## Special Functions for Five-Point One-Mass Scattering in QCD

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based on Chicherin, VS, Zoia [arXiv:2110.10111] Abreu, Chicherin, Ita, Page, VS, Tschernow, Zoia [arXiv:2306.15431]

QCD meets gravity 2023, CERN

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## Introduction

### Motivation

- LHC today is a precision machine
- 20x more data to be taken at HL-LHC, future colliders
- Theoretical understanding of SM predictions is key to interpret data
- At least NNLO QCD and NLO EW corrections ( $\oplus$  parton shower, resummation, ...) must be included to achieve percent level theory uncertainties

$$d\sigma_{h_1h_2 \to X}(p_1, p_2) = \sum_{i,j} \int dx_1 dx_2 f_i(x_1, \mu) f_j(x_2, \mu) \frac{d\hat{\sigma}_{ij \to X}(x_1p_1, x_2p_2, \mu)}{|\mathsf{ntrinsic uncertainty}} + \mathcal{O}(\Lambda_{\mathsf{QCD}}/Q)$$

$$d\hat{\sigma}_0 \left(1 + \alpha_s \sigma^{(1,0)} + \alpha_s^2 \sigma^{(2,0)} + \alpha \sigma^{(0,1)} + \alpha_s^3 \sigma^{(3,0)} + \alpha \alpha_s \sigma^{(1,1)} + \dots \right) \qquad \alpha_s(M_Z) \sim 0.1$$

$$\alpha(M_Z) \sim 0.01$$

## NNLO QCD multiplicity frontier





• NNLO QCD beyond  $2 \rightarrow 2$  remarakably challenging



$$F+X_{NNLO} = \sigma_{NLO}^{F+X} + \int_{\Phi_{F(+2)}} d\sigma_{RR} + \int_{\Phi_{F(+1)}} d\sigma_{RV} + \int_{\Phi_{F}} d\sigma_{VV}$$
IR divergences
Two-loop
amplitudes

 $\sigma$ 

This talk:

 $2\to 3$  processes with one external mass  $pp\to Vjj,\ pp\to Hjj,\ e^+e^-\to 4j$ 

## Analytic multi-loop amplitude calculations



## Setup of the computation

### Integral topologies & kinematics



#### **Previous work**



[Badger, Hartanto, Zoia '21] color-ordered

planar one-mass pentagon functions [Chicherin, VS, Zoia '21]



Precious numerical data:

- Initial (boundary) conditions
- Validation

## **Canonical differential equations**

## Pure integrals and canonical differential equations



🚹 Canonical DE very challenging to obtain for multi-scale integrals

other cutting edge examples: [Febres Cordero, Figueiredo, Kraus, Page, Reina '23] [Badger, Becchetti, Chaubey, Marzucca '22] [Henn, Peraro, Xu, Zhang '21]

We succeed in deriving this form for complete set of integrals

## The alphabet

Hexa-box alphabet [Abreu, Ita, Page, Tschernow '21], no new letters from DP

| $A = \sum^{204}$        | $d \log \frac{W_i}{W_i}$ | $A_i$      | c.f. 31 letters,               | Algebraic letters, odd under root sign flip |   |                   |                                   |  |  |
|-------------------------|--------------------------|------------|--------------------------------|---|---|-------------------|-----------------------------------|--|--|
| i=1                     | $\sum_{i=1}^{2}$         |            | 1 square root<br>for massless! |   | e.g. $W_{118} = rac{p_1^2 - s_{23} + s_{45} + \sqrt{\Delta_3^{(1)}}}{p_1^2 - s_{23} + s_{45} - \sqrt{\Delta_3^{(1)}}}$ |                   |                                   |  |  |
| Degree                  | Letter                   | s          |                                |   |   |                   |                                   |  |  |
| linear                  | 27                       | <u> </u>   |                                |   | Roots   | Letters           |                                   |  |  |
| quadrat<br>qubic        | 1C 66<br>24              | > 117 rati | onal                           |   | $\sqrt{\Delta_5}$   | 32                |                                   |  |  |
|                         |                          | ,<br>,     |                                |   | $\sqrt{\Delta_3^{(i)}}$   | 12                | square root                       |  |  |
|                         |                          |            |                                |   | $\sqrt{\Sigma_5^{(i)}}$   | <sub>24</sub> )   | ·                                 |  |  |
| Post                    | Degrae                   | Perms./    |                                |   | $\sqrt{\Delta_5}, \sqrt{\Delta_3^{(i)}}$  | 3)                | 9 two                             |  |  |
| Root                    | Degree                   | Letters    | -                              |   | $\sqrt{\Delta_5}, \sqrt{\Sigma_5^{(i)}}$  | 6                 | square roots                      |  |  |
| $\sqrt{\Delta_5}$       | 4                        | 1          |                                |   | • 0, V 3  | )                 |                                   |  |  |
| $\sqrt{\Delta_3^{(i)}}$ | 2                        | 3          | > 10 square                    | $\Sigma_{5}^{(1)} =$                        | $=(s_{12}s_{15}-s_{12}s_{23})$  | $-s_{15}s_{45} +$ | $(s_{34}s_{45} + s_{23}s_{34})^2$ |  |  |
| $\sqrt{\Sigma_5^{(i)}}$ | 4                        | 6)         | TOOLS                          | -   | $-4s_{23}s_{34}s_{45}(s_{34} -$   |                   |                                   |  |  |







## **Function basis**

#### Chen's iterated integrals

[Chen '77] (see also "Iterated integrals in QFT" [Brown '11])

 $\epsilon$ -factorized DE can be readily solved through Chen's iterated integrals [Chen '77], along a path  $\gamma \in \mathcal{P}$  (phase space) connecting  $s_0$  and s,

$$\vec{g}(\mathbf{s}) = \mathbb{P} \exp\left[\epsilon \int_{\gamma} A\right] \vec{g}(\mathbf{s}_0) = \vec{g}^{(0)}(\mathbf{s}_0) + \sum_i \epsilon^i \vec{g}^{(i)}(\mathbf{s}),$$

 $\vec{g}^{(n)}$  are linear combinations of  $g_i^{(n_1)}(\mathbf{s}_0) \cdot [\omega_{i_1}, \dots, \omega_{i_{n_2}}]_{\gamma}$ ,  $n_1 + n_2 = n$ .

Let  $\omega_1, \ldots, \omega_n$  be differential 1-forms on  $\mathcal{P}$ , and path  $\gamma : [0,1] \to \mathcal{P}$ . Pull the forms back on the path  $\omega_i(\mathbf{s}) \xrightarrow{\gamma^*} w_i(t) \, \mathrm{d}t$ . Iterated integrals are

$$\underbrace{ \left[ \omega_{1}, \dots, \omega_{n} \right]_{\gamma} }_{M = 0} \int_{0}^{1} w_{n}(t_{n}) \, \mathrm{d}t_{n} \dots \int_{0}^{t_{2}} w_{1}(t_{1}) \, \mathrm{d}t_{1}$$
 (ii)

Here we need only logarithmic forms  $\omega_i = d \log W_i$ .

Weight = number of integrations = order of  $\epsilon$ 

#### Linear independence

Iterated integrals with distinct words  $[\omega_1, \ldots, \omega_n]$  are  $\mathbb{Q}$ -linear independent (if  $\{\omega_i\}$  are).  $\implies$  graded vector space



# Symbol map S Let $dF = \sum_i d \log W_i$ $F_i$ (recall $d[\omega_1, \dots, \omega_n]_{\gamma} = \omega_n \ [\omega_1, \dots, \omega_{n-1}]_{\gamma}$ ) $S([\omega_i]_{\gamma}) = W_i.$

Effectively discards initial values and path in DE solution.

## Pentagon functions construction

[Abreu, Chicherin, Ita, Page, VS, Tschernow, Zoia '23] (see also [Chicherin, VS '20] [Badger, Hartanto, Zoia '21] [Chicherin, VS, Zoia '21])



## Promoting symbol-level basis

Full functions are defined by iterated integrals, including terms with transcendental constants (initial values  $\vec{\chi} \coloneqq \vec{g}(\mathbf{s}_0)$ )



We want to work in a vector space  $\implies$  we must know all algebraic identities between  $\vec{\chi}^{(w-w')}.$ 

This turns out to be difficult [Chicherin, VS, Zoia '21] (need very high precision  $\vec{\chi}$  for PSLQ).

#### New approach

- 1. Use relation of  $f_i^{(w)}$  to  $\vec{g}$  to define lifts of  $f_i^{(w)}$  to functions (as iterated integrals).
- 2. Insist that symbol-level decomposition of  $\vec{g}$  through polynomials of  $f_i^{(w)}$  also holds as functions, modulo  $\zeta$  values.
- This is possible if \$\vec{\car{x}}\$(w-w')\$ satisfy certain algebraic identities. We check (numerically) that they indeed do!

 $\hat{g}^{(i)} : \begin{pmatrix} [\omega_i] \\ 2[\omega_2] \end{pmatrix} \rightarrow \chi^{(i)}$ Weight 1 -[w1] - 5[W2] symbol level basis [ω]]  $\frac{1}{1} = \begin{pmatrix} -\frac{1}{f_2^{(1)}} \\ -\frac{1}{f_1^{(1)}} & \frac{1}{2} & \frac{1}{2} \\ -\frac{1}{f_1^{(1)}} & \frac{1}{2} & \frac{1}{2} & \frac{1}{2} \end{pmatrix}$  $\begin{array}{c} f_{1}^{(1)} := g_{1}^{(1)} \\ f_{2}^{(0)} := g_{2}^{(1)} \end{array} = 2 \qquad \overrightarrow{g}_{2}^{(1)} \end{array}$ possible if  $\chi^{6_j}_{\iota^{(j)}}$  $\begin{array}{c} \chi_{1}^{(c)} \\ \chi_{2}^{(c)} \\ \chi_{3}^{(c)} \end{array}$  $= \begin{pmatrix} -\chi_1^{(i)} - \frac{\zeta}{2}\chi_2^{(i)} \\ \chi_1^{(i)} \end{pmatrix}$ -χ.<sup>(1)</sup>-

$$Weight 2$$

$$\frac{1}{2} \left(2\right) = \begin{pmatrix} \left[\alpha_{i}, \omega_{i}\right]^{2} + \chi_{i}^{(0)}\left[\omega_{i}\right]^{2} \\ 2\left[\omega_{z}, \omega_{z}\right]^{2} + \chi_{1}^{(0)}\left[\omega_{z}\right]^{2} \\ 2\left[\omega_{z}, \omega_{z}\right]^{2} + \chi_{1}^{(0)}\left[\omega_{z}\right]^{2} +$$

$$\begin{array}{c} \left(f_{i}^{(1)}\right)^{2} = 2 \left[\omega_{i}, \omega_{i}\right] + 2 \chi_{i}^{(1)} \left[\omega_{i}\right] + \left(\chi_{j}^{(1)}\right)^{2} \\ \left(f_{2}^{(1)}\right)^{2} = 8 \left[\omega_{2}, \omega_{2}\right] + 2 \chi_{i}^{(2)} \left[\omega_{2}\right] + \left(\chi_{2}^{(1)}\right)^{2} \\ \left(f_{1}^{(1)}\right)^{2} = 2 \left[\omega_{2}, \omega_{i}\right] + 2 \left[\omega_{2}, \omega_{2}\right] + 2 \chi_{i}^{(1)} \left[\omega_{2}\right] + \chi_{i}^{(2)} \left[\omega_{2}\right] + \chi_{i}^{(2)} \left[\omega_{2}\right] \\ \left(f_{1}^{(1)}\right)^{2} \left(f_{1}^{(1)}\right)^{2} \left(f_{2}^{(1)}\right)^{2} + 2 \chi_{i}^{(1)} \left[\omega_{2}\right] + \chi_{i}^{(2)} \left[\omega_{2}\right] \\ \end{array} \right) \\ Now consider span \left\{\left(f_{1}^{(1)}\right)^{2} \left(f_{2}^{(1)}\right)^{2} + \left(f_{1}^{(1)}\right)^{2} \left(f_{i}^{(1)}\right)^{2} + \left(f_{i}^{(1)}\right)^{2} + \left(f_{i}^{(1)}\right)^{2} + \left(f_{i}^{(2)}\right)^{2} +$$

$$\frac{3}{9} = \begin{pmatrix} \frac{1}{2} \left(f_{1}^{(i)}\right)^{2} \\ \frac{1}{4} \left(f_{2}^{(i)}\right)^{2} \\ \frac{1}{4} \left(f_{2}^{(i)}\right)^{2} \\ \frac{1}{4} \left(f_{2}^{(i)}\right)^{2} \\ \frac{1}{2} \left(f_{1}^{(i)}\right)^{2} - \frac{3}{8} \left(f_{2}^{(i)}\right)^{2} - f_{1}^{(2)} \end{pmatrix} \xrightarrow{\text{Symbol level}}$$

$$\frac{1}{9055ible if}$$

$$\chi_{1}^{(i)} \stackrel{!}{=} \frac{1}{2} \left(\chi_{1}^{(i)}\right)^{2} + C \stackrel{>}{>}_{2}$$

$$\chi_{4}^{(i)} \stackrel{!}{=} \frac{3}{2} \left(\chi_{1}^{(i)}\right)^{2} - \frac{3}{8} \left(\chi_{2}^{(i)}\right)^{2} - \chi_{3}^{(2)} + C \stackrel{>}{>}_{2}$$

$$We \quad \text{find these are always satisfied !}$$

## Features of the function space

### Anomalous thresholds in massless scattering?

Consider iterated integral along  $\gamma:t\in[0,1]\to \mathcal{P}_{\rm phys},$  and  $W_i(t^\star)=0,$ 

$$\int_{\gamma} \mathrm{d}\log W_i \ h = \int_{\gamma} \frac{\mathrm{d}W_i}{W_i} h \xrightarrow{t \to t^*} \frac{W'(t)}{t - t^*} \left( h^{(0)} + h^{(1)}(t - t^*) + \mathcal{O}\left((t - t^*)^2\right) \right)$$

#### Planar scattering

Only linear or quadratic letters vanish in  $\mathcal{P}_{\mathsf{phys}}$ , poles always canceled, i.e.  $h^{(0)}=0$ 

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New feature of nonplanar scattering Square roots of quartic polynomials  $\sqrt{\Sigma_5}$  can vanish in  $\mathcal{P}_{phys} \implies$  new types of divergences 1. Integrable square root:  $d \log \frac{a + \sqrt{\Sigma_5}}{a - \sqrt{\Sigma_5}} \xrightarrow{\Sigma_5 \to 0} \frac{d\Sigma_5}{a \sqrt{\Sigma_5}} \xrightarrow{t \to t^*} \frac{C}{\sqrt{t - t^*}} + \dots$ 2. Uncompensated poles:  $d \log \sqrt{\Sigma_5} \xrightarrow{\Sigma_5 \to 0} \frac{d\Sigma_5}{2\Sigma_5} \xrightarrow{t \to t^*} \frac{C}{t - t^*} + \dots \implies \log$  divergence!

- · Choose basis functions to localize non-analytic behavior
- Functions with type 2 divergence cancel out in physical results?
- Numerical evaluation more challenging

| Weight | $P \cup PB$ | +HB | +DP | Total  |
|--------|-------------|-----|-----|--------|
| 1      | 11          | 0   | 0   | 11     |
| 2      | 25          | 10  | 0   | 35     |
| 3      | 145         | 72  | 0   | 217    |
| 4      | 675         | 305 | 48  | 1028 🔫 |
| #MIs   | 1361        | 542 | 345 | 2248 - |
|        |             |     |     |        |

Permutation closed  $\sigma\left(f_{i}^{(w)}\right) \rightarrow \sum_{j} c_{ij} f_{j}^{(w)} + \dots$ 



# Numerical evaluation

## Numerical evaluation

### Weights 1 and 2

Well-defined combinations of  $\log$ ,  $Li_2$  functions

$$f_{13}^{(2)} = \operatorname{Li}_2\left(1 - \frac{s_{15} - s_{23} - s_{34}}{s_{15}}\right) > 0$$

### Weights 3 and 4



- No crossing of physical thresholds  $\implies$  no analytic continuation needed
- Dedicated series expansions around (spurious) singularities

## Numerical performance



- Sample over physical phase space for NLO Wjj production at the LHC
- Evaluate all functions on each point, plot the worst accuracy per point
- Timing for all functions on one CPU

 $\label{eq:available} Available in PentagonFunctions++ \\ gitlab.com/pentagon-functions/PentagonFunctions-cpp$ 

# Conclusions

#### Conclusions

- Basis of special functions for two-loop five-point one-mass processes is available. Hopefully exciting phenomenology in near future!
- Existence of the basis "mysteriously" implies algebraic identities between initial values.
- Interesting feature discovered: anomalous thresholds in nonplanar massless scattering.
- All we need is iterated integrals with nice kernels.

#### Outlook

- Ideas generally useful for multi-scale problems with many square roots, e.g. EW corrections and (quantum) gravity amplitudes.
- $\bullet$  Dream: extension beyond  $d\log$  forms.

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# Backup



Weight 3 functions are one-fold integrals of weight 2 functions by definition

$$f_i^{(3)}(X) = \sum_{j,k} c_{i,j,k} \int_0^1 \mathrm{d}\log W_j(t) \, h_k^{(2)}(t) + \tau_i^{(3)}$$

Integrands analytic on the integration domain  $\implies$  integration well-defined.

- Efficient numerical integration possible
- Some care to avoid numerical cancellations if  $d \log(W_j)$  can vanish along the path

Change order of integration [Caron-Huot, Henn '14]  

$$I_{\gamma}[\omega_{1}, \dots, \omega_{n}] = \int_{0}^{1} (\gamma^{*} \circ \omega_{n})(t) \int_{0}^{t} (\gamma^{*} \circ \omega_{n-1})(u) I_{\gamma(u)}[\omega_{1}, \dots, \omega_{n-2}] = \int_{0}^{1} (\gamma^{*} \circ \omega_{n-1})(u) \left( \int_{u}^{1} (\gamma^{*} \circ \omega_{n})(t) \right) I_{\gamma(u)}[\omega_{1}, \dots, \omega_{n-2}] = 0$$

For logarithmic forms the last integration is trivial

$$\int_{u}^{1} (\gamma^{\star} \circ \omega_n)(t) = \int_{u}^{1} \mathrm{d}\log\left(W_n(t)\right) = \log(W_n(1)) - \log(W_n(u))$$

## DE reconstruction strategy

Hope: the result is pure functions of uniform transcendentality [Henn '13]



### Physical region geometry



- Nontrivial geometry due to degree 4 polynomial boundary  $\Delta_5=0$
- Not convex
- Not star shaped

- Positivity properties of the alphabet important for deriving well-defined functions in physical region
- Can be established by expressing through Gram determinants
- Non-sign-definite letters  $\implies$  spurious singularities

[Chicherin, VS, Zoia '21]

We choose an initial point  $X_0 \in \mathcal{P}_{45}^+$ ,

$$X_0 := \left( p_1^2 = 1, s_{12} = 3, s_{23} = 2, s_{34} = -2, s_{45} = 7, s_{15} = -2 \right),$$

which satisfies the following requirements:

- 1.  $X_0$  introduces the minimal number of distinct prime factors.
- 2.  $X_0$  is invariant under the exchanges of momenta  $2 \leftrightarrow 3$  and  $4 \leftrightarrow 5$  (automorphisms of  $\mathcal{P}_{45}$ ).

| Algebraic relations between initial                                       |        |             |     |             |    |
|---|--------|-------------|-----|-------------|----|
| values required.  |        | Linear span |     | Irreducible |    |
| <ul> <li>Numerical evaluation of available<br/>GPL expressions</li> </ul> | Weight | Re          | Im  | Re          | Im |
| [Canko, Papadopoulos, Syrrakos '20].                                      | 1      | 4*          | 1   | 4*          | 1  |
| [Syrrakos '20] to 3000 digits   | 2      | 12          | 4   | 5           | 0  |
|   | 3      | 67          | 23  | 23          | 7  |
| • Relations from $PSLQ \implies$  | 4      | 305         | 135 | 90          | 40 |
| generating set  |        |             |     |             |    |

3. The four linear letters which have indefinite sign vanish at  $X_0$ .

Pushing the limits of most advanced PSLQ algorithms [Bailey, Broadhurst '01]

[Bailey, Borwein, Kimberley, Ladd '17]