All Two-Loop Feynman Integrals for Five-Point One-Mass Scattering

Samuel Abreu,[1,2] Dmitry Chicherin,[3] Harald Ita,[4,5] Ben Page,[1] Vasily Sotnikov,[6,7]
Wladimir Tschernow,[8] and Simone Zoia[9]
[1]*CERN, Theoretical Physics Department, CH-1211 Geneva 23, Switzerland*
[2]*Higgs Centre for Theoretical Physics, School of Physics and Astronomy, The University of Edinburgh, Edinburgh EH9 3FD, Scotland, United Kingdom*
[3]*LAPTh, Université Savoie Mont Blanc, CNRS, B.P. 110, F-74941 Annecy-le-Vieux, France*
[4]*Paul Scherrer Institut, Forschungsstrasse 111, 5232 Villigen, Switzerland*
[5]*ICS, University of Zurich, Winterthurerstrasse 190, Zurich, Switzerland*
[6]*Physik-Institut, University of Zurich, Winterthurerstrasse 190, 8057 Zurich, Switzerland*
[7]*Department of Physics and Astronomy, Michigan State University, 567 Wilson Road, East Lansing, Michigan 48824, USA*
[8]*Physikalisches Institut, Albert-Ludwigs-Universität Freiburg, D-79104 Freiburg, Germany*
[9]*Dipartimento di Fisica and Arnold-Regge Center, Università di Torino, and INFN, Sezione di Torino, Via P. Giuria 1, I-10125 Torino, Italy*

(Received 19 July 2023; revised 16 February 2024; accepted 4 March 2024; published 1 April 2024)

We compute the complete set of two-loop master integrals for the scattering of four massless particles and a massive one. Our results are ready for phenomenological applications, removing a major obstacle to the computation of complete next-to-next-to-leading order QCD corrections to processes such as the production of a $H/Z/W$ boson in association with two jets at the LHC. Furthermore, they open the door to new investigations into the structure of quantum-field theories and provide precious analytic data for studying the mathematical properties of Feynman integrals.

DOI: 10.1103/PhysRevLett.132.141601

Feynman integrals play a central role in obtaining precise predictions in quantum-field theory (QFT). They are also of great mathematical interest, giving rise to noteworthy classes of special functions. Advances in the calculation of Feynman integrals have led to new insights into the mathematical properties of these functions, as well as to new results in formal studies of QFTs and (beyond) standard-model phenomenology. While the calculation of two-loop five-point Feynman integrals is an active area of research [1–12], a complete set of integrals is only available for massless particles [1–7]. In this Letter, we advance the state of the art by computing all Feynman integrals necessary to describe the scattering of four massless particles and a massive one at two loops.

We obtain a representation for the Feynman integrals in dimensional regularization that exhibits their analytic structure and allows for a stable and efficient numerical evaluation. This is achieved by finding bases of pure integrals [13] that satisfy differential equations (DEs) [14–18] in canonical form [19], explicitly displaying all singularities of the integrals. Despite recent progress [5,20–25], finding a pure basis is still a major bottleneck. We followed the approach of Refs. [3,6], building on modular arithmetic to bypass intermediate computational bottlenecks [26,27]. Using Chen iterated integrals [28], we solve the DEs at each order in the dimensional regulator in terms of a minimal set of functions, called "(one-mass) pentagon functions." We demonstrate that this solution is efficient and numerically stable over phase space and therefore ready for phenomenological application. A C++ library [29] for the evaluation of the pentagon functions makes our results accessible to the whole community. Previous approaches for constructing such solutions [7,30–32] relied on the possibility of representing them through multiple polylogarithms [33], but it is generally unclear if such a representation exists [34]. We show that this is not required, and only one evaluation of the integrals at a precision comparable to that at which we evaluate the pentagon functions is sufficient. Nonplanar integrals introduce added complexity: some exhibit nonanalytic behavior or a logarithmic singularity within the physical scattering region. We isolate this behavior in the pentagon functions, and extend the numerical methods of Refs. [7,32] to deal with it.

Our results open the door to new explorations in many different directions. On the analytic side, this is the first complete set of two-loop integrals allowing us to explore the (extended) Steinmann relations [35–41]. Moreover, these integrals make it possible to study how unexplained observations of analytic cancellations in gauge-theory

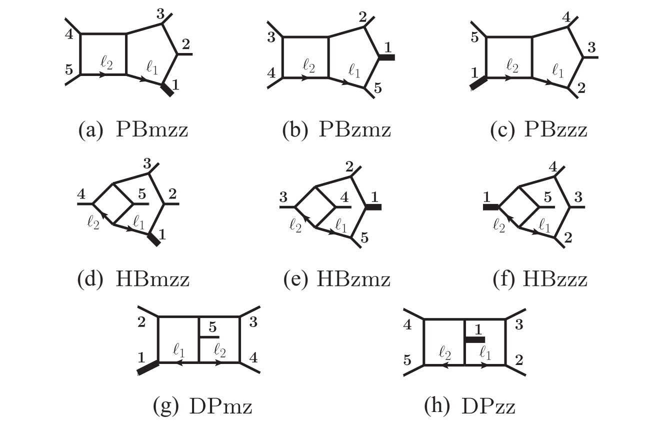


FIG. 1. Two-loop five-point one-mass families. The thick external line denotes the massive external leg.

amplitudes [31,42–44] extend beyond the leading-color approximation. In formal studies of QFTs, they have already been central in bootstrapping results in $\mathcal{N}=4$ super Yang-Mills theory, leading to new conjectures [45,46]. Finally, all two-loop Feynman integrals for the production of a massive boson in association with two jets at hadron colliders are now readily available, removing a main bottleneck for these important processes in LHC physics for which more precise theoretical predictions are urgently needed. Indeed, it is now possible to go beyond the leading-color approximation for $W+2$-jet processes [31,43,47–49], and obtain two-loop results for crucial processes such as $H+2$ jets that are intrinsically nonplanar.

Notations and conventions.—We define the momenta of external particles as p_i, $i=1,\ldots,5$, where $p_1^2\neq 0$ and $p_i^2=0$ for $i=2,\ldots,5$. For a fixed ordering of the massless legs, there are three planar pentabox (PB) families, three nonplanar hexabox (HB) families, and two nonplanar double-pentagon (DP) families that we depict in Fig. 1, as well as a factorizable planar topology. The factorizable, PB and HB families have already been studied in the literature [2,6,8–10]. Here, we define the DP families. Integrals in these families can generically be written as

$$I[\vec{\nu}]=e^{2\epsilon\gamma_{\mathrm{E}}}\int\frac{\mathrm{d}^D\ell_1}{\mathrm{i}\pi^{D/2}}\frac{\mathrm{d}^D\ell_2}{\mathrm{i}\pi^{D/2}}\frac{\rho_9^{-\nu_9}\rho_{10}^{-\nu_{10}}\rho_{11}^{-\nu_{11}}}{\rho_1^{\nu_1}\cdots\rho_8^{\nu_8}},\qquad(1)$$

where we set $D=4-2\epsilon$, and $\vec{\nu}$ is a vector of integers with the restriction that $\nu_9,\nu_{10},\nu_{11}\leq 0$. Explicit expressions for the ρ_i are given in ancillary files [50].

There are six independent variables $s_{ij}=(p_i+p_j)^2$, which we choose to be

$$\vec{s}=\{p_1^2,s_{12},s_{23},s_{34},s_{45},s_{15}\}.\qquad(2)$$

Together with the parity-odd object

$$\mathrm{tr}_5=4\mathrm{i}\varepsilon_{\alpha\beta\gamma\delta}p_1^\alpha p_2^\beta p_3^\gamma p_4^\delta,\qquad(3)$$

they fully specify a point in the five-particle phase space. Singularities of Feynman integrals are located at zeroes of certain determinants; see, e.g., Refs. [51–55]. Three cases play a special role here: the three- and five-point Gram determinants

$$\begin{aligned}\Delta_3&=-\det G(p_1,p_2+p_3),\\ \Delta_5&=\det G(p_1,p_2,p_3,p_4),\end{aligned}\qquad(4)$$

where $G(q_1,\ldots,q_n)=2\{q_i\cdot q_j\}_{i,j\in\{1,\ldots,n\}}$, and the polynomial [9]

$$\begin{aligned}\Sigma_5=&(s_{12}s_{15}-s_{12}s_{23}-s_{15}s_{45}+s_{34}s_{45}+s_{23}s_{34})^2\\ &-4s_{23}s_{34}s_{45}(s_{34}-s_{12}-s_{15}).\end{aligned}\qquad(5)$$

While $\Delta_5=\mathrm{tr}_5^2$, relating tr_5 to $\sqrt{\Delta_5}$ precisely is a subtle issue. We adopt the convention of Ref. [9] to only use $\sqrt{\Delta_5}$ in the pure integrals' definitions.

Figure 1 shows a fixed ordering of the massless legs, but we consider the set of integrals closed under all permutations of these legs. While Δ_5 is invariant under these permutations, there are three different permutations of Δ_3, denoted $\Delta_3^{(k)}$, and six different permutations of Σ_5, denoted by $\Sigma_5^{(k)}$. Expressions for the $\Delta_3^{(k)}$, $\Sigma_5^{(k)}$, and Δ_5 are given in ancillary files [50].

Analytic differential equations.—We follow Refs. [3,4,6,9], where analytic DEs [14–18] in canonical form [19] are obtained from numerical samples. We focus on the DPmz and DPzz families, for which we obtain canonical DEs for the first time. Any integral in the DPmz (DPzz) family can be written as a linear combination of 142 (179) master integrals. The top sectors, with eight propagators and nine master integrals each, were previously unknown. All integration-by-parts reductions [56–58] are performed within FiniteFlow [59] (interfaced to LiteRed [60,61]), and checked with KIRA2.0 [62] and FIRE6 [63].

Let $\vec{g}_\tau$ denote a vector whose entries form a pure [13] basis of master integrals for a family of integrals τ. It satisfies a DE in canonical form [19]

$$\mathrm{d}\vec{g}_\tau=\epsilon\mathbf{M}\cdot\vec{g}_\tau,\qquad\mathbf{M}=\sum_i\mathbf{M}_i\mathrm{d}\log W_i,\qquad(6)$$

where the W_i are the letters of the (symbol) alphabet [33] associated with $\vec{g}_\tau$. While the W_i are algebraic functions of $\vec{s}$, the matrices $\mathbf{M}_i$ are matrices of rational numbers. Finding a pure basis is still the most challenging aspect in obtaining DEs in canonical form. We construct educated guesses for pure bases following the ideas of Refs. [4–6,9], and test candidate bases by evaluating their derivatives at numerical points and verifying the factorization of ϵ. Once a pure basis is found, we proceed as in Sec. 4 of Ref. [6] to determine that the alphabet for the DPmz and DPzz families is contained within the one obtained in Ref. [9]. DPmz and DPzz have 62 and 74 letters, respectively. As in Ref. [6], we fit the matrices $\mathbf{M}_i$ from numerical evaluations on a finite field. Our results for the pure bases, the alphabet (closed under all permutations of the massless legs), and the analytic DEs can be found in ancillary files [50]. Some pure integrals were simplified with ideas from Ref. [64].

Construction of one-mass pentagon functions.—The *(one-mass) pentagon functions* are a basis of special functions to express all one- and two-loop five-point integrals with an external massive leg, up to the order in ϵ required to compute two-loop corrections. The one-loop and planar two-loop integrals have been previously considered in Ref. [32]. Here, we discuss a novel approach, suitable for the nonplanar families, that overcomes bottlenecks of previous strategies.

We start by considering the ϵ expansion of the master integrals for each family τ in Fig. 1. To cover all integrals relevant for an amplitude, we consider all 4! permutations σ of the massless momenta, denoting the corresponding master integrals by $\vec{g}_{\tau,\sigma}$. We normalize the $\vec{g}_{\tau,\sigma}$ so that they have the expansion

$$\vec{g}_{\tau,\sigma}(\vec{s}) = \sum_{w\geq 0} \epsilon^w \vec{g}^{(w)}_{\tau,\sigma}(\vec{s}). \tag{7}$$

We obtain the DEs for all $\vec{g}_{\tau,\sigma}$ by permuting those in the standard ordering, and use them to write the $\vec{g}^{(w)}_{\tau,\sigma}(\vec{s})$ as $\mathbb{Q}$-linear combinations of Chen iterated integrals [28],

$$[W_{i_1}, \ldots, W_{i_w}]_{\vec{s}_0}(\vec{s}) = \int_\gamma [W_{i_1}, \ldots, W_{i_{w-1}}]_{\vec{s}_0} \mathrm{d}\log W_{i_w}, \tag{8}$$

and boundary values at a point $\vec{s}_0$, $\vec{g}^{(w)}_{\tau,\sigma}(\vec{s}_0)$. The path γ connects $\vec{s}_0$ and $\vec{s}$, and the iteration starts with $[]_{\vec{s}_0} = 1$. The number of integrations w is called the transcendental weight. Up to two loops, it suffices to restrict our focus to $w \leq 4$. We choose [32]

$$\vec{s}_0 = (1, 3, 2, -2, 7, -2), \tag{9}$$

which is in the physical s_{45} channel: particles 4 and 5 are in the initial state, and the remaining particles are in the final state. The $\vec{g}^{(0)}_{\tau,\sigma}(\vec{s}_0)$ are rational numbers and are determined by the first-entry condition [65] up to an overall normalization. For $w \geq 1$, we compute the $\vec{g}^{(w)}_{\tau,\sigma}(\vec{s}_0)$ with 60-digit precision using AMFlow [66], interfaced to FiniteFlow [59] and LiteRed [60,61].

The structure of the iterated integrals in Eq. (8) is very well understood [28]: integrals involving different letters are linearly independent, and products of integrals are controlled by a shuffle algebra. This enables an algorithmic construction of a minimal set of functions in which to express the $\vec{g}^{(w)}_{\tau,\sigma}(\vec{s})$: the one-mass pentagon functions. To construct this minimal set, we follow the procedure in Refs. [7,32]. We begin by considering the $\vec{g}^{(w)}_{\tau,\sigma}(\vec{s})$ at symbol level [33] and select a minimal set of the $\vec{g}^{(w)}_{\tau,\sigma}(\vec{s})$ from the symbol-level solutions, starting at weight 1 and proceeding iteratively up to weight 4. To this end, we consider the set of coefficients $\vec{g}^{(w)}_{\tau,\sigma}(\vec{s})$ for all τ and σ, as well as all weight-w products of lower-weight functions, and select a subset of linearly independent elements, preferring products of lower-weight pentagon functions. This minimizes the number of "irreducible functions": functions that cannot be expressed in terms of products of lower-weight functions. In this way, at each weight we construct a set of algebraically independent $\vec{g}^{(w)}_{\tau,\sigma}(\vec{s})$, which we call the pentagon functions and denote by $\{f^{(w)}_i\}$. We find 11 irreducible functions of weight 1, 35 of weight 2, 217 of weight 3, and 1028 of weight 4. The total number is substantially lower than 2304, the number of independent master integrals.

We now turn to expressing the $\vec{g}^{(w)}_{\tau,\sigma}(\vec{s})$ in terms of pentagon functions. The approach that we use bypasses the determination of the relations between the boundary values $\vec{g}^{(w)}_{\tau,\sigma}(\vec{s}_0)$, a bottleneck of previous approaches. To this end, we make the following ansatz: we assume that the $\vec{g}^{(w)}_{\tau,\sigma}$ are graded polynomials in the pentagon functions and two transcendental constants, ζ_2 and ζ_3, over the field of rational numbers. Let us consider a weight-2 coefficient $g^{(2)}_{\tau,\sigma}$ as an example. Our ansatz is

$$g^{(2)}_{\tau,\sigma} = \sum_i a^i_{\tau,\sigma} f^{(2)}_i + \sum_{i,j} a^{i,j}_{\tau,\sigma} f^{(1)}_i f^{(1)}_j + \tilde{a}_{\tau,\sigma}\zeta_2. \tag{10}$$

We determine the rational numbers $a^i_{\tau,\sigma}$ and $a^{i,j}_{\tau,\sigma}$ from symbol-level manipulations, and the $\tilde{a}_{\tau,\sigma}$ by numerically evaluating the coefficients on both sides of the equation at $\vec{s}_0$. In this way, we explicitly write all $\vec{g}^{(w)}_{\tau,\sigma}(\vec{s})$ in terms of ζ values and a minimal set of pentagon functions, for which we have an iterated-integral representation and a boundary condition valid to 60 digits.

We emphasize that the ansatz of Eq. (10) implies nontrivial polynomial relations among the $\vec{g}^{(w)}_{\tau,\sigma}(\vec{s}_0)$. Previous approaches [7,31,32] to determine these relations required PSLQ [67] studies of high-precision numerical evaluations [$\mathcal{O}(3000)$ digits] that were obtained from MPL expressions [8]. Bypassing the need for high-precision evaluations, which are not available for nonplanar topologies, is therefore a substantial improvement.

To validate our results, we checked that they agree with those of Refs. [6,32] for the factorizable and PB families. For HB families, we compared our results with evaluations from DiffExp [68] starting at the boundary values of Ref. [9]. We find numerical agreement with the results of Ref. [10]

for the HBmzz family but were unable to evaluate their results for HBzzz and HBzmz. For the two DP families, we started from an evaluation of the pentagon functions, and used DiffExp to verify that the integrals are regular at all Euclidean spurious singularities. We further checked selected permutations of the DP integrals against AMFlow at random phase-space points.

Numerical evaluation and analytic structure.—The algorithm given above leaves freedom in the definition of pentagon functions. We leverage it to build a basis of functions that can be evaluated in an efficient and stable way, and is informed by the singularities that are expected in physical quantities. Nonplanar families bring considerable new challenges, highlighted below.

The general approach to the evaluation of pentagon functions follows Refs. [7,30,32,69]. We focus on the phase-space region corresponding to the s_{45} channel defined below Eq. (9), which is sufficient for hadron-collider processes (other $2 \to 3$ channels are obtained through appropriate permutations [32]). We construct the path γ in Eq. (8) so that it never leaves the s_{45} channel, following the algorithm of Ref. [32]. Up to weight 2, we obtain expressions in terms of logarithms and dilogarithms [70] with no logarithmic branch points within the s_{45} channel. At weights 3 and 4 we construct one-fold integral representations [69] and perform the integration numerically. We refer to Ref. [32] for a thorough discussion, and highlight here novel cases where the one-fold integral representation has a singularity at some point on γ.

We exemplify our approach with weight-3 pentagon functions, but generalization to weight 4 is straightforward. The one-fold integral representations of the pentagon functions are combinations of terms of the form

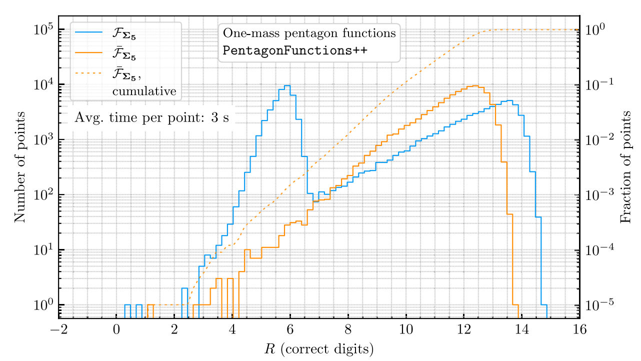
$$I(h, W) = \int_\gamma h(t)\partial_t \log(W[t])\mathrm{d}t. \qquad (11)$$

For simplicity, we parametrize γ in terms of t so that $\partial_t \log(W[t])$ diverges at $t = 0$ (if it does diverge on γ). To construct a numerically stable algorithm for evaluating the pentagon functions, we consider the analytic structure of Eq. (11) in detail. In many instances the singularity at $t = 0$ cancels in the sum of the contributions of the form of Eq. (11). We arrange these cancellations analytically as in Refs. [7,32], and such pentagon functions are infinitely differentiable in the physical region. The novel behavior in this work is a feature of five-point one-mass nonplanar pentagon functions, related to $\Sigma_5^{(i)} = 0$ surfaces. All cases are summarized in Table I, and can be organized in terms of the local behavior of h and W. In all cases the integrands diverge. For cases a and b, the singularity is integrable. In case a, $W = \Sigma_5^{(i\neq 3)}$; in case b, $\mathrm{d}\log W$ is odd with respect to $\sqrt{\Sigma_5^{(3)}}$ and, as h_0 is known, we handle the integrable singularity with an analytic subtraction. In case c, $W = \Sigma_5^{(3)}$ and the integral has a logarithmic singularity. We introduce a subtraction term and analytically integrate the $1/t$ singularity, resulting in a numerical integration over the remaining integrable singularity. We discuss the analytic continuation across $\Sigma_5^{(3)} = 0$ in the Appendix. The distinguished role played by $\Sigma_5^{(3)}$ is a consequence of working in the s_{45} channel.

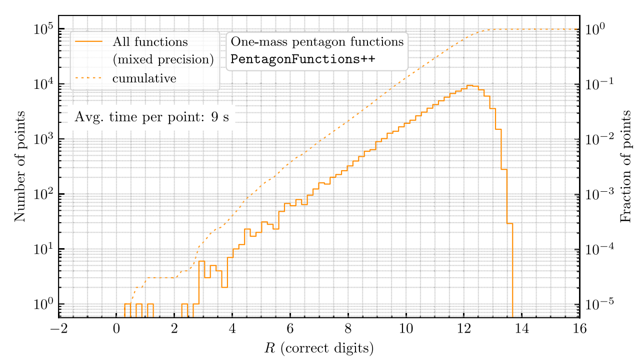
TABLE I. Nondifferentiable integral functions due to divergent integrands in Eq. (11) at singularity of $\partial_t \log(W[t])$, which cause discontinuities (right column).

Case	$\partial_t \log(W[t])$	$h(t)$	Continuous
a	$(\omega_1/t) + \mathcal{O}(t^0)$	$h_{1/2}\sqrt{t} + \mathcal{O}(t)$	✓
b	$(\omega_{1/2}/\sqrt{t}) + \mathcal{O}(t^0)$	$h_0 + \mathcal{O}(\sqrt{t})$	✓
c	$(\omega_1/t) + \mathcal{O}(t^0)$	$h_0 + \mathcal{O}(\sqrt{t})$	✗

Integrable singularities in Eq. (11) complicate the application of the numerical algorithms of Refs. [7,32]. Since all problematic cases have $W = \Sigma_5^{(i)}$, we dub the subset of pentagon functions with this behavior as $\mathcal{F}_{\Sigma_5}$. Integrating over the integrable singularities in cases a and c



(a) Functions $\mathcal{F}_{\mathbf{\Sigma_5}}$ shown in blue and $\bar{\mathcal{F}}_{\mathbf{\Sigma_5}}$ in orange. Dashed line represents the latter's cumulative distribution.



(b) All one-mass pentagon functions. The functions $\mathcal{F}_{\mathbf{\Sigma_5}}$ are evaluated in higher precision when the numerical integration path crosses the $\Sigma_5 = 0$ surface.

FIG. 2. Distribution of correct digits compared to quadruple-precision evaluations over 100 000 points.

demands higher intermediate precision, at the cost of performance. This motivates the construction of the pentagon functions so that the set $\mathcal{F}_{\boldsymbol{\Sigma}_5}$ is as small as possible, which also isolates the logarithmic singularity at $\Sigma_5^{(3)} = 0$ (case c) in as few functions as possible. More generally, we can organize the construction of the pentagon functions to make analytic properties manifest. For instance, a conjecture about the absence of the letter Δ_5 in the properly defined finite remainders of scattering amplitudes has been put forward for the massless case (see [71–73] for possible explanations), and we thus isolate the Δ_5 dependence in as few functions as possible.

The numerical evaluation of the one-mass pentagon functions is available through the C++ library PentagonFunctions++ [29]. To assess its numerical performance, we evaluate all functions on a sample of 10^5 points as in Ref. [32]. We present the distributions of correct digits with standard intermediate precision for the functions in $\mathcal{F}_{\boldsymbol{\Sigma}_5}$ [blue line in Fig. 2(a)] and the ones that do not involve the letters $\Sigma_5^{(i)}$ [orange line in Fig. 2(a)], denoted $\bar{\mathcal{F}}_{\boldsymbol{\Sigma}_5}$. The blue peak at six digits in Fig. 2(a) is generated by phase-space points that use integration paths that intersect the surfaces $\Sigma_5^{(i)} = 0$. As expected, it is absent for the orange line as well as in Fig. 2(b), where higher intermediate precision is employed to rescue the cases contributing to the blue peak mentioned above. Given the evaluation times of a few seconds per point and the overall good numerical stability, our results are suitable for immediate phenomenological applications.

Discussion and outlook.—We complete the calculation of all two-loop five-point integrals with massless propagators and a single massive external leg. Our results allow us to study their analytic structure, and to efficiently evaluate them numerically through weight 4, as needed for current phenomenological applications. The numerical evaluation is readily available as a C++ library [29].

The new algorithm we present for constructing pentagon functions provides a substantial improvement over previous ones, only relying on the knowledge of pure bases and the evaluation of the functions at a single point to moderate precision [12,66]. This robust algorithm will certainly find applications in other classes of integrals.

Our results open the door to further explorations of the analytic structure of this class of integrals, for instance along the direction of Refs. [53–55]. An undoubtedly important question to explore in more detail is the presence of logarithmic singularities within the physical region associated with the letter $\Sigma_5^{(i)}$ for some master integrals. Furthermore, our results can be used in the very active area of bootstrapping in $\mathcal{N} = 4$ super Yang-Mills (see, e.g., Refs. [45,46,74–76]). Finally, they will be central to the calculation of the next-to-next-to-leading-order corrections to processes such as the production of a massive boson in association with two jets at hadron colliders, as well as the ongoing N^{3}LO calculations [77,78] of processes involving a massive external particle and three massless ones.

D. C., V. S., and S. Z. gratefully acknowledge the computing resources provided by the Max Planck Institute for Physics. We thank Nikolaos Syrrakos for communications regarding the results of Ref. [10], and Andrew McLeod and Sebastian Mizera for discussions related to the singularities at $\Sigma_5 = 0$. This project received funding from the European Union's Horizon 2020 research and innovation programme "High precision multi-jet dynamics at the LHC" (Grant Agreement No. 772099). V. S. has received funding from the European Research Council (ERC) under the European Union's Horizon 2020 research and innovation programme Grant Agreement No. 101019620 (ERC Advanced Grant TOPUP). The work of B. P. was supported by the European Union's Horizon 2020 research and innovation program under the Marie Sklodowska-Curie Grant Agreement No. 896690 (LoopAnsatz). D. C. is supported by the French National Research Agency in the framework of the *Investissements d'avenir* program (ANR-15-IDEX-02).

Appendix: Analytic continuation across $\Sigma_5^{(3)} = 0$ surface.—The analytic continuation of Feynman integrals across singularities that do not correspond to normal thresholds is known to be a subtle issue. In this appendix, we discuss how it was addressed in constructing the pentagon functions defined in this Letter. More precisely, we focus on the $\Sigma_5^{(3)} = 0$ surface, which, as noted in the main text, introduces a logarithmic singularity in the physical region corresponding to the s_{45} channel. Other similar polynomials, such as $\Delta_3^{(i)}$ and Δ_5, have a well-defined sign within this region and so do not lead to singularities [32].

Let us start by commenting on a problem that is related to all square roots that appear in our alphabet, that is with both $\Sigma_5^{(i)}$ as well as $\Delta_3^{(i)}$ and Δ_5. There are several letters involving the square root of these polynomials. These square roots are introduced as normalizations of otherwise rational integrands and, in practice, we must choose a branch for them. This choice is spurious by construction, and should be made consistently in the definition of the pentagon functions and in the definition of the pure basis of integrals. Therefore, without loss of generality, we choose the standard principal square root branch, i.e., square roots are either real positive or have a positive imaginary part. This choice dictates how we evaluate the logarithms of algebraic letters in the one-fold integral representations. We verified that these logarithms are continuous along the integration path and cannot pick up any monodromy contributions. As expected, the dependence on this prescription cancels out in all quantities that are even under square-root sign changes, such as scattering amplitudes.

Let us now return to the main issue that we wish to clarify in this appendix, namely how to handle integrals that diverge on $\Sigma_5^{(3)} = 0$ surfaces (case c of Table I). We start from the iterated integral representation of the pentagon functions and manipulate them so that all divergent terms are explicitly written in terms of $\log \Sigma_5^{(3)}$ [79]. We must then have a prescription to analytically continue such terms through the $\Sigma_5^{(3)} = 0$ surface. We define the logarithm as

$$\log \Sigma_5^{(3)} = \log\left|\Sigma_5^{(3)}\right| + i\pi\Theta\left(-\Sigma_5^{(3)}\right), \tag{A1}$$

where Θ is the Heaviside step function, which is consistent with our definition of square roots discussed above. We proved that this prescription is uniquely fixed by assigning small positive imaginary parts to all Mandelstam invariants. More precisely, we verified that $\Sigma_5^{(3)}$ receives a small positive imaginary for an arbitrary path approaching the $\Sigma_5^{(3)} = 0$ surface within the s_{45} channel. The nontrivial part of the proof involves showing that all derivatives of $\Sigma_5^{(3)}$ evaluated at $\Sigma_5^{(3)} = 0$ are positive in the s_{45} channel. The details of this proof are rather lengthy so we do not reproduce them here.

Equation (A1) completely determines the analytic continuation of the integrals and the pentagon functions through the $\Sigma_5^{(3)} = 0$ surface. It is, however, instructive to present further evidence for the correctness of this procedure. We focus on the simplest integral family that contains integrals that are singular at $\Sigma_5^{(3)} = 0$, namely HBzmz in the permutation $(3 \to 4, 4 \to 5, 5 \to 3)$ of the external legs (see Fig. 1). First, we use AMFlow to evaluate the master integrals at several points on a path approaching the $\Sigma_5^{(3)} = 0$ surface within the s_{45} channel. We observe numerically the onset of the divergence, and that the evaluation of the pentagon functions is in agreement and stable also near the singularity. We further evaluate the master integrals at points on the other side of the $\Sigma_5^{(3)} = 0$ surface with respect to the base point $\vec{s}_0$ in Eq. (9), confirming the validity of our prescription in Eq. (A1). Second, we use DiffExp [68] to solve the differential equations along a specially constructed set of paths, which are illustrated by Fig. 3. Starting from P_+, where $\Sigma_5^{(3)} > 0$, we evolve the master integrals along a path segment P_+E_+ into the Euclidean region without crossing the $\Sigma_5^{(3)} = 0$ surface. We then cross the surface along a path segment E_+E_-, while staying within the Euclidean region where $\Sigma_5^{(3)} = 0$ does not lead to singularities, which guarantees that no analytic continuation through this surface is required. Finally, we return to the physical region via a path segment E_-P_-, along which $\Sigma_5^{(3)} < 0$. As noted in [9], this allows one to circumvent the singular surface, showing that the result of continuing across it is uniquely defined. We then confirmed that the evaluations of the pentagon functions at the points P_+ and P_- agree with the results from DiffExp.

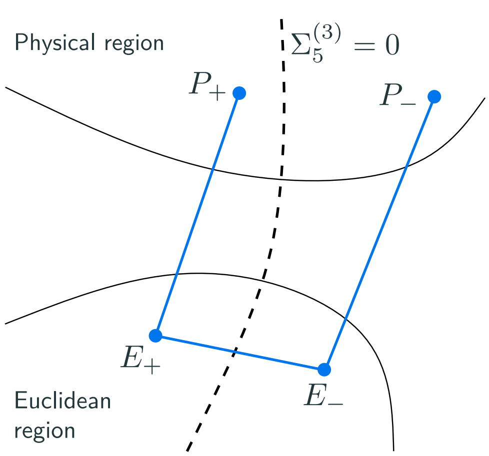


FIG. 3. A path that connects phase-space points with opposite $\Sigma_5^{(3)}$ signs without encountering the singularity at the $\Sigma_5^{(3)} = 0$ surface.

[1] T. Gehrmann, J. M. Henn, and N. A. Lo Presti, Phys. Rev. Lett. **116**, 062001 (2016); **116**, 189903(E) (2016).

[2] C. G. Papadopoulos, D. Tommasini, and C. Wever, J. High Energy Phys. 04 (2016) 078.

[3] S. Abreu, B. Page, and M. Zeng, J. High Energy Phys. 01 (2019) 006.

[4] S. Abreu, L. J. Dixon, E. Herrmann, B. Page, and M. Zeng, Phys. Rev. Lett. **122**, 121603 (2019).

[5] D. Chicherin, T. Gehrmann, J. M. Henn, P. Wasser, Y. Zhang, and S. Zoia, Phys. Rev. Lett. **123**, 041603 (2019).

[6] S. Abreu, H. Ita, F. Moriello, B. Page, W. Tschernow, and M. Zeng, J. High Energy Phys. 11 (2020) 117.

[7] D. Chicherin and V. Sotnikov, J. High Energy Phys. 12 (2020) 167.

[8] D. D. Canko, C. G. Papadopoulos, and N. Syrrakos, J. High Energy Phys. 01 (2021) 199.

[9] S. Abreu, H. Ita, B. Page, and W. Tschernow, J. High Energy Phys. 03 (2022) 182.

[10] A. Kardos, C. G. Papadopoulos, A. V. Smirnov, N. Syrrakos, and C. Wever, J. High Energy Phys. 05 (2022) 033.

[11] S. Badger, M. Becchetti, E. Chaubey, and R. Marzucca, J. High Energy Phys. 01 (2023) 156.

[12] M. Hidding and J. Usovitsch, Phys. Rev. D **108**, 036024 (2023).

[13] N. Arkani-Hamed, J. L. Bourjaily, F. Cachazo, and J. Trnka, J. High Energy Phys. 06 (2012) 125.

[14] A. V. Kotikov, Phys. Lett. B **254**, 158 (1991).

[15] A. V. Kotikov, Phys. Lett. B **267**, 123 (1991); **295**, 409(E) (1992).

[16] Z. Bern, L. J. Dixon, and D. A. Kosower, Nucl. Phys. **B412**, 751 (1994).

[17] E. Remiddi, Nuovo Cimento Soc. Ital. Fis. A **110**, 1435 (1997).
[18] T. Gehrmann and E. Remiddi, Nucl. Phys. **B580**, 485 (2000).
[19] J. M. Henn, Phys. Rev. Lett. **110**, 251601 (2013).
[20] C. Dlapa, J. Henn, and K. Yan, J. High Energy Phys. 05 (2020) 025.
[21] J. Henn, B. Mistlberger, V. A. Smirnov, and P. Wasser, J. High Energy Phys. 04 (2020) 167.
[22] C. Dlapa, J. M. Henn, and F. J. Wagner, J. High Energy Phys. 08 (2023) 120.
[23] L. Görges, C. Nega, L. Tancredi, and F. J. Wagner, J. High Energy Phys. 07 (2023) 206.
[24] C. Dlapa, X. Li, and Y. Zhang, J. High Energy Phys. 07 (2021) 227.
[25] J. Chen, X. Jiang, C. Ma, X. Xu, and L. L. Yang, J. High Energy Phys. 07 (2022) 066.
[26] A. von Manteuffel and R. M. Schabinger, Phys. Lett. B **744**, 101 (2015).
[27] T. Peraro, J. High Energy Phys. 12 (2016) 030.
[28] K.-T. Chen, Bull. Am. Math. Soc. **83**, 831 (1977).
[29] https://gitlab.com/pentagon-functions/PentagonFunctions-cpp.
[30] T. Gehrmann, J. M. Henn, and N. A. Lo Presti, J. High Energy Phys. 10 (2018) 103.
[31] S. Badger, H. B. Hartanto, and S. Zoia, Phys. Rev. Lett. **127**, 012001 (2021).
[32] D. Chicherin, V. Sotnikov, and S. Zoia, J. High Energy Phys. 01 (2022) 096.
[33] A. B. Goncharov, M. Spradlin, C. Vergu, and A. Volovich, Phys. Rev. Lett. **105**, 151605 (2010).
[34] C. Duhr and F. Brown, *Proc. Sci.*, MA2019 (2022) 005 [arXiv:2006.09413].
[35] O. Steinmann, Doctoral thesis, ETH Zürich, Zürich, 1960.
[36] O. Steinmann, Helv. Phys. Acta **33**, 347 (1960).
[37] K. E. Cahill and H. P. Stapp, Ann. Phys. (N.Y.) **90**, 438 (1975).
[38] S. Caron-Huot, L. J. Dixon, A. McLeod, and M. von Hippel, Phys. Rev. Lett. **117**, 241601 (2016).
[39] L. J. Dixon, J. Drummond, T. Harrington, A. J. McLeod, G. Papathanasiou, and M. Spradlin, J. High Energy Phys. 02 (2017) 137.
[40] S. Caron-Huot, L. J. Dixon, M. von Hippel, A. J. McLeod, and G. Papathanasiou, J. High Energy Phys. 07 (2018) 170.
[41] H. S. Hannesdottir, A. J. McLeod, M. D. Schwartz, and C. Vergu, J. High Energy Phys. 07 (2023) 236.
[42] S. Badger, H. B. Hartanto, J. Kryś, and S. Zoia, J. High Energy Phys. 11 (2021) 012.
[43] S. Abreu, F. Febres Cordero, H. Ita, M. Klinkert, B. Page, and V. Sotnikov, J. High Energy Phys. 04 (2022) 042.
[44] S. Badger, H. B. Hartanto, J. Kryś, and S. Zoia, J. High Energy Phys. 05 (2022) 035.
[45] L. J. Dixon, O. Gurdogan, A. J. McLeod, and M. Wilhelm, Phys. Rev. Lett. **128**, 111602 (2022).
[46] L. J. Dixon, O. Gürdoğan, Y.-T. Liu, A. J. McLeod, and M. Wilhelm, Phys. Rev. Lett. **130**, 111601 (2023).
[47] H. B. Hartanto, R. Poncelet, A. Popescu, and S. Zoia, Phys. Rev. D **106**, 074016 (2022).
[48] H. B. Hartanto, R. Poncelet, A. Popescu, and S. Zoia, arXiv:2209.03280.
[49] L. Buonocore, S. Devoto, S. Kallweit, J. Mazzitelli, L. Rottoli, and C. Savoini, Phys. Rev. D **107**, 074032 (2023).
[50] S. Abreu, D. Chicherin, H. Ita, B. Page, V. Sotnikov, and S. Zoia, Supplementary material for "All Two-Loop Feynman Integrals for Five-Point One-Mass Scattering", 10.5281/zenodo.8082811 (2023).
[51] S. Abreu, R. Britto, C. Duhr, and E. Gardi, J. High Energy Phys. 06 (2017) 114.
[52] N. Arkani-Hamed and E. Y. Yuan, arXiv:1712.09991.
[53] H. S. Hannesdottir, A. J. McLeod, M. D. Schwartz, and C. Vergu, Phys. Rev. D **105**, L061701 (2022).
[54] H. S. Hannesdottir and S. Mizera, arXiv:2204.02988.
[55] J. L. Bourjaily, C. Vergu, and M. von Hippel, Phys. Rev. D **108**, 085021 (2023).
[56] F. V. Tkachov, Phys. Lett. **100B**, 65 (1981).
[57] K. G. Chetyrkin and F. V. Tkachov, Nucl. Phys. **B192**, 159 (1981).
[58] S. Laporta, Int. J. Mod. Phys. A **15**, 5087 (2000).
[59] T. Peraro, J. High Energy Phys. 07 (2019) 031.
[60] R. N. Lee, arXiv:1212.2685.
[61] R. N. Lee, J. Phys. Conf. Ser. **523**, 012059 (2014).
[62] J. Klappert, F. Lange, P. Maierhöfer, and J. Usovitsch, Comput. Phys. Commun. **266**, 108024 (2021).
[63] A. V. Smirnov and F. S. Chuharev, Comput. Phys. Commun. **247**, 106877 (2020).
[64] J. L. Bourjaily, C. Langer, and Y. Zhang, J. High Energy Phys. 08 (2022) 176.
[65] D. Gaiotto, J. Maldacena, A. Sever, and P. Vieira, J. High Energy Phys. 12 (2011) 011.
[66] X. Liu and Y.-Q. Ma, Comput. Phys. Commun. **283**, 108565 (2023).
[67] H. R. P. Ferguson and D. H. Bailey, RNR Technical Report No. RNR-91-032, 1992.
[68] M. Hidding, Comput. Phys. Commun. **269**, 108125 (2021).
[69] S. Caron-Huot and J. M. Henn, J. High Energy Phys. 06 (2014) 114.
[70] C. Duhr, H. Gangl, and J. R. Rhodes, J. High Energy Phys. 10 (2012) 075.
[71] D. Chicherin, J. M. Henn, and G. Papathanasiou, Phys. Rev. Lett. **126**, 091603 (2021).
[72] S. He, J. Liu, Y. Tang, and Q. Yang, Sci. China Phys. Mech. Astron. **67**, 231011 (2024).
[73] L. Bossinger, J. M. Drummond, and R. Glew, J. High Energy Phys. 11 (2023) 002.
[74] Y. Guo, L. Wang, and G. Yang, Phys. Rev. Lett. **127**, 151602 (2021).
[75] Y. Guo, L. Wang, and G. Yang, arXiv:2209.06816.
[76] T. Gopalka and E. Herrmann, arXiv:2306.13640.
[77] D. D. Canko and N. Syrrakos, J. High Energy Phys. 04 (2022) 134.
[78] J. M. Henn, J. Lim, and W. J. Torres Bobadilla, J. High Energy Phys. 05 (2023) 026.
[79] S. Abreu, D. Chicherin, H. Ita, B. Page, V. Sotnikov, W. Tschernow, and S. Zoia (to be published).