Progress on two-loop integrals for top-pair production plus a W boson

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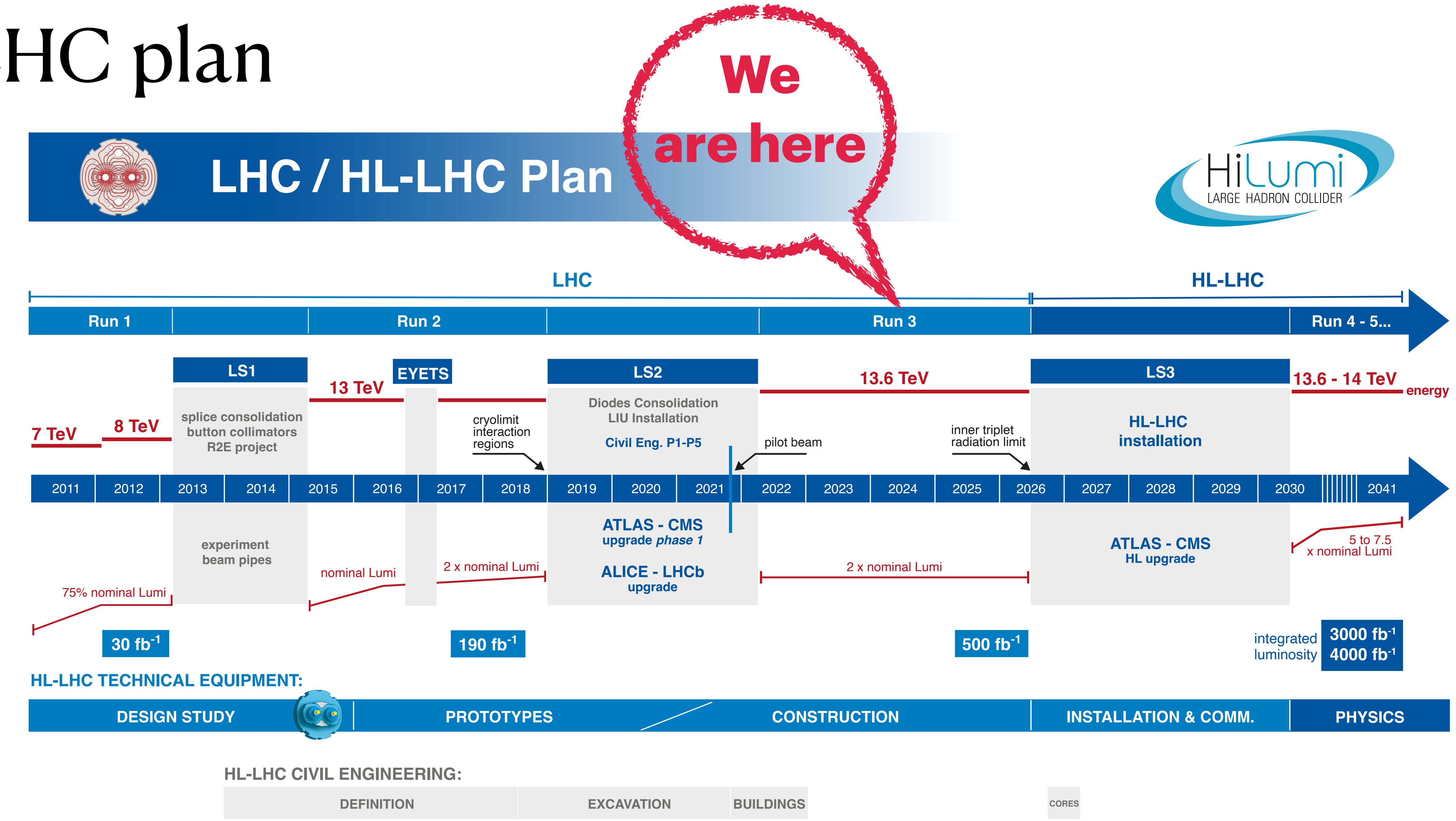
University of Bologna, 20/03/2025

Motivation

- High luminosity LHC plan



- Experimental precision for HL-LHC of $\mathcal{O}(1\%)$ for many observables
- Theoretical predictions at higher orders are required to match experimental precision. Typically: at least NNLO QCD

Precision demands at least NNLO QCD

$$\mathrm{d}\sigma = \boxed{\mathrm{d}\sigma^{\mathrm{LO}}} + \boxed{\alpha_S\, \mathrm{d}\sigma^{\mathrm{NLO}}} + \boxed{\alpha_S^2\, \mathrm{d}\sigma^{\mathrm{NNLO}}} + \ldots$$

$\approx 10 - 30\,\%$ $\approx 1 - 10\,\%$

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loops

The difficulty grows with

- order in the coupling (# loops)
- number of particles

particles

$2 \to n$

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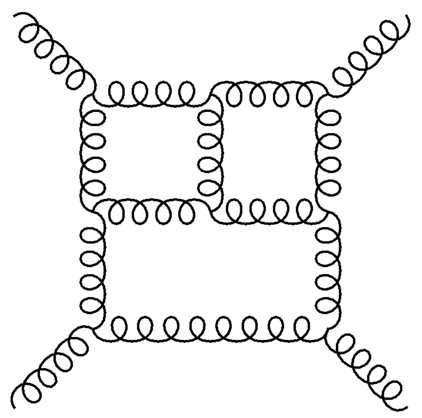
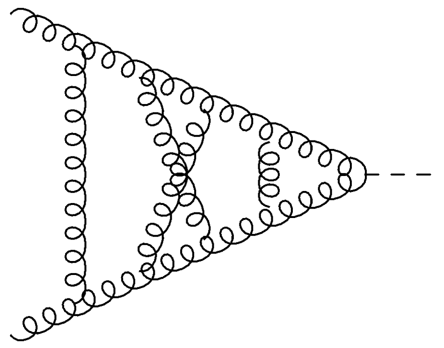
Loop frontier

N3LO $2 \to 2$



N4LO $2 \to 1$



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Precision demands at least NNLO QCD

$$d\sigma = d\sigma^{\mathrm{LO}} + \alpha_S\, d\sigma^{\mathrm{NLO}} + \alpha_S^2\, d\sigma^{\mathrm{NNLO}} + \ldots$$

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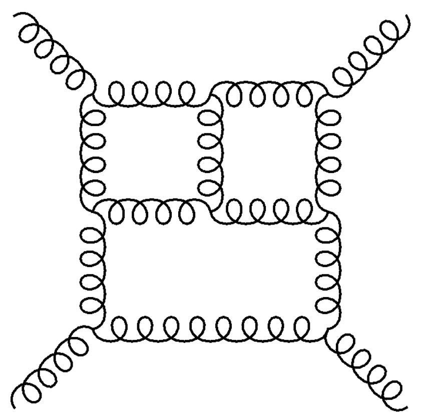
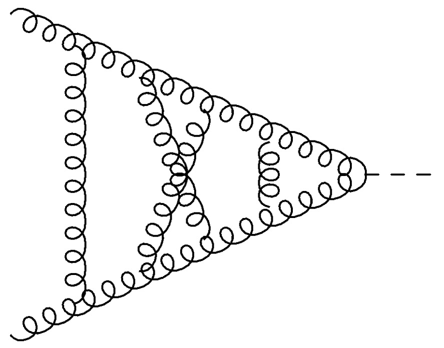


N4LO $2 \to 1$



loops

The difficulty grows with

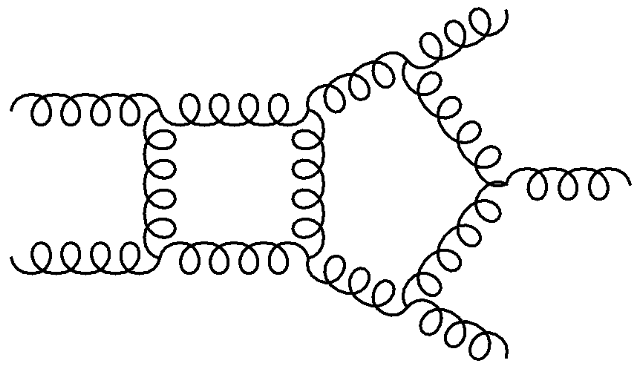
- order in the coupling (# loops)
- number of particles

particles

$2 \to n$

Multiplicity frontier

NNLO $2 \to 3$



Ingredients for theoretical predictions

Scattering amplitudes

IR subtraction

PDFs

Parton showers

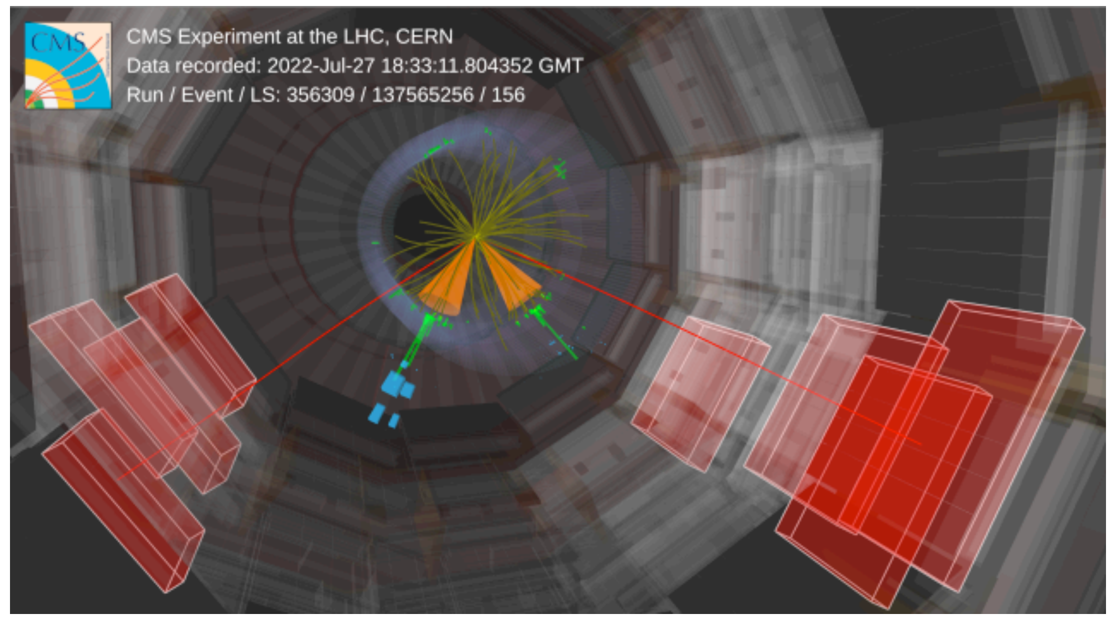
Resummation

Hadronisation

Monte Carlo event generator

Detector simulation

Experimental data



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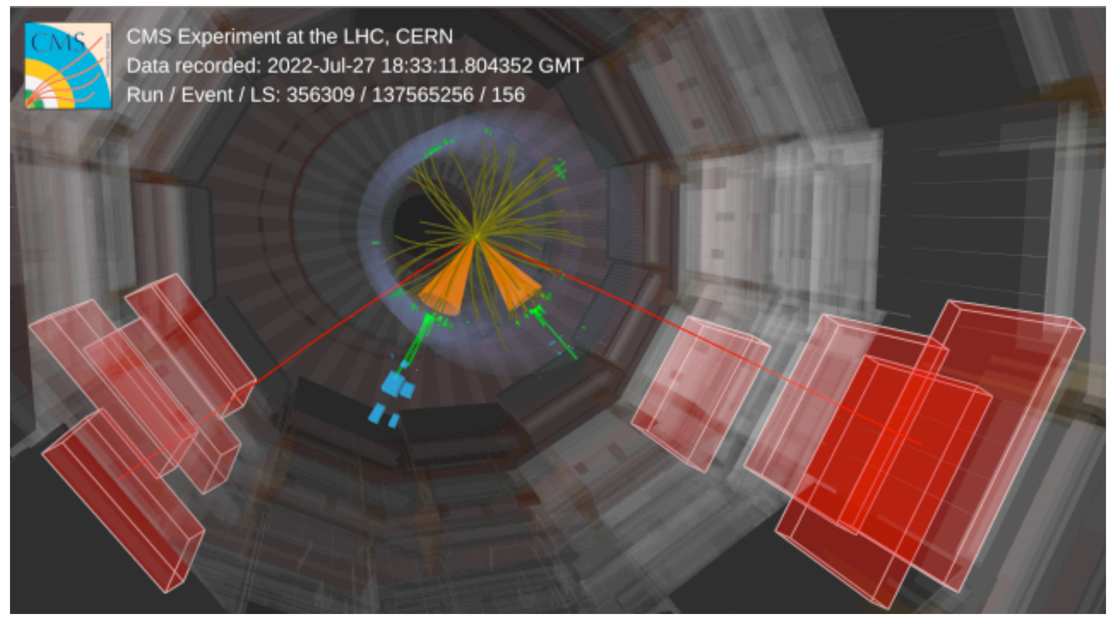


Main bottleneck: 2-loop 5-point scattering amplitudes

Cross sections for $h_1 h_2 \longrightarrow f$:

$$\mathrm{d}\sigma_{h_1h_2\to f} = \sum_{i,j=q,\bar{q},g} \int\int \mathrm{d}x_1 \mathrm{d}x_2\, \mathcal{F}_{i/h_1}(x_1,\mu^2)\mathcal{F}_{j/h_2}(x_2,\mu^2)\, \mathrm{d}\hat{\sigma}_{ij\to f}(\vec{s},\mu^2)$$

Partonic cross section:

$$\mathrm{d}\hat{\sigma}_{ij\to f} \backsim \int \mathrm{d}\Phi\, |\mathcal{A}|^2$$

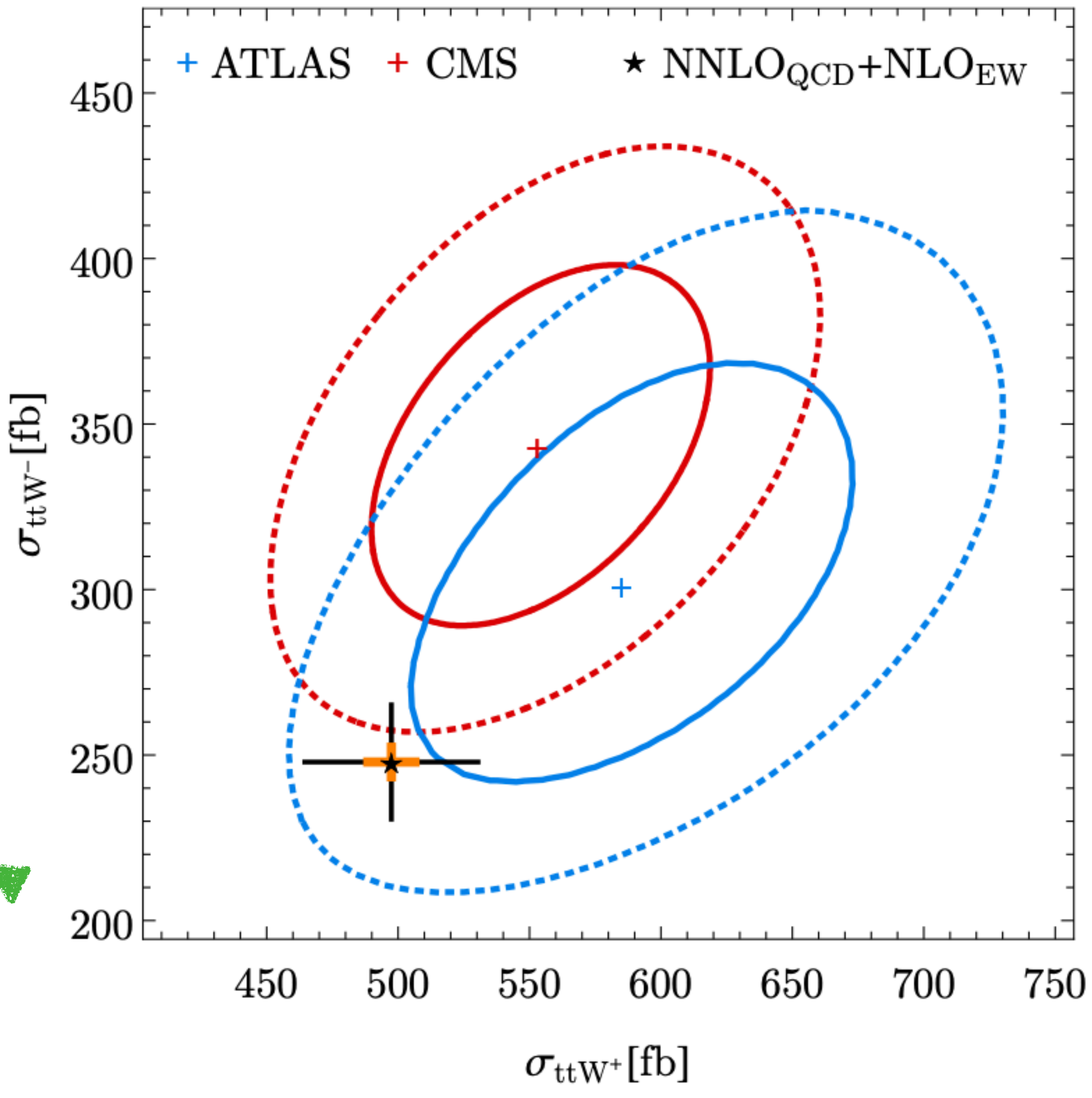
Amplitude:

$$\mathcal{A} \backsim \sum_i F_i(\vec{s};\varepsilon)\, G_i(\vec{s};\varepsilon)$$

Feynman Integrals

Motivation

- $t\bar{t}W$ production is relevant for BSM searches and constitutes a significant background for $t\bar{t}H$ and $t\bar{t}t\bar{t}$ production in Standard Model
- Theoretical predictions systematically underestimate measured rates [ATLAS 2024 and CMS 2023]. Currently within uncertainties, but experimental precision is set to increase
- NNLO: 2-loop amplitude approximated with soft-W and massification [Buonocore et al. 2023]
- Exact 2-loop amplitude is needed to remove uncertainty of approximation



What's the challenge?

- Complexity originates from:
  - Massive internal propagators
  - Five external legs, two different external scales
- Analytic complexity
  - Functions beyond the polylogarithmic case
- Algebraic complexity
  - State of the art calculations: usually localised in the amplitude part of the calculation
  - Here: large expressions already in the differential equations for the integrals

Status of related calculations

- $t\bar{t}$: complete NNLO QCD corrections [Czakon et al. 2012, 2013 and 2016; Catani et al. 2019 and 2020]

- $t\bar{t}j$: NLO QCD corrections up to $\mathcal{O}(\varepsilon^2)$ [Badger et al. 2022], two-loop integrals in the leading colour approximation [Badger et al. 2023 and 2024; Becchetti et al. 2025] and numerical evaluation of the amplitude [Badger et al. 2024]

- $t\bar{t}H$: NLO QCD corrections up to $\mathcal{O}(\varepsilon^2)$ [Buccioni et al. 2024]. Numerical results for a set of two-loop Feynman integrals [Febres Cordero et al. 2024] and two-loop N_f part of the quark-initiated scattering amplitudes [Agarwal et al. 2024]

- $t\bar{t}Z$: NLO QCD corrections [Lazopoulos et al. 2008, Kardos et al. 2012], NLO QCD and EW corrections [Frixione et al. 2015]

Kinematics

$\bar{t}(p_1) + t(p_2) + \bar{d}(p_3) + W(p_4) + u(p_5) \longrightarrow 0$

- Momentum conservation:

  $p_1 + p_2 + p_3 + p_4 + p_5 = 0$

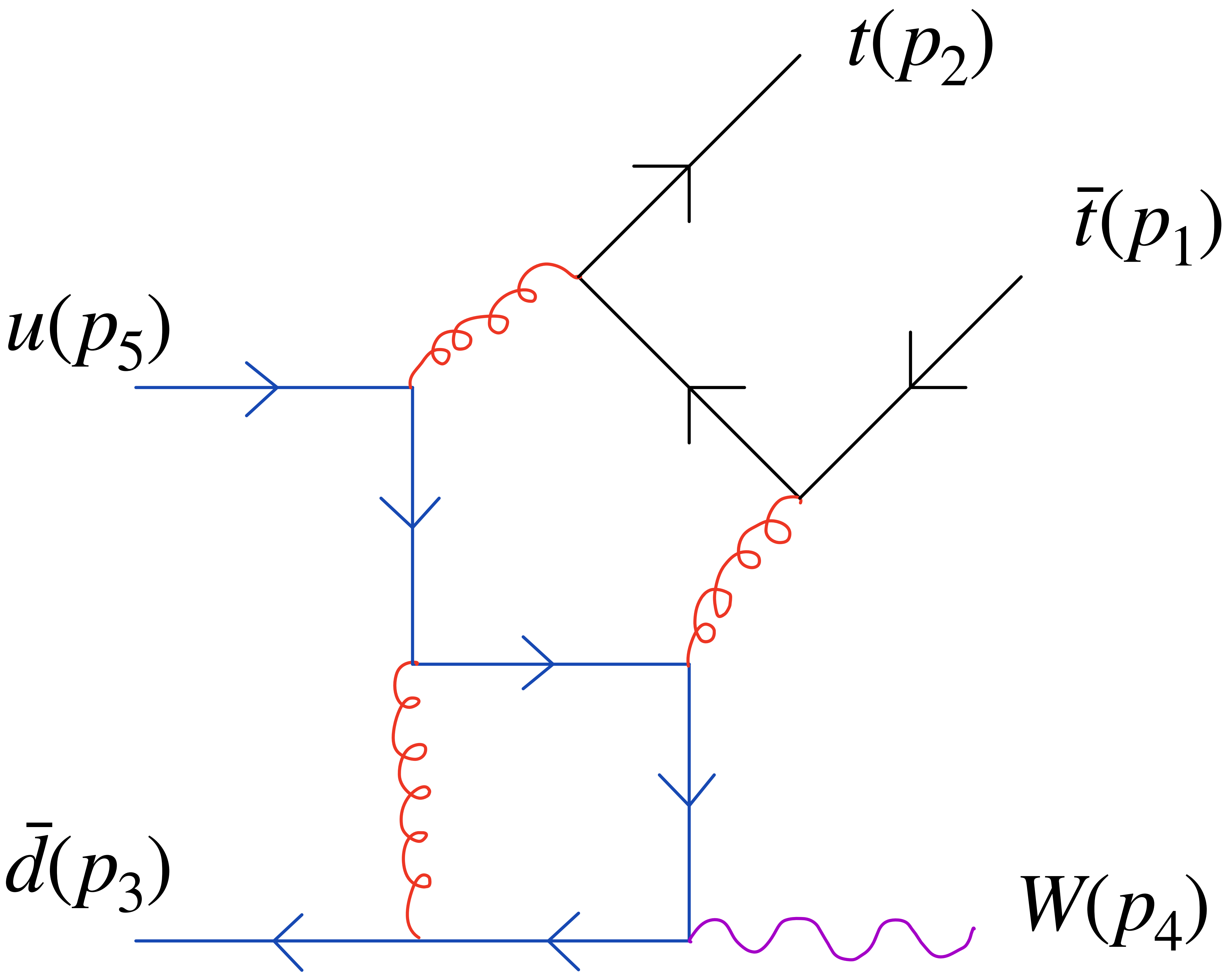
- $p_1^2 = p_2^2 = m_t^2, \quad p_3^2 = p_5^2 = 0, \quad p_4^2 = m_W^2$

- 7 Invariants:

  $\vec{x} := \{s_{12}, s_{23}, s_{34}, s_{45}, s_{15}, m_t^2, m_w^2\}$, with

  $s_{ij} = (p_i + p_j)^2$

- Dimensional regularisation: $d = 4 - 2\varepsilon$



Integral families

$$G_{a_1,\ldots,a_{11}} = \int \mathrm{d}^d k_1 \mathrm{d}^d k_2 \frac{1}{D_1^{a_1} \cdots D_{11}^{a_{11}}}, \qquad (a_1, \ldots, a_{11}) \in \mathbb{Z}^{11}$$

Propagators of Feynman integrals

- Sectors: same non-negative exponents
- Top sector: maximum number of non-negative exponents
- Amplitude calculations: express $k_i \cdot p_j$ and $k_i \cdot k_j$ in terms of propagators

$\Longrightarrow$ Beyond one-loop we need irreducible scalar products (ISPs). Here: 3 ISPs

Integral families: example

$$G_{a_1,\ldots,a_{11}} = \int \mathrm{d}^d k_1 \mathrm{d}^d k_2 \frac{1}{D_1^{a_1}\ldots D_{11}^{a_{11}}}, \qquad (a_1,\ldots,a_{11}) \in \mathbb{Z}^{11}$$

$$D_1 = k_1^2 - m_t^2, \quad D_2 = (k_1 - p_2)^2$$

$$D_3 = (k_1 - p_{23})^2, \quad D_4 = (k_1 - p_{234})^2$$

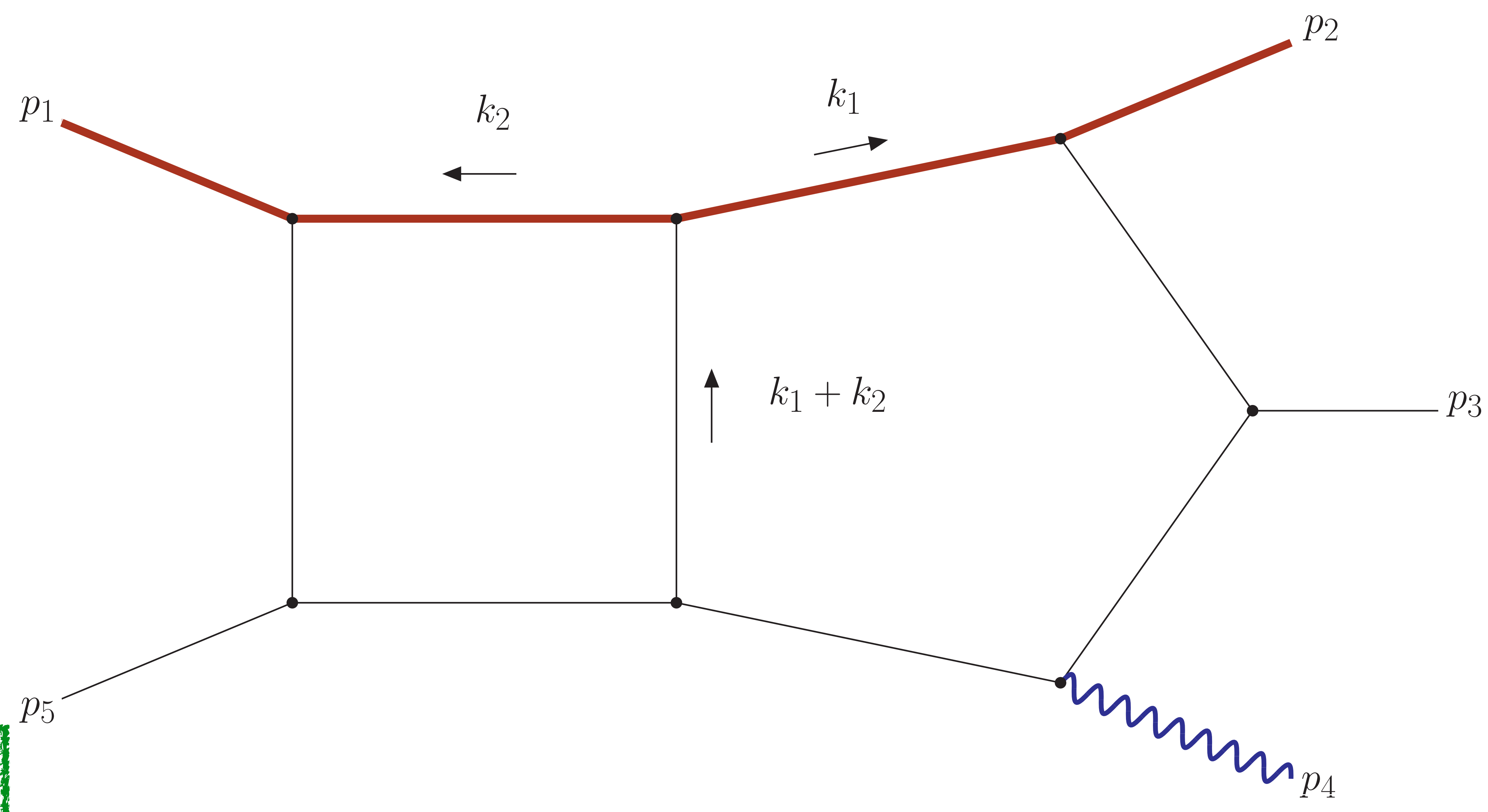
$$D_5 = k_2^2 - m_t^2, \quad D_6 = (k_2 - p_1)^2$$

$$D_7 = (k_2 + p_{234})^2, \quad D_8 = (k_1 + k_2)^2$$

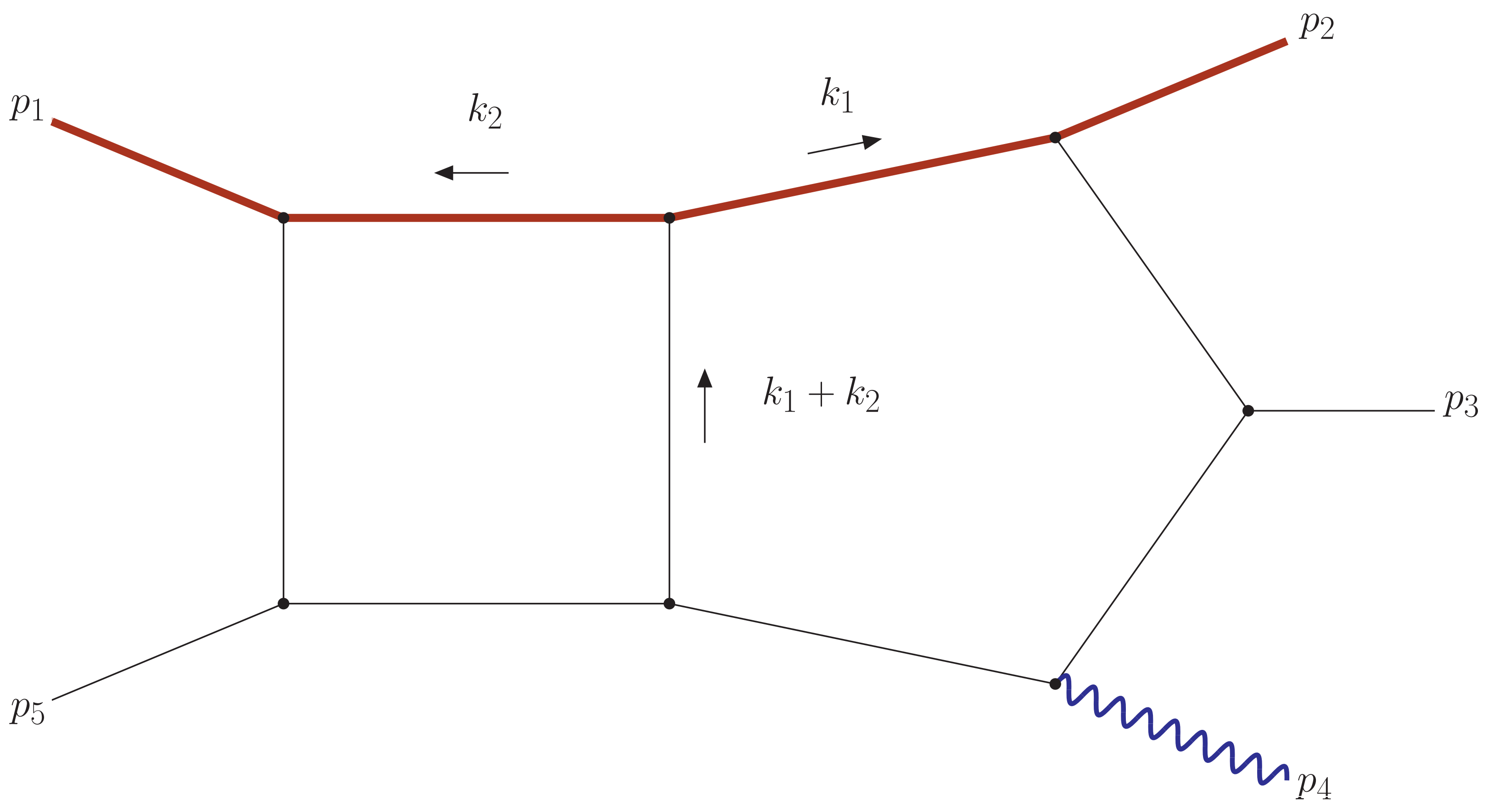
$$D_9 = (k_1 + p_1)^2 - m_t^2, \quad D_{10} = (k_2 + p_2)^2 - m_t^2$$

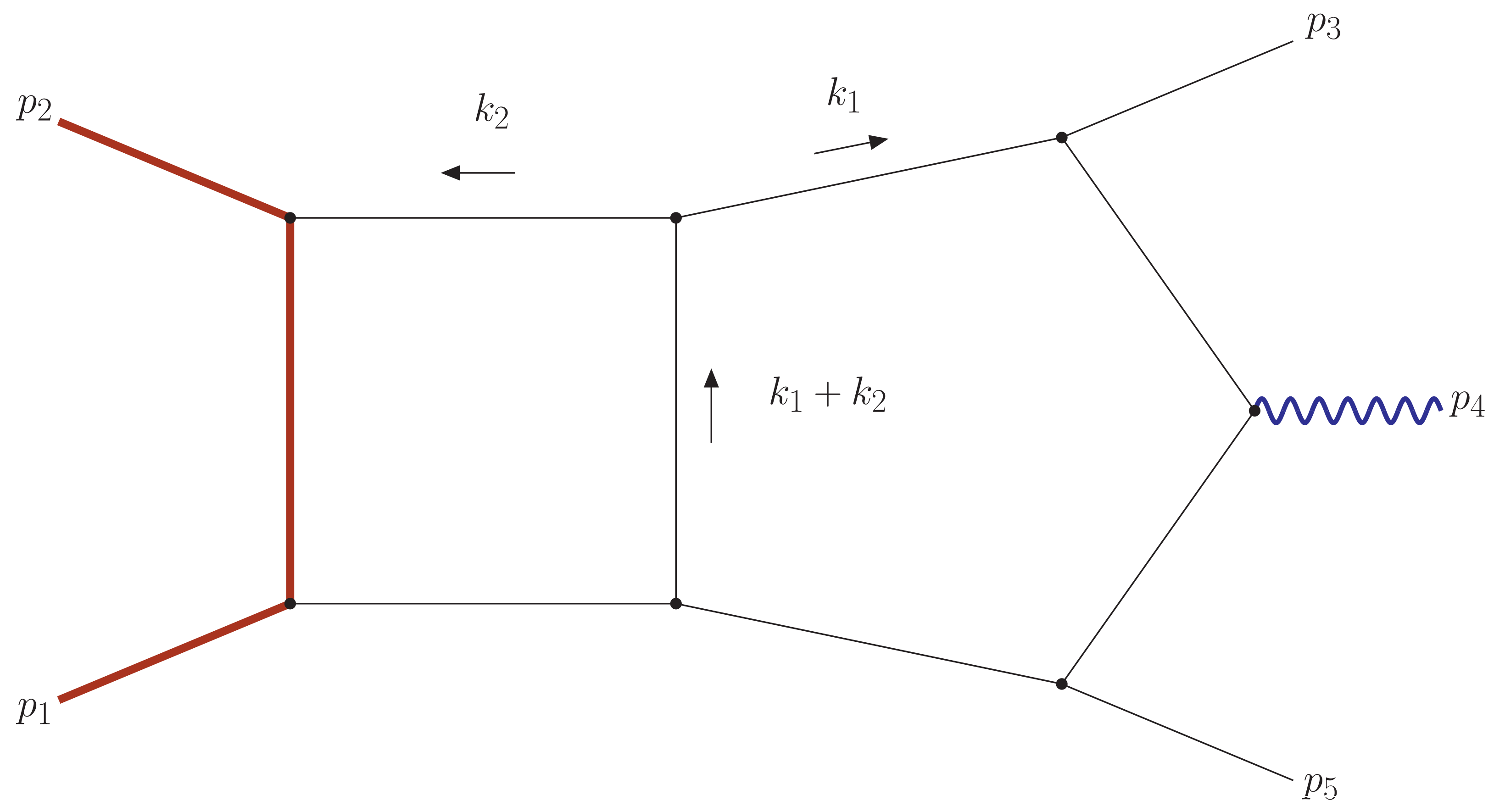
$$D_{11} = (k_2 + p_{23})^2 - m_t^2$$

ISPs



$t\bar{t}W$ integral families

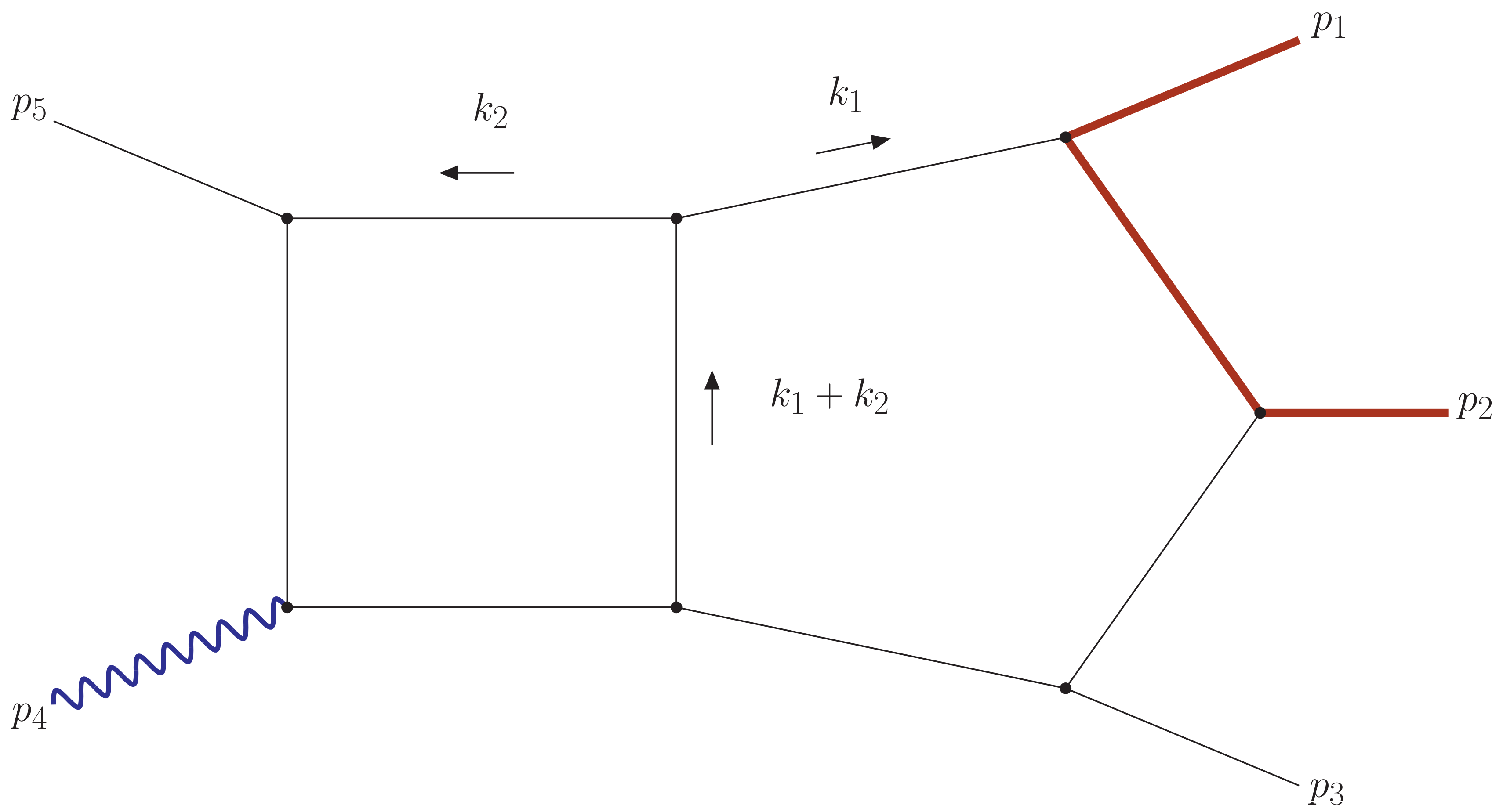




Family F_1: 141 MIs

Family F_2: 122 MIs

Family F_3: 131 MIs



IBPs and reduction to Master Integrals

- Feynman integrals satisfy linear relations: integration by part identities (IBPs) [Chetyrkin, Tkachov '81]

$$0 = \int \mathrm{d}^d k_1 \mathrm{d}^d k_2 \frac{\partial}{\partial k_l^\mu} \frac{v^\mu}{D_1^{a_1} \cdots D_{11}^{a_{11}}}, \quad v^\mu \in \{k_j^\mu, p_j^\mu\}$$

Master Integrals (MIs) $\vec{I}(\vec{x})$

- Reduction to master integrals

$$\sum_{\vec{a}_k} c_{\vec{a}_k}(\vec{x};\varepsilon) G_{\vec{a}_k}(\vec{x};\varepsilon) = 0 \Longrightarrow G_{\vec{a}}(\vec{x};\varepsilon) = \sum_j c_{\vec{a},j}(\vec{x};\varepsilon)\, I_j(\vec{x};\varepsilon)$$

- Laporta algorithm: IBPs generated for some seeding [Laporta 2000]
- Finite Fields techniques [von Manteuffel, Schabinger 2014; Peraro 2016] to tackle algebraic complexity
- `NeatIBP` [Wu et al. 2023] and `FiniteFlow` [Peraro 2019] to generate and solve an optimised system of IBPs

Finite field revolution

[von Manteuffel, Schabinger 2014; Peraro 2016]

- Evaluate rational functions at numerical rational points $(\{p\}, \epsilon)$ modulo prime number $\longrightarrow$ finite field/modular arithmetic
- Perform all intermediate rational operations numerically
- Reconstruct the analytic expression of the final result from multiple numerical evaluations

Mathematica/C++ framework **FiniteFlow** [Peraro 2019]

```
In[1]:= << FiniteFlow`;

In[2]:= prime = FFPrimeNo[1]

Out[2]= 9 223 372 036 854 775 643

In[3]:= c1 = FFRatMod[3 / 4, prime]
        c2 = FFRatMod[-7, prime]

Out[3]= 6 917 529 027 641 081 733

Out[4]= 9 223 372 036 854 775 636

In[5]:= FFRatRec[c1 * c2, prime]

Out[5]= - 21/4
```

Method of differential equations

[Kotikov '91; Bern, Dixon, Kosower '94; Gehrmann, Remiddi 2000]

- Using IBPs we can construct linear differential equations (DEs) for the MIs

$$\forall\ \xi \in \vec{x}: \quad \partial_\xi I_i(\vec{x};\varepsilon) = \sum_{\vec{a}} c_{i,\vec{a}}(\vec{x};\varepsilon) G_{\vec{a}}(\vec{x};\varepsilon)$$

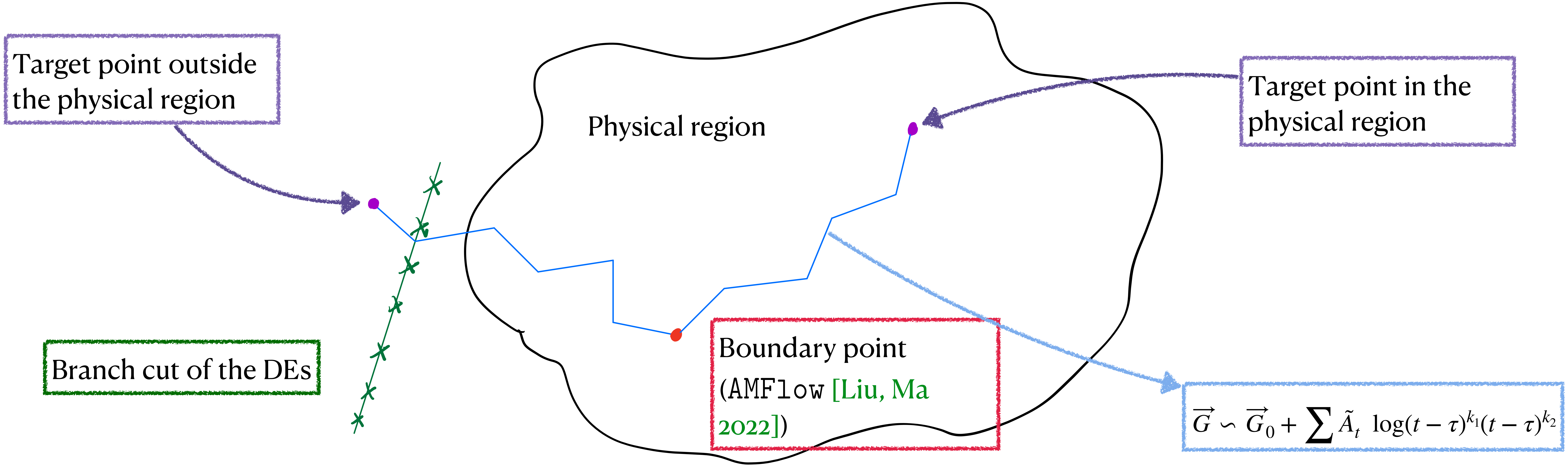
$$\Longrightarrow \partial_\xi \vec{I}(\vec{x};\varepsilon) = B_\xi(\vec{x};\varepsilon)\cdot \vec{I}(\vec{x};\varepsilon)$$

IBP reduction

- Many strategies to solve the differential equation. Our choice: semi-numerical approach using `DiffExp` [Hidding 2020]
  - Suitable for very general problems
  - The implementation supports only rational functions and simple square roots

Semi-numerical evaluation

- Generalised series expansion method [Moriello 2019]: approximate the solution in terms of logs along the integration path



- Work in the physical region: no analytic continuation needed!

What is a good choice of basis of MIs?

- The basis of MIs is not unique. A good choice of basis can greatly simplify the DEs
- [Henn 2014]: DEs in canonical form (no general algorithm)

$$\mathrm{d}\vec{I}(\vec{x};\varepsilon) = \varepsilon\, \mathrm{d}\tilde{A}(\vec{x})\, \vec{I}(\vec{x};\varepsilon)$$

one-forms with at most simple poles

- In the best understood cases the one-forms are logarithmic

$$\mathrm{d}\tilde{A}(\vec{x}) = \sum_i a_i\, \mathrm{d}\log W_i(\vec{x})$$

Letters

  - ε dependence factorises: solution at each order depends only on previous order
  - Full control over linear relations through iterated integrals representation of the solution $\Longrightarrow$ Construction of a minimal basis of special functions, which simplifies the representation of the amplitude
  - Well-established techniques to handle the solution of the DEs

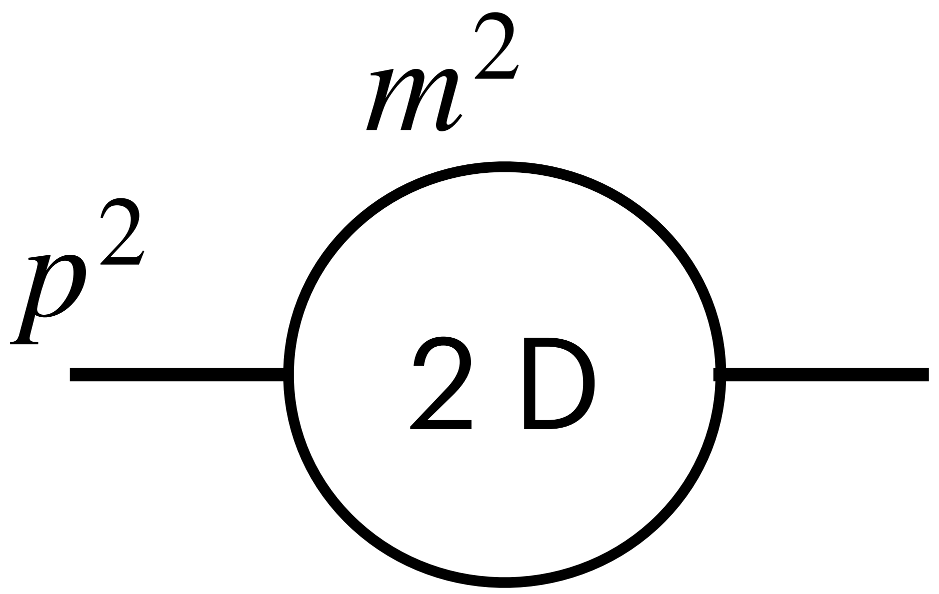
How do we construct a canonical basis?

[Arkani-Hamed, Bourjaily, Cachazo, Trnka 2012]

Dlog-integrands and leading singularities

- Conjecture: integrals with a loop-integrand with at most simple poles and a constant leading singularity are good MIs

$$\mathrm{d}\log(z+c) = \frac{\mathrm{d}z}{z+c}$$



$$\propto \int \frac{\mathrm{d}\alpha_1 \wedge \mathrm{d}\alpha_2}{p^2(\alpha_1\alpha_2 - z)[(1+\alpha_1)(1+\alpha_2) - z]}$$

$$= \int \frac{\mathrm{d}\alpha_1}{p^2(\alpha_1^2 + \alpha_1 + z)} \left[\mathrm{d}\log(\alpha_1\alpha_2 - z) - \mathrm{d}\log(1+\alpha_1+\alpha_2+\alpha_1\alpha_2 - z)\right]$$

$$= \frac{1}{p^2\sqrt{1-4z}} \int \mathrm{d}\log(\ldots) \wedge \mathrm{d}\log(\ldots)$$

Leading singularity (LS) → $\frac{1}{p^2\sqrt{1-4z}}$

dlog-form → $\mathrm{d}\log(\ldots) \wedge \mathrm{d}\log(\ldots)$

- Commonly: rational functions and simple square roots

Beyond the *dlog*-case: elliptic integrals

- During the computation of the leading singularity, we can also bump into an elliptic curve

$$\int \frac{\mathrm{d}z}{\sqrt{\mathscr{P}_4(z)}} \wedge \mathrm{d}\log(\ldots), \qquad \mathscr{P}_4(z) = (z-a_1)(z-a_2)(z-a_3)(z-a_4)$$

- The leading singularity contains elliptic functions

$$\int \frac{\mathrm{d}z}{\sqrt{\mathscr{P}_4(z)}} \propto K(\ldots)$$

Elliptic integral of the first kind

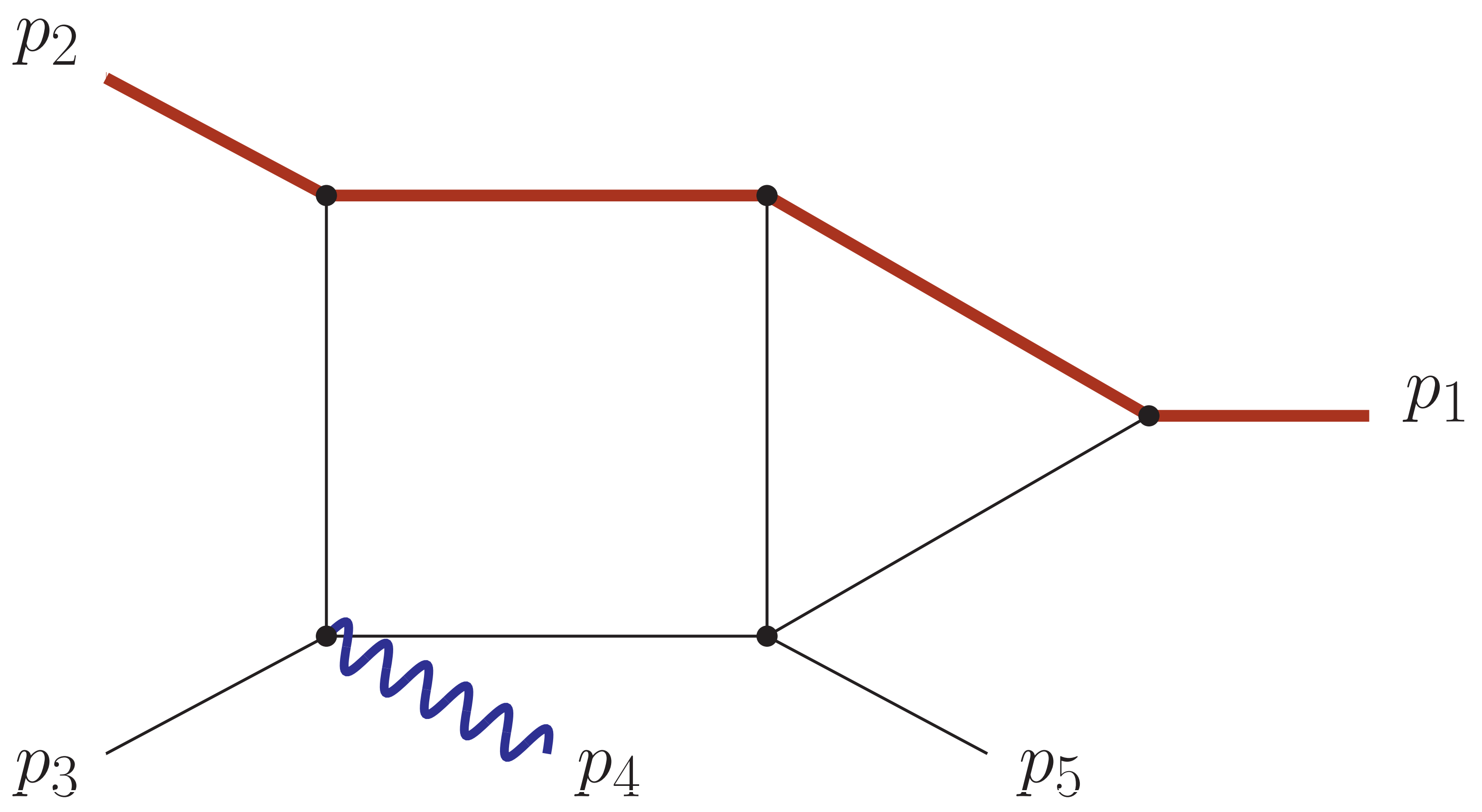
- Transcendental functions are needed to put the differential equation in canonical form
  - Progress on general strategy in recent years (see e.g. [Görges et al. 2023])
  - Still no general method to efficiently evaluate these functions

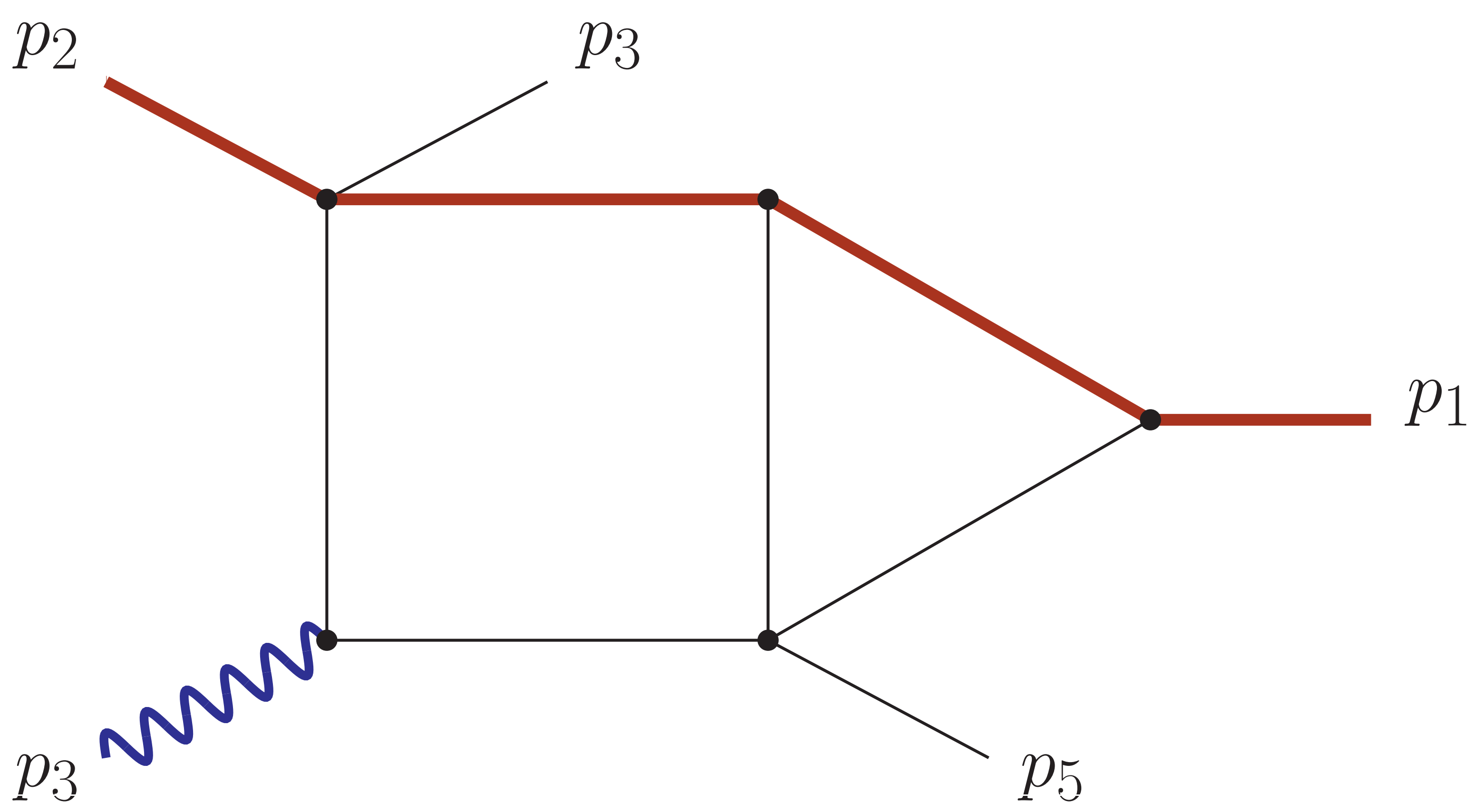
The “simple” $t\bar{t}W$ elliptic curves

- Comparable with known elliptic curves (e.g. [Badger et al. 2024])
- 4-point kinematics ⇒ depend on less than 7 variables
- 3 MIs for each sector
- Elliptic curve of the form

$$\mathscr{P}_4(z) = (z - m_t^2)(z - 3m_t^2)\mathscr{P}_2(z)$$

- The curves are disctinct, as we checked by computing the j-invariant

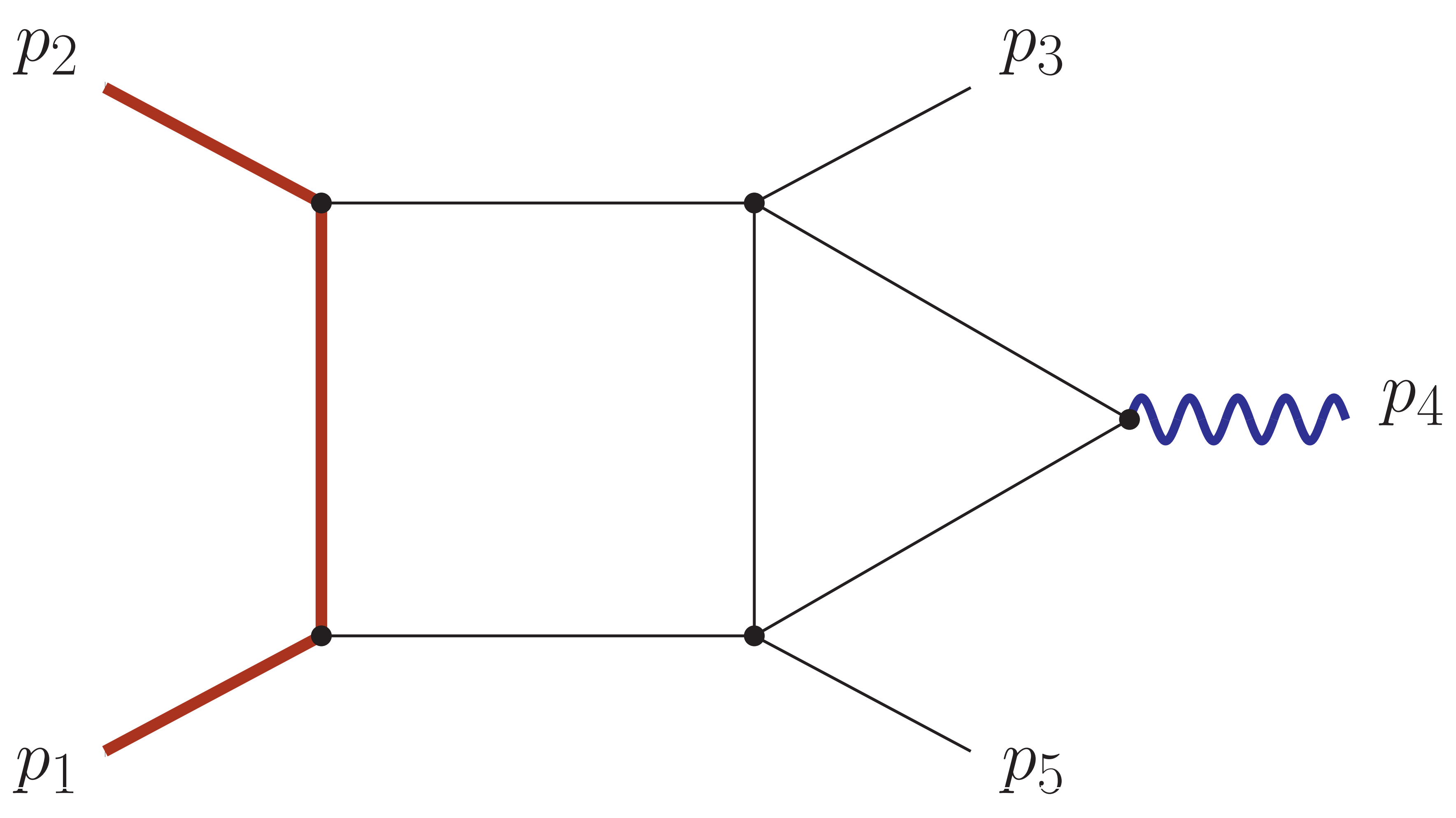




The "monster" $t\bar{t}W$ elliptic curve

- First ever study of an elliptic curve for a 5-point kinematics ⇒ dependence on all 7 invariants
- 7 MIs in the sector
- Computation of LS leads to

$$\int \left(\frac{\mathrm{d}z}{\sqrt{\mathcal{Q}_4(z)}} \wedge \mathrm{d}\log(\alpha(y,z)) - \frac{\mathrm{d}z}{\sqrt{\mathcal{Q}_4(z)^\dagger}} \wedge \mathrm{d}\log(\alpha(y,z)^\dagger) \right)$$



Same j-invariant ⇒ same elliptic curve

$$f^\dagger \equiv f|_{r_1 \to -r_1}, \quad r_1 = \sqrt{G(p_1,p_2,p_3,p_4)}$$

Algebraic complexity of the monster curve

- $\mathcal{Q}_4(z)$ has degree 4 in z and degree 14 in $\vec{x}$, involves r_1 and 2787 terms
- Discriminant of the elliptic curve contains a degree 14 polynomial in $\vec{x}$
  - 2547 terms
  - File size is 94 KB
  - Appears in the denominators of the DEs $\Longrightarrow$ one of the singularities of the solution
- ε-factorised DEs challenging even with known techniques

How we deal with elliptics

Aims: obtain a good basis compatible with `DiffExp`

- Simple ε-dependence
  - No ε-poles in the differential equation
  - Maximum degree as low as possible (2 in this case)
- Elliptic MIs finite
  - Poles of the amplitude dictated by tree-level and 1-loop: no elliptic functions
  - Allows to apply the method of [Badger et al. 2025] to construct a basis of special functions up to the finite part

⚠ Apparent trade-off between the above criteria and the algebraic complexity:

We allow for a spurious degree-9 polynomial in the denominators

Beyond (?) the *dlog*-case: nested square roots

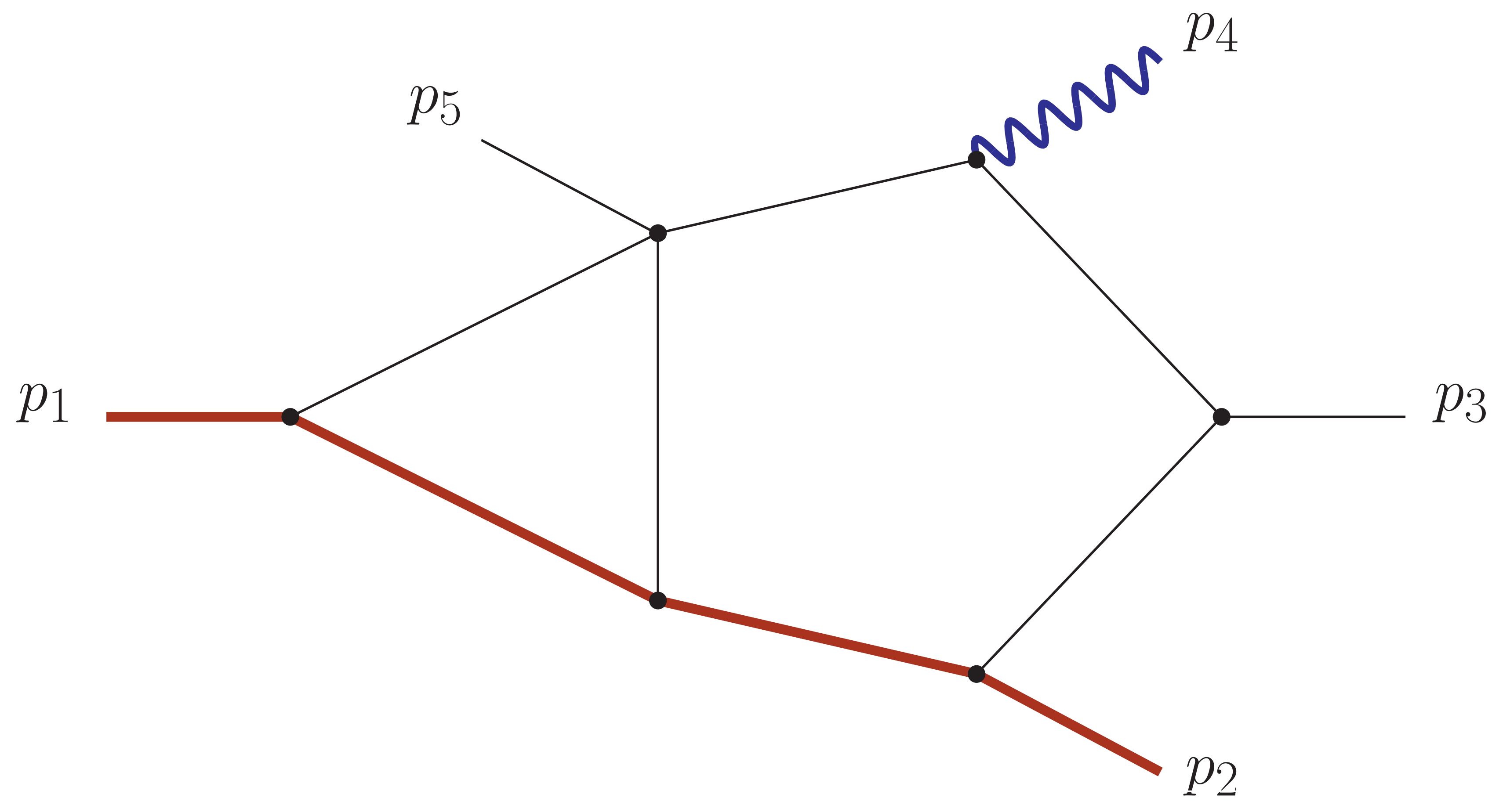
- For $t\bar{t}H$ [Febres Cordero et al. 2024] and $t\bar{t}j$ [Badger et al. 2024] leading singularities involving nested square roots were observed. This is the case also here

$$NR_\pm = \sqrt{q_1(\vec{x}) \pm q_2(\vec{x}) r_1}, \quad r_1 = \sqrt{G(p_1, p_2, p_3, p_4)}$$

$$NR_+ \xrightarrow{r_1 \to -r_1} NR_-$$

- Nested square roots are not supported by DiffExp
- Due to the elliptics, the differential equation will not be ε-factorised anyway

$\Longrightarrow$ keep the differential equation linear in ε



Final representation of the differential equation

- We selected a basis
  - ε factorised as much as possible
  - Linear in ε for the nested square root sectors and at most quadratic in the elliptic sectors
  - Elliptic integrals finite
- Write connection matrix in terms of independent one-forms

$$\mathrm{d}\vec{I}(\vec{x};\varepsilon) = \mathrm{d}A^{(F)}(\vec{x};\varepsilon)\cdot\vec{I}(\vec{x};\varepsilon), \qquad \mathrm{d}A^{(F)}(\vec{x};\varepsilon) = \sum_{k=0}^{2}\varepsilon^k\Big[\sum_{\alpha} c_{k\alpha}^{(F)}\mathrm{d}\log(W_\alpha(\vec{x})) + \sum_{\beta} d_{k\beta}^{(F)}\omega_\beta(\vec{x})\Big]$$

Some numbers…

	Nested square root sectors	"Simple" elliptic sectors	Monster elliptic sector	# square roots	# letters	# one-forms	Dimension one-forms file
Family 1	Yes	2	No	8	101	119	6.7 MB
Family 2	No	1	Yes	11	122	84	311 MB
Family 3	No	1	Yes	12	137	96	316.5 MB

Numerical checks

- `DiffExp` implementation with in-house path-parametrisation
- Checked against `AMFlow` at 10 physical phase-space points, to 25 digits accuracy
- We verified that we can integrate between any of these 10 points with `DiffExp`

Summary and Outlook

- Basis and differential equation for all the integral families relevant for $t\bar{t}W$ production at 2-loop at leading color
- Addressed complications arising from nested square roots and elliptic integrals
- Semi-numerical solution using `DiffExp`
- Next steps
  1. 2-loop amplitude
  2. ε-factorised differential equation

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Thank you!

Backup slides

Definitions for elliptic curves

- Cross ratio

$$\lambda = \frac{(a_1 - a_4)(a_2 - a_3)}{(a_1 - a_3)(a_2 - a_4)}$$

- Elliptic integral of the first kind

$$K(\lambda) = \int_0^1 \frac{\mathrm{d}t}{\sqrt{(1 - t^2)(1 - \lambda t^2)}}$$

- Periods of the elliptic curve

$$\omega_1 = 2c_4 \int_{a_2}^{a_3} \frac{\mathrm{d}z}{y} = 2K(\lambda), \quad \omega_2 = 2c_4 \int_{a_1}^{a_2} \frac{\mathrm{d}z}{y} = 2\mathrm{i}K(1 - \lambda),$$

$$\text{with } c_4 = \frac{1}{2}\sqrt{(a_1 - a_3)(a_2 - a_4)}$$

- J-invariant

$$j = 256 \frac{(1 - \lambda(1 - \lambda))^3}{\lambda^2 (1 - \lambda)^2}$$