_{\rm finite}(k,l) := \left[\frac{1}{l^2(l+k)^2} - \frac{1}{(l^2 - M_{UV}^2)^2}\right] \mathscr{M}^{(1)}_{\rm finite}(k)$$

$\mathscr{M}_{\rm finite}$ integration numerically in D=4 **in the physical region** cannot happen unless we have a way of extracting the discontinuities arising from threshold singularities.

▷In other words, what do we do about the $i\epsilon$ prescription in a numerical program?

Subtracted amplitude in D=4

$\mathcal{M}_{\text{finite}}$ integration numerically in D=4 **in the physical region** cannot happen unless we have a way of extracting its discontinuities arising from threshold singularities.

Several possibilities:

Numerical contour deformation

Feynman parameters

0004013, Binoth, Heinrich
0703282, Anastasiou, Beerli, Daleo
0703273, Lazopoulos, Melnikov, Petriello
1011.5493, Carter, Heinrich
1703.09692, Borowka, Heinrich, Jahn, Jones, Kerner, Schlenk,..
2302.08955, Borinsky, Munch, Tellander
…

Loop Momentum space

9804454, Soper
0812.3686, Gong, Nagy, Soper
1010.4187, Becker, Reuschle, Weinzierl
1111.1733, Becker, Goetz, Reuschle, Schwan, Weinzierl
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What we use:

Numerical threshold subtraction

- 0912.3495, Kilian, Kleinschmidt
- 2110.06869, Kermanschah

To remove threshold singularities in momentum space:

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- expose threshold singularities

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integrate over dk^0

To remove threshold singularities in momentum space:

- expose threshold singularities

integrate over dk^0

- regulate threshold singularities

To remove threshold singularities in momentum space:

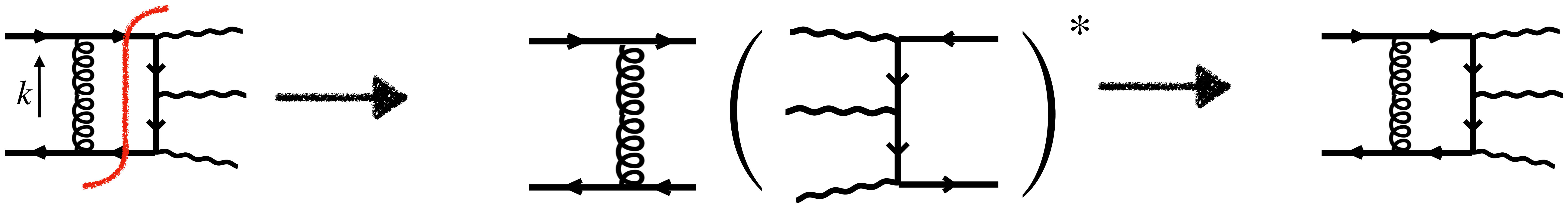
- expose threshold singularities — integrate over dk^0
- regulate threshold singularities — construct local counterterms

Exposing threshold singularities in loop momentum space

Example of threshold singularity:

corresponds to physical subprocesses

discontinuity of



when cut propagators go on-shell

To expose all the threshold singularities and their overlaps in loop momentum space:

$$\int dk^4 \mathscr{M}_{\text{finite}}(k) = \int d^3\vec{k}\, f^{3\text{d}}\left(\mathscr{M}_{\text{finite}}(k)\right) \sim \int d^3\vec{k} \left\{ \frac{1}{E_1 + E_3 - p_1^0 - p_2^0} \frac{1}{E_0 + E_1 - p_1^0} \cdots + \cdots \right\}$$

E_i **: on-shell energy of propagator** i

$\int dk^0$ **via residue theorem**

f^{3d} **: 3d representation of the integrand, several options:**

- **Loop-Tree-Duality (LTD)**
- **Cross-Free Family (CFF)**

CFF

2211.09653, Capatti

LTD

0804.3170, Catani, Gleisberg, Krauss, Rodrigo, Winter

1904.08389, Aguilera-Verdugo, Driencourt-Mangin, Plenter, Ramírez-Uribe, Rodrigo, Sborlini et al.,

1906.06138, Capatti, Hirschi, Kermanschah, Ruijl

2009.05509, Capatti, Hirschi, Kermanschah, Pelloni, Ruijl

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Numerical threshold subtraction

Setting each denominator = 0 identifies a bounded region in $\vec{k}$ space

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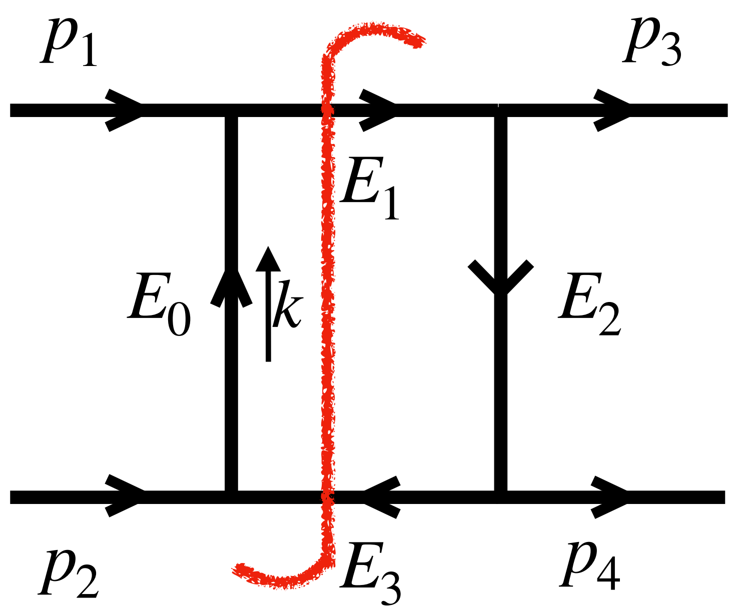
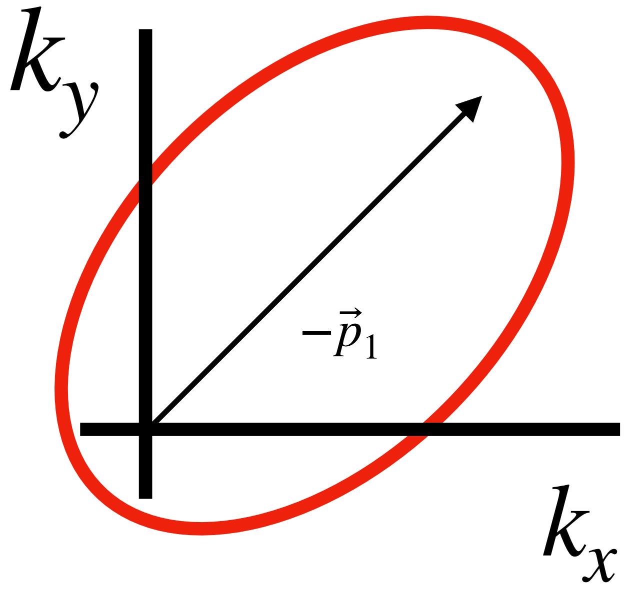


$$E_1 + E_3 - p_1^0 - p_2^0 = 0$$

for some $\vec{k} = \vec{k}^*$

if $(p_1 + p_2)^2 > 0\,, (p_1^0 + p_2^0) > 0$



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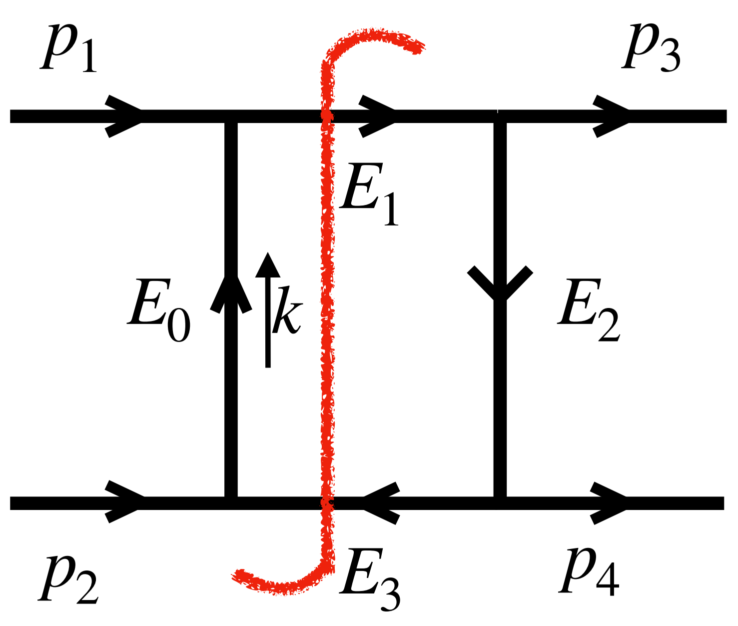

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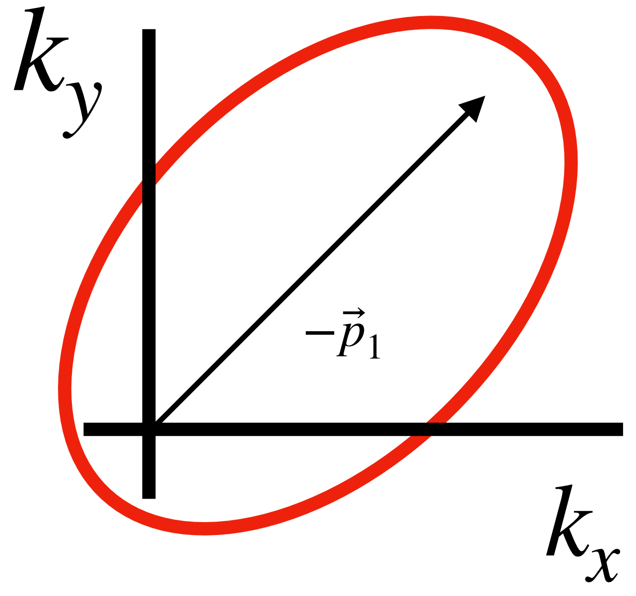

2110.06869, Kermanschah

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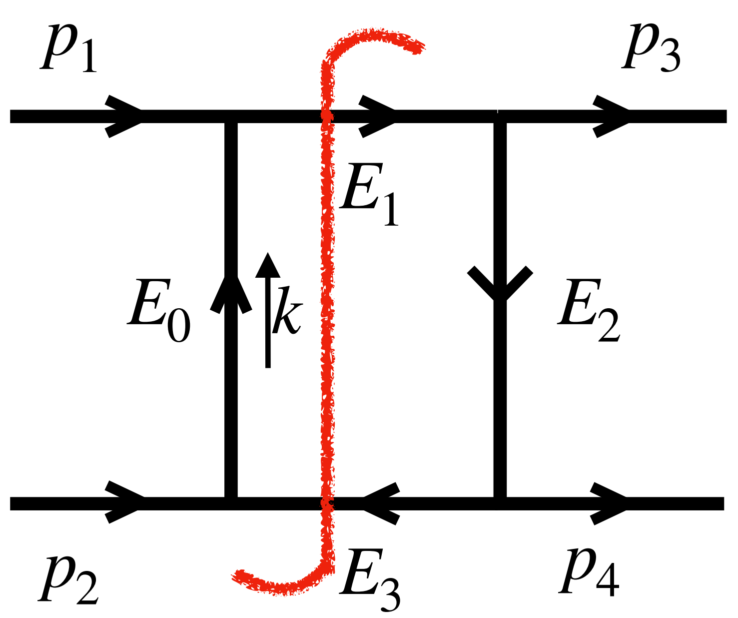

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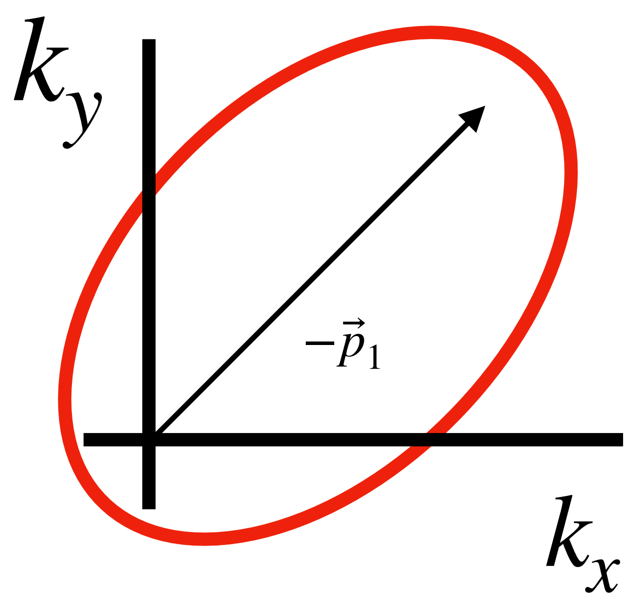
⟷



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around the threshold singularity at $\vec{k} = \vec{k}^*$ the integrand behaves as:

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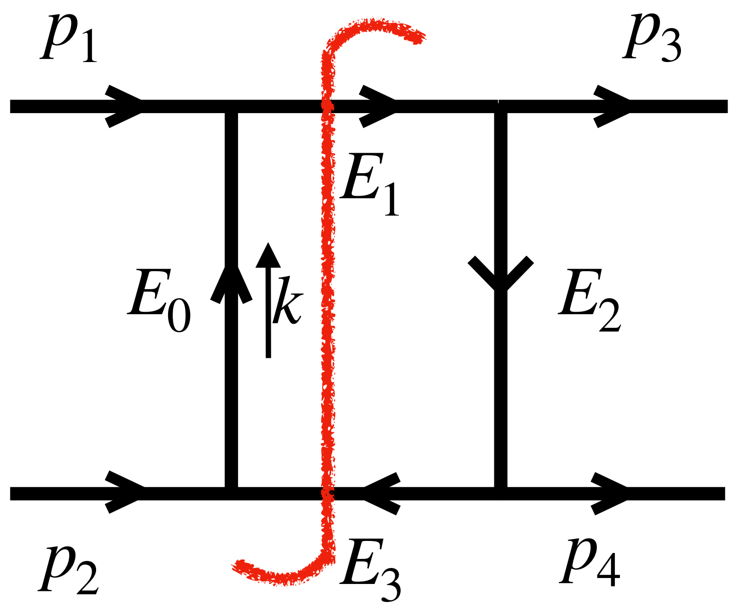

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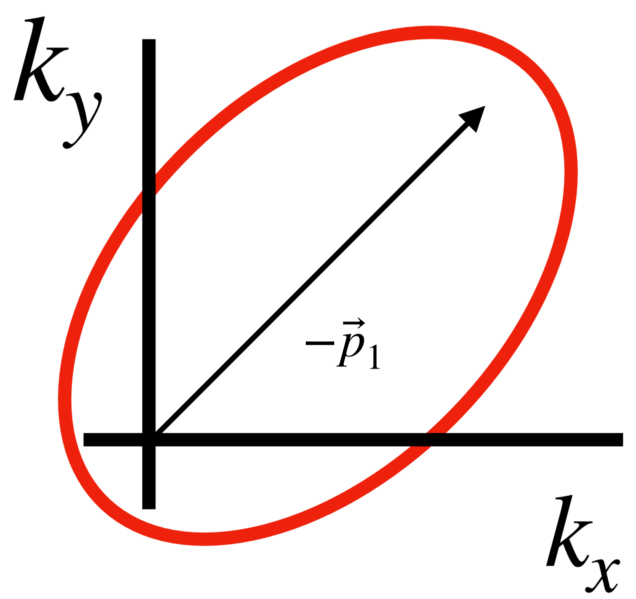

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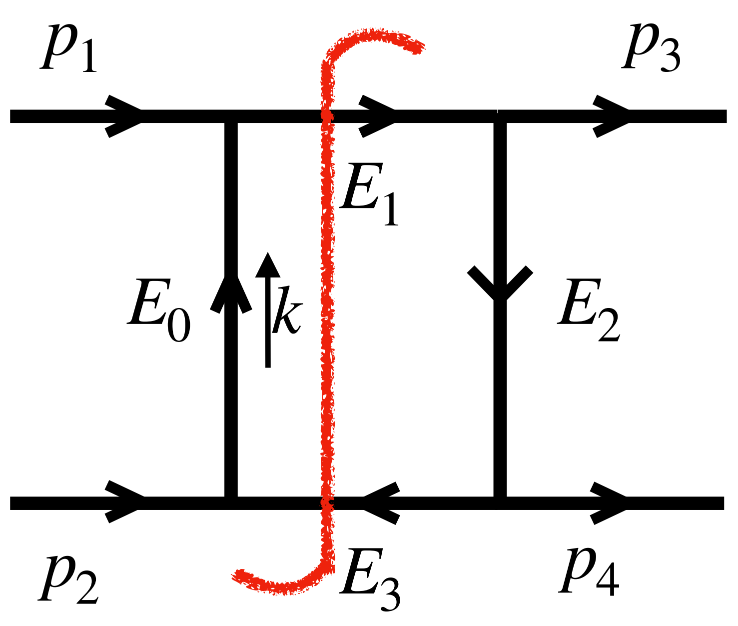

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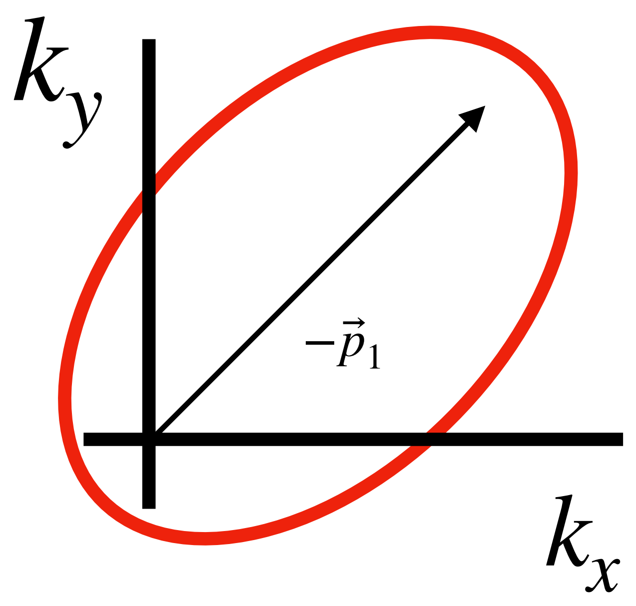

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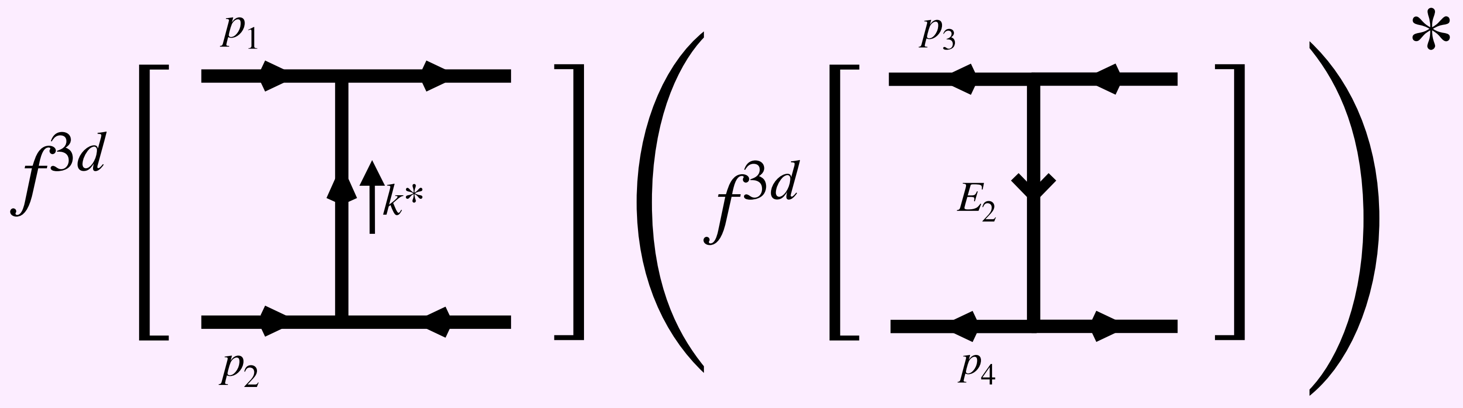

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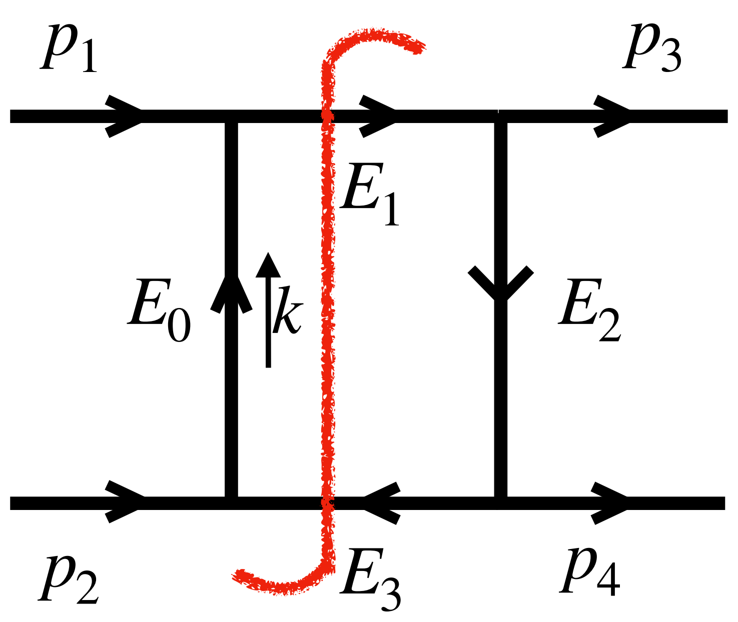

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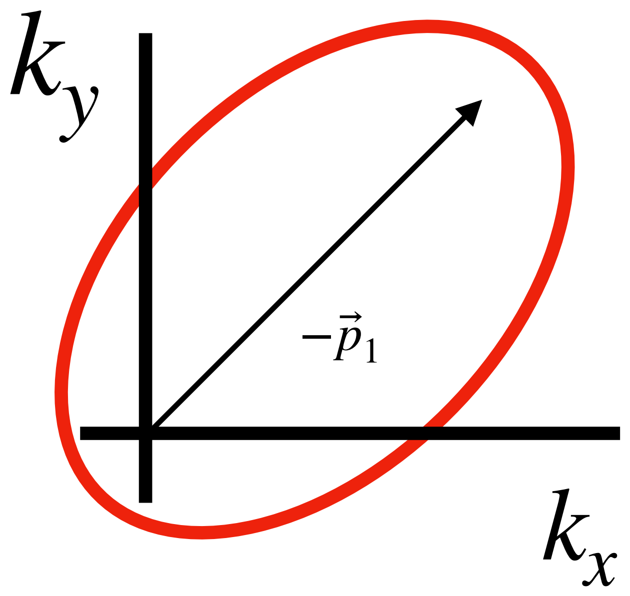

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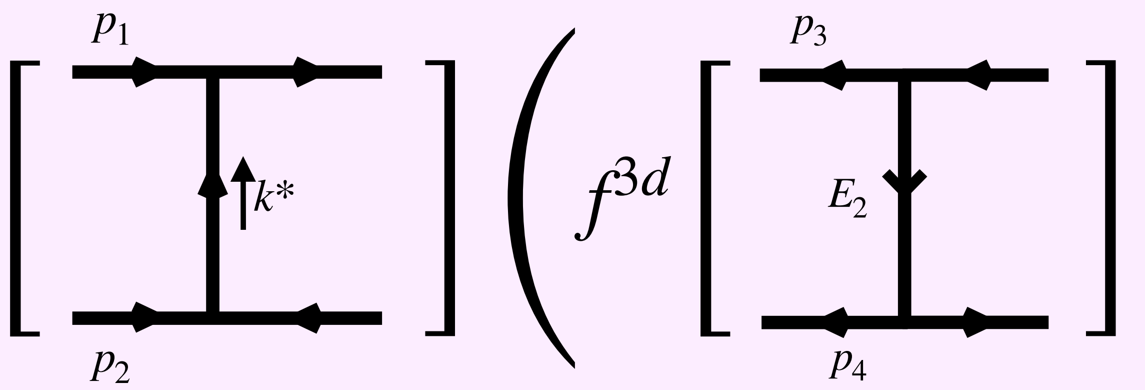

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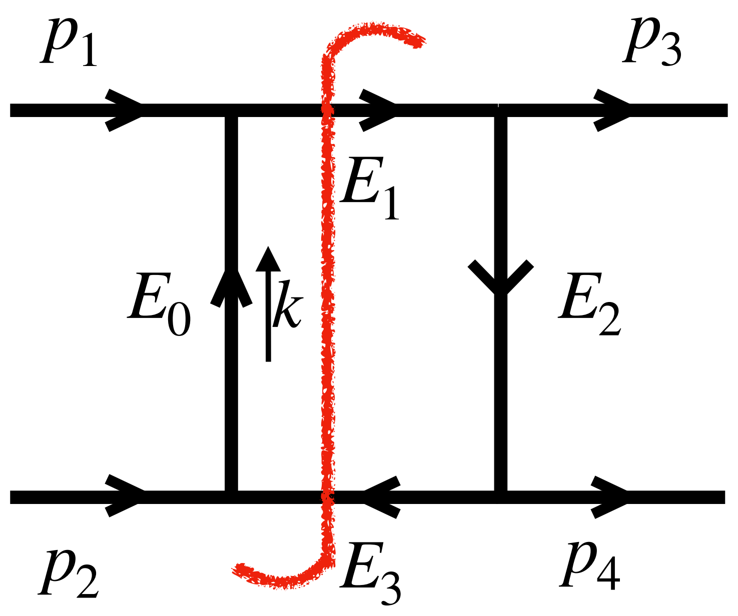
e.g.:



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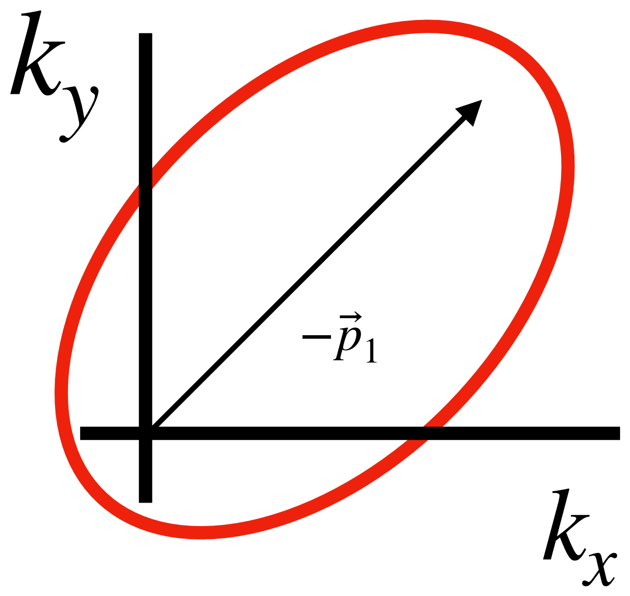
$\longleftrightarrow$



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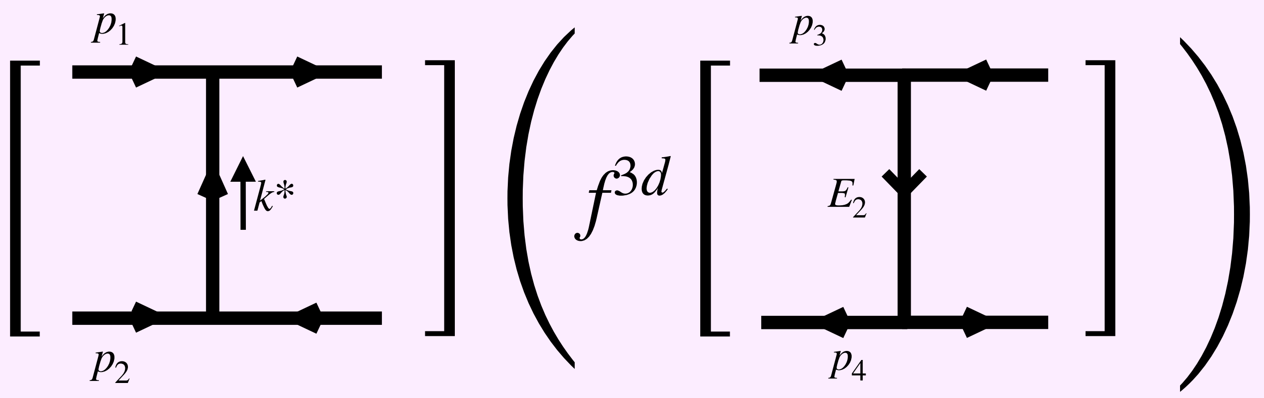

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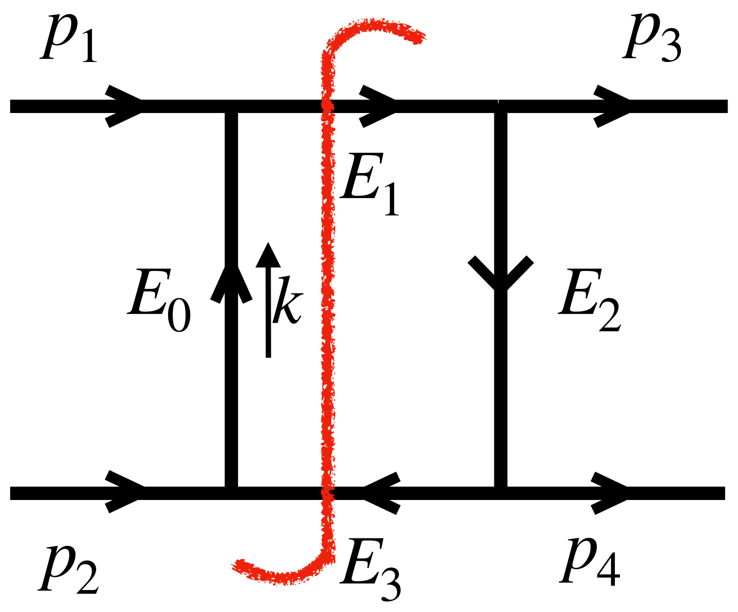

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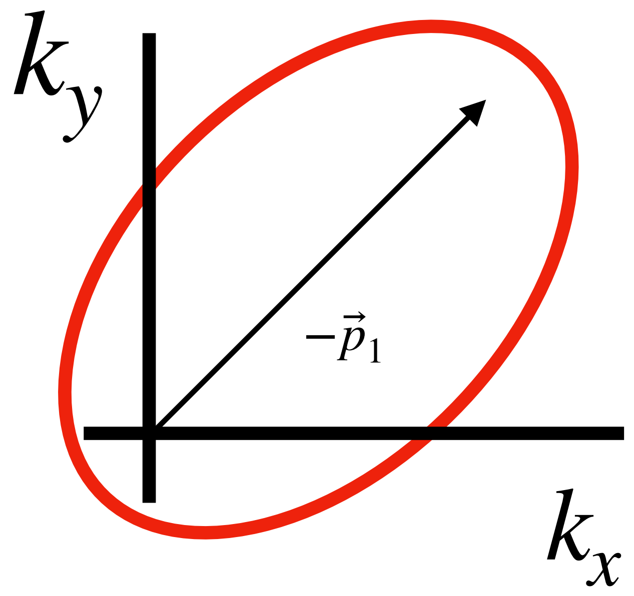

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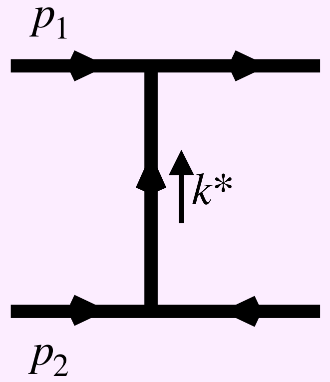
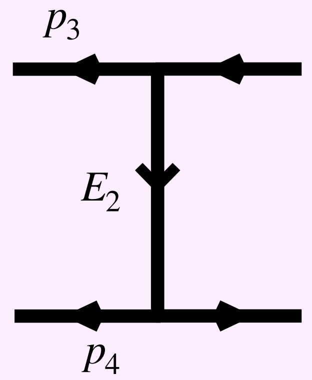
χ **: suppression function,** $\text{Res}_{\vec{k}=\vec{k}^*}[f^{3d}(\mathcal{M})] \sim f^{3d}$ [] $\left(f^{3d} \right.$ [] $\left. \right)^*$

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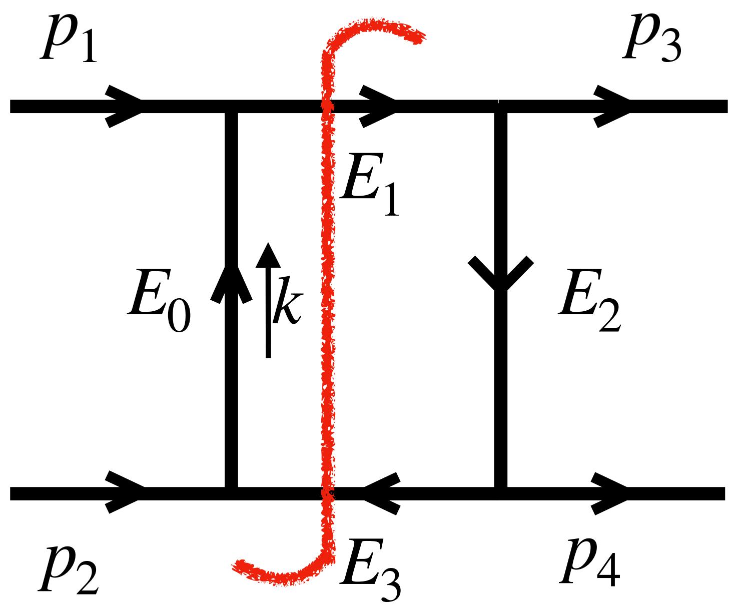

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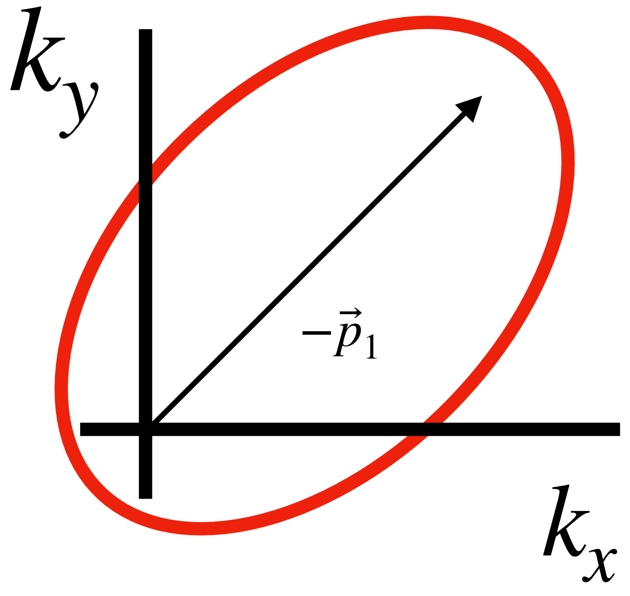

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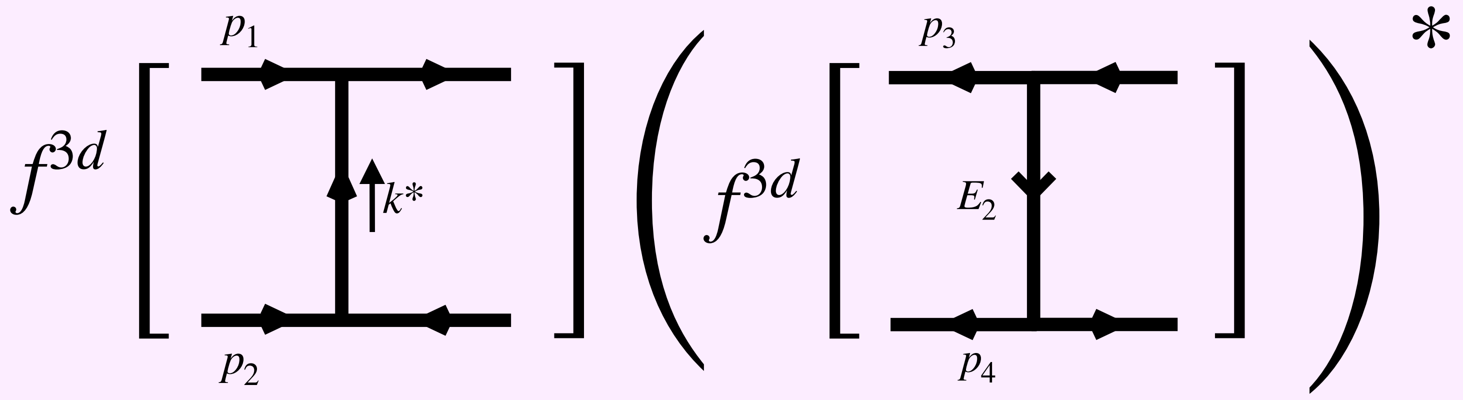

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$$\lim_{\epsilon\to 0}\frac{1}{x-a\pm i\epsilon}=PV\frac{1}{x-a}\mp i\pi\delta(x-a)$$

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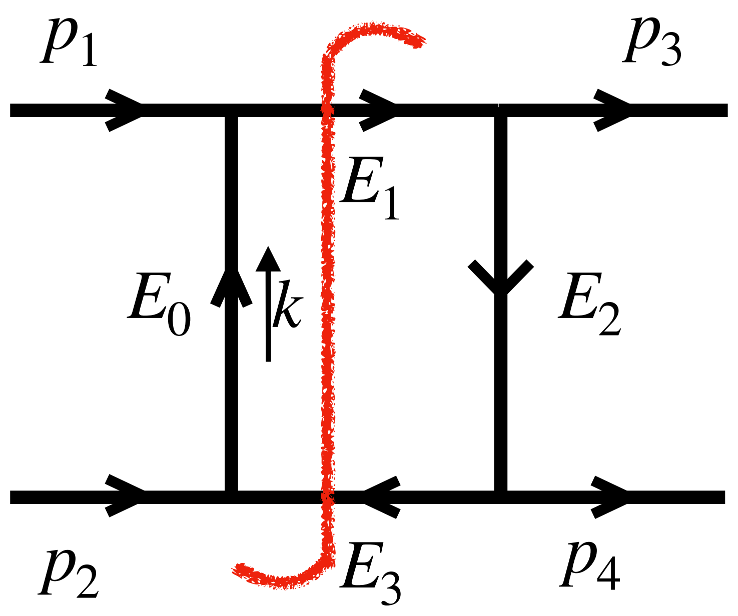

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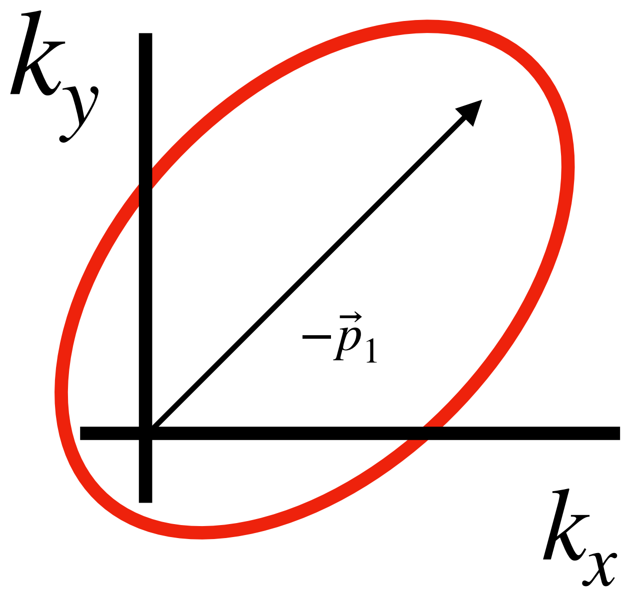

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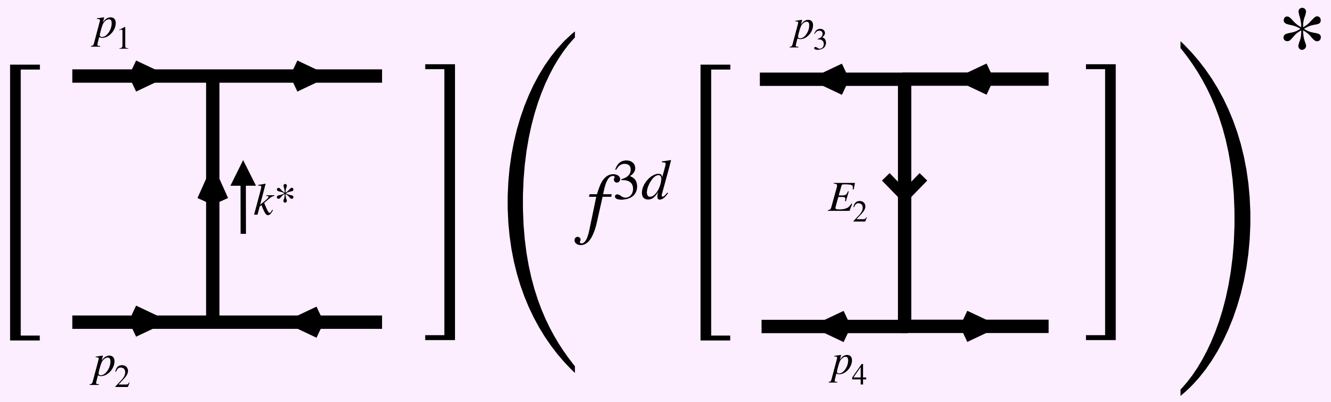
$\text{Res}_{\vec{k}=\vec{k}^*}[f^{3d}(\mathcal{M})] \sim f^{3d}$ 

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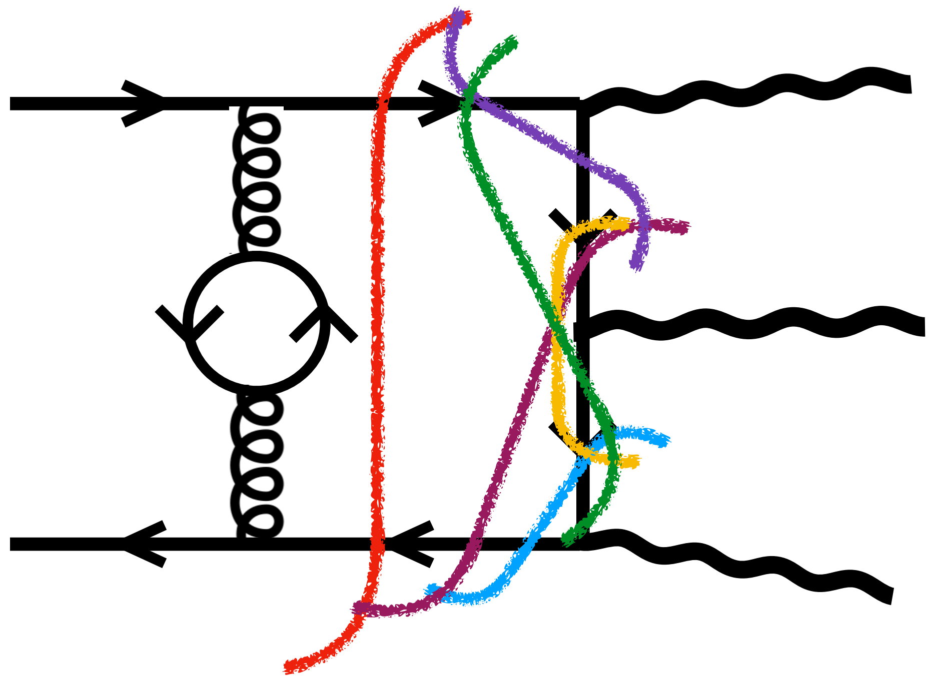
$$\lim_{\epsilon \to 0} \frac{1}{x - a \pm i\epsilon} = PV \frac{1}{x-a} \mp i\pi\delta(x-a) \implies \int CT_* = \mp i\pi \int d^2\hat{k}\, \text{Res}_*(\hat{k})$$

for smart choice of χ

Overlapping thresholds

Back to our example:



- here 6 threshold surfaces are active,
- some intersections can lead to higher-order poles!

Add a local threshold counterterm for each possible threshold singularity

$$CT_* = \frac{\mathbf{Res}_{\vec{k}=\vec{k}^*}[f^{3d}(\mathscr{M})]}{|\vec{k}| - k^* \pm i\varepsilon}\chi(\vec{k}, \vec{k}^*)$$

The CFF representation gives constraints on which overlapping thresholds lead to higher order poles.

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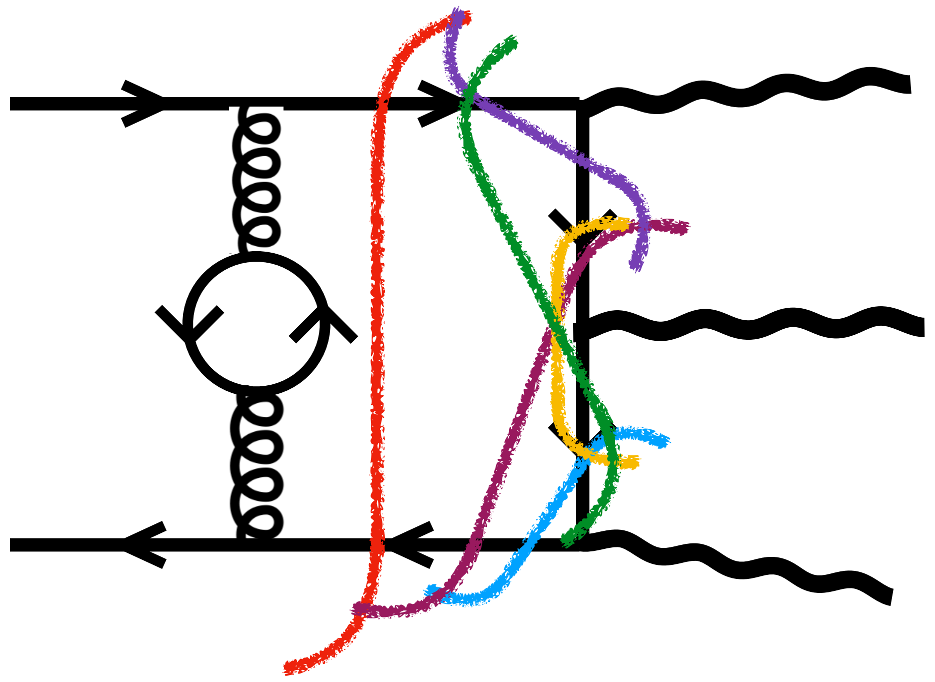

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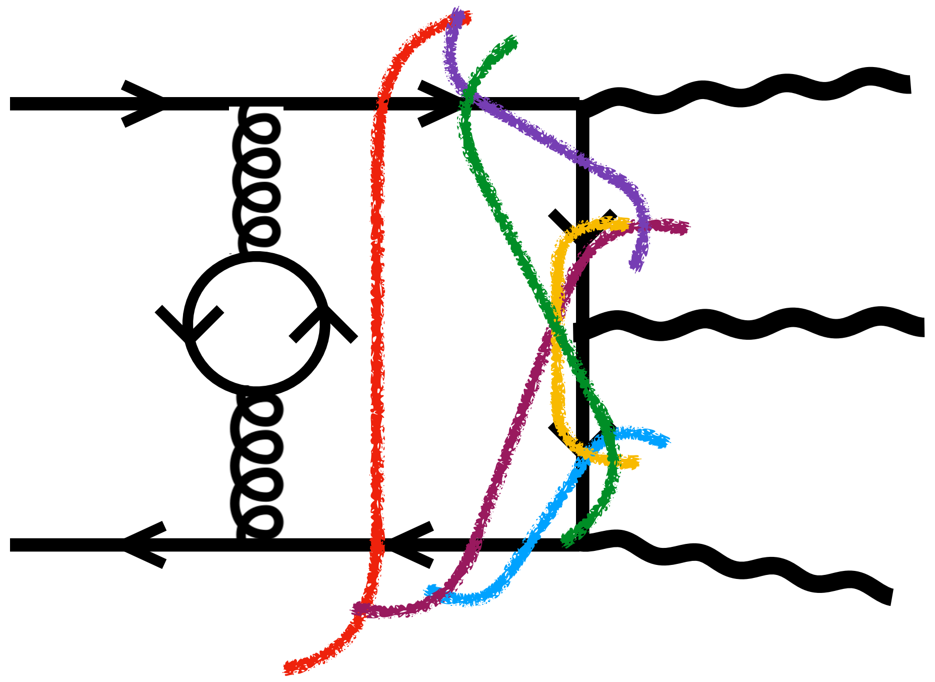

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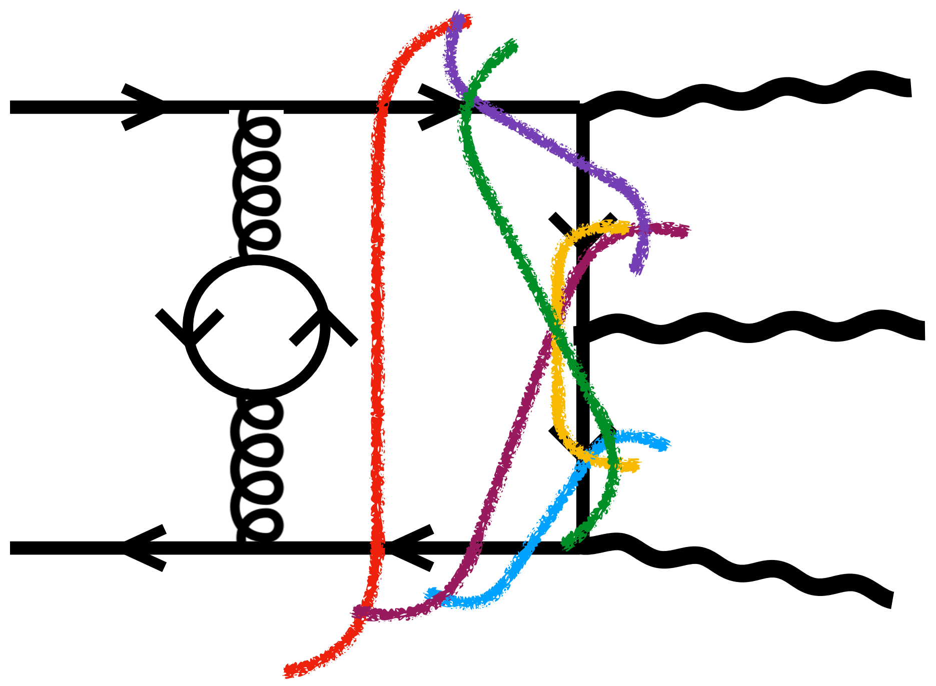

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The CFF representation gives constraints on which overlapping thresholds lead to higher order poles.

For higher order poles the same $i\epsilon$ prescription needs to appear in the counterterms

$\Longrightarrow$achieved by imposing same parametrisation of loop momentum space for overlapping threshold counterterms!

Does threshold structure change with phase space points?

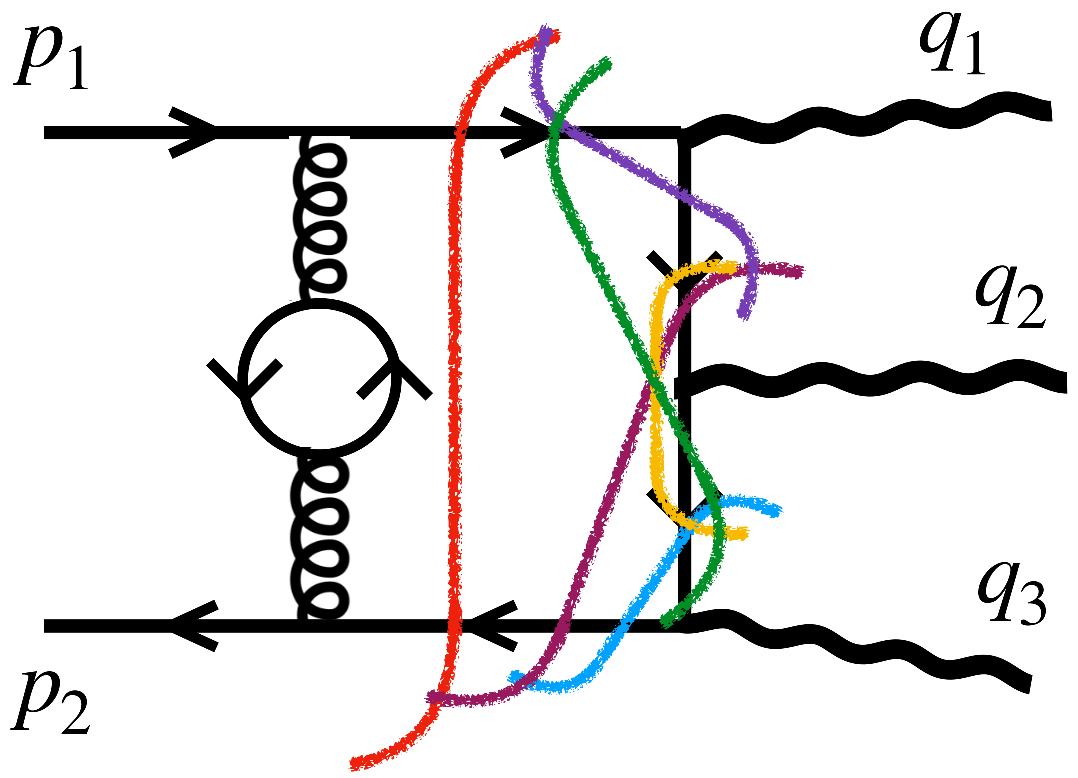
Now $$\int d^3\vec{k}\, f^{3\mathrm{d}}\left(\mathscr{M}(k)\right) = \int d^3\vec{k}\, \left\{ f^{3\mathrm{d}}\left(\mathscr{M}(k)\right) - \sum_{*} \frac{\mathbf{Res}_{\vec{k}=\vec{k}*}[f^{3d}(\mathscr{M})]}{|\vec{k}| - k* \pm i\varepsilon} \chi(\vec{k}, \vec{k}*) \right\} + \sum_{*} \int CT_{*}$$

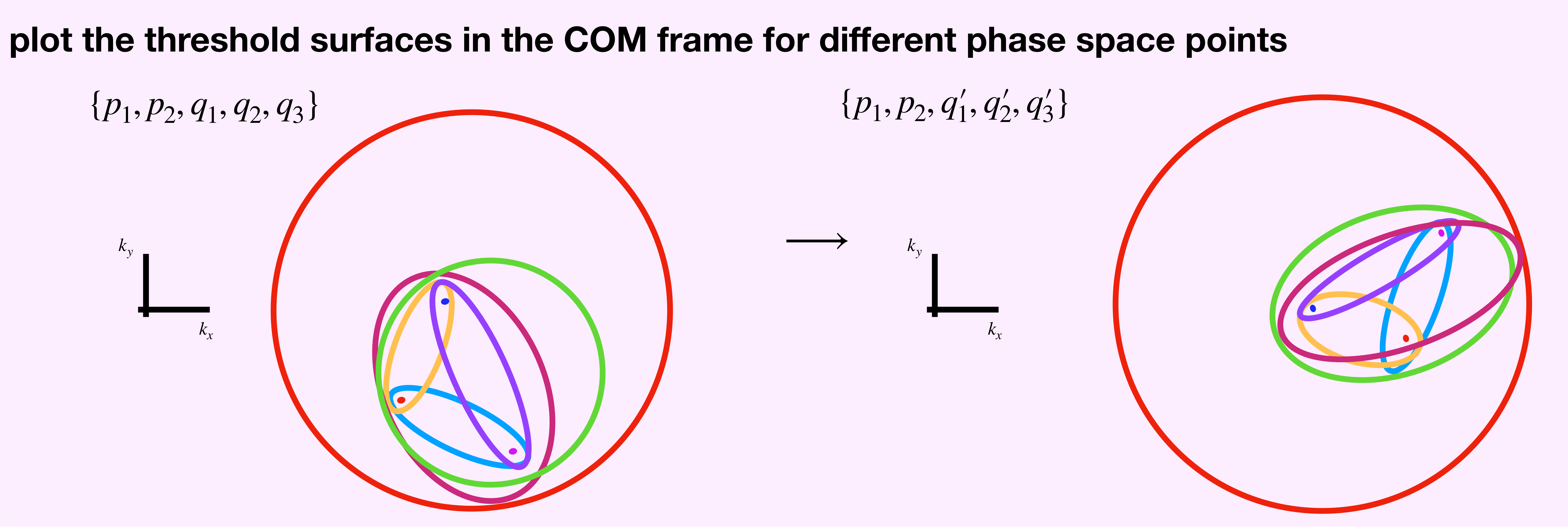
is locally finite for each set of external momenta in the physical region.

If we keep the Lorentz frame constant, does the intersection of threshold surfaces change?

Integration over phase space

For this specific example, threshold structure varies with q_1, q_2, q_3 sampled from the phase space generation in this way:





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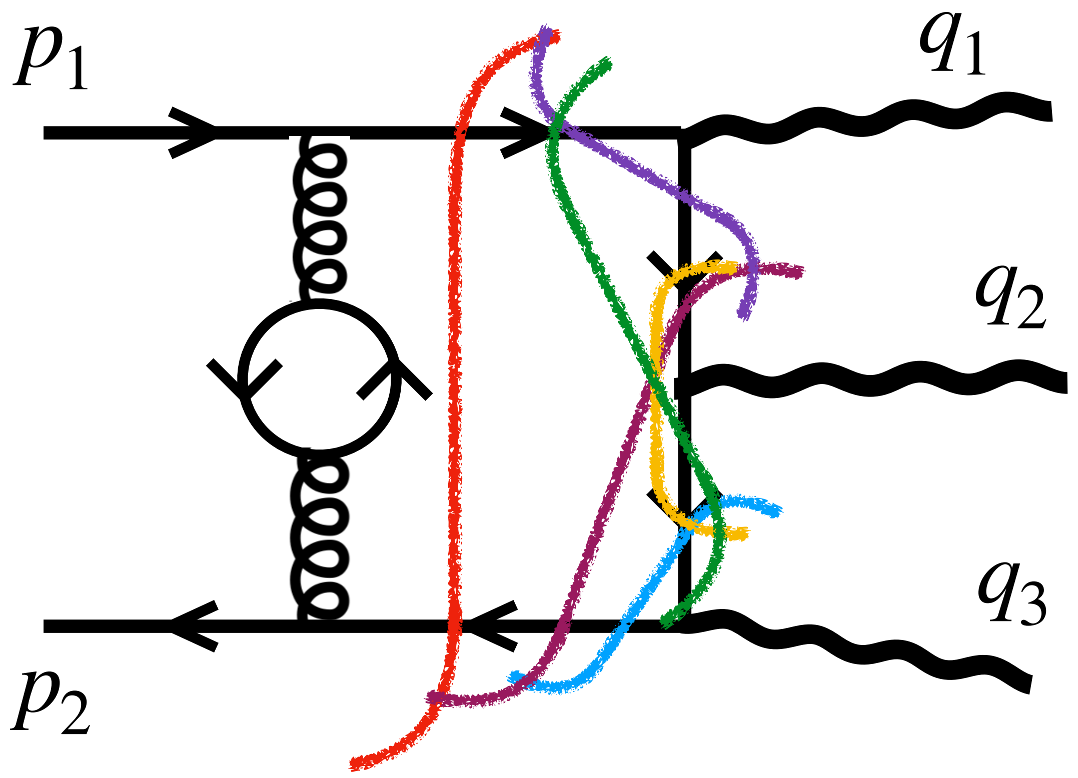

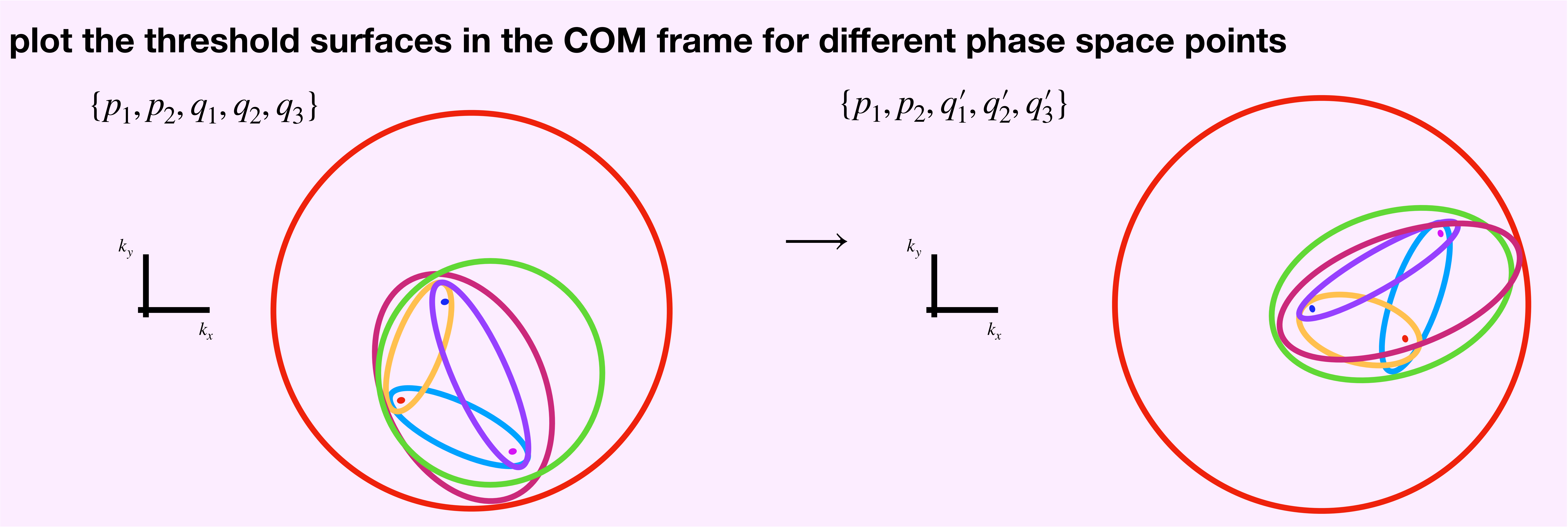

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$\Longrightarrow$

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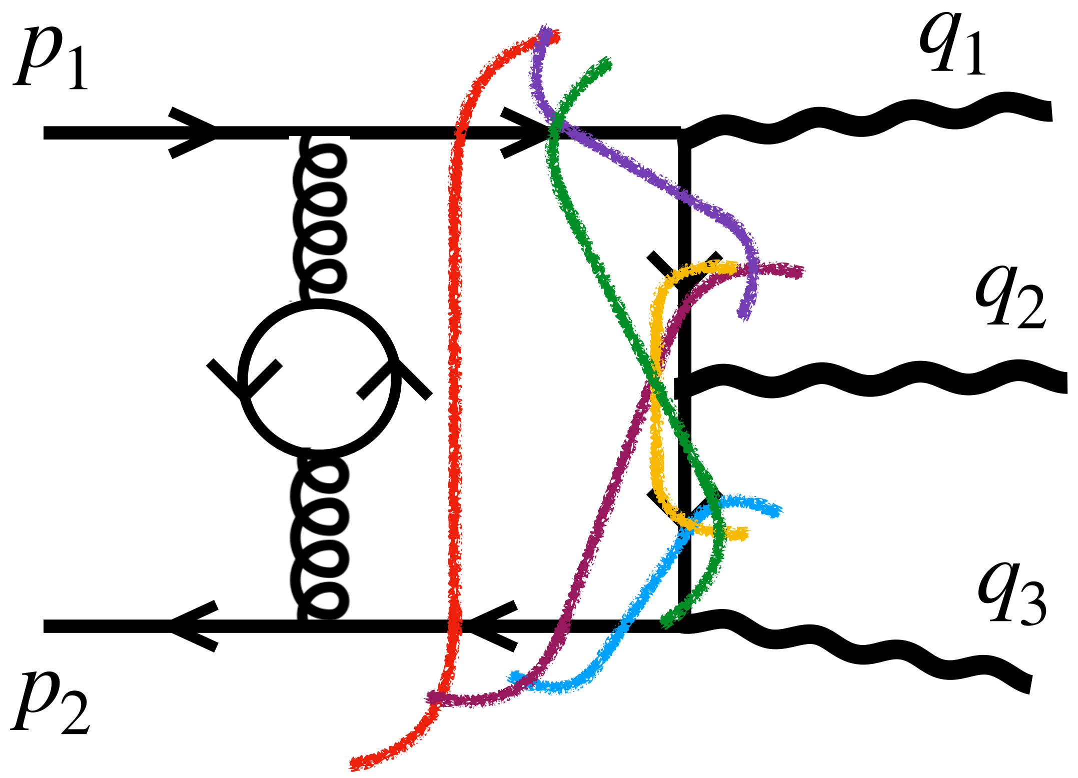
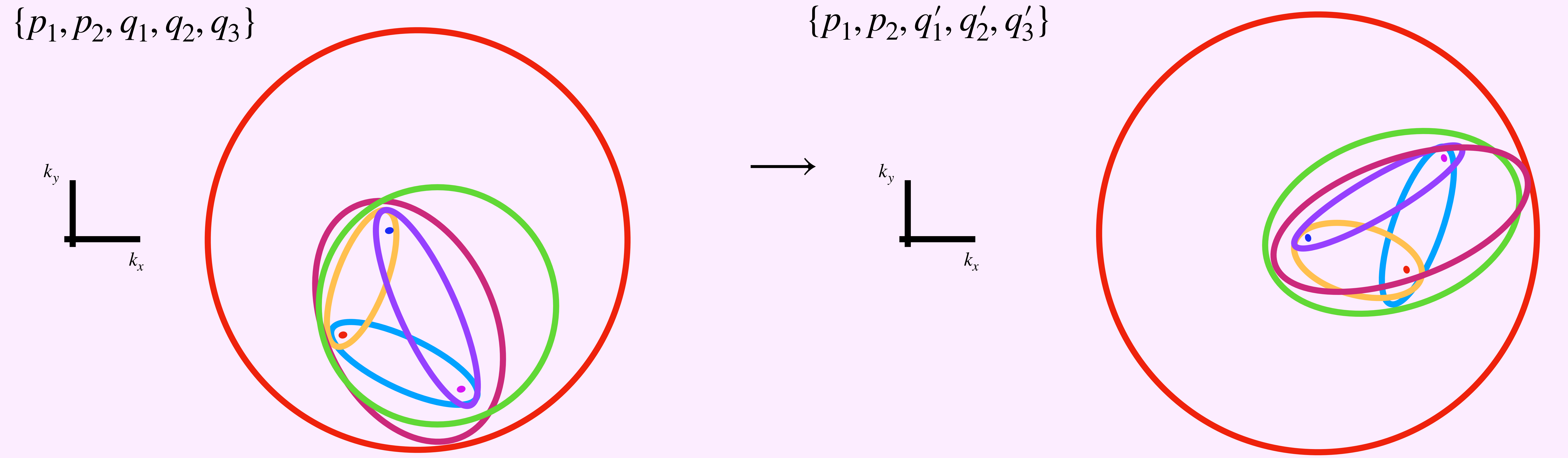


plot the threshold surfaces in the COM frame for different phase space points

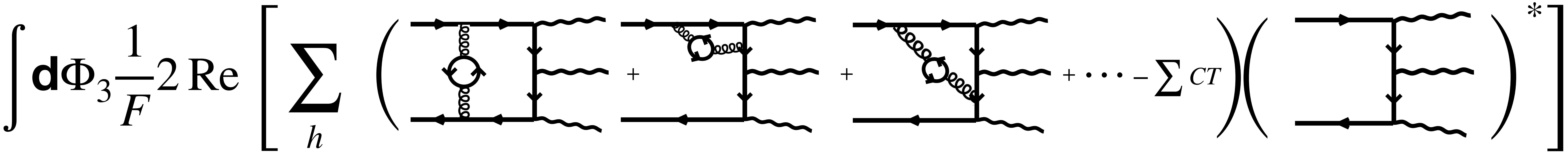


The structure of the intersections is constant

$\Longrightarrow$ the higher-order poles are the same over whole phase space!

This allows to…

- Perform simultaneous Monte-Carlo integration $\mathrm{d}\Phi_3 d^3\vec{k} d^3\vec{l}$ in:



- present gauge-invariant finite corrections to the virtual cross section!
- save computing time!

Finally, we add back the integrated counterterms

The integration that we need to perform analytically for the IR and UV counterterms are much simpler than those needed for the full amplitude! The master integrals needed for N external γ^* are:

$$\frac{\text{TadP}(M^2)}{M^2} := i(e^{\gamma_E}\mu^2)^\varepsilon \int \frac{dk^D}{i\pi^{D/2}} \frac{1}{k^2 - M^2} = -ie^{\gamma_E\varepsilon}\Gamma(\varepsilon - 1)\left(\frac{\mu^2}{M^2}\right)^\varepsilon$$

$$\frac{\text{Tad2P}(M^2)}{M^2} := i^2(e^{\gamma_E}\mu^2)^{2\varepsilon} \int \frac{dk^D}{i\pi^{D/2}} \frac{dl^D}{i\pi^{D/2}} \frac{1}{l^2(l+k)^2(k^2 - M^2)} = -i^2 e^{2\varepsilon\gamma_E} \frac{\Gamma(1-\varepsilon)^2\Gamma(2\varepsilon - 1)\Gamma(\varepsilon)}{\Gamma(2-\varepsilon)}\left(\frac{\mu^2}{M^2}\right)^{2\varepsilon}$$

$$\text{Bub}(s_{12}) := i(e^{\gamma_E}\mu^2)^\varepsilon \int \frac{dk^D}{i\pi^{D/2}} \frac{1}{(k+p_1)^2(k-p_2)^2} = i\frac{e^{\gamma_E\varepsilon}\Gamma(1+\varepsilon)\Gamma(1-\varepsilon)^2}{\Gamma(2-2\varepsilon)\varepsilon}\left(-\frac{\mu^2}{s_{12}}\right)^\varepsilon$$

$$\text{Tri}(s_{12}) := i^2(e^{\gamma_E}\mu^2)^{2\varepsilon} \int \frac{dk^D}{i\pi^{D/2}} \frac{dl^D}{i\pi^{D/2}} \frac{1}{l^2(l+k)^2(k+p_1)^2(k-p_2)^2}$$

$$= i^2 e^{2\varepsilon\gamma_E}\Gamma(1+\varepsilon)^2\left(-\frac{\mu^2}{s_{12}}\right)^{2\varepsilon}\left[\frac{1}{2\varepsilon^2} + \frac{5}{2\varepsilon} + \frac{19}{2} + \left(\frac{65}{2} - 4\zeta_3\right)\varepsilon + \left(\frac{211}{2} - 20\zeta_3 - \frac{1}{15}\pi^4\right)\varepsilon^2 + O(\varepsilon^3)\right]$$

Results

virtual finite remainder with Catani-Seymour poles subtraction in $\overline{\text{MS}}$ convention

	$\sigma_{\text{virt}}^{(2,N_f)}$	time/sample
$pp \to \gamma^*\gamma^*\gamma^*$	$N_f C_F T_F(-8.12 \pm 0.16) \times 10^{-5}$ pb preliminary	1.3 ms

$C_F = 4/3\,, \quad T_F = 1/2\,, \quad N_f = 5$
with max 10^{10} MC samples on 48 cores
$\sqrt{s} = 13$TeV
$\mu_F = \mu_r = M_Z = 91.1876$ GeV
5 flavours of quarks in PDFs
$m_{\gamma^*,1} = 20.0$ GeV $\quad m_{\gamma^*,2} = 50.0$ GeV $\quad m_{\gamma^*,3} = M_Z$
$p_{T,\gamma^*} > 10.0$ GeV

CT1nlo set (11000) LHAPDF [1412.7420 Buckley, Ferrando, Lloyd, Nordstrom, Page, Ruefenacht, Schoenherr, Watt]

Results

virtual finite remainder with Catani-Seymour poles subtraction in $\overline{\text{MS}}$ convention

	$\sigma_{\text{virt}}^{(2,N_f)}$	time/sample	Δ [%]	
$pp \to \gamma\gamma\gamma$	$N_f C_F T_F (-2.42 \pm 0.03) \times 10^{-3}$ pb preliminary	0.03 ms	0.8	cross-check: [2010.15834, Abreu, Page, Pascual, Sotnikov] FivePointAmplitudes-cpp

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one-loop results

virtual finite remainder in BLHA convention
cross-checked with MadGraph [1405.0301]
thanks to Valentin Hirschi

preliminary	$\sigma^{(1)}_{\text{virt}}$		$\Delta\,[\%]$	time/sample
$p\,p \to \gamma\,\gamma$	$(-1.6277 \pm 0.0002) \times 10^{2}$	pb	0.4	0.005 ms
$pp \to ZZ$ **(only d quark in PDFs)**	$(9.8599 \pm 0.0007) \times 10^{-1}$	pb	0.3	0.03 ms
$pp \to \gamma\,\gamma\,\gamma$	$(4.02 \pm 0.06) \times 10^{-2}$	pb	0.3	0.014 ms
$pp \to \gamma^*\gamma^*\gamma^*$ $(m_{\gamma^*} = M_Z)$	$(2.446 \pm 0.012) \times 10^{-4}$	pb	0.3	0.3 ms

Conclusions

- Numerical computation of the N_f contribution to $\sigma^{\text{virtual}}_{NNLO}(pp \to \gamma^*\gamma^*\gamma^*)$.

- We can't wait to tackle with the same method the full two-loop numerical integration.