An Introduction to Integrals with Uniformally Transcendental Weights, Canonical Differential Equation, Symbols and Polylogarithms

Yang Zhang

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In both the phenomenological and formal studies of fundamental physics, the central research focus is on high-order perturbative corrections (loop expansion). The computation and analysis of Feynman integrals, especially the multiloop ones, is thus crucial in theoretical physics.

In this lecture, we study the *milestone* method for Feynman integral computation: canonical differential equation for Feynman integrals with uniformally transcendental (UT) weights [1]. It was invented by Henn in 2013, and soon led to a revolution in the field of Feynman integral computation. A lot of previously untouchable Feynman integrals were analytically computed in this way. UT method for loop amplitudes, is like the "Dreadnought" battleship (1906) in the naval history, which classified all previous battleships as "pre-Dreadnoughts".

The outline of this method is,

- The ϵ^{n} -order of UT Feynman integrals is the integration of (ϵ^{n-1}) -order of these integrals, and then the Feynman integrals are analytically expressed as *iterative integrals*.
- The mathematical properties of iterative integrals were studied long time ago, by the Mathematician Kuo-Tsai Chen.
- Specifically, many beautiful properties of iterative integrals can be captured by the so-called Symbol [2]., which was invented in the context of $\mathcal{N} = 4$ super-Yang-Mills theory.
- If the iterative integrals have certain simple integration kernels, the result would be *polylog-arithm* functions.

In practice, if order-by-order in ϵ , a Feynman integral is expressed as *polylogarithm* functions, we say that this Feynman integral is computed analytically.

In this lectures, we provides an introduction of UT integrals, canonical differential equation, symbols and polylogarithms. The main references are [3, 4].

I. UT INTEGRALS AND POLYLOGARITHMS

We begin with the simplest example massless bubble integral.

Example I.1. This is one of the simplest loop integrals. The propagators are

$$D_1 = l_1^2, \quad D_2 = (l_1 - p)^2.$$
 (1)

with $p^2 = s$. From the Symanzik polynomials, $U = z_1 + z_2$, $F = -sz_1z_2$, s < 0 is the Euclidean region, and s > 0 is the physical region. By a direction computation,

$$G[\alpha_1, \alpha_2] = \frac{(-1)^{\alpha_1 + \alpha_2} \Gamma\left(\frac{d}{2} - \alpha_1\right) \Gamma\left(\frac{d}{2} - \alpha_2\right) \Gamma\left(-\frac{d}{2} + \alpha_1 + \alpha_2\right) (-s)^{\frac{1}{2}(d-2(\alpha_1 + \alpha_2))}}{\Gamma\left(\alpha_1\right) \Gamma\left(\alpha_2\right) \Gamma\left(d - \alpha_1 - \alpha_2\right)} \,. \tag{2}$$

The apparently simplest integral in this sector is $(d = 4 - 2\epsilon)$,

$$I_{bub} \equiv e^{\epsilon\gamma} (-s)^{\epsilon} G[1,1] = \frac{1}{\epsilon} + 2 + \left(4 - \frac{\pi^2}{12}\right) \epsilon + \left(-\frac{7\zeta(3)}{3} + 8 - \frac{\pi^2}{6}\right) \epsilon^2 + \left(-\frac{14\zeta(3)}{3} + 16 - \frac{\pi^2}{3} - \frac{47\pi^4}{1440}\right) \epsilon^3 + O\left(\epsilon^4\right)$$
(3)

where γ is the Euler gamma constant. The Riemann Zeta function is defined as,

$$\zeta(z) \equiv \sum_{n=1}^{\infty} \frac{1}{n^z} \tag{4}$$

Since this is an one-scale integral, $(-s)^{\epsilon}$ factor removed the s dependence. $e^{\epsilon \gamma}$ removed Euler constants.

However, the "simplest" integral is not G[1,1] but the magic uniformly transcendental (UT) integral ([1]),

$$I_{bub}' \equiv e^{\epsilon\gamma}(-s)^{\epsilon} sG[1,2] = -\frac{1}{\epsilon} + \frac{\pi^2 \epsilon}{12} + \frac{7\zeta(3)\epsilon^2}{3} + \frac{47\pi^4 \epsilon^3}{1440} + O\left(\epsilon^4\right) \,. \tag{5}$$

This expression is much more concise than (I.1). If we define π to have the transcendental degree one, and ζ_n has the transcental degree n, then the ϵ^n order of this expression has the transcendental degree n + 1.

So why is I_{bub} complicated? The IBP relation between the two integrals is that

$$I_{bub} = \frac{1}{-1+2\epsilon} I'_{bub} \,. \tag{6}$$

The factor $1/(-1+2\epsilon)$ messed up the ϵ expansion. We say that I'_{bub} is an integral with uniform transcendental weights.

Here we have a feeling that UT integral has a simpler analytic expression, while the non-UT integral of the same sector tends to have a more complicated expression. For the analytic computation, we would like to aim at UT integrals. The formal definition of UT integrals is given by Henn [1]: First, the transcedental degree \mathcal{T} is defined as,

$$\mathcal{T}(\text{rational number}) = 0, \quad \mathcal{T}(\text{rational function}) = 0$$
$$\mathcal{T}(\pi) = 1, \quad \mathcal{T}(\zeta(n)) = n, \quad \mathcal{T}(\log x) = 1, \quad \mathcal{T}(\text{Li}_n(x)) = n$$
$$\mathcal{T}(H(a_1, \dots a_n; x)) = n, \quad \mathcal{T}(G(a_1, \dots a_n; x)) = n, \quad (7)$$

where $\operatorname{Li}_n(\ldots)$, $H(\{a_1, \ldots a_n\}, x)$ and $G(\{a_1, \ldots a_n\}, x)$ are the weight *n* classical, harmonic and Goncharov polylogarithm functions respectively:

• Classical polylogarithms

$$\operatorname{Li}_{1}(z) \equiv -\log(1-z), \quad \operatorname{Li}_{n}(z) \equiv \int_{0}^{z} \frac{dt}{t} \operatorname{Li}_{n-1}(t)$$
(8)

Note that Li_n has the branch cut from 1 to $+\infty$. When z < 1, $\operatorname{Li}_n(z)$ is real. This integral is convergent since $\operatorname{Li}_n(z) = 0$, $\forall n$. The pole 1/t does not provide a monodromy group around z = 0 again because $\operatorname{Li}_n(0) = 0$.

$$\frac{\partial}{\partial z} \operatorname{Li}_{n}(z) = \frac{1}{z} \operatorname{Li}_{n-1}(z) \tag{9}$$

• Harmonic polylogarithms (HPLs). We first define three rational functions,

$$f_{-1}(z) = \frac{1}{z+1}, \quad f_0(z) = \frac{1}{z}, \quad f_1(z) = \frac{1}{1-z}$$
 (10)

Then define,

$$H(-1;z) \equiv \int_{0}^{z} dt f_{-1}(t) = \log(1+z),$$

$$H(0;z) \equiv \log(z),$$

$$H(1;z) \equiv \int_{0}^{z} dt f_{1}(t) = -\log(1-z),$$
(11)

H(0, z)'s definition seems a bit strange, however, all of these functions satisfy $\partial_z H(a; z) = f_a(z), a = -1, 0, 1.$

Then we recursively define that

$$H(a_1, \dots, a_n; z) \equiv \int_0^z dt f_{a_1}(t) H(a_2, \dots, a_n; t)$$
(12)

with the special case when $a_1 = \ldots = a_n = 0$

$$H(\vec{0}_n; z) \equiv \frac{1}{n!} \log^n(z) \tag{13}$$

 (a_1, \ldots, a_n) is called the *weight vector* and $H(a_1, \ldots, a_n; z)$ has the weight n. They satisfy,

$$\partial_z H(a_1, \dots, a_n; z) = f_{a_1}(z) H(a_2, \dots, a_n; z) \tag{14}$$

It is easy to check that,

$$H(\vec{0}_{n-1}, 1; z) = \text{Li}_n(z) \tag{15}$$

Except for the case when $a_1 = \ldots = a_n = 0$,

$$H(a_1, \dots, a_n; 0) = 0 \tag{16}$$

All HPLs are real in the range $z \in (0, 1)$. Depending on the weight vector, it may have the branch cuts $(-\infty, 0)$, $(-\infty, -1)$, $(1, \infty)$ or a union of these.

HPLs are very useful common functions in the field of scattering amplitudes. With the weight $n \leq 3$, all HPLs can be converted to classical polylogarithms. But when n > 3, this property does not hold. Mathematica cannot deal with generic HPLs, however, these functions can be easily handled by the Mathematica package HPL [5].

• Goncharov polylogarithms (GPLs). These are more complicated functions than HPLs, and also common in scattering amplitudes, especially for complicated kinematics. Like HPLs,

$$G(a_1, \dots, a_n; z) \equiv \int_0^z dt \frac{1}{t - a_1} G(a_2, \dots, a_n; t)$$
(17)

with the exception

$$G(\vec{0}_n; z) = \frac{1}{n!} \log^n(z) \tag{18}$$

Different from the HPLs, here the weight vector $(a_1, \ldots a_n)$ can take arbitrary values. If $a_n \neq 0$, then by simple calculus,

$$G(\lambda \vec{a}_n; \lambda z) = G(\vec{a}_n; z) \tag{19}$$

The integration of rational functions to GPLs can be nicely treated with the Maple package HYPINT [6], while the numeric evaluation of GPLs can be done with the C package GINAC [7].

Note that as in any graded algebra, the element 0 can be associated with arbitrary transcedental weight.

Second, a function f with uniformal transcendental weight n is *pure*, if

$$\mathcal{T}(f) = n, \quad \mathcal{T}(\partial_x f) = n - 1$$
 (20)

for any kinematic variable x. For example, $\log^2(x)$ is UT and pure, while $x \log(1 - x)$ is UT but not pure. Nowadays, in the literature, by the abuse of notation, "UT" usually means UT and pure.

Third, a UT Feynman integral has the ϵ expansion:

$$I = \epsilon^k \sum_{i=0}^{\infty} I^{(n)} \epsilon^n \tag{21}$$

with

$$\mathcal{T}(I^{(n)}) = n \tag{22}$$

Again, usually we require that $I^{(n)}$ is pure also. Here k is an integer to make the series formally from the order ϵ^0 .

We comment that the Euler's gamma constant, γ 's transcendental weight is not defined. By multiplying an *L*-loop Feynman integral by $e^{\epsilon L \gamma}$, γ is cancelled out at all orders of ϵ .

II. CANONICAL DIFFERENTIAL EQUATION

Consider an integral basis \vec{J} of an integral family, we know that \vec{J} satisifies a first-order differential equation,

$$\partial_i \vec{J} = M_i(x,\epsilon) \vec{J},\tag{23}$$

where M_i is a $m \times m$ square matrix. Recall that under a basis transformation $\vec{J} \to T\vec{J}$, the DE matrix transform as a connection,

$$M_i \to T M_i T^{-1} + (\partial_i T) T^{-1} \,. \tag{24}$$

(23) is called a *canonical differential equation* if M_i is proportional to ϵ .

$$M_i(x,\epsilon) = \epsilon m_i(x) \tag{25}$$

A UT (and pure) integral basis

$$\vec{I} = \epsilon^k \sum_{n=0}^{\infty} \vec{I}^{(n)} \epsilon^n, \tag{26}$$

such that $\mathcal{T}(\vec{I}^{(n)}) = n$ and $\mathcal{T}(\partial \vec{I}^{(n)}) = n - 1$, must be associated with a canonical DE.

To see this, assume that $\partial_i \vec{I} = A_i(x,\epsilon)\vec{I}$ and

$$A_i(x,\epsilon) = \sum_{j=-\infty}^{0} \epsilon^j \bar{A}_i^{(j)}(x) + \epsilon A_i^{(1)}(x) + \sum_{j=2}^{\infty} \epsilon^j \bar{A}_i^{(j)}(x)$$
(27)

The differential equation for integral basis in the sense of Laporta can only have rational functions in the kinematic variables. Here to get a UT basis, we further request that the transformation from the Laporta basis to a UT basis can only have algebraic functions in the kinematic variables.

Compare the ϵ^n order of the differential equation: for the left hand side,

$$\mathcal{T}(\partial_i \vec{I}^{(n)}) = n - 1.$$
⁽²⁸⁾

for the right the only weight-(n-1) term is $A_i^{(1)}(x)\vec{I}^{(n-1)}$. Therefore,

$$\partial_i \vec{I}^{(n)} = A_i^{(1)}(x) \vec{I}^{(n-1)} \,. \tag{29}$$

Then sum over $n = 0, ... \infty$ and rename $A_i^{(1)}(x)$ as $A_i(x)$, we see that

$$\partial_i \vec{I} = \epsilon A_i(x) \vec{I} \,. \tag{30}$$

For a canonical DE, the proportionality in ϵ provides great advantages, since this differential equation can be solved perturbatively in ϵ .

• The integrability condition for the differential equation splits as,

$$\partial_j A_i = \partial_i A_j, \quad [A_i, A_j] = 0 \tag{31}$$

That means A_i s are total derivitives,

$$A_i = \partial_i \tilde{A} \tag{32}$$

So the canonical DE can be combined as the exterior differential form,

$$d\vec{I} = \epsilon(d\tilde{A}(x))\vec{I}.$$
(33)

where $d\tilde{A}(x)$ is an $m \times m$ matrix whose entires are one forms.

• $\tilde{A}(x)$ should have a further decomposition

$$\tilde{A}(x) = \sum_{l=1}^{N} a_l \log(W_l)$$
(34)

where each a_l is $m \times m$ is a constant matrix and W_l 's are rational or algebraic functions of the kinematic variables. W_l is called a *symbol letter* or simply *letter*. The set of all W_l is called the *alphabet*. As the name suggests, symbol letters are the building blocks of Feynman integrals, as we will see. • With the canonical DE, order-by-order in ϵ , we see the beautiful structure,

$$\partial_i \vec{I}^{(0)} = 0$$

$$\partial_i \vec{I}^{(1)} = A_i(x) \vec{I}^{(0)}$$

$$\partial_i \vec{I}^{(2)} = A_i(x) \vec{I}^{(1)}$$

$$\partial_i \vec{I}^{(3)} = A_i(x) \vec{I}^{(2)}$$

....
(35)

Hence I^n is simply the integration of $A_i(x)I^{(n-1)}$. From the structure of \tilde{A} , A_i should be "simple", so the iterative integration is likely to be done analytically and the UT Feynman integral can be calculated analytically to an arbitrary order of ϵ .

In particular, we see that the leading order $I^{(0)}$ is a constant vector. In practice, they are usually rational numbers.

• There are advantages to choose a UT basis for the IBP reduction. Let I_i 's be a UT basis and J an integral in the family,

$$J = \sum_{i} c_i(\bar{x}, \epsilon) I_i \tag{36}$$

If J is also a UT integral with the matched degree of transcendental weights, then $c_i(\bar{x}, \epsilon)$'s are *rational numbers*. This property is important since we can use it to "optimize" a UT basis. Do an IBP reduction of a large list of Feynman integrals to the UT basis, and if c_i 's are all rational numbers, then we find new UT integrals. Then we replace some of the I_i 's by simpler UT integrals to get a simpler basis.

For generic J's, the reduction coefficients also have nice features [8]. In particular, c_i ' corresponding to a UT basis can be dramatically simplified with a multivariate partial fraction.

However, there is still a doubt: if from the expression of Feynman integrals we know that they are UT, then we do not need to solve the canonical DE. The real power of canonical DE is that we can predict (guess) a UT integral basis, set up a canonical DE and then solve it. This is the content of the next section.

III. TO DETERMINE A UT BASIS, I

There are many ways to determine a UT basis. Roughly speaking, the ideas come from two directions: (1) hints from formal theory studies like $\mathcal{N} = 4$ Super-Yang-Mills theory and modern field theory methods like generalized unitarity; (2) the mathematical theory of differential equations. In practice, they are both useful.

A. Leading singularity analysis

For years in the study of the planar $\mathcal{N} = 4$ Super-Yang-Mills theory, people preferred "nice" Feynman integrals with *constant leading singularity*. The amplitudes in this theory can usually be expressed as,

$$\mathcal{A} = \sum (\text{color factor}) \times (\text{Parker-Taylor factor}) \\ \times (\text{integral with constant leading singularity})$$
(37)

After the invention of UT integrals and canonical differential equations, it was discovered that integrals with constant leading singularity are likely to be UT integrals.

Leading singularity can be calculated from 4D generalized unitarity analysis, i.e., setting the propagators on-shell and compute the residue [9, 10]. This computation is simple and provides valuable information for the UT integral searching.

Example III.1. Consider the one-loop massless box diagram with

$$D_1 = l_1^2, \quad D_2 = (l_1 - p_1)^2, \quad D_3 = (l_1 - p_1 - p_2)^2, \quad D_4 = (l_1 + p_4)^2$$
 (38)

with $p_i^2 = 0$, i = 1, 2, 3, 4. $(p_1 + p_2)^2 = s$, $(p_1 + p_4)^2 = t$ and $(p_2 + p_4)^2 = -s - t$. The master integrals in the Laporta sense are,

$$G[1,1,1,1], \quad G[1,0,1,0], \quad G[0,1,0,1]$$
(39)

The differential equation matrices are,

$$A'_{s} = \begin{pmatrix} -\frac{s+t\epsilon+t}{s(s+t)} & -\frac{2(2\epsilon-1)}{s^{2}(s+t)} & \frac{2(2\epsilon-1)}{st(s+t)} \\ 0 & -\frac{\epsilon}{s} & 0 \\ 0 & 0 & 0 \end{pmatrix}, \quad A'_{t} = \begin{pmatrix} -\frac{s\epsilon+s+t}{t(s+t)} & \frac{2(2\epsilon-1)}{st(s+t)} & -\frac{2(2\epsilon-1)}{t^{2}(s+t)} \\ 0 & 0 & 0 \\ 0 & 0 & -\frac{\epsilon}{t} \end{pmatrix}$$
(40)

• Sector (1,1,1,1). We first check the leading singularity of G[1,1,1,1] by the generalized unitarity cut. The cut equation

$$D_1 = D_2 = D_3 = D_4 = 0 \tag{41}$$

has two solutions at $l_1 = l^*$ and $l_1 = \overline{l^*}$. It is useful to apply spinor-helicity formalism to express the two solutions and compute the residue.

$$l_1 = a_1 p_1 + a_2 p_2 + a_3 \frac{\langle 43 \rangle}{\langle 13 \rangle} \lambda_1 \tilde{\lambda}_4 + a_4 \frac{\langle 13 \rangle}{\langle 43 \rangle} \lambda_4 \tilde{\lambda}_1 \,. \tag{42}$$

There are two maximal cut solutions at,

$$l^*: \quad a_1 = 0, \quad a_2 = 0, \quad a_3 = -1, \quad a_4 = 0$$

$$\bar{l}^*: \quad a_1 = 0, \quad a_2 = 0, \quad a_4 = 0, \quad a_4 = \frac{s}{s+t}$$
(43)

The multivariate residues are,

$$\pm \frac{1}{st} \tag{44}$$

Therefore we guess that stG[1, 1, 1, 1] is a UT integral.

• Sector (1,0,1,0). We try to compute the 4D leading singularity like the box. However, a short computation ends up with

$$\oint da_2 \oint da_3 \frac{1}{a_3} \tag{45}$$

There is no multivariate residue defined for a_2 and a_3 . It is difficult convert G[1, 0, 1, 0] to a UT integral by multiplying a function in s and t.

However, for the bubble diagram, or any kind of two-point Feynman integral, the trick is to consider 2D leading singularity. Consider the bubble integral with $d = 2 - 2\epsilon$. The 2D leading singularity computation is similar: we can parameterize $l_1^{[2D]}$ as,

$$l_1^{[2D]} = c_1(p_1 + p_2) + c_2 p^{\perp}$$
(46)

where p^{\perp} is a 2D vector such that $p^{\perp} \cdot (p_1 + p_2) = 0$. It is convenient to set $(p^{\perp})^2 = -s$. A two-fold computation provides that $G^{(2-2\epsilon)}[1,0,1,0]$ has the leading singularity,

$$\pm \frac{1}{s} \tag{47}$$

So we guess the $sG^{(2-2\epsilon)}[1,0,1,0]$ is a UT integral. By the dimension recursion relation,

$$sG^{(2-2\epsilon)}[1,0,1,0] = -2sG^{(4-2\epsilon)}[2,0,1,0] = 2(1-2\epsilon)G^{(4-2\epsilon)}[1,0,1,0]$$
(48)

So we guess that $(1 - 2\epsilon)G[1, 0, 1, 0]$ is a UT.

• Sector (0, 1, 0, 1). We guess that $(1 - 2\epsilon)G[0, 1, 0, 1]$ is a UT.

By using the three UT canidates stG[1,1,1,1], $(1-2\epsilon)G[1,0,1,0]$ and $(1-2\epsilon)G[0,1,0,1]$, unfortunately the new DE is still not proportional to ϵ . This is from the fact that each candidate is a UT but their transcedental weights do not match at the same ϵ order. It is easily fixed by considering,

$$stG[1,1,1,1], \quad \frac{1-2\epsilon}{\epsilon}G[1,0,1,0], \quad \frac{1-2\epsilon}{\epsilon}G[0,1,0,1]$$
 (49)

We can do some "cosmetic" work to get dimensionless UT integrals,

$$I_{1} = e^{\epsilon\gamma}(-s)^{\epsilon} stG[1,1,1,1], \quad I_{2} = e^{\epsilon\gamma}(-s)^{\epsilon} \frac{1-2\epsilon}{\epsilon} G[1,0,1,0], \quad I_{3} = e^{\epsilon\gamma}(-s)^{\epsilon} \frac{1-2\epsilon}{\epsilon} G[0,1,0,1].$$
(50)

Indeed the new DE is canonical. With $x \equiv t/s$,

$$A_x = \begin{pmatrix} -\frac{\epsilon}{x(x+1)} & -\frac{2\epsilon}{x+1} & \frac{2\epsilon}{x(x+1)} \\ 0 & 0 & 0 \\ 0 & 0 & -\frac{\epsilon}{x} \end{pmatrix}.$$
 (51)

It is a classical trick to double the propagator of bubble-type integrals to get UT integrals. However the new fashion is to consider reducible integrals to replace bubble-type integrals. In this example,

$$sG[1,0,1,1], \quad tG[0,1,1,1]$$
 (52)

are also UT integrals, based on the leading singularity computations.

Example III.2. Consider the two-loop massless box family with inversed propapators,

$$D_1 = l_1^2, \quad D_2 = (l_1 - p_1)^2, \quad D_3 = (l_1 - p_1 - p_2)^2, \quad D_4 = (l_2 + p_1 + p_2)^2$$
$$D_5 = (l_2 - p_4)^2, \quad D_6 = l_2^2, \quad D_7 = (l_1 + l_2)^2, \quad D_8 = (l_1 + p_4)^2, \quad D_9 = (l_2 + p_1)^2, \tag{53}$$

The last two are irreducible scalar products and we consider the sector (1, 1, 1, 1, 1, 1, 1, 0, 0) and all its subsector. By the standard IBP process (with the symmetry), there are 8 master integrals. We consider the UT searching sector-by-sector,

• Sector (1,1,1,1,1,1,0,0). There are two master integrals and we need to find two UT integrals.

Note that the two-loop 4D integration is 8-fold, while in this sector we only have 7 denominators. With the abuse of multivariate residue definition, we can pick up 7 integration variables first, and treat the rest one as a free variable "y". If for generic values of y,

$$D_1 = \dots = D_7 = 0 \tag{54}$$

has a solution, then we compute the 7-fold residue as a function of y. Then we continue to compute the residue in y. This kind of computation for G[1, 1, 1, 1, 1, 1, 1, 0, 0] provides values:

$$\frac{1}{s^2 t}, \quad -\frac{1}{s^2 t}, \quad 0,$$
 (55)

So the leading singularity of G[1, 1, 1, 1, 1, 1, 1, 0, 0] can be defined as $\frac{1}{s^2 t}$.

Note that in this step, we have to exhaust all possible way of computing the multivariate residues. Obviously this is a complicated procedure, and the complete treatment is given [10]. We comment that this multivariate residue computation is a typical algebraic geometry problem, and the leading singularity computation can be efficiently carried out with the so-called "primary decomposition" and "transformation law" [11].

We guess that $s^2 tG[1,1,1,1,1,1,0,0]$ is a UT integral. Similarly, $s^2 G[1,1,1,1,1,1,1,0,0]$ is also a UT integral candidate.

Alternatively, we can compute the leading singularity in a loop-by-loop fashion. The left loop is a massless box with external legs $p_1, p_2, -l_2 - p_1 - p_2, l_2$, which is the so-called "hard" two-mass box. The leading singularity of this box is

$$\frac{1}{s(l_2+p_1)^2} \tag{56}$$

For the right loop with the propagators l_2^2 , $(l_2 - p_4)^2$ and $(l_2 + p_1 + p_2)^2$. Note that from (56), we get a new box in l_2 . Taking the singularity again, we see that the leading singularity of G[1, 1, 1, 1, 1, 1, 1, 0, 0] is $1/(s^2t)$. This analysis is much easier than the full leading singularity analysis.

- Sector (0, 1, 0, 1, 1, 1, 1, 0, 0). This is a box-bubble diagram. We can perform a loop-by-loop analysis to compute the right box residue first, and get a bubble. For the one-loop bubble analysis, we know that it would be a UT if one of its propagator is doubled. Therefore we guess that stG[0, 2, 0, 1, 1, 1, 1, 0, 0]/ε is a UT.
- Sector (0, 1, 1, 0, 1, 1, 1, 0, 0). This is a slashed box diagram. This one is tricky. It is not easy to find the leading singularity from the 4D residue computation. It can be determined by other methods. The UT candidate is (s + t)G[0, 1, 1, 0, 1, 1, 1, 0, 0].
- Sector (0, 1, 0, 1, 0, 1, 1, 0, 0). This is a trianglar-bubble diagram. The analysis would be similar to the box-bubble diagram, and the UT candidate is sG[0, 2, 0, 1, 0, 1, 1, 0, 0]/ε.

- Sector (1, 0, 1, 1, 0, 1, 0, 0, 0). This is a factorized bubble-bubble diagram. From the one-loop result, we know that G[2,0,1,2,0,1,0,0,0]/ε² must be a UT integral.
- Sector (0, 0, 1, 0, 0, 1, 1, 0, 0) and (0, 1, 0, 0, 1, 0, 1, 0, 0). These are the sunset integrals. From the 2D leading singularity analysis, we see that sG[0,0,2,0,0,2,1,0,0]/ε² and tG[0,2,0,0,2,0,1,0,0]/ε² are UT candidates.

With some cosmetic work, the UT candidates are,

$$I_{1} = s^{2} e^{2\gamma\epsilon} G[1, 1, 1, 1, 1, 1, 1, -1, 0](-s)^{2\epsilon},$$

$$I_{2} = s^{3} x e^{2\gamma\epsilon} G[1, 1, 1, 1, 1, 1, 1, 0, 0](-s)^{2\epsilon},$$

$$I_{3} = s(x+1) e^{2\gamma\epsilon} G[0, 1, 1, 0, 1, 1, 1, 0, 0](-s)^{2\epsilon},$$

$$I_{4} = -\frac{s^{2} x e^{2\gamma\epsilon} G[0, 2, 0, 1, 1, 1, 1, 0, 0](-s)^{2\epsilon}}{\epsilon},$$

$$I_{5} = \frac{s^{2} e^{2\gamma\epsilon} G[2, 0, 1, 2, 0, 1, 0, 0, 0](-s)^{2\epsilon}}{\epsilon^{2}},$$

$$I_{6} = -\frac{s e^{2\gamma\epsilon} G[0, 2, 0, 1, 0, 1, 1, 0, 0](-s)^{2\epsilon}}{\epsilon},$$

$$I_{7} = -\frac{s e^{2\gamma\epsilon} G[0, 2, 0, 0, 2, 1, 0, 0](-s)^{2\epsilon}}{\epsilon^{2}},$$

$$I_{8} = \frac{s x e^{2\gamma\epsilon} G[0, 2, 0, 0, 2, 0, 1, 0, 0](-s)^{2\epsilon}}{\epsilon^{2}},$$
(57)

and the canonical DE is

$$A_x = \epsilon \left(\frac{a_{-1}}{x+1} + \frac{a_0}{x} \right) \tag{58}$$

with

and

In practice, if we guess a MI I_k which may be proportional to a UT integral by a ϵ -independent factor, we can make a transformation ansatz

$$I_k \to f(\bar{x})I_k \tag{61}$$

and then collect all ϵ^0 terms in the DE matrix. Cancel the ϵ^0 terms, and we are able to determine $f(\bar{x})$ analytically. This trial and error way is convenient and saves the time for finding the leading singularity.

Note that for a complicated integral, the leading singularities may be a list of rational functions, which do not differ between each other by constant factors. In this case, it is impossible to construct a UT integral from this integral directly and we have to consider a linear combination.

B. Lee's algorithm

Another approach to find UT integrals, is to convert a non-canonical DE to a canonical DE. With a canonical DE, it is highly likely that the corresponding integrals are UT. However, we comment that a canonical DE does *not* not guarantee that the integrals are UT. For example, if \vec{I} is a UT basis which satisfies,

$$d\vec{I} = \epsilon(d\tilde{A})\vec{I} \tag{62}$$

Then a basis $\vec{J} = f(\epsilon)\vec{I}$ has the same DE. However, with a nontrivial function $f(\epsilon)$, J is in general not a UT basis. This subtlety can usually be fixed by evaluating the simplest integral in the basis analytically, or compute the leading singularity of some integrals, and then remove possible $f(\epsilon)$ factor.

Here we introduce Roman Lee's algorithm [12] of finding the canonical DE. There are basically three steps. For simplicity, we consider the one-variable case, 1. Make the differential equation to a Fuchsian form. This step is based on Moser's algorithm, which lowers DE matrix's pole degree in a sequence of rational transformations.

It is not guranteed that any differential equation of Feynman integrals can always be transformed to a Fuchsian form by Moser's algorithm. When it is the case, pick up the residue matrices like,

$$\partial_x I' = \Big(\sum_i \frac{A_i(x,\epsilon)}{x-a_i}\Big)I' \tag{63}$$

2. $A_i(x, \epsilon)$ are in general not proportional to ϵ . Find the eigenvalues of $A_i(x, \epsilon)$. (We also need to consider the residue matrix at the infinity.) If the eigenvalues are all in the form $\mathbb{Z} + \mathbb{Q}\epsilon$, then apply the so-called *balance transformation*. For $i \neq j$, pick one eigenvalue λ_{ik} of A_i and one eigenvalue λ_{jl} of A_j . A balance transformation is

$$(\mathbb{I} - P) + \frac{x - x_i}{x - x_j}P \tag{64}$$

with

$$P = \frac{1}{vu} \left(uv \right), \quad A_i u = \lambda_{ik} u, \quad vA_j = \lambda_{jl} v \tag{65}$$

where u is a right eigenvector of A_i and v is a left eigenvector of A_j . A balance transformation increases A_i 's eigenvalue λ_{ik} by one and decrease A_j 's eigenvalue λ_{jl} by one.

Repeat this steps, until all eigenvalues are proportional to ϵ . Name the total transformation as $I'' = T_1 I'$.

3. Now the differential equation reads

$$\partial_x I'' = \left(\sum_i \frac{A_i(x,\epsilon)}{x-a_i}\right) I'' \tag{66}$$

with all $A_i(x, \epsilon)$'s eigenvalues proportional to ϵ . Note that A_i 's in general do not commute, so a simultaneous diagonalization does not work. Then here is the brilliant trick of Lee, to make all entries of $A_i(x, \epsilon)$ proportional to ϵ .

Suppose there is a transformation matrix $T(x, \epsilon)$ such that

$$T(x,\epsilon)A_i(x,\epsilon)T^{-1}(x,\epsilon) = \epsilon B_i(x), \quad \forall i$$
(67)

then we introduce an auxiliary variable μ . It is clear,

$$T(x,\epsilon)A_i(x,\epsilon)T^{-1}(x,\epsilon)/\epsilon = T(x,\mu)A_i(x,\mu)T^{-1}(x,\mu)/\mu$$
(68)

Define $S(x,\epsilon,\mu) = T(x,\mu)^{-1}T(x,\epsilon)$, and

$$S(x,\epsilon,\mu)\frac{A_i(x,\epsilon)}{\epsilon} = \frac{A_i(x,\mu)}{\mu}S(x,\epsilon,\mu) \quad \forall i$$
(69)

This is a linear equation in $S(x, \epsilon, \mu)$ and in principle we can solve it for $S(x, \epsilon, \mu)$ with x, ϵ, μ treated as parameters. If for the solution, $S(x, \epsilon, \mu)$ is finite and invertible when $\mu \to \mu_0$ with some constant μ_0 , then

$$S(x,\epsilon,\mu_0)A_i(x,\epsilon)S(x,\epsilon,\mu_0)^{-1} = \epsilon \frac{A_i(x,\mu_0)}{\mu_0}$$
(70)

Let $T = S(x, \epsilon, \mu_0)$ and this makes all entries proportional ϵ . The canonical DE is obtained.

Lee's algorithm is implemented as an interactive Mathematica package *Libra* [13], or the automatic packages *epsilon* and *fuchsia* [14, 15].

We comment that sometimes in the second step, the eigenvalues do not have the form $\mathbb{Z} + \mathbb{Q}\epsilon$. This is usually caused by the variable choice x and implies the UT integrals have a square root factor over the original MIs. In this case, we need to rationalize the square root and then use Lee's algorithm.

Sometimes, we could not find a non-singular balance transformation to make all eigenvalues proportional to ϵ . Usually, this means the UT basis does not exist and the Feynman integrals contain elliptic functions.

IV. INTEGRATION TO SYMBOLS

Before we consider solving the canonical DE analytically, we introduce the solution of DE in the symbol level. Symbol is a great tool for the loop-level scattering amplitudes which captures many features of the analytic Feynman integrals.

We see that all polylogarithm functions has the form: an integration of a simple rational function multiplied by a lower weight polylogarithm. To illustrate this structure, the symbol [2] is defined recursively as, if

$$dF = \sum_{i} F_i d\log R_i \tag{71}$$

with rational functions R_i , then the symbol of F is

$$\mathcal{S}(F) \equiv \sum_{i} \mathcal{S}(F_i) \otimes R_i \tag{72}$$

Here S is the \mathbb{Q} linear map from the function space to the symbol space. \otimes is the notation for noncommutative tensor product. Each entry of the tensor is called a symbol letter.

For the simplest function,

$$\mathcal{S}(\log(z)) = z \tag{73}$$

The original symbol definition treats

$$\mathcal{S}(\pi) = 0, \quad \mathcal{S}(\zeta_n) = 0, \tag{74}$$

to ignore these constants. Note that against the intuition, $S(\pi \log(z)) = 0$.

Note that $d\log(R_1R_2) = d\log R_1 + d\log R_2$, $d\log(cR) = d\log(R)$, $d\log(R^{-1}) = -d\log(R)$, so we demand the symbol to have the distributivity,

$$\dots \otimes (R_1 R_2) \otimes \dots = \dots \otimes R_1 \otimes \dots + \dots \otimes R_2 \otimes \dots$$
$$\dots \otimes (cR) \otimes \dots = \dots \otimes R \otimes \dots$$
$$\dots \otimes (R^{-1}) \otimes \dots = - \dots \otimes R \otimes \dots$$
(75)

Example IV.1. By the definition,

$$\mathcal{S}(\text{Li}_2(z)) = -(1-z) \otimes z, \quad \mathcal{S}(\text{Li}_4(z)) = -(1-z) \otimes z \otimes z \otimes z$$
$$S\left(\text{Li}_2(\frac{x}{y})\right) = -(1-\frac{x}{y}) \otimes \frac{x}{y}, \quad \mathcal{S}(H(1,-1;z)) = -(z+1) \otimes (1-z) \tag{76}$$

For the second line, we do not need to decompose $d(x/y) = dx/y - xdy/y^2$ but just treat d(x/y) as one object.

Note that in $-(1-z) \otimes z$, the overall minus sign cannot be dropped. However, it is quite risky to confuse it with $(z-1) \otimes z$. Therefore, frequently, especially for the programming, we write

$$\mathcal{S}(\mathrm{Li}_2(z)) = -S[1-z,z] \tag{77}$$

and the overall factor is emphasized.

The map S is a simple representation of polylogarithm functions, and can be used to check function identities. If a function combination is zero, then its symbol must be zero.

Example IV.2. (Abel's identity)

$$\operatorname{Li}_{2}\left(\frac{x}{1-y}\right) + \operatorname{Li}_{2}\left(\frac{y}{1-x}\right) - \operatorname{Li}_{2}\left(\frac{xy}{(1-x)(1-y)}\right) = \operatorname{Li}_{2}(x) + \operatorname{Li}_{2}(y) + \log(1-x)\log(1-y)$$
(78)

We use symbol to check this identity.

$$S[l.h.s] = -S[1 - \frac{x}{1 - y}, \frac{x}{1 - y}] - S[1 - \frac{y}{1 - x}, \frac{y}{1 - x}] + S[1 - \frac{xy}{(1 - x)(1 - y)}, \frac{xy}{(1 - x)(1 - y)}]$$

= -S[1 - x, x] + S[1 - x, 1 - y] + S[1 - y, 1 - x] - S[1 - y, y] (79)

which is obviously the same as the letters of the right hand side, since

$$d(\log(1-x)\log(1-y)) = \log(1-x)d\log(1-y) + \log(1-y)d\log(1-x)$$
(80)

However, note that even if the corresponding symbol is zero, we still could not claim the function is zero. The reason is that constants like π or ζ_n are dropped in the symbol map S. S is not an injective map. It is possible to make an ansatz which proportional to π or ζ_n for the missing part, and then use numeric evaluation to check a function relation completely.

Given a symbol $S[R_1, \ldots, R_n]$, can we find a function F such that $S(F) = S[R_1, \ldots, R_n]$? Naively, we define the *iterative integral* like this: Let M be the space (manifold) of variables and choose o a base point. For any point $p \in M$, $p = (x_1, \ldots, x_m)$, we find a smooth map $\gamma : [0, 1] \to M$ such that

$$\gamma(0) = o, \quad \gamma(1) = p \tag{81}$$

With the abuse of notation $R_i(t) \equiv R_i(\gamma(t))$, we define

$$F(p) = \int_0^1 dt_n \frac{R'_n(t_n)}{R_n(t_n)} \left(\int_0^{t_n} dt_{n-1} \frac{R'_{n-1}(t_{n-1})}{R_{n-1}(t_{n-1})} \left(\int_0^{t_{n-1}} dt_{n-2} \frac{R'_{n-2}(t_{n-2})}{R_{n-2}(t_{n-2})} \left(\dots \right) \right) \right)$$
(82)

This definition is clearly extended to the linear combination of symbols. For a connect region containing o, it seems F is defined. However, we need to check if the definition is homotopically invariant under an infinitesimal deformation of γ .

Example IV.3. Consider the symbol $(1 + x) \otimes (1 + y)$. In the x-y plane, choose the base point o = (0,0). For p = (1,1), choose a path (x(t), y(t)) such that (x(0), y(0)) = (0,0) and (x(1), y(1)) = (1,1). The "function" F at p has the expression,

$$F(p) = \int_0^1 dt_2 \frac{y'(t_2)}{1+y(t_2)} \int_0^{t_2} dt_1 \frac{x'(t_1)}{1+x(t_1)}$$
(83)

With x(t) = t, y(t) = t we get $F(p) = \log(2)^2/2$, while for $x(t) = t, y(t) = t^2$ we get $F(p) = \log(2)^2/4 + \pi^2/48$. The two paths are hotomopically equivalent, so this function is not well defined.

The validity condition of the iterative integral is solved by Chen's iterative integral theory [16]. The integral 82 is well defined if and only if the symbol is *integrable*: Let A be a weight-m symbol in letters $\{R_1 \ldots R_l\},\$

$$A = \sum_{I} c_I S[R_{i_1}, \dots R_{i_m}] \tag{84}$$

where each $I = \{i_1, \dots, i_m\}$ is *m*-tuple whose entries are integers in [1, l]. A is integrable if for any $1 \le j \le m - 1$

$$\sum_{I} c_{I} \left(d \log R_{i_{j}} \wedge d \log R_{i_{j+1}} \right) S[R_{i_{1}}, \dots, \widehat{R_{i_{j}}}, \widehat{R_{i_{j+1}}}, \dots, R_{i_{m}}] = 0$$
(85)

Example IV.4. The symbol

$$S[1-x,x] + S[1-x,1-y] + S[1-y,1-x]S[1-y,y]$$
(86)

is integrable. Since it is clear that

$$-d\log(1-x) \wedge d\log(x) + d\log(1-x) \wedge d\log(1-y) + d\log(1-y) \wedge d\log(1-x) - d\log(1-y) \wedge d\log(y) = 0$$
(87)

by the anti-commutative wedge product. This is the symbol from the well-defined function in the example (IV.2).

The symbol

$$S[x+y, 1-y, y] + S[1-y, x+y, y] + S[1-y, y, x+y]$$
(88)

is also integrable. To see this, with j = 1 for the condition in (85), we can check

$$d\log(x+y) \wedge d\log(1-y)S[y] + d\log(1-y) \wedge d\log(x+y)S[y] + d\log(1-y) \wedge d\log(y)S[x+y] = 0$$
(89)

The check with j = 2 is similar.

When a symbol A is integrable, the iterative integral (82) F is well-defined. By Newton-Leibniz theorem and the symbol definition

$$\mathcal{S}(F) = A. \tag{90}$$

So we see that a integrable symbol corresponds to a function. Note the iterative integral is homotopically invariant, but if the variable space is not simply connected (because of singular points), the iterative integral can have branch cuts.

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Integrable symbols can be used to calculate an amplitude in the approach of *bootstrap*, for example see ref. [17–19]. In practice, the integrable symbols with fixed weights can be found by the package [20].

Back to the canonical differential equation, with the background knowledge of Chen's theory, it is clear that the solution would be an iterative integral. In many cases, we first want to know the symbol of the solution, instead of the analytic solution. By the definition, the symbol of the solution can be obtained without much effort.

Consider the canonical differential equation for UT integrals,

$$d\vec{I} = \epsilon(d\tilde{A})\vec{I} = \epsilon\left(\sum_{i=1}^{N} a_i d\log W_i\right)\vec{I}$$
(91)

with

$$\vec{I} = \epsilon^k \sum_{n=0}^{\infty} \vec{I}^{(n)} \epsilon^n \tag{92}$$

Recall the canonical DE splits to differential orders of ϵ in (35): each derivate of $I^{(n)}$ is the product of dlog's and $I^{(n-1)}$. This immediately indicts that

$$\mathcal{S}(I^{(m)}) = \left(\sum_{i_m=1}^N \sum_{i_{m-1}=1}^N \dots \sum_{i_1=1}^N a_{i_m} a_{i_{m-1}} \dots a_{i_1} I^{(0)}\right) S[W_{i_1}, \dots, W_{i_m}]$$
(93)

where $I^{(0)}$ is the leading order of the UT basis, which is a constant (rational number) vector. The correctness of (93) is simply from the definition of symbols.

Note that this forumla only needs the leading order of UT, $I^{(0)}$, which can be easily obtained from an infrared/ultraviolet structure analysis or a numeric computation. In practice, to evaluate the big sum in (93), we always compute $a_{i_1}I^{(0)}$ first, then $a_{i_2}a_{i_1}I^{(0)}$ and likewise for the rest multiplication to speed up the computation. This computation should be simple.

An interesting consequence of (93) is that if the two matrices satisfy,

$$a_i a_j = 0, \tag{94}$$

Then the symbol can never have W_j and W_i in the adjacent position.

V. INTEGRATION TO FUNCTIONS

From the study of symbols, the idea of solving canonical differential equation in terms of iterative integrals becomes clear. However, in practice, we need the analytic function form of Feynman integrals. The new ingredient is the *boundary condition*. The solution of a canonical differential equation is completely determined by UT integral at one boundary point o,

$$\vec{I}^{(n)}(o) \equiv B^{(n)} \tag{95}$$

Let γ be a smooth starting from o. Then along the curve γ , the solution corresponding to the UT Feynman integral is

$$I^{(0)} = B^{(0)}$$

$$I^{(1)} = B^{(1)} + \int_{\gamma} (d\tilde{A}) I^{(0)}$$

$$I^{(2)} = B^{(2)} + \int_{\gamma} (d\tilde{A}) I^{(1)}$$
...
$$I^{(n)} = B^{(n)} + \int_{\gamma} (d\tilde{A}) I^{(n-1)}$$
(96)

Here the notation \int_{γ} can be explicitly written as an integration over a *t*-parameterized curve from o to an arbitrary point p.

The main difference between (93) and (96) is that the higher order boundary values $B^{(i)}$'s are also taken into account. That means the computation is significantly harder than the previous section.

About the integration in (96), note that $(d\tilde{A})$ contains only dlog's of the symbol letters. If all letters are rational functions, then $(d\tilde{A})$ contain rational function only. Along the curve γ , the pull back of $(d\tilde{A})$ would become rational function in t. By a factorization, each rational function only have linear denominators in t. The power of each linear factor would be at most one, because of the dlog form. Therefore, the integration, by the definition, produces GPLs only if all symbol letters are rational. Of course, in many cases the integration only gives HPLs or classical polylogarithms.

If the symbol letters contain square root and cannot be rationalized simultaneously, then the integration may provide more complicated function other than GPLs.

Here the main problem is to find the higher order boundary values. This step is tricky: unfortunately, there is no automatic algorithm to do this. There are two types of strategies for determining the boundary values:

1. Direct evaluation of the boundary values at a special point. The special point can have accidental kinematic symmetries or some special physical meaning. For integrals with internal masses, we often consider the special point to be the limit mass $\rightarrow \infty$. For integrals with multiple legs, we often consider the point with the permutation symmetry of the legs.

At the special point, the number of master integral may drop dramatically and we do not need to evaluate all UT integrals at that point. One example is the so-called two-loop fivepoint nonplanar "double-pentagon" integral family at the kinematic point, where p_3 , p_4 and p_5 are symmetric under permutations, the number of master integrals dropped from 108 to 49.

Then we try to directly evaluate the independent UT integrals at that point. The methods could be Feynman parametrization with Cheng-Wu theorem, dimension recursion relation, expansion by regions or direct integration with HYPINT. However, there is no automatic way for this computation.

2. Set an Ansatz for the boundary values and determine them later against the consistency condition. There are many types of consistency conditions. For example, for the massless four-point kinematics, a *planar* UT integral should be finite in the limit $u \rightarrow 0$. More generically, a UT integral is likely to be finite when one of the symbol letter is zero and $\epsilon < 0$. Thos generic consistency condition was systematically studied in []. Furthermore, it is also useful to consider the soft/collinear/Regge limit of the UT integrals.

In solving a canonical DE in the function level, one may need to use both of the strategies.

Example V.1. (One-loop massless box) The UT basis and the canonical DE of one-loop massless box integral family are given in (50) and (51).

The canonical DE has the symbol letter decomposition,

$$A_x = \epsilon \left(\frac{a_{-1}}{x+1} + \frac{a_0}{x} \right) \tag{97}$$

with

$$a_{-1} = \begin{pmatrix} 1 & -2 & -2 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \quad a_0 = \begin{pmatrix} -1 & 0 & 2 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix}.$$
 (98)

We choose the point x = 1. At this point, $I_2 = I_3$ and by a simple Feynman parametrization computation,

$$I_2|_{x=1} = I_3|_{x=1} = \epsilon^{-2} \left(1 - \frac{\pi^2 \epsilon^2}{12} - \frac{7\zeta(3)\epsilon^3}{3} - \frac{47\pi^4 \epsilon^4}{1440} + \dots \right)$$
(99)

For the convenience, we define,

$$\vec{I} = \epsilon^{-2} \sum_{n=0}^{\infty} \vec{I}^{(n)}(x) \epsilon^n \,. \tag{100}$$

The boundary value is then

$$\sum_{n} \vec{B}^{(n)} \epsilon^{n} = \begin{pmatrix} c^{(0)} \\ 1 \\ 1 \end{pmatrix} + \begin{pmatrix} c^{(1)} \\ 0 \\ 0 \end{pmatrix} \epsilon + \begin{pmatrix} c^{(2)} \\ -\frac{\pi^{2}}{12} \\ -\frac{\pi^{2}}{12} \end{pmatrix} \epsilon^{2} + \begin{pmatrix} c^{(3)} \\ -\frac{7\zeta(3)}{3} \\ -\frac{7\zeta(3)}{3} \end{pmatrix} \epsilon^{3} + \dots$$
(101)

c's are to be fixed by the condition that planar Feynman integral should not diverge at x = -1(u = 0). Note that the DE itself has the pole x = -1 does not mean the solution must diverge there.

The condition $\lim_{x\to -1} \vec{I}^{(n+1)}(x) < \infty$ is translated as,

$$\lim_{x \to -1} a_{-1} \vec{I}^{(n)}(x) = \vec{0}$$
(102)

• Weight-0. (102) determines that $c_0 = 4$ and (96) provides,

$$\vec{I}^{(0)} = \left(4, 1, 1\right)^{T} \tag{103}$$

• Weight-1. (102) determines that $c_1 = 0$ and (96) provides,

$$\vec{I}^{(1)} = \left(-2\log(x), \ 0, \ -\log(x)\right)^T \tag{104}$$

Note that in using the logarithm function, we impose the branch cut $(-\infty, 0)$ on the x-plane.

• Weight-2. The condition (102) reads

$$\lim_{x \to -1} c_2 - \log(x)^2 + \frac{\pi^2}{3} = 0$$
(105)

It appears subtle because $\log(x)$ has different values above and below the point x = -1. However, this subtlety is cleared because of the square, and we get $c_2 = -4\pi^2/3$. By (96),

$$\vec{I}^{(2)} = \left(-\frac{4\pi^2}{3}, -\frac{\pi^2}{12}, \frac{\log^2(x)}{2} - \frac{\pi^2}{12}\right)^T$$
(106)

• Weight-3. The condition (102) determines that

$$c_3 = \frac{1}{6} \left(-77\zeta(3) - 6\pi^2 \log(2) \right) \tag{107}$$

$$\begin{pmatrix} \frac{1}{6} (12 \text{Li}_{3}(-x) - 12 \text{Li}_{2}(-x) \log x + 2 \log^{3} x - 6 \log(x+1) \log^{2} x + 7\pi^{2} \log x - 6\pi^{2} \log(x+1) - 68\zeta_{3}) \\ -\frac{7\zeta_{3}}{3} \\ \frac{1}{12} (-2 \log^{3} x + \pi^{2} \log x - 28\zeta_{3}) \end{cases}$$
(108)

Note that these functions also have the branch cut $(-\infty, 0)$.

Higher orders can be analytically computed in the similar way. After the analytic computation, it is important to check it with numeric computations. With s = -1 and t = -1, from the package pySecdec we have

$$I_1|_{x\to 1} = 4.00000\epsilon^{-2} - (1.74986 \times 10^{-7})\epsilon^{-1} - 13.1595 - 22.2675\epsilon$$
(109)

which is consistent with our analytic boundary condition. Furthermore, we can check the integrated result on a generic physical point. For example, consider the point s = -1 and t = +3, pySecdec gives

$$I_1|_{x \to -3} = \frac{4.00000}{\epsilon^2} - \frac{2.19725 - 6.28323i}{\epsilon} - (13.15975 - 0.00021i) + (-9.8244 - 10.2675i)\epsilon \quad (110)$$

which is consistent with our analytic computation. Note that in the physical region, we have to shift the value as,

$$s \to -1, \quad t \to 3 + i\delta, \quad \delta > 0$$
 (111)

in order to get the correct value for functions like $\log x$ and $\operatorname{Li}_2(-z)$. Otherwise, we are using the wrong branch.

Example V.2. (Two-loop massless box) The UT basis and the canonical DE were given in (57) and (58). Again the UT basis is dimensionless and we consider x = 1 as our boundary. Here we see that this example has new features, comparing with the one-loop box family.

The last four UT integrals in (57) can be easily computed from Feynman parameterization. The UT integrals I_3 and I_4 can also be computed from Feynman parameterization, however, the cost is heavier. We leave the boundary values for the first four UT integrals undetermined.

We use the convention

$$\vec{I} = \epsilon^{-4} \sum_{n=0}^{\infty} \vec{I}^{(n)}(x) \epsilon^n \,.$$
(112)

The boundary condition for the 8 UT integrals is

$$\sum_{n=0}^{\infty} \vec{B}^{(n)} \epsilon^{n} = \begin{pmatrix} c_{1}^{(0)} + \epsilon c_{1}^{(1)} + \epsilon^{2} c_{1}^{(2)} + \epsilon^{3} c_{1}^{(3)} + \epsilon^{4} c_{1}^{(4)} + O(\epsilon^{5}) \\ c_{2}^{(0)} + \epsilon c_{2}^{(1)} + \epsilon^{2} c_{2}^{(2)} + \epsilon^{3} c_{2}^{(3)} + \epsilon^{4} c_{2}^{(4)} + O(\epsilon^{5}) \\ c_{3}^{(0)} + \epsilon c_{3}^{(1)} + \epsilon^{2} c_{3}^{(2)} + \epsilon^{3} c_{3}^{(3)} + \epsilon^{4} c_{3}^{(4)} + O(\epsilon^{5}) \\ c_{4}^{(0)} + \epsilon c_{4}^{(1)} + \epsilon^{2} c_{4}^{(2)} + \epsilon^{3} c_{4}^{(3)} + \epsilon^{4} c_{4}^{(4)} + O(\epsilon^{5}) \\ 1 - \frac{\pi^{2} \epsilon^{2}}{6} - \frac{14 \zeta(3) \epsilon^{3}}{3} - \frac{7\pi^{4} \epsilon^{4}}{120} + O(\epsilon^{5}) \\ \frac{1}{4} + \frac{\pi^{2} \epsilon^{2}}{24} - \frac{13 \zeta(3) \epsilon^{3}}{6} - \frac{41\pi^{4} \epsilon^{4}}{120} + O(\epsilon^{5}) \\ -1 + \frac{\pi^{2} \epsilon^{2}}{6} - \frac{32 \zeta(3) \epsilon^{3}}{3} - \frac{19\pi^{4} \epsilon^{4}}{120} + O(\epsilon^{5}) \\ 1 - \frac{\pi^{2} \epsilon^{2}}{6} - \frac{32 \zeta(3) \epsilon^{3}}{3} - \frac{19\pi^{4} \epsilon^{4}}{120} + O(\epsilon^{5}) \end{pmatrix}$$

$$(113)$$

We may use the planar consistency condition $\lim_{x\to -1}\vec{I}^{n+1}(x)<\infty$ or

$$\lim_{x \to -1} a_{-1} \vec{I}^n(x) = 0 \tag{114}$$

• Weight 0. In this case, (114) means,

$$c_2^{(0)} = \frac{7}{4} + c_1^{(0)}, \quad c_3^{(0)} = 0, \quad c_4^{(0)} = \frac{9}{4}$$
 (115)

It does not look good because $c_1^{(0)}$ is still undetermined. We leave $c_1^{(0)}$ as a free parameter and turn to the next order.

• Weight 1. We integrate $\vec{I}^{(0)}$ to get $\vec{I}^{(1)}$. Then (114) reads,

$$c_2^{(1)} = c_1^{(1)} + \lim_{x \to -1} (2c_1^{(0)} - \frac{9}{2})\log x, \quad c_3^{(1)} = 0, \quad c_4^{(1)} = 0$$
(116)

No matter we approach the point x = -1 from the above or the below, $\log x$ would be complex. However $c_2^{(1)}$ and $c_1^{(1)}$ should be real, since the boundary point is in the Euclidean region. Hence,

$$c_1^{(0)} = \frac{9}{4} \tag{117}$$

At the weight-1 order, we fixed the weight-0 boundary condition. Here the value of $c_1^{(1)}$ is undetermined yet.

• Weight 2. We integrate $\vec{I}^{(1)}$ to get $\vec{I}^{(2)}$. Then (114) reads,

$$c_2^{(2)} \to \frac{1}{24} \left(48c_1^{(1)} \lim_{x \to -1} (\log(x)) + 24c_1^{(2)} - 13\pi^2 \right) \quad c_3^{(2)} \to \frac{\pi^2}{2} \quad c_4^{(2)} = -\frac{13\pi^2}{8}$$
(118)

Again by the Euclidean region argument,

$$c_1^{(1)} = 0 \tag{119}$$

So we completely obtained the UT basis up to weight 1, and the result is,

$$\vec{I}^{(0)} + \epsilon \vec{I}^{(1)} = \begin{pmatrix} \frac{9}{4} - 2\epsilon \log(x) \\ 4 - 5\epsilon \log(x) \\ 0 \\ \frac{9}{4} - 3\epsilon \log(x) \\ 1 \\ \frac{1}{4} \\ -1 \\ 1 - 2\epsilon \log(x) \end{pmatrix}$$
(120)

All order boundary values can be fixed by (1) the planar integral consistency condition (2) Euclidean region condition. The rest computation is left as homework.

We remark that for solving canonical DE, it may be cumbersome to use the "Integrate" command in Mathematica, even if a result contains only classical polylogarithm. It is more convenient to define the iterative integration rules and formal function like HPLs or GPLs in the computer algebra system. Then call a package like HPL to simplify the result.

To simplify polylogarithms combinations, the main tool is the *shuffle identity*.

Example V.3. To understand shuffle identity, it is good to start from a simple example. Consider $f_1(z) = H(1, -1; z)$ and $f_2(z) = H(-1, 1; z)$. Assume that 0 < z < 1, and they both have the iterative integral form,

$$f_1(z) = \int_0^z dt_2 \frac{1}{1 - t_2} \int_0^{t_2} dt_1 \frac{1}{1 + t_1}$$

$$f_2(z) = \int_0^z dt_2 \frac{1}{1 + t_2} \int_0^{t_2} dt_1 \frac{1}{1 - t_1}$$
(121)

In the second integral, rename the variables $t_1 \leftrightarrow t_2$, and we get

$$H(1,-1;z) + H(-1,1;z) = \int_0^z dt_1 \frac{1}{1+t_1} \int_0^z dt_2 \frac{1}{1-t_2} = -\log(1+z)\log(1-z)$$
(122)

We see that

$$S(\log(1+z)) = S[1+z], \quad S(-\log(1-z)) = -S[1-z]$$

$$S(H(1,-1;z) + H(-1,1;z)) = -S[1+z,1-z] - S[1-z,1+z]$$
(123)

So for the symbol of two products $\log(1+z)$ and $\log(1-z)$, is the sum of the shuffle product of two letters.

We also comment that all terms in (122) have the same branch cuts $(-\infty, -1)$ and $(1, \infty)$, and by analytic continuation, the identity holds everywhere on the complex plane except for $z = \pm 1$.

For the product of two polylogarithms, the shuffle identity can be derived by a simplex decomposition. For GPLs,

$$G(a_1 \dots a_n; z)G(a_{n+1}, \dots a_{n+m}; z) = \sum_{\sigma \in \Sigma_{n,m}} G(a_{\sigma(1)} \dots a_{\sigma(n+m)}; z)$$
(124)

where $\Sigma_{n,m}$ is a subset of the permutation group Σ_{n+m} consists all permutations such that

$$\sigma^{-1}(1) < \ldots < \sigma^{-1}(n), \text{ and, } \sigma^{-1}(n+1) < \ldots < \sigma^{-1}(n+m),$$
 (125)

For HPLs, the shuffle identity is the same with $G \to H$.

The shuffle identity means that GPLs (HPLs) of the same weights in z are not independent. So we can use the shuffle identity to simplify polylogarithms, and extract the divergence.

Example V.4. Consider the function f(z) = H(1, 0, -1, 0; z). This function is divergent when $z \to 1$. Find the leading divergence. We use the shuffle identity,

$$H(1;z)H(0,-1,0;z) = H(1,0,-1,0;z) + H(0,1,-1,0;z) + H(0,-1,1,0;z) + H(0,-1,0,1;z)$$
(126)

The last three functions are not divergent at $z \to 1$. Hence we see that,

$$H(1,0,-1,0;z)|_{z\to 0} \to -H(0,-1,0;z)\log(1-z) \sim \frac{3}{2}\zeta(3)\log(1-z)$$
(127)

VI. SIMPLIFIED CANONICAL DIFFERENTIAL EQUATION

Sometimes, for a real-world problem, we do not need to solve *all* the integrals in a family. Instead, we are only interesed in a subset of integrals to a certain ϵ order. In this case, a canonical DE can be simplified [21].

We illustrate the idea with a concrete example in the ref. [21],

Example VI.1. (One-loop box with internal mass).

$$D_1 = l_1^2 - m^2, \quad D_2 = (l_1 - p_1)^2 - m^2, \quad D_3 = (l_1 - p_1 - p_2)^2 - m^2, \quad D_4 = (l_1 + p_4)^2 - m^2$$
(128)

with $p_i^2 = 0$, i = 1, 2, 3, 4. $(p_1 + p_2)^2 = s$, $(p_1 + p_4)^2 = t$ and $(p_2 + p_4)^2 = -s - t$. There are 6 master integrals in this family. With the leading singularity analysis and some reasonable guessing, the UT basis is,

$$I_{1} = e^{\epsilon \gamma} (m^{2})^{\epsilon} \sqrt{st (st - 4m^{2}(s+t))} G[1, 1, 1, 1]$$

$$I_{2} = e^{\epsilon \gamma} s (m^{2})^{\epsilon} G[1, 0, 1, 1]$$

$$I_{3} = e^{\epsilon \gamma} t (m^{2})^{\epsilon} G[0, 1, 1, 1]$$

$$I_{4} = e^{\epsilon \gamma} \frac{\sqrt{s(s - 4m^{2})} (m^{2})^{\epsilon}}{\epsilon} G[1, 0, 2, 0]$$

$$I_{5} = e^{\epsilon \gamma} \frac{\sqrt{t(t - 4m^{2})} (m^{2})^{\epsilon}}{\epsilon} G[0, 1, 0, 2]$$

$$I_{6} = e^{\epsilon \gamma} \frac{(m^{2})^{\epsilon + 1}}{\epsilon^{2}} G[0, 0, 0, 3]$$
(129)

It is convenient to define

$$u = -\frac{4m^2}{s}, \quad v = -\frac{4m^2}{t}$$
(130)

and,

$$\beta_u = \sqrt{1+u}, \quad \beta_v = \sqrt{1+v}, \quad \beta_{uv} = \sqrt{1+u+v}, \tag{131}$$

The alphabet $\{W_1, \ldots, W_8\}$ is

$$\left\{\frac{u}{1+u}, \frac{v}{1+v}, \frac{u+v}{1+u+v}, \frac{\beta_u-1}{\beta_u+1}, \frac{\beta_v-1}{\beta_v+1}, \frac{\beta_{uv}-\beta_u}{\beta_{uv}+\beta_u}, \frac{\beta_{uv}-\beta_v}{\beta_{uv}+\beta_v}, \frac{\beta_{uv}-1}{\beta_{uv}+1}\right\}$$
(132)

By a numerical fitting, the canonical differential equation has the \tilde{A} matrix (homework):

$$\tilde{A} = \begin{pmatrix} \log(W_3) & -2\log(W_8) & -2\log(W_8) & -2\log(W_6) & -2\log(W_7) & 0 \\ 0 & 0 & 0 & -\log(W_4) & 0 & 0 \\ 0 & 0 & 0 & 0 & -\log(W_5) & 0 \\ 0 & 0 & 0 & \log(W_1) & 0 & 2\log(W_4) \\ 0 & 0 & 0 & 0 & \log(W_2) & 2\log(W_5) \\ 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix}$$
(133)

It is easy to find the boundary value at $m \to \infty$

$$u \to \infty, \quad v \to \infty$$
 (134)

and solve the canonical DE. However, if we only need the I_1 's ϵ^0 order, there is a short cut.

Note that from the UV/IR analysis, in the UT list

$$I_1, I_2, I_3 \sim O(\epsilon^0), \quad I_4, I_5 \sim O(\epsilon^{-1}), \quad I_6 \sim O(\epsilon^{-2})$$
 (135)

Then we define

$$J_1 = I_1, \quad J_2 = I_2, \quad J_3 = I_3, \quad J_4 = \epsilon I_4, \qquad J_5 = \epsilon I_5, \qquad J_6 = \epsilon^2 I_5,$$
 (136)

So J_i 's are finite as $\epsilon \to 0$. The DE for J's is,

$$d\vec{J} = d \begin{pmatrix} \epsilon \log(W_3) & -2\epsilon \log(W_8) & -2\epsilon \log(W_8) & -2\log(W_6) & -2\log(W_7) & 0 \\ 0 & 0 & 0 & -\log(W_4) & 0 & 0 \\ 0 & 0 & 0 & 0 & -\log(W_5) & 0 \\ 0 & 0 & 0 & \epsilon \log(W_1) & 0 & 2\log(W_4) \\ 0 & 0 & 0 & 0 & \epsilon \log(W_2) & 2\log(W_5) \\ 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix} \vec{J} \quad (137)$$

If we are only interested in the ϵ^0 order of J, then

$$d\vec{J}^{(0)} = d \begin{pmatrix} 0 & 0 & 0 & -2\log(W_6) & -2\log(W_7) & 0 \\ 0 & 0 & 0 & -\log(W_4) & 0 & 0 \\ 0 & 0 & 0 & 0 & -\log(W_5) & 0 \\ 0 & 0 & 0 & 0 & 0 & 2\log(W_4) \\ 0 & 0 & 0 & 0 & 0 & 2\log(W_5) \\ 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix} \vec{J}^{(0)}$$
(138)

The DE is significantly simplified. Especially,

$$d \begin{pmatrix} J_1^{(0)} \\ J_4^{(0)} \\ J_5^{(0)} \\ J_6^{(0)} \end{pmatrix} = d \begin{pmatrix} 0 & -2\log(W_6) & -2\log(W_7) & 0 \\ 0 & 0 & 0 & 2\log(W_4) \\ 0 & 0 & 0 & 2\log(W_5) \\ 0 & 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} J_1^{(0)} \\ J_4^{(0)} \\ J_5^{(0)} \\ J_6^{(0)} \end{pmatrix}$$
(139)

That means $J_1^{(0)}$ is an integration of $J_4^{(0)}$ and $J_5^{(0)}$, where the latter two are the integration of $J_6^{(0)}$. We then have a simple iterative integration, unlike the standard canonical DE, here the iterative structure is over different integrals.

From Feynman parameterization,

$$J_6^{(0)} = -\frac{1}{2} \tag{140}$$

 $and \ then$

$$J_4^{(0)} = -\log(W_4) + c_4 = -\log(\frac{\beta_u - 1}{\beta_u + 1}) + c_4, \quad J_5^{(0)} = -\log(W_5) + c_5 = -\log(\frac{\beta_v - 1}{\beta_v + 1}) + c_5 \quad (141)$$

From the boundary condition at $s \to 0$ and $t \to 0$, we see that $c_4 = c_5 = 0$. Then, the symbol of $J_1^{(0)}$ is clear,

$$\mathcal{S}(J_1^{(0)}) = 2S[W_4, W_6] + 2S[W_5, W_7] = 2\left(S[\frac{\beta_u - 1}{\beta_u + 1}, \frac{\beta_{uv} - \beta_u}{\beta_{uv} + \beta_u}] + S[\frac{\beta_v - 1}{\beta_v + 1}, \frac{\beta_{uv} - \beta_v}{\beta_{uv} + \beta_v}]\right).$$
(142)

If we pick up a boundary point where $J_1^{(0)} \to 0$, then $J_1^{(0)}$ has a compact expression in terms of iterative integral

$$J_1^{(0)} = 2\int_{\gamma} \log\left(\frac{\beta_u - 1}{\beta_u + 1}\right) d\log\left(\frac{\beta_{uv} - \beta_u}{\beta_{uv} + \beta_u}\right) + \log\left(\frac{\beta_v - 1}{\beta_v + 1}\right) d\log\left(\frac{\beta_{uv} - \beta_v}{\beta_{uv} + \beta_v}\right)$$
(143)

This is a perfect answer.

However, in practice, we may want the expression in terms of polylogarithms. In general, Chen's iterative integral may not be a combination of polylogrithm, but the integral (143) is, because all three square roots can be rationalized simultaneously:

$$u = \frac{(1 - w^2)(1 - z^2)}{(w - z)^2}, \quad v = \frac{4wz}{(w - z)^2}$$
(144)

For the simplicity, we choose the Euclidean region,

$$u = -\frac{4m^2}{s} > 0, \quad v = -\frac{4m^2}{t} > 0 \tag{145}$$

and correspondingly 0 < w < z < 1. In this region,

$$\beta_u = \frac{1 - wz}{z - w}, \quad \beta_v = \frac{z + w}{z - w}, \quad \beta_{uv} = \frac{1 + wz}{z - w}$$
(146)

Then

$$W_4 = \frac{(w+1)(1-z)}{(1-w)(z+1)}, \quad W_5 = \frac{w}{z}, \quad W_6 = wz, \quad W_7 = \frac{(1-w)(1-z)}{(w+1)(z+1)}$$
(147)

Here we see that in the new coordinates, the relevant symbol letters become $\{z, w, 1 \pm z, 1 \pm w\}$. For a generic point (z, w), 0 < w < z < 1, we pick the boundary point as (w, w) and γ to be the straight line from (w, w) to (z, w). At (w, w), $J_1^{(0)}$ is zero. Then the computation of (143) is straightforward, and the result is

$$J_{1}^{(0)} = -2\text{Li}_{2}(1-w) - 4\text{Li}_{2}(-w) + 2\text{Li}_{2}(w) + 2\text{Li}_{2}(1-z) + 4\text{Li}_{2}(-z) - 2\text{Li}_{2}(z) + 2\log(w+1)\log(z) + 2\log(w)\log(z+1)\log(z) + 2\log(w)\log(z+1) + 2\log(z)\log(z+1) + 2\log(z)\log(z)\log(z+1) + 2\log(z)\log(z+1) + 2\log(z)\log(z)\log(z+1) + 2\log(z)\log(z)\log($$

This result is consistent with PYSECDEC.

The lesson here is that we do not need to compute the two triangles but directly get the box from the integration of bubbles. The equation (139) is not just upper triangular, but has all diagonal elements zero. Then the iterative integration structure over UT integrals is manifest.

This kind of treatment certainly simplified the canonical DE a lot. However, it would be greater if one can completely skip the full canonical DE and directly get a simple DE like (139). This is possible and the key idea is find integral relations only valid to a fixed order of ϵ .

VII. UT DETERMINATION, II

The UT determination for multiloop Feynman integrals, especially with multiple legs, is not a easy task. In this section, we give an overview of some more recent methods.

A. Integrand dlog construction

Roughly speaking, integrand dlog construction can be understood as an advanced version of the leading singularity analysis. Again, it was invented in the study of N = 4 Super-Yang-Mills theory [22, 23].

A 4D dlog integrand has the form

$$\int d\log f_1 \wedge \dots d\log f_{4L} \tag{149}$$

We can consider f_1, \ldots, f_{4L} as variables and thus any residue would be ± 1 . Note that this argument is actually stronger than the leading singularity based on cuts, since here no cut is taken. A Feynman integral with 4D dlog integrand is likely to be UT, while a Feynman integral with constant leading singularity tends to be a UT up to some lower sector integrals.

Example VII.1. (one loop massless box's dlog form). The inverse propagators are

$$D_1 = l_1^2, \quad D_2 = (l_1 - p_1)^2, \quad D_3 = (l_1 - p_1 - p_2)^2, \quad D_4 = (l_4 + p_4)^2$$
 (150)

We define a "magic factor",

$$F = (l - l_*)^2 \tag{151}$$

where l_* is one of the maximal cut solution for l. Then it is easy to check

$$\int d\log\left(\frac{F}{D_1}\right) \wedge d\log\left(\frac{F}{D_2}\right) \wedge d\log\left(\frac{F}{D_3}\right) \wedge d\log\left(\frac{F}{D_4}\right)$$

$$\propto st \int d^4 l \frac{1}{D_1 D_2 D_3 D_4}$$
(152)

therefore stG[1,1,1,1] is a dlog integral. We already know that this is a UT integral.

In practice, it is not easy to find an elegant dlog integrand like (VII.1). However, for the purpose of UT determination, a linear combination of several dlog integrand is equally good. Such a linear combination can be found with Wasser's package DLOG [24].

B. Baikov leading singularity

Baikov representation is convenient for the leading singularity computation, and has been used recently in the UT determination [25–28]. In Baikov representation, the ϵ parameter is preserved while the integration is over an integer number of variables.

Example VII.2. (two-loop massless slashed box). With the notation in the previous examples, the integral G[0, 1, 1, 0, 1, 1, 1, 0, 0] is the so-called slashed box integral.

$$G[0,1,1,0,1,1,1,0,0] = \int \frac{d^d l_1}{i\pi^{d/2}} \int \frac{1}{(l-p_1)^2 (l-p_1-p_2)^2} \int \frac{d^d l_2}{i\pi^{d/2}} \frac{1}{(l_2)^2 (l_2-p_4)^2 (l_2+l_1)^2}$$
(153)

We can do a right-to-left Baikov analysis. For the loop with l_2 , the external lines are l_1 and p_4 , so the Baikov representation is

$$G\left(\begin{array}{cc}l_{1} & p_{4}\\ l_{1} & p_{4}\end{array}\right)^{\frac{3-d}{2}} \int dz_{1}dz_{2}dz_{3} \ G\left(\begin{array}{cc}l_{2} & l_{1} & p_{4}\\ l_{2} & l_{1} & p_{4}\end{array}\right)^{\frac{d-4}{2}} \frac{1}{z_{1}z_{2}z_{3}}$$
(154)

with the Baikov variable definition,

$$l_2^2 = z_1, \quad l_1 \cdot l_2 = \frac{1}{2}(-l_1^2 - z_1 + z_3), \quad l_2 \cdot p_4 = \frac{1}{2}(z_1 - z_2).$$
 (155)

Consider the residue at $\{z_1, z_2, z_3\} \rightarrow \{0, 0, 0\}$ of 154 with $d \rightarrow 4$, we get,

$$\frac{1}{l_1 \cdot p_4} \tag{156}$$

For the left loop with external lines p_2 , the Baikov representation is

$$G\begin{pmatrix} p_2 & p_4 \\ p_2 & p_4 \end{pmatrix}^{\frac{3-d}{2}} \int dw_1 dw_2 dw_3 \ G\begin{pmatrix} l_1 - p_1 & p_2 & p_4 \\ l_1 - p_1 & p_2 & p_4 \end{pmatrix}^{\frac{d-4}{2}} \frac{1}{w_1 w_2 w_3}$$
(157)

with the Baikov variable definition,

$$(l_1 - p_1)^2 = w_1, \quad (l_1 - p_1 - p_2)^2 = \frac{1}{2}(w_1 - w_2), \quad l_1 \cdot p_4 = w_3 - \frac{t}{2}$$
 (158)

Note that from the right loop analysis we have a new propagator $(l_1 \cdot p_4)^{-1}$. We have to add p_4 as an external line. The residue of (157) is then,

$$\frac{1}{s+t} \tag{159}$$

From the loop-by-loop Baikov representation we can see the leading singularity of G[0, 1, 1, 0, 1, 1, 1, 0, 0] is 1/(s + t).

More important, in multi-leg cases, an *integrand* may be explicitly zero in the 4D limit, but the integral does not vanish. In such cases, 4D UT determination method completely failed but the Baikov method works.

Example VII.3. (*Two-loop five-point nonplanar UT integral*). *The propagators of this integral family are,*

$$D_{1} = l_{1}^{2}, \quad D_{2} = (l_{1} - p_{1})^{2}, \quad D_{3} = (l_{1} - p_{12})^{2}, \quad D_{4} = l_{2}^{2},$$

$$D_{5} = (l_{2} - p_{123})^{2}, \quad D_{6} = (l_{2} - p_{1234})^{2}, \quad D_{7} = (l_{1} - l_{2})^{2},$$

$$D_{8} = (l_{1} - l_{2} + p_{3})^{2}, \quad D_{9} = (l_{1} - p_{1234})^{2}, \quad D_{10} = (l_{2} - p_{1})^{2},$$

$$D_{11} = (l_{2} - p_{12})^{2}.$$
(160)

Consider the integral,

$$I[\mu_{12}] \equiv \int \frac{d^d l_1 d^d l_2}{(i\pi^{d/2})^2} \frac{G\left(\begin{array}{cccc} l_1 & p_1 & p_2 & p_4 & p_5 \\ l_2 & p_1 & p_2 & p_4 & p_5 \end{array}\right)}{D_1 \dots D_8}$$
(161)

This one has no 4D leading singularity, since in the 4D limit the numerator is vanishing. However, the integral itself is not zero. A Baikov leading singularity analysis finds nonzero residues of $I[\mu_{12}]$, and we can predict that,

$$\frac{s_{12} - s_{45}}{\epsilon_{1245}} I[\mu_{12}]. \tag{162}$$

would be a UT integral [25]. Indeed it is, by the check of the differential equation.

C. Module lift method

Sometimes the search of UT integrals has a flavour of algebraic geometry: we need to combine several integrals to satisfy some condition (leading singularity, dlog form ...). However, the coefficients must be "nice", without certain poles. The double constraints tend to form an algebraic geometry problem.

$$Mv = b \tag{163}$$

where the $m \times n$ matrix M and the m-dimensional vector b are known. The vector v is to be solved for. Sometimes, we want v's entries are all polynomials. Then it is a classical problem in algebraic geometry. Each column of M is a generator in the module R^m so M defines a submodule S in R^m . To find a polynomial vector solution v, is equivalent to lift S to b [25]. This can be done by a Groebner basis computation for S.

Example VII.4. (Module Lift to find UT integrals) Again, consider the integral family in Example VII.3. The sector (1, 1, 1, 1, 1, 1, 1, 0, 0, 0) contains 9 master integrals. It is then a tough problem to construct 9 UT integrals for this sector. To simplify the discussion, we only look at the maximal cut level. The building blocks are the integrals,

$$G[1, 1, 1, 1, 1, 1, 1, 1, a_9, a_{10}, a_{11}]$$
(164)

with

$$-2 \le a_9 + a_{10} + a_{11} \le 0, \quad a_j \le 0, \quad j = 9, 10, 11$$
(165)

There 10 such kind of integrals, which are denoted as I_1, \ldots, I_{10} . A UT anasatz on the maximal cut level is given by,

$$\sum_{j=1}^{10} c_j I_j \tag{166}$$

Here we simply consider the 4D leading singularities. There are 8 solutions for the maximal cut, say $p_1, \ldots p_8$. Define the residues,

$$Res_{p_i}[I_j] \equiv M_{ij} \tag{167}$$

And we have the 4D leading singularity requirement,

$$\sum_{j=1}^{10} M_{ij} c_j = b_i \tag{168}$$

where b_i must be rational numbers. The (8×10) matrix M contains large expressions, so it would not be explicitly listed here. What a pity!

In this example, it is clear that from the viewpoint of linear algebra, for a fixed vector b, the solution for c is not unique even if the solution exists. If we naively pick up a solution of c for

the UT Ansatz, unfortunately, we do not get a canonical DE in the end. The problem is that most solutions of c contains complicated unphysical poles, which can hardly make a UT, even if the 4Dleading singularities are all constants.

Here we impose a radical condition, for even integrals the c's must be a polynomial of Mandelstam variables, while for odd integrals the c's must be a polynomial of Mandelstam variables over ϵ_{1234} .

For the even case, c's are polynomial but note that M itself contains fractions. This subtlety can be easily solved by a rescaling $\tilde{M} = FM$, where F is a known polynomial of Mandelstam variables to ensure that \tilde{M} contains polynomials only. Then,

$$\tilde{M}c = Fb \tag{169}$$

is a module lift problem in the module \mathbb{R}^8 , with $\mathbb{R} = \mathbb{Q}[s_{12}, s_{23}, s_{34}, s_{45}, s_{15}]$. For a given b, an algebraic geometry software like SINGULAR can find the lift solution c within a second.

For example, with $b = (1, 0, 0, -1, 0, 0, 0, 0)^T$, SINGULAR provides the solution for c,

$$c = \begin{pmatrix} 0 \\ 4s_{12}s_{23}(s_{12} - 2s_{45}) \\ 4s_{12}s_{34}s_{45} \\ 4s_{12}s_{15}(s_{12} - s_{45}) \\ 0 \\ 0 \\ -4s_{12}s_{15} \\ -4s_{12}(s_{12} - s_{45}) \\ -4s_{12}(s_{23} + s_{45}) \\ -4s_{12}(s_{12} - s_{34}) \end{pmatrix}$$
(170)

The solution is surprisingly simple and such kind of solutions can be used to build a 9×9 canonical DE on the maximal cut [25]. After fitting the lower subsector contributions, this solution really turns to a UT integral.

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