A fully numerical approach to perturbative computations in QFT

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For the position of Group Leader in Numerics

at the

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Self.me

2009 **Ph.D.** on the automation of NLO computations

@EPFL, Lausanne supervisor : S. Frixione

2013 **Post-doc #1**

@SLAC, Stanford SNF mobility grants

2017 **Post-doc #2**

@ETHZ, Zurich in the group of C. Anastasiou

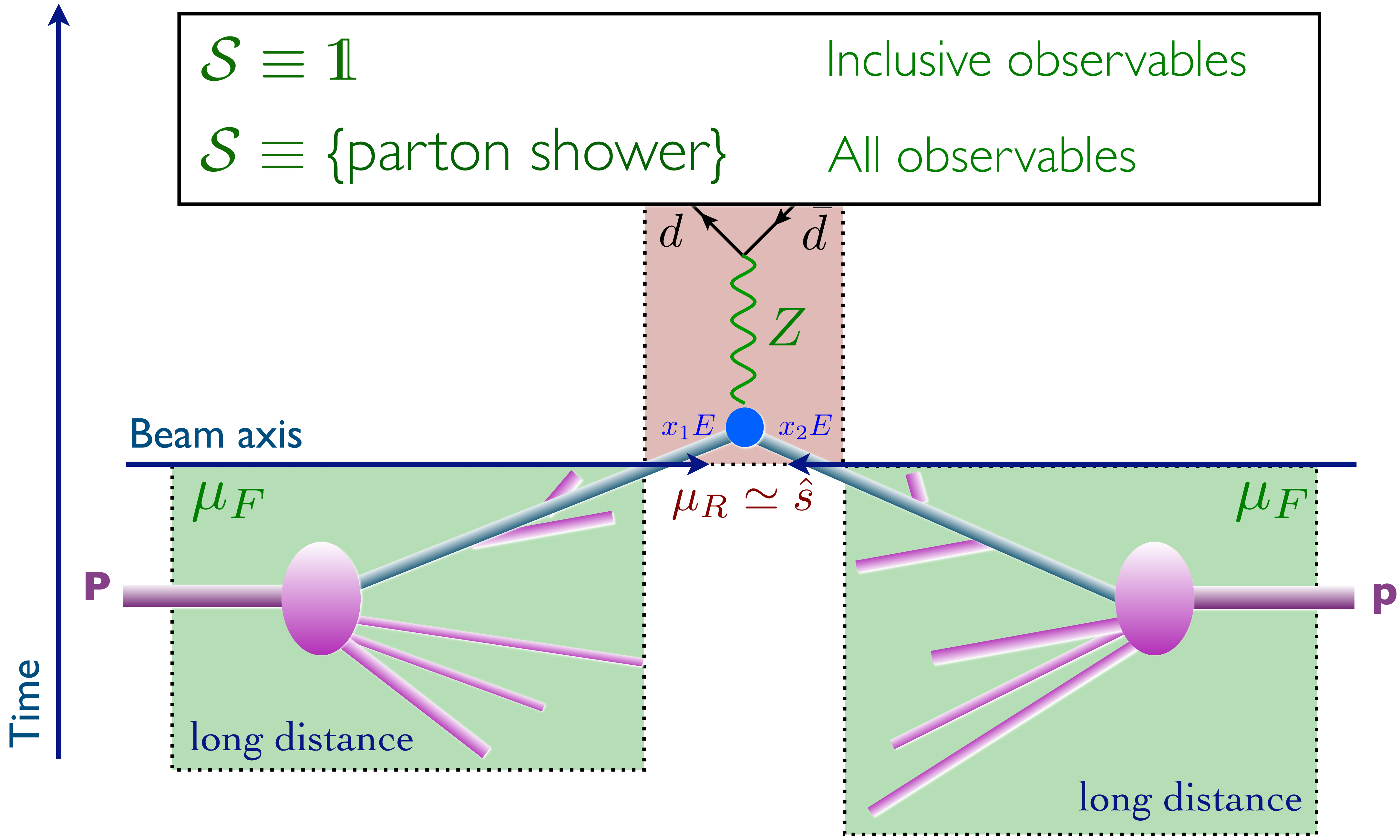
Oct. 2020 **CERN Fellow**

Broad context of my research

$$\sum_{a,b} \int dx_1 dx_2 d\Phi_{\rm FS}\, f_a(x_1,\mu_F) f_b(x_2,\mu_F)\, \hat{\sigma}_{pp\rightarrow\{P\}}(\mu_F,\mu_R,\mu_S)\, \mathcal{S}_{\{P\}\rightarrow\{H\}}(\mu_S)$$

Phase-space integral — Parton density functions — Parton-level differential cross section — Parton evolution operator

$\mathcal{S} \equiv \mathbb{1}$	Inclusive observables
$\mathcal{S} \equiv$ {parton shower}	All observables



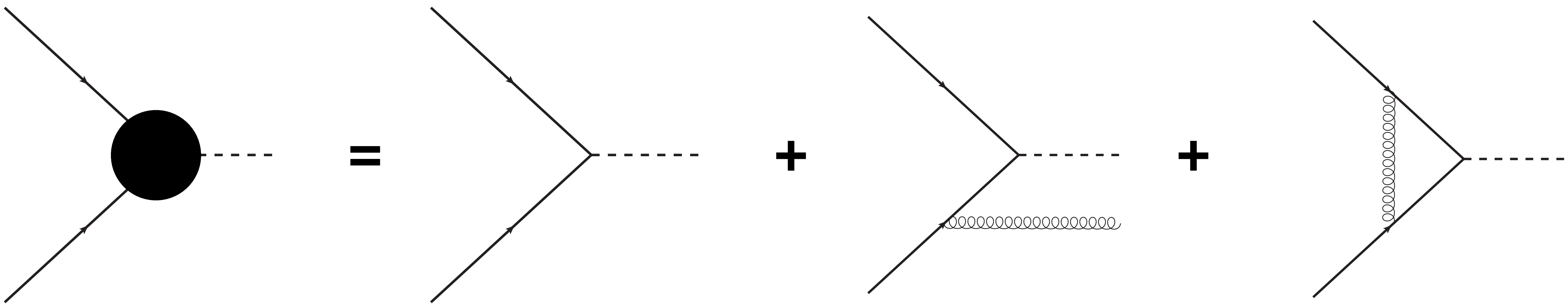
PERTURBATIVE EXPANSIONS

The differential cross section can be written as a perturbation series, using the coupling constant as an expansion parameter :

$$\hat{\sigma} = \sigma^{\text{Born}}\left(1 + \frac{\alpha_s}{2\pi}\sigma^{(1)} + \left(\frac{\alpha_s}{2\pi}\right)^2\sigma^{(2)} + \left(\frac{\alpha_s}{2\pi}\right)^3\sigma^{(3)} + \dots\right)$$

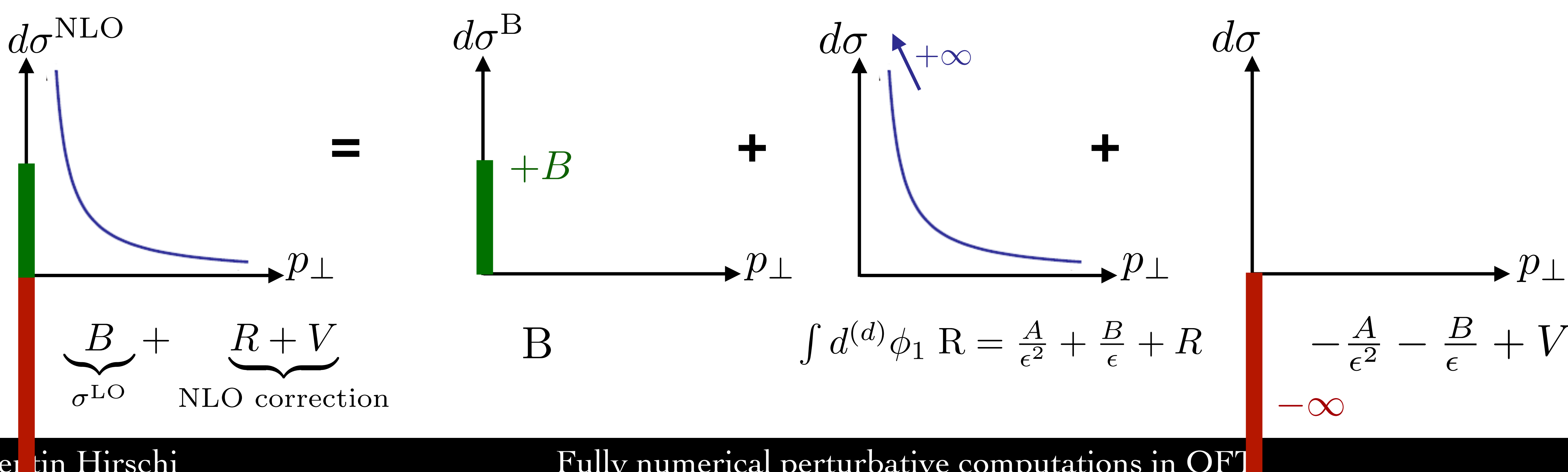
LO predictions	NLO corrections	NNLO corrections	NNNLO corrections
Easy	Difficult but **automated.** My past research MadGraph5	Case-by-case only Automation at this order and beyond is the goal of my current research	pp → V/H only

NLO Anatomy



$$\sigma^{\rm NLO} = \int_m d^{(4)}\sigma^B + \int_{m+1} d^{(d)}\sigma^R + \int_m d^{(4)} \int_1 d^{(d)}\sigma^V$$

NLO inclusive — Born (B) — Real-emission (R) — Virtual (V)



$\underbrace{B}_{\sigma^{\rm LO}} + \underbrace{R+V}_{\text{NLO correction}}$

B

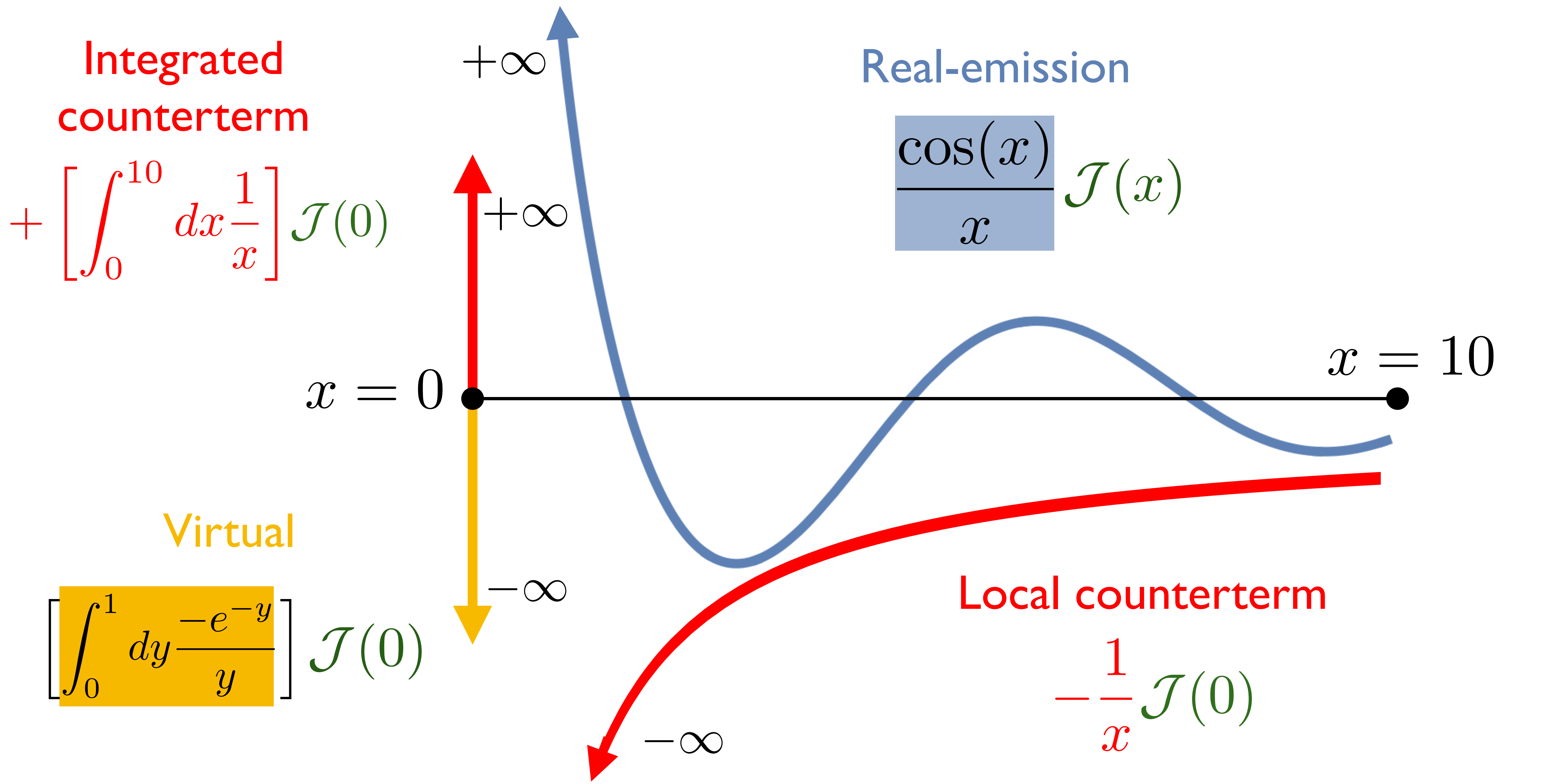
$\int d^{(d)}\phi_1 \, \mathrm{R} = \frac{A}{\epsilon^2} + \frac{B}{\epsilon} + R$

$-\frac{A}{\epsilon^2} - \frac{B}{\epsilon} + V$

One-dimensional toy example

- Toy expression with $\mathcal{J}$ a measurement function, over $x \in [0, 10]$

$$\sigma^{(R+V)}(\mathcal{J}) = \int_0^{10} dx \left[\frac{\cos(x)}{x} \mathcal{J}(x) - \frac{1}{x} \mathcal{J}(0) \right] + \left[\int_0^1 dy \frac{-e^{-y}}{y} \right] \mathcal{J}(0) + \left[\int_0^{10} dx \frac{1}{x} \right] \mathcal{J}(0)$$



Subtraction vs Local Unitarity

- One can introduce the following local (in x) **counterterm**:

$$\sigma^{(R+V)}(\mathcal{J}) = \int_0^{10} dx \left[\frac{\cos(x)}{x}\mathcal{J}(x) - \frac{1}{x}\mathcal{J}(0)\right] + \left(\left[\int_0^1 dy \frac{-e^{-y}}{y}\right] + \left[\int_0^{10} dx \frac{1}{x}\right]\right)\mathcal{J}(0)$$

- And a **regulator** to evaluate the divergent integrals

$$\sigma^{(R+V)}(\mathcal{J}) = \int_0^{10} dx \left[\frac{\cos(x)}{x}\mathcal{J}(x) - \frac{1}{x}\mathcal{J}(0)\right] + \lim_{\epsilon\to 0}\left(\left[\int_\epsilon^1 dy \frac{-e^{-y}}{y}\right] + \left[\int_\epsilon^{10} dx \frac{1}{x}\right]\right)\mathcal{J}(0)$$

- To finally arrive at a **finite** result, differential in $x \in [0, 10]$

$$= \int_0^{10} dx \left[\frac{\cos(x)}{x}\mathcal{J}(x) - \frac{1}{x}\mathcal{J}(0)\right] + \lim_{\epsilon\to 0}\left(\log(\epsilon) + \gamma - \text{Ei}(-1) + \log(10) - \log(\epsilon)\right)\mathcal{J}(0)$$

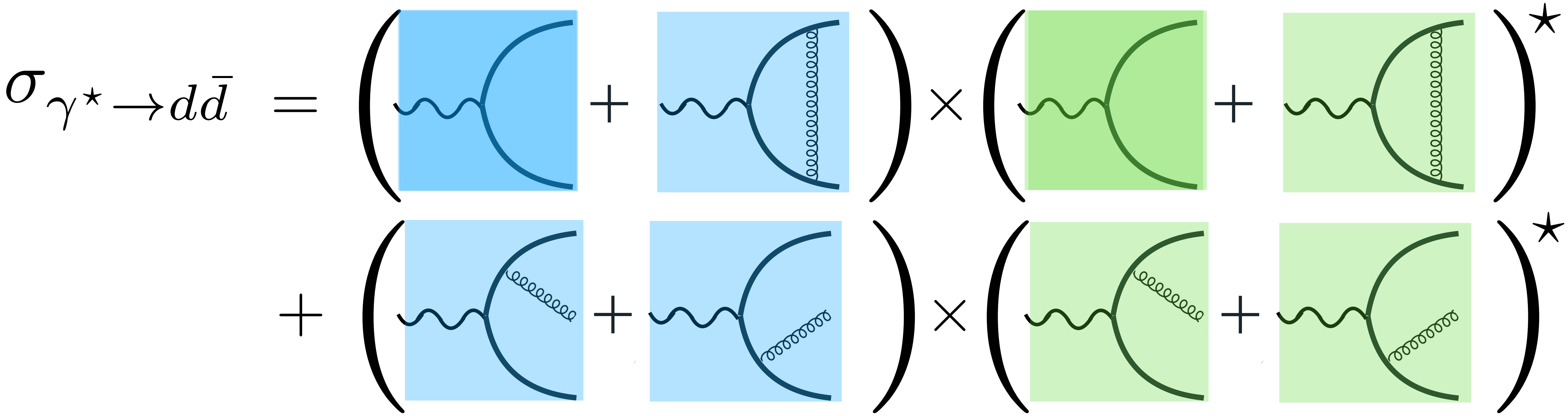
NUMERICAL | ANALYTIC

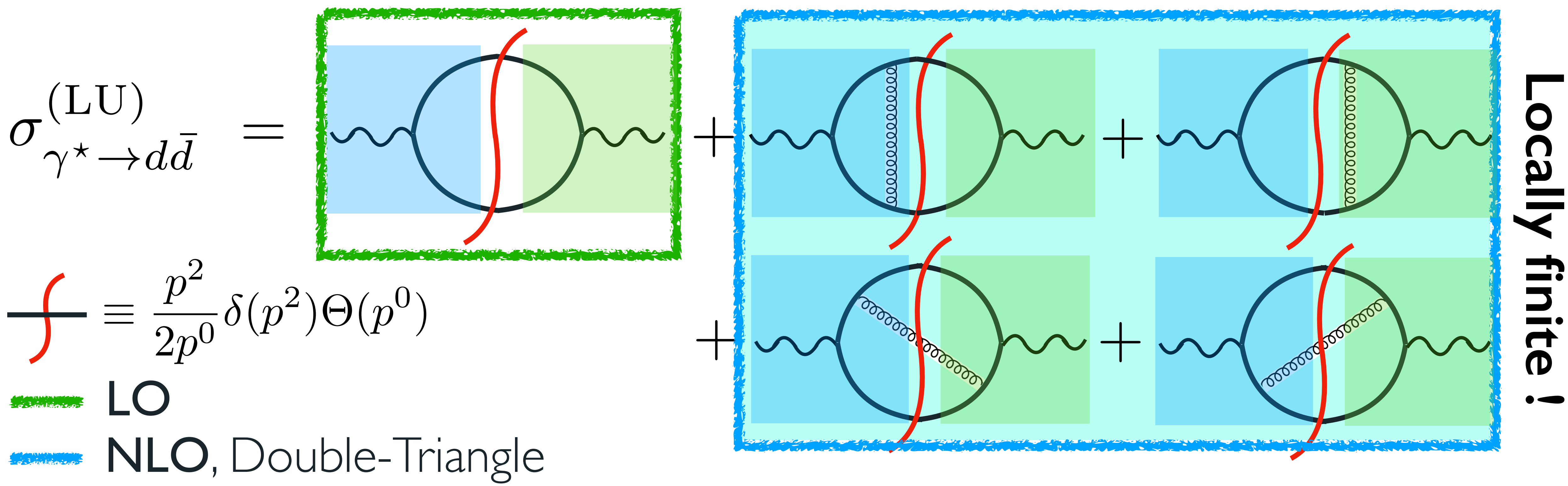
- My research introduces a new paradigm, **Local Unitarity**, whereby :

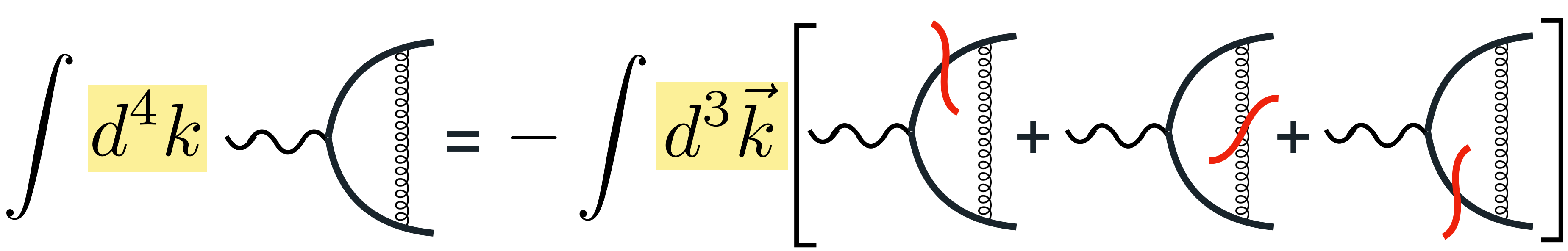
$$\sigma^{(R+V)}(\mathcal{J}) = \int_0^{10} dx \left[\frac{\cos(x)}{x}\mathcal{J}(x) + \frac{-e^{-x}}{x}\mathcal{J}(0)\Theta(1-x)\right]$$

Local Unitarity: supergraphs

[Z. Capatti, VH, A. Pelloni, B. Ruijl, arXiv : 2010.01068]   [Also more details in my recent CERN Seminar talk]







Loop-Tree Duality

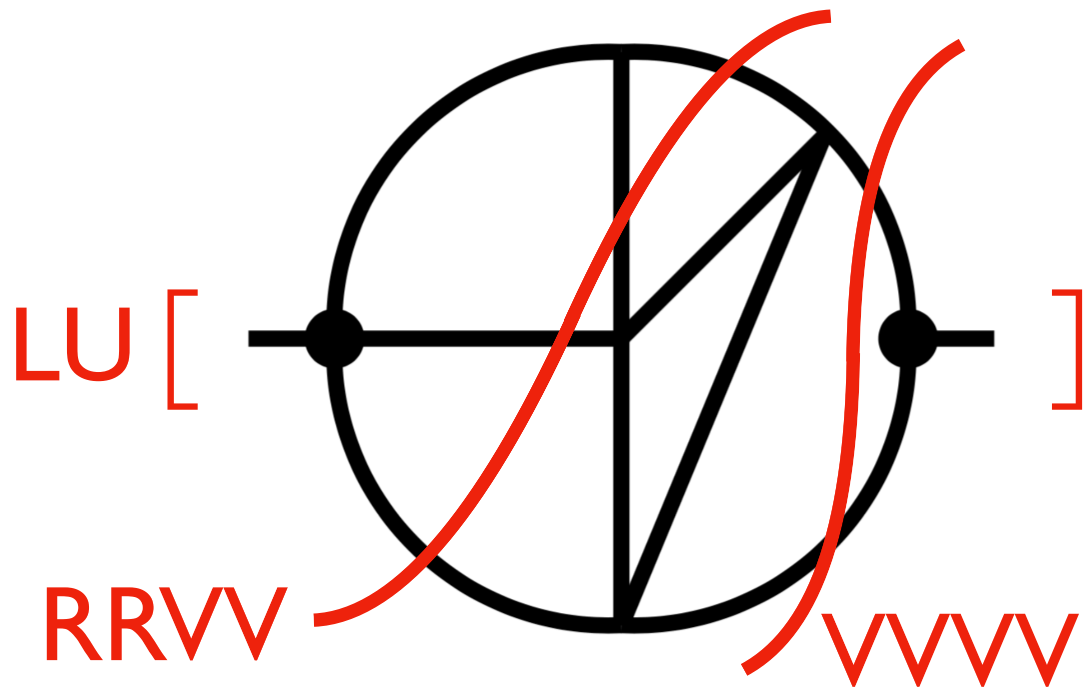
[arXiv: 1906.06138]
[arXiv: 1912.09291]
[arXiv: 2009.05509]

Numerical results from αLoop

[Capatti, VH, Pelloni, Ruijl, arxiv: 2010.01068]

Piece of the "N⁴LO" correction to $\phi^\star \to \phi\phi$ within $\{\phi^3, \phi^4\}$-theory

One individual **5-loop supergraph** :



$$= \frac{5\pi}{(16\pi)^5}\frac{441}{40}\zeta(7)$$

[**FORCER** B. Ruijl, T. Ueda, J. Vermaseren arxiv: 1704.06650]

[**R*** F. Herzog, B. Ruijl arxiv: 1703.03776]

without **contour deformation** (doing it differentially would have required one)

Γ	N_p [10^6]	t/p [μs] min	t/p [μs] avg	N_{ch}	FORCER [GeV²]	αLoop [GeV²]	exp.	Δ [σ]	Δ [%]
c.3	1	1600	69000	130	1.77832	1.7797(33)	-9	0.42	0.00077

SOFTWARE AND COMPUTING ACHIEVEMENTS I

MadGraph5_aMC@NLO

[arXiv: 1103.0621 first NLO QCD automaton]

[arXiv: 1405.0301 each year in top-ten hep cite]

C++ / Python / Fortran

Core contributor: ~100k lines

[2009 - 2017]

- Experience with development in large collaboration and iterative design (Agile coding)
- Numerous users with different technical skills and needs:
  - Automated code with a high-level of abstraction with user-friendly interface
  - Frequent releases with robust testing suite (unit, acceptance, parallel, I/O tests,...)
  - Accommodate multiple computing infrastructures (slurm, LSF, condor, multicore, MPI,...)
  - Automation of NLO EW corrections and MSSM (CMS, photon isolation, multi-couplings,...)
- Widely used by experiments, so that efficiency matters:
  - Advanced parallelisation paradigms (multi-channels, work-stealing, async,...)
  - Optimised algorithms (MadLoop, diagram generation, phase-space generation,...)
  - Variance minimisation in Monte-Carlo (adaptive sampling, dynamic approximations,...)
- Expertise in interfacing with a vast ecosystem of HEP softwares:
  - Loop computations (GoSam, Recola, OpenLoops, COLLIER, Ninja, QCDLoop, LoopTools, OneLOop,...)
  - Event generation (FastJet, Pythia8, LHAPDF, Vegas3, Cuba, reweighting, MadSpin, MadOS, biasing,...)
  - Collider analysis (HepMC, Rivet, MadAnalysis, HwU,...)
- Organised tutorials at many schools and workshops (TASI, CERN, MG schools,...)

Software and computing achievements II

MadN^{k}LO

[arXiv: 2010.09451, 1902.10167 private code]

Python / Rust

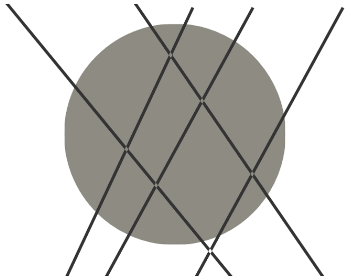
MG5aMC for beyond-NLO predictions
Lead developer

[2016 - now]

- Higher level abstraction suited to beyond-NLO subtraction formalisms:
  - Flexible customisation of each fixed-order piece (NLO loop-induced,…)
  - Generalised PS supports and process generation (RRR, RVV, ISR convolutions,…)
  - Multi-loop through effective vertices in UFO models (WAMP, gg>Hg 2-loop EW,…)
  - Containerisation of dependencies in Docker images for ease of deployment
  - Integrator abstracted away, opening up to ML-based approach (iFlow, Zünis,…)
  - Generalised color and spin correlators to arbitrary perturbative orders
  - Interfaced multi-loop computation tools (Chaplin, GINAC, pySecDec,…)

While very **useful**, this work is not addressing the root cause of **complexity growth** of fixed-order predictions: IR singularities

Software and computing achievements III



α-Loop

[arXiv: 1906.06138, 1912.09291, 2009.05509, 2010.01068 private code]

Python / Rust / C / FORM / Mathematica

Fully numerical computation of cross-sections

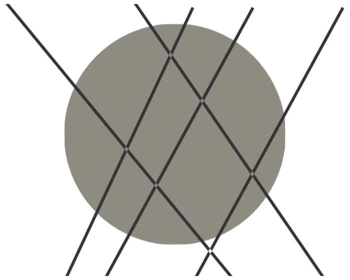
Co-leader of a team of junior scientists

[2019 - now]

- High loop count algorithms (up to six loops):
  - Heavy graph manipulations (QGRAF, isomorphisms, spanning trees, BPHZ forest, topology reduction,…)
  - Efficient code meta-generation (Fast Lorentz and colour algebra, polynomial optimisation in FORM,…)
  - Generalised Loop Tree Duality algorithms in Python standalone codes

- Contour deformation:
  - Solving NP hard problem with custom domain-specific heuristics
  - Conic solvers for numerical optimisiation under convex constraints (ECOS, SCS,…)
  - Automatic differentiation using dual numbers

Software and computing achievements III



α-Loop

[arXiv: 1906.06138, 1912.09291, 2009.05509, 2010.01068 private code]

`Python / Rust / C / FORM / Mathematica`

Fully numerical computation of cross-sections

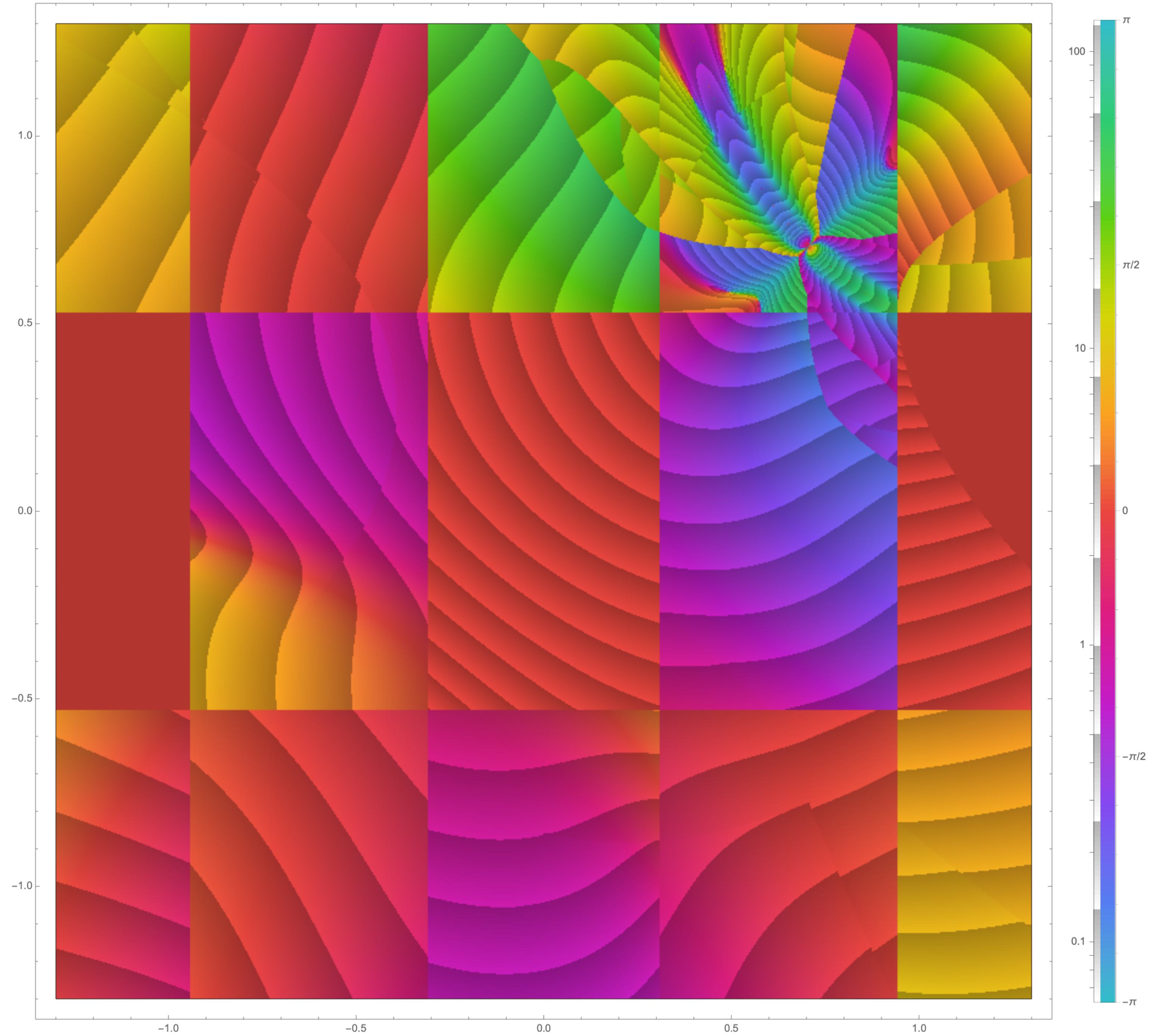
Co-leader of a team of junior scientists

[2019 - now]

- Numerical stability:
  - Rescue pipeline involving f128 arithmetics and a new more stable cLTD representation
  - Automated Python sampler of all UV limits using Rust-Python bindings
- Advanced Monte-Carlo and parallelisation techniques
  - New nested adaptive sampling involving multiple discrete and continuous dimensions
  - Semi-autonomous search for optimal hyperparameters distributed over clusters
  - Custom parameterisations and multi-channeling for taming integrable singularities
- Analytic multi-(up to three)loop vacuum integrals
  - Integration by part identities with high rank numerator reduction
  - Consistent combination with $\overline{\mathrm{MS}}$ NNLO renormalisation

Differential Local Unitary Integrand

$$e^+e^- \rightarrow \gamma^\star \rightarrow d\bar{d}$$



" Cut what you cannot compute "