

Analytic computation of three-loop five-point Feynman integrals

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We evaluate the three-loop five-point pentagon-box-box massless integral family in the dimensional regularization scheme, via canonical differential equation. We use tools from computational algebraic geometry to enable the necessary integral reductions. The boundary values of the differential equation are determined analytically in the Euclidean region. To express the final result, we introduce a new representation of weight six functions in terms of one-fold integrals over the product of weight-three functions with weight-two kernels that are derived from the differential equation. Our work paves the way to the analytic computation of three-loop multileg Feynman integrals.

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I. INTRODUCTION

High-precision predictions for scattering amplitudes are essential for data analysis at particle colliders. These predictions enable the exploration of fundamental questions, including the structure of the Standard Model and the search for new physics. The High-Luminosity Large Hadron Collider (HL-LHC) upgrade [1], along with upcoming colliders such as the Future Circular Collider (FCC) [2], International Linear Collider (ILC) [3], and Circular Electron Positron Collider (CEPC) [4], will achieve unprecedented experimental precision. This progress drives the need for advancements in theoretical methods.

To meet the demands of this accuracy, multiloop perturbative computations are crucial for refining theoretical predictions [5–9]. At the LHC energy scales, the strong coupling constant, α_s , is the largest of the Standard Model

coupling constants but remains small enough for perturbative calculations. Its uncertainty significantly affects the precision of theoretical predictions for cross sections. Jet production observables, such as the ratio of two- to three-jet cross sections, provide key opportunities to measure α_s with high precision. These measurements not only refine collider predictions but also enhance our understanding of potential new physics. Higher-order corrections in α_s for complex processes require more precise multiloop evaluations, a task which becomes challenging with increasing loop orders and external legs.

One of the challenging parts of a multiloop perturbative computation is the calculation of the appearing Feynman integrals. Significant progress has been made in this direction, with innovative techniques developed, such as differential equations [10–12], sector decomposition [13], auxiliary mass flow [14,15], difference equation [16], etc. In particular, many multiloop Feynman integrals with four, five, and even six external legs, important for phenomenology and theory, were calculated analytically [17–33]. The analytic expressions, when coded in public packages, make the phenomenology computation highly efficient. Analytic results of Feynman integrals also provide the basis for theoretical studies in perturbative quantum field theory.

Despite significant advances, the analytic computation of multiloop, multileg Feynman integrals in the dimensional regularization (DR) scheme remains a major challenge. Notably, in the literature, no analytic solutions exist for three-loop five-point integral families in DR. Furthermore,

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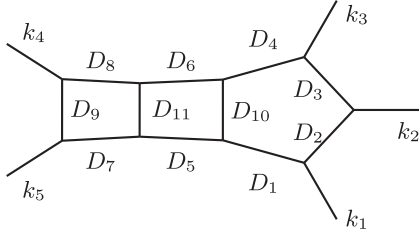


FIG. 1. Pentagon-box-box Feynman integral.

for three-loop integrals with more than four external legs, even existing numerical methods struggle to provide efficient results.

In this paper, we present the first analytic evaluation of a three-loop five-point Feynman integral family shown in Fig. 1. The solutions to the canonical differential equation (CDE) are expressed in terms of classical polylogarithms up to weight three, while the higher weight parts, up to weight six, are expressed as one-fold integrals.

A major difficulty is the complexity of integration-by-parts (IBP) reduction. For typical three-loop integrals with more than four external legs, standard reduction tools [34,35] encounter great difficulties. We overcome this by using computational algebraic geometry-based IBP methods and the NeatIBP package [36], enabling the reduction of three-loop five-point integrals.

Another significant challenge is to find an integral basis with uniform transcendental (UT) weights. We apply the latest leading singularity analysis [26,37], the INITIAL algorithm [38] and d log integrand construction [39] to get a UT basis and thus the canonical differential equation.

In order to get the weight-six solution to the differential equation, we introduce a novel iterated integral representation. The solutions at weights four to six are all expressed as one-fold integrations over products of classical polylogarithms. Our solutions agree with standard numerical program pySecDec [13,40,41] for all integrals, and with AMFLow [14,15] for the integrals calculable in the current version of AMFLow.

Our approach marks a significant advancement in the analytic computation of three-loop multileg Feynman integrals. We expect our result to play a crucial role in next-to-next-to-next-to-leading order (N³LO) cross section computations for processes like three-jet production, three-photon production, jet-two-photon production, and the high-precision determination of α_s . The result is also important for theoretical studies.

This paper is organized as follows: In Sec. II, we introduce the definition of the integral family. Section III explains how computational algebraic geometry methods enable the integral reduction. In Sec. IV, we construct the UT basis, which is then used in Sec. V to achieve the CDE. In Sec. VI, we express the integrals via simple functions at lower weight, which we supplement with the boundary values in Sec. VII. In Sec. VIII, a new representation of

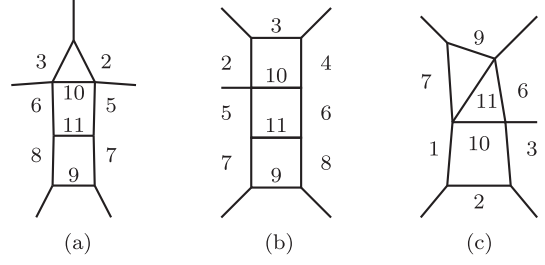


FIG. 2. Typical subfamily for PBB. (a) Rocket. (b) Five-point ladder. (c) Box-triangle-triangle.

iterative integrals is used to express the higher weight integrals. Finally, Sec. IX provides concluding remarks and an outlook for future work.

II. FAMILY DEFINITION

The three-loop five-point integral family considered in this article is the so-called pentagon-box-box (PBB) shown in Fig. 1, while some subfamilies are shown in Fig. 2. All integrals from the family take the form

$$I_{\nu_1, \dots, \nu_{18}}(\mathcal{N}) = e^{3\epsilon\gamma_E} \int \prod_{j=1}^3 \frac{d^{4-2\epsilon} \ell_j}{(i\pi)^{2-\epsilon}} \frac{\mathcal{N}(\ell, k)}{\prod_{k=1}^{18} D_k^{\nu_k}} \quad (1)$$

where ϵ is the dimensional regulator, γ_E is the Euler-Mascheroni constant, ν_k are the propagator powers and $\mathcal{N}$ is a kinematic numerator. The inverse propagators are defined as follows:

$$\begin{aligned} D_1 &= \ell_1^2, & D_2 &= (\ell_1 - k_1)^2, \\ D_3 &= (\ell_1 - k_1 - k_2)^2, & D_4 &= (\ell_1 - k_1 - k_2 - k_3)^2, \\ D_5 &= \ell_2^2, & D_6 &= (\ell_2 - k_1 - k_2 - k_3)^2, \\ D_7 &= \ell_3^2, & D_8 &= (\ell_3 - k_1 - k_2 - k_3)^2, \\ D_9 &= (\ell_3 + k_5)^2, & D_{10} &= (\ell_1 - \ell_2)^2, \\ D_{11} &= (\ell_2 - \ell_3)^2, & D_{12} &= (\ell_1 + k_5)^2, \\ D_{13} &= (\ell_2 - k_1)^2, & D_{14} &= (\ell_2 - k_1 - k_2)^2, \\ D_{15} &= (\ell_2 + k_5)^2, & D_{16} &= (\ell_3 - k_1)^2, \\ D_{17} &= (\ell_3 - k_1 - k_2)^2, & D_{18} &= (\ell_1 - \ell_3)^2, \end{aligned}$$

where $\{D_i | 12 \leq i \leq 18\}$ serve as irreducible scalar products ($\nu_i < 0, i = 12, \dots, 18$) and k_j are the external momenta of the scattering process.

We use standard kinematic variables, $s_{12}, s_{23}, s_{34}, s_{45}, s_{15}$, where $s_{ij} = 2k_i \cdot k_j$, and the parity-odd invariant

$$\epsilon_5 = 4i\epsilon_{\mu\nu\rho\sigma} k_1^\mu k_2^\nu k_3^\rho k_4^\sigma, \quad (2)$$

which is related to the Gram determinant as: $\epsilon_5^2 = G(p_1, p_2, p_3, p_4)$.

III. USING COMPUTATIONAL ALGEBRAIC GEOMETRY FOR IBP REDUCTION

IBP reductions are currently a crucial step in constructing a differential equation for an integral family. However, their computational complexity poses a bottleneck for most cutting-edge calculations both in terms of memory and computation time. To facilitate the computation of the PBB family, we thus turn to computational algebraic geometry methods [42–49] and the public code NeatIBP [36]. NeatIBP leverages computational algebraic geometry techniques, such as syzygy methods, to impose additional constraints on IBP identities. By utilizing the module intersection approach, these constraints are systematically combined, effectively preventing the increase of propagator indices and gets a much shorter IBP linear system than that from the traditional IBP identities [50].

On a laptop, NeatIBP finds about 85000 IBP identities in full kinematics dependence within several hours. These relations are sufficient to derive the differential equation. As a comparison, standard IBP tools would generate three orders of magnitude more IBP relations, which make the reduction computation impossible.

The PBB family as shown in Fig. 1 consists of 316 master integrals, while details for some subfamilies are shown in Table I.

We use the packages Rational Tracer [51] and FiniteFlow [52] to solve the IBP system from NeatIBP over finite fields. Once the UT basis and alphabet are determined, the canonical differential equation can be reconstructed from the alphabet.

IV. UT INTEGRAL DETERMINATION

In this section, we use several computational techniques to complete the UT basis for a family of 316 master integrals. Here is the basic strategy we took to search for the UT integrals:

- (i) Classify the master integrals by the number of-shell external legs resulting from pinching propagators. Among the 168 topologies of the PBB family, 14 correspond to two-point, 44 to three-point, 80 to four-point and 30 to genuine five-point topologies.
- (ii) The two- and three-point UT topologies are quite straightforward. Moreover, from the works on three-loop four-point Feynman integrals with one off-shell

leg [27,28,53], we can find UT integrals for the four-point topologies.

- (iii) For the genuine five-point topologies with bubbles, we first integrate out the dotted bubble loop [54] to get an effective two loop integral, and then look for the well-studied two-loop five-point UT integrals [17,55]. For the remaining five-point topologies, we use Dlogbasis [39] algorithm to search for dlog integrals. However, after this step, there are still some missing UT integrals.
- (iv) Those missing UT integrals are found case by case. One can make use of the INITIAL algorithm, the Magnus series [56,57], and some empirical rules to get the cut DE matrix, which refers to the differential equation matrix derived under a specific cut (i.e., ignoring certain sectors of the Feynman integrals), in an ε -factorized form. If the off-diagonal parts are linear in ε , the $\mathcal{O}(\varepsilon^0)$ term can often be eliminated by subtracting tail integrals from lower sectors [58–60].

To define the integrals in the novel genuine five-point sectors, we provide numerator factors that feature in (1).

Pentagon-box-box (Fig. 1): There are five UT integrals in the PBB sector given by

$$\mathcal{N}_1 = s_{12}s_{23}s_{45}^2 D_{12}, \quad (3)$$

$$\mathcal{N}_2 = s_{12}s_{23}s_{45}^2 D_{15} - s_{23}s_{45}^2 D_1 - s_{12}s_{45}^2 D_4, \quad (4)$$

$$\mathcal{N}_3 = \frac{s_{45}^2}{\varepsilon_5} G(\ell_1, k_1, k_2, k_3, k_4), \quad (5)$$

$$\mathcal{N}_4 = \frac{s_{45}^2}{\varepsilon_5} G\left(\begin{matrix} \ell_1, k_1, k_2, k_3, k_4 \\ \ell_2, k_1, k_2, k_3, k_4 \end{matrix}\right), \quad (6)$$

$$\mathcal{N}_5 = \frac{s_{45}^2}{\varepsilon_5} G\left(\begin{matrix} \ell_1, k_1, k_2, k_3, k_4 \\ \ell_3, k_1, k_2, k_3, k_4 \end{matrix}\right), \quad (7)$$

where G denotes the Gram determinant. Note that for the integral (4), we need to introduce a correction from a lower sector to make it a UT integral.

Five-point ladder [Fig. 2(b)]: There are six UT integrals given by

$$\mathcal{N}_1 = s_{23}s_{34}s_{45}^2, \quad (8)$$

$$\mathcal{N}_2 = s_{23}s_{45}^2 D_{12}, \quad (9)$$

$$\mathcal{N}_3 = s_{23}s_{45}^2 D_{14}, \quad (10)$$

$$\mathcal{N}_4 = s_{23}s_{45}(s_{45} - s_{12})D_{15}, \quad (11)$$

$$\mathcal{N}_5 = \frac{s_{45}}{\varepsilon_5} G\left(\begin{matrix} \ell_1, k_1, k_2, k_3, k_4 \\ \ell_2, k_1, k_2, k_3, k_4 \end{matrix}\right), \quad (12)$$

TABLE I. Typical number of master integrals.

Family	Master integrals	Own sector
The PBB	316	5
The rocket	80	6
Five-point ladder	175	6
Box-triangle-triangle	49	8

$$\mathcal{N}_6 = \frac{s_{45}}{\epsilon_5} G\left(\ell_1, k_1, k_2, k_3, k_4\right). \quad (13)$$

The rocket [Fig. 2(a)]: Out of the six UT integrals in this sector, only five are constructed by Dlogbasis . The last one can be found as follows. First, we observe that the DE matrix on cut is linear to ϵ , so the $\mathcal{O}(\epsilon^0)$ -term can be eliminated via Magnus series. After that, we turn to the full DE matrix and eliminate the $\mathcal{O}(\epsilon^0)$ -term by adding tail integrals.

Box-triangle-triangle [Fig. 2(c)]: We need eight UT integrals in this sector, while Dlogbasis returns only three candidates. If we double some propagators on triangle [61] and manually adjust an ansatz, it is not difficult to get the cut DE matrix in ϵ -form. After that, the off diagonal parts $\mathcal{O}(\epsilon^0)$ -terms can be eliminated by adding tail integrals.

The full UT basis for the PPB family can be found in the auxiliary file `Canonical_Basis.m`, see the Appendix.

V. DIFFERENTIAL EQUATION AND SYMBOL ALPHABET

The pentagon alphabet has been extensively studied at two-loop order [62], and it was suggested that additional letters would appear at three-loop order [63]. However, for the PBB family, the 31 pentagon letters listed in Ref. [62] are sufficient. Specifically, for the PBB family, only the planar pentagon letters $\mathbb{A}_p$ appear, while the nonplanar letters W_{20+i} , ($1 \leq i \leq 5$) are absent. The relevant letters are defined as follows:

$$\begin{aligned} W_i &= s_{i,i+1}, & W_{5+i} &= s_{i+2,i+3} + s_{i+3,i+4} \\ W_{10+i} &= s_{i,i+1} - s_{i+3,i+4}, \\ W_{15+i} &= s_{i,i+1} + s_{i+1,i+2} - s_{i+3,i+4}, \\ W_{25+i} &= \frac{a_{i,i+1,i+2,i+3} - \epsilon_5}{a_{i,i+1,i+2,i+3} + \epsilon_5}, & W_{31} &= \epsilon_5, \end{aligned}$$

where $a_{1,2,3,4} = s_{12}s_{23} - s_{23}s_{34} + s_{34}s_{45} - s_{12}s_{15} - s_{45}s_{15}$ and the index $i = 1, \dots, 5$. The corresponding CDE can be decomposed as

$$d\mathbf{I} = \epsilon d\tilde{\mathbf{A}}\mathbf{I}, \quad d\tilde{\mathbf{A}} = \sum_{i=1}^{31} a_i d\log W_i, \quad (14)$$

where W_i are algebraic functions of the kinematic variables and the a_i are $\mathbb{Q}$ -valued constant 316×316 matrices.

The knowledge of the CDE allows us to derive an ϵ -expansion for any integral in the family

$$\mathbf{I} = \sum_{j=-6}^0 \epsilon^j \mathbf{I}^{(j+6)} + \mathcal{O}(\epsilon), \quad (15)$$

where the coefficients $\mathbf{I}^{(n)}$ are referred to as the weight- n part of the solution. In this paper, we are interested in the

functions up to weight six that are relevant for applications to three-loop scattering processes. Together with the weight-zero boundary value discussed in the succeeding section, one can also calculate the symbol solution up to weight-six, which we provided in the Appendix.

VI. PENTAGON FUNCTIONS

Instead of solving the CDE directly, it is constructive to express the integrals in terms of a minimal set of transcendental functions. At five points, they are referred to as pentagon functions. They have been extensively studied at two-loop order [19–25, 62, 64, 65].

For the PBB family, the weight-one and weight-two functions are simply

$$\log(-W_i), \quad \text{Li}_2 \frac{W_{10+i}}{W_i}, \quad 1 \leq i \leq 5. \quad (16)$$

These functions are well defined in the full Euclidean region $s_{i,1+(i)_5} < 0$, ($1 \leq i \leq 5$). They are exactly the same as the functions that appear in the two-loop pentagon box integrals [65].

At weight-three, the structure of the functions becomes more intricate. To express the integrals, logarithms with additional arguments are needed,

$$\log(-W_{15+i}), \quad 1 \leq i \leq 5, \quad (17)$$

as well as Li_2 and Li_3 functions with the following arguments

$$\begin{aligned} &\text{Li}_n\left(-\frac{W_{11+(1+i)_5}}{W_i}\right), \quad \text{Li}_n\left(\frac{W_{11+(2+i)_5}}{W_i}\right), \\ &\text{Li}_n\left(-\frac{W_{11+(3+i)_5}}{W_i}\right), \quad \text{Li}_n\left(-\frac{W_{11+(2+i)_5}}{W_{16+(4+i)_5}}\right), \\ &\text{Li}_n\left(\frac{W_{11+(4+i)_5}}{W_{16+(4+i)_5}}\right), \quad \text{Li}_n\left(-\frac{W_{11+(2+i)_5} W_{11+(4+i)_5}}{W_i W_{1+(1+i)_5}}\right), \\ &\text{Li}_n\left(-\frac{W_{11+(1+i)_5} W_{11+(4+i)_5}}{W_i W_{16+(1+i)_5}}\right), \quad 1 \leq i \leq 5, n \in \{2, 3\}. \end{aligned} \quad (18)$$

We use a subscript-5 notation, $(x)_5 \equiv \text{mod}(x, 5)$, to denote that the pentagon functions in Euclidean region form a group with S_5 cyclic permutation symmetry. To obtain such functions, we used the algorithm implemented in [66] to construct parity-even arguments for the Li_n function, then integrals can be fitted onto these pentagon functions by numerically fitting the integrand after taking the derivative.

The space formed by these functions is large enough to describe the entire family at weight-three except for one parity-odd integral, which is discussed in the following subsection.

A. Matching the parity-odd weight-three symbol

In the Euclidean region, the square root ϵ_5 first appears at weight three. Initially, several integrals seem to involve parity-odd components at this weight. However, the choice of a UT basis for an integral family is not unique. It is possible to introduce $\mathbb{Q}$ -linear combinations for these UT integrals. Therefore, the parity-odd components at weight three share one single parity-odd function, which we denote as $\mathcal{P}(s_{12}, s_{23}, s_{34}, s_{45}, s_{15})$.

However, even with this simplification, performing the integration remains challenging. Naive rationalization of the square root leads to a cumbersome expression with a complex branch cut structure, making it difficult to manipulate.

The function $\mathcal{P}$ was found to coincide with those of the one-loop pentagon at weight-three, which was written as a one-fold integration or MPL functions [67–69]. To derive explicit function representation for more efficient numerical evaluation, recall that only classical polylogarithms are involved at weight-three, and their symbol structure indicates that we shall search for $\text{Li}_n(x)$ such that both x and $1-x$ factorize over the symbol alphabet [70–72]. This approach motivates a search for solutions over $\mathbb{Q}$ for the coefficients q_i that satisfy

$$\text{dlog}(1-x) = \sum_{i=1}^{31} q_i \text{dlog} W_i, \quad \text{dlog}(x) = \sum_{i=1}^{31} q_i \text{dlog} W_i. \quad (19)$$

We use a heuristic algorithm to find all the necessary arguments to match the symbol $\text{SB}(\mathcal{P})$. First, we perform the integration with rationalized square root via PolyLogTools [73] and express the function $\mathcal{P}$ as multiple polylogarithms (MPLs). Next, we reduce the MPLs in terms of classical polylogarithms [74,75] and extract the arguments which respect the condition (19). We eventually reach identities like

$$\begin{aligned} & 2\text{dlog}\left(\frac{W_2 W_3 (W_{28} - 1)}{W_{31} W_{28}}\right) \\ &= -\text{dlog} W_1 + \text{dlog} W_2 + \text{dlog} W_3 - \text{dlog} W_{19} - \text{dlog} W_{28}, \\ & 2\text{dlog}\left(1 - \frac{W_2 W_3 (W_{28} - 1)}{W_{31} W_{28}}\right) \\ &= -\text{dlog} W_1 + \text{dlog} W_4 \\ &\quad - \text{dlog} W_{19} + \text{dlog} W_{20} - \text{dlog} W_{28} - \text{dlog} W_{29}. \end{aligned} \quad (20)$$

With these arguments and the determined even part, we can find a function $\tilde{\mathcal{P}}$

$$\begin{aligned} \tilde{\mathcal{P}} = & \dots + 2\text{Li}_3\left(\frac{W_2 W_3 (W_{28} - 1)}{W_{31} W_{28}}\right) \\ & + 2\text{Li}_3\left(\frac{\frac{2W_{28}W_{31}}{W_{28}-1} - 2W_2(W_1 + W_5)}{\frac{2W_{27}W_{31}}{W_{27}-1} - 2W_1(W_2 + W_3)}\right) + \dots \\ & - 2\text{Li}_2\left(\frac{W_{14}(W_1 W_2 - \frac{W_{27}W_{31}}{W_{27}-1})}{W_1 W_2 W_{19}}\right) \log(-W_1) + \dots, \end{aligned} \quad (21)$$

such that $\text{SB}(\tilde{\mathcal{P}}) = \text{SB}(\mathcal{P})$. Note that although there are only 40 terms in $\text{SB}(\mathcal{P})$, more than 2800 weight-three functions have to be combined in order to fit the $\text{SB}(\mathcal{P})$. Also, we have to restrict the computation to a smaller region, where the arguments have definitive signs. To define $\tilde{\mathcal{P}}$ in other regions, one has to construct a basis for such a region or perform analytic continuation [76].

We determine $\tilde{\mathcal{P}}$ by introducing 10 additional log arguments, namely $\log W_i$, with $\{11 \leq i \leq 15\} \cup \{16 \leq i \leq 20\}$, as well as 14 new arguments for Li_2 , and 23 arguments for Li_3 . Furthermore, the “beyond-the-symbol” term $\mathcal{P} - \tilde{\mathcal{P}}$ can be determined up to the boundary constant by differentiating a basis of $\pi^2 \log$ functions, and subsequently performing a numerical fit to the integrand of CDE.

Finally, following these steps, we reach the function representation for the odd integral $\mathcal{P}$

$$\begin{aligned} \mathcal{P} = & \underbrace{\tilde{\mathcal{P}}}_{526 \text{ terms}} - \frac{\pi^2}{6} (\log(-W_1) - 2 \log(-W_2) + \log(-W_3) \\ & + 3 \log(-W_4) - 2 \log(-W_{16}) - \log(-W_{20}) \\ & + \log(-W_{26}) + \log(-W_{27}) + \log(-W_{28}) \\ & + 2 \log(-W_{29}) - \log(-W_{30})) + \zeta_3. \end{aligned} \quad (22)$$

The constant ζ_3 is found by the method described in the following section. At this point, we have already expressed all pentagon functions and thus all integrals in PBB family, up to weight-three, in terms of classical polylogarithms.

VII. BOUNDARY VALUES

While the basis should remain regular throughout the Euclidean region, this is not necessarily the case for the differential equation matrices. As a result, certain spurious poles can appear. The boundary values of the differential equation can be determined from the cancellation of spurious poles [65,77,78]. To illustrate this idea, we adopt the following integral representation:

$$\mathbf{I}^{(n)}(x) = \underbrace{\mathbf{I}^{(n)}(x_0)}_{\text{Boundary Values}} + \underbrace{\int_{x_0}^x d\tilde{A} \cdot \mathbf{I}^{(n-1)}(x)}_{\text{Function Part}}. \quad (23)$$

We denote the position of the spurious poles as x_i . If we require that the weight- $(n+1)$ integral should be finite at

the spurious poles, then the integrand should vanish at these points

$$\text{Res}\left(\frac{d\tilde{A}}{dx}\right)\Big|_{x_i} \cdot \mathbf{I}^{(n)}(x_i) = 0. \quad (24)$$

We require that all integrals in the basis remain finite at the following locations of spurious poles: $x_0 = \{-1, -1, -1, -1, -1\}$, which is also chosen as the boundary point, $x_1 = \{-2, -1, -1, -1, -1\}$ along with its cyclic permutations, and $x_6 = \{1/4, -1, -1, -1, -1\}$, where ϵ_5 vanishes. With these conditions, one can formally express all boundary values, at all orders in ϵ , as a $\mathbb{Q}$ -combination of the transcendental functions that appear in the second term of (23) evaluated at these spurious poles, up to one trivial integral

$$I_1(x_0) = -1 + \frac{\pi^2}{4}\epsilon^2 + 7\zeta_3\epsilon^3 + \frac{37\pi^4}{480}\epsilon^4 + \left(\frac{93\zeta_5}{5} - \frac{7\pi^2\zeta_3}{4}\right)\epsilon^5 + \left(\frac{943\pi^6}{120960} - \frac{49\zeta_3^2}{2}\right)\epsilon^6 + O(\epsilon^7). \quad (25)$$

By performing line integrations from x_0 to other x_i along a path which rationalize the ϵ_5 [65], one can express the boundary values in terms of special values of MPLs. Intriguingly, together with the Li_3 representation for $\mathcal{P}$, we found that the corresponding boundary value, originally written in terms of hundreds of MPLs [65], can be analytically simplified to only four terms

$$\begin{aligned} \mathcal{P}(-1, -1, -1, -1, -1) \\ = -14\text{Li}_3(-\phi) - \frac{14}{3}\log^3\phi - \frac{46}{15}\pi^2\log\phi + \frac{7}{5}\zeta_3, \end{aligned} \quad (26)$$

where $\phi = (1 + \sqrt{5})/2$ is the golden ratio.

Employing the above strategy, we analytically compute the boundary values up to weight-six for the entire PBB family. The package NumPolyLog [79] and PSLQ algorithm have been used to numerically evaluate and simplify the boundary values.

VIII. AUXILIARY MATRIX FOR HIGHER WEIGHT INTEGRATION

With the analytic weight three solutions and the boundary constants at hand, we can turn toward the computation of the integrals up to weight six. However, beyond weight three, classical polylogarithms are no longer sufficient and the number and complexity of the functions grow significantly. For multiscale problems with square roots, obtaining higher weight expressions in terms of MPLs is still a highly nontrivial task. Moreover, such explicit MPL representations are not always good for efficient numerical evaluations. Therefore, it is more practical to express the

higher weight iterative integrals in terms of a one-fold integral representation [23,65,80,81].

Starting from the iterative representation of the solution of CDE

$$\mathbf{I}^{(n+1)}(x) = \mathbf{I}^{(n+1)}(x_0) + \int_0^1 \frac{d\tilde{A}(t)}{dt} \mathbf{I}^{(n)}(t) dt, \quad (27)$$

we can reach the one-fold integration formula, which is widely used at two-loop order to reach weight-four solution from weight-two functions

$$\begin{aligned} \mathbf{I}^{(n+2)}(x) = \mathbf{I}^{(n+2)}(x_0) + \int_0^1 \frac{d\tilde{A}(t)}{dt} \mathbf{I}^{(n+1)}(x_0) dt \\ + \int_0^1 (\tilde{A}(1) - \tilde{A}(t)) \frac{d\tilde{A}(t)}{dt} \mathbf{I}^{(n)}(t) dt. \end{aligned} \quad (28)$$

If we wanted to apply this technique to calculate the weight six part of the PBB family, we would require analytic knowledge of the weight-four functions. To circumvent this requirement, we introduce a novel formula to write higher weight parts as one-fold integrals. By defining a weight-two *auxiliary matrix* $\tilde{B}$ as the integration kernel, which satisfies a matrix differential equation

$$d\tilde{B} = (d\tilde{A})\tilde{A}, \quad (29)$$

one can decompose a weight- $(n+3)$ function into a one-fold integration,

$$\begin{aligned} \mathbf{I}^{(n+3)}(x) = \mathbf{I}^{(n+3)}(x_0) + \int_0^1 \frac{d\tilde{A}}{dt} \mathbf{I}^{(n+2)}(x_0) dt \\ + \int_0^1 (\tilde{A}(1) - \tilde{A}(t)) \frac{d\tilde{A}}{dt} \mathbf{I}^{(n+1)}(x_0) dt \\ + \int_0^1 (\tilde{A}(t) - \tilde{A}(1)) \tilde{A}(t) \frac{d\tilde{A}}{dt} \mathbf{I}^{(n)}(t) dt \\ + \int_0^1 (\tilde{B}(1) - \tilde{B}(t)) \frac{d\tilde{A}}{dt} \mathbf{I}^{(n)}(t) dt. \end{aligned} \quad (30)$$

This formula can be derived by using the Eqs. (27) and (28) and changing the integration order. $\tilde{B}$ is guaranteed to exist because of the integrability condition

$$d((d\tilde{A})\tilde{A}) = -\frac{1}{2}[A_i, A_j]dx^i \wedge dx^j = 0, \quad (31)$$

from the property of canonical differential equation. Note that the matrix $\tilde{A}$ and $\tilde{B}$ are not unique, the former is up to a constant matrix, and the latter is up to a matrix of logarithmic functions. This is consistent due to the fact that only their difference will contribute to Eq. (30).

In our case, we use this formula with $n = 3$ to express the weight-six part in terms of one fold integration. Based

on the same symbol matching techniques as in Sec. VI A, it is straightforward to express the $\tilde{B}$ -kernel in terms of $\log^2$ and Li_2 . The explicit $\tilde{B}$ -matrix is provided in the auxiliary files, see Appendix.

Similarly, one can further change the integration order and introduce more auxiliary matrix, for example one can express the weight-six part as a one-fold integration over the weight-two integrals and a new weight-three auxiliary matrix $\tilde{C}$ defined as $d\tilde{C} = (d\tilde{A})\tilde{B}$. The $\tilde{C}$ matrix can be used as the kernel of one-fold integration to calculate the weight- n part from analytic expressions of weight- $(n-4)$ integrals. However, we do not adopt this approach in this work, as the expression for $\tilde{C}$ has a higher transcendental weight and involves more algebraically dependent arguments, making it more intricate.

IX. CONCLUSION AND OUTLOOK

In this paper, we initiate the analytic computation of three-loop five-point Feynman integrals in dimensional regularization. The pentagon-box-box integral family is calculated up to weight six via the canonical differential equation method. Powered by a novel iterated integral formula, we achieve the explicit function representation up to weight three and the one-fold integration representation up to weight six in the Euclidean region, with only $\log$, Li_2 and Li_3 functions. The boundary values for this integral family up to weight six are analytically expressed as special values of MPLs. A proof-of-concept implementation of one-fold integration is provided to calculate this integral family with high efficiency, see Appendix.

Our results initiate the computation of the Feynman integrals for massless $2 \rightarrow 3$ processes at $N^3\text{LO}$, and thereby open a new level of precision for collider phenomenology. With the developments in the IBP reduction and iterative integrals, we expect the full computation of all planar three-loop five-point integrals to finish in the near future.

We anticipate that the methods and the results we have presented will have numerous applications, for example to 3-jet and 3-photon production, and to the precision determination of the strong coupling constant. Our work, together with the recent computation of two-loop six-point Feynman integrals [30,31], will serve as an important ingredient in the massless $2 \rightarrow 3$ $N^3\text{LO}$ computations.

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DATA AVAILABILITY

The data that support the findings of this article are openly available [82], embargo periods may apply.

APPENDIX

In this appendix, we first briefly introduce some of the auxiliary files mentioned in this paper. Then we show how to validate our computation by the numerical cross check.

- (i) `Canonical_Basis.m`, the UT basis for the PBB family.
- (ii) `Atilde.m`, the CDE matrix $\tilde{A}$ defined in Eq. (14).
- (iii) `Weight-<i>-Integrals.m`, analytic functions for the UT integrals from weight-one to weight-three.
- (iv) `Weight-<i>-Symbol.tar.xz`, compress file for the symbol of the UT integrals.
- (v) `Boundary-Values-Analytics.m`, analytic boundary values from weight-one to weight-six.
- (vi) `Btilde.m`, the $\tilde{B}$ kernel matrix define in Eq. (29).
- (vii) `Evaluate-All-Integrals.wl`, a proof-of-concept implementation of the one-fold integration to numerically evaluate the UT integrals.

These auxiliary files can be accessed at [82].

For a generic point in the Euclidean region

$$\left\{ -\frac{79}{46}, -\frac{129}{29}, -\frac{89}{36}, -\frac{87}{55}, -\frac{51}{13} \right\} \quad (\text{A1})$$

TABLE II. Numerical cross check.

ϵ -order	pySecDec results	Analytic results
ϵ^0	$+1.1666667 \pm 3.80 \times 10^{-8}$	$+1.1666666$
ϵ^1	$-3.2652194 \pm 1.20 \times 10^{-6}$	-3.2652203
ϵ^2	$-3.2525854 \pm 9.30 \times 10^{-6}$	-3.2525818
ϵ^3	$-3.3833398 \pm 4.82 \times 10^{-5}$	-3.3833422
ϵ^4	$-37.8523289 \pm 1.96 \times 10^{-4}$	-37.8523988
ϵ^5	$-122.2098436 \pm 7.81 \times 10^{-4}$	-122.2104218
ϵ^6	$-71.5043735 \pm 6.72 \times 10^{-3}$	-71.5031577

our proof-of-concept implementation for one-fold integration is sufficient to produce the numeric results with 32 digits for all UT integrals in less than one hour with 30 cores. For comparison, it takes around 38 h for pySecDec

with four A100 GPUs to generate a result for a single UT integral (3) in the top sector with several digits, which is shown in Table II. Evaluating the full family with the current version of AMFLow is not yet feasible.

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