

Solving differential equations for 3-loop diagrams: relation to hyperbolic geometry and knot theory

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Abstract In hep-th/9805025, a result for the symmetric 3-loop massive tetrahedron in 3 dimensions was found, using the lattice algorithm PSLQ. Here we give a more general formula, involving 3 distinct masses. A proof is devised, though it cannot be accounted as a derivation; rather it certifies that an Ansatz found by PSLQ satisfies a more easily derived pair of partial differential equations. The result is similar to Schläfli's formula for the volume of a bi-rectangular hyperbolic tetrahedron, revealing a novel connection between 3-loop diagrams and 1-loop boxes. We show that each reduces to a common basis: volumes of ideal tetrahedra, corresponding to 1-loop massless triangle diagrams. Ideal tetrahedra are also obtained when evaluating the volume complementary to a hyperbolic knot. In the case that the knot is positive, and hence implicated in field theory, ease of ideal reduction correlates with likely appearance in counterterms. Volumes of knots relevant to the number content of multi-loop diagrams are evaluated; as the loop number goes to infinity, we obtain the hyperbolic volume of a simple 1-loop box.

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1 Introduction

In [1] we studied the 3-loop 3-dimensional tetrahedral Feynman diagram

$$C(a, b) := \frac{1}{\pi^6} \int \int \int \frac{d^3\mathbf{k}_1 d^3\mathbf{k}_2 d^3\mathbf{k}_3}{(k_1^2 + a^2)(k_2^2 + 1)(k_3^2 + 1)(k_{2,3}^2 + b^2)(k_{1,3}^2 + 1)(k_{1,2}^2 + 1)} \quad (1)$$

with $k_n^2 := |\mathbf{k}_n|^2$ and $k_{i,j}^2 := |\mathbf{k}_i - \mathbf{k}_j|^2$. For the totally symmetric tetrahedron, with $a = b = 1$, we found a simple reduction to a Clausen integral:

$$\frac{C(1, 1)}{2^{5/2}} = - \int_{2\alpha}^{4\alpha} d\theta \log(2 \sin \frac{1}{2}\theta); \quad \alpha := \arcsin \frac{1}{3}, \quad (2)$$

thus obtaining an exact dilogarithmic result for the diagram evaluated numerically in [2].

The discovery route for (2) was based on a dispersion relation for the more general Feynman tetrahedron (1), with masses a and b on non-adjacent lines and unit masses on the other 4 lines. This was derived by applying the methods of [3, 4] in 3 dimensions. In this paper, we reduce $C(a, b)$ to 7 dilogarithms, for $a^2 + b^2 > 4$, and to 8 Clausen values, for $a^2 + b^2 < 4$. In the latter case, (2) results by use of the classical formula [5]

$$\pi = 2 \arcsin \frac{1}{3} + 4 \arcsin \frac{1}{\sqrt{3}}, \quad (3)$$

which reduces the Clausen values to only 2.

Section 2 gives the 3-loop results. In Sections 3 and 4 we examine connections, via hyperbolic geometry, to very different types of diagrams, in 4 dimensions: massive box diagrams, with only 1 loop, studied in [6], and massless diagrams with more than 6 loops, studied in [7, 8]. Remarkably, the infinite-loop limit of the hyperbolic volumes of knots entailed by the latter recovers a simple case of the former. Section 5 gives our conclusions.

2 Solving the vacuum differential equations

In [1], we reduced (1) to dispersive integrals of the form $\int dx P(x, X) \log Q(x, X)$ where P and Q are rational algebraic functions of x and of the square root, X , of a quadratic function of x . Section 8.1.2 of [9] shows that every integral of this form may be reduced to dilogarithms, albeit with the possibility of complex arguments. Pursuing the methods of [9], one readily establishes that $C(a, b)$ is reducible to real dilogarithms for $a^2 + b^2 > 4$. Implementing the algorithm of [9], in REDUCE, we obtained a formidably complicated result, involving 2 square roots: $\sqrt{a^2 + b^2 - 4}$ and $\sqrt{2b(b+2)}$. The appearance of the former is to be expected; the characteristics of the result clearly change when $a^2 + b^2 - 4$ changes sign. The appearance of the latter is a gratuitous consequence of the dispersive derivation; it may be removed by consideration of $C(b, a) = C(a, b)$, but then $\sqrt{2a(a+2)}$ appears. Clearly there must exist a result involving neither $\sqrt{2a(a+2)}$ nor $\sqrt{2b(b+2)}$. How to achieve this is problematic.

One strategy for removing a bogus square root is to differentiate the dilogarithms that involve it and then to combine the resultant logarithms, to show that the differential is free of the unwanted square root. In this case, REDUCE showed that the dispersion relation for the Feynman tetrahedron $C(a, b)$ yields the partial differential equation

$$\frac{b\sqrt{a^2 + b^2 - 4}}{4} \frac{\partial}{\partial a} \frac{a\sqrt{a^2 + b^2 - 4}}{4} C(a, b) = \log\left(\frac{a+2}{a+b+2}\right) + \frac{b}{a+2} \log\left(\frac{a+b+2}{b+2}\right) + \frac{2b}{a^2-4} \log\left(\frac{a+2}{4}\right), \quad (4)$$

which entails only the physical square root, easily traceable to a tree diagram for elastic scattering [1]. A second partial differential equation immediately follows from the symmetry $C(a, b) = C(b, a)$ of the diagram. We checked that the pair agrees with results in [10], obtained by the methods of [11], more recently espoused in [12].

Systematic re-integration of (4), by the methods of [9], still produced 20 dilogarithms, with 8 of these entailing the unwanted square root $\sqrt{2b(b+2)}$. Accordingly, we resorted to an alternative strategy, by evaluating $C(a, b)$ numerically at an arbitrarily chosen transcendental point, $a = \exp(1)$, $b = \pi$, and then using the lattice algorithm PSLQ [13] to search for a rational linear combination of dilogarithms of a character suggested by those parts of the analytical 20-dilogarithm result that did not involve the bogus square root $\sqrt{2b(b+2)}$. After much trial and error, in search spaces of dimensions as large as 80, to accommodate the possibility of many products of logs, we found a simple log-free fit to the single numerical datum:

$$\begin{aligned} \frac{1}{8} abc C(a, b) &= \text{Li}_2\left(-\frac{p}{m}\right) + \text{Li}_2\left(1 - \frac{4}{m}\right) + \text{Li}_2\left(1 - \frac{m}{a+2}\right) + \text{Li}_2\left(1 - \frac{m}{b+2}\right) \\ &- \text{Li}_2\left(-\frac{m}{p}\right) - \text{Li}_2\left(1 - \frac{4}{p}\right) - \text{Li}_2\left(1 - \frac{p}{a+2}\right) - \text{Li}_2\left(1 - \frac{p}{b+2}\right) \end{aligned} \quad (5)$$

with a dilogarithm $\text{Li}_2(x) := -\int_0^x (dy/y) \log(1-y)$ and

$$c := \sqrt{a^2 + b^2 - 4}, \quad p := a + b + 2 + c, \quad m := a + b + 2 - c. \quad (6)$$

Ansatz (5) is manifestly symmetric in (a, b) and fits the datum to 360-digit precision.

It was then a routine application of computer algebra to prove that (5) is correct, by showing that it satisfies the partial differential equation (4). Hence the r.h.s. of (5) may differ from the required result only by a function of b . But by symmetry it thus differs only by a function of a , and hence only by a constant. Since the r.h.s. and l.h.s. both vanish when $c = 0$, the constant must vanish. Hence (5) is proven to be correct, though no analytical *derivation* of it has yet been obtained. To our knowledge, this is the first time that a lattice algorithm, such as PSLQ, has been used to find a previously unknown solution to a pair of partial differential equations.

We note that one of the 8 dilogarithms in (5) may be removed, using [9]

$$0 = \text{Li}_2(-p/m) + \text{Li}_2(-m/p) + \frac{1}{6}\pi^2 + \frac{1}{2}\log^2(p/m). \quad (7)$$

No further reduction was found by PSLQ, with transcendental values of a and b . With rational values of $\{a, b, c\}$, considerable simplification was obtained. For example

$$224 C(14, 8) = \text{Li}_2\left(\frac{3}{5}\right) + \frac{1}{12}\pi^2 - \log 5 \log \frac{9}{5} \quad (8)$$

was spectacularly reduced by PSLQ to a single dilogarithm. It remains an open question whether (5) may be reduced to fewer than 7 dilogs, in the general case. We suspect not.

2.1 Reduction to Clausen values

The result (5) clearly entails only real dilogarithms when $a^2 + b^2 > 4$. When $a^2 + b^2 < 4$, it may be reduced, by application of Eq (A.2.5.1) of [9], to Clausen values of the form

$$\text{Cl}_2(\theta) := - \int_0^\theta d\phi \log \left| 2 \sin \frac{1}{2}\phi \right| = \sum_{n>0} \frac{\sin(n\theta)}{n^2}. \quad (9)$$

Since the imaginary part of a dilog yields 3 Clausen values, plus the product of an angle and log, the result (5) might be expected to be rather complicated, involving up to 16 terms. Transforming to the regime where $\gamma := \sqrt{4 - a^2 - b^2}$ is real, one finds that

$$\begin{aligned} \frac{1}{16} ab\gamma C(a, b) &= \frac{1}{2} \{ \text{Cl}_2(4\phi) + \text{Cl}_2(2\phi_a + 2\phi_b - 2\phi) + \text{Cl}_2(2\phi_a - 2\phi) + \text{Cl}_2(2\phi_b - 2\phi) \\ &\quad - \text{Cl}_2(2\phi_a + 2\phi_b - 4\phi) - \text{Cl}_2(2\phi_a) - \text{Cl}_2(2\phi_b) - \text{Cl}_2(2\phi) \} \end{aligned} \quad (10)$$

is log-free and involves only 8 Clausen values, with arguments formed from

$$\phi := \arctan \frac{\gamma}{a+b+2}, \quad \phi_a := \arctan \frac{\gamma}{a}, \quad \phi_b := \arctan \frac{\gamma}{b}, \quad (11)$$

which are related by

$$\cos \phi_a \cos \phi_b = \cos(\phi_a + \phi_b - 2\phi). \quad (12)$$

The freedom from logs is highly non-trivial, entailing the multiplicative relation

$$\left(1 - \frac{4}{m}\right) \left(1 - \frac{4}{p}\right) = \left(1 - \frac{m}{a+2}\right) \left(1 - \frac{m}{b+2}\right) \left(1 - \frac{p}{a+2}\right) \left(1 - \frac{p}{b+2}\right) \quad (13)$$

between 6 of the arguments of the 8 dilogarithms of (5). Had it been known in advance that neither (5) nor (10) entails logs, while each reduces to only 8 terms, the process of constructing a viable symmetric Ansatz would have been greatly simplified. We offer this observation as a guide to future work.

2.2 The symmetric tetrahedron

To obtain a result for $C(1, 1)$, we use the specific values of the angles (11), namely $\phi = \alpha$, $\phi_a = \phi_b = \frac{1}{4}\pi + \frac{1}{2}\alpha$, with $\alpha := \arcsin \frac{1}{3}$ appearing as the only non-trivial angle, by virtue of (3). Then using $\text{Cl}_2(\pi) = 0$, and the general identity [9]

$$\frac{1}{2}\text{Cl}_2(\pi - 2\alpha) = \text{Cl}_2\left(\frac{1}{2}\pi - \alpha\right) - \text{Cl}_2\left(\frac{1}{2}\pi + \alpha\right), \quad (14)$$

one finds that only the first and last terms in (10) survive, giving

$$\frac{C(1,1)}{8\sqrt{2}} = \frac{1}{2} \{\text{Cl}_2(4\alpha) - \text{Cl}_2(2\alpha)\} \approx 0.01537, \quad (15)$$

in agreement with (2). The tiny value will be seen to be significant.

3 Connection to 1-loop diagrams

In [6], Andrei Davydychev and Bob Delbourgo considered an apparently very different problem, namely the massive 1-loop box diagram in 4 dimensions, which yields a result uncannily similar to (5,10), in the case of a common mass on the internal lines and a common norm for the external 4-momenta. Then there are three kinematic variables, which may be taken as Mandelstam's $\{s, t, u\}$. The internal mass provides the scale, here set to unity. In certain kinematic regimes, $\{s, t, u\}$ may be transformed to the 3 non-trivial dihedral angles, $\{\psi_1, \psi_2, \psi_3\}$, of a bi-rectangular tetrahedron in a 3-space of constant curvature [6]. This is one of the 4 congruent parts that result from dissection of a tetrahedron with a symmetry that derives from the common internal mass. The result then entails its volume, which is a Schläfli [14, 15] function.

After the results (5) and (10), for the 3-loop vacuum diagram, were communicated to Andrei Davydychev, he made the intriguing suggestion that (10), for the case $a^2 + b^2 < 4$, might be reducible from 8 real Clausen values to 7, as is the case [6] for the box diagram, in restricted kinematic regimes. If this were the case, one might hope to cap the ‘magic’ feat in [16], where a 2-loop vacuum diagram was transformed to a massless 1-loop triangle diagram, in a dimension differing by 2 units. In the present case, such a conjuring act would entail a more remarkable connection, between diagrams whose loop numbers differ by 2, while their spacetime dimensions differ only by unity. We now examine this issue.

3.1 Geometric and non-geometric boxes

From [6], we obtained a simple conversion of $\{s, t, u\}$ to $\{\psi_1, \psi_2, \psi_3\}$ as follows. Let

$$v := \frac{4}{s}, \quad w := \frac{4}{t}, \quad x := \frac{8}{s + t + u - 8} \quad (16)$$

be a re-parametrization of Mandelstam space. Then the dihedral angles satisfy

$$\frac{1-w}{\tan^2 \psi_1} = \frac{\tan^2 \psi_2}{1-x^2} = \frac{1-v}{\tan^2 \psi_3} = \frac{1}{\tan^2 \delta} = G := \frac{vw}{x^2} - (1-v)(1-w) \quad (17)$$

where G derives from a Gram determinant and δ is an auxiliary angle, with

$$\tan \delta \cos \psi_1 \cos \psi_3 = D(\psi_1, \psi_2, \psi_3) := \sqrt{\cos^2 \psi_2 - \sin^2 \psi_1 \sin^2 \psi_3}. \quad (18)$$

The box diagram evaluates to

$$B(s, t, u) := \frac{N(\psi_1, \psi_2, \psi_3)}{D(\psi_1, \psi_2, \psi_3)}, \quad (19)$$

with a numerator that is a Schläfli function [6]:

$$N(\psi_1, \psi_2, \psi_3) := \frac{1}{2} \{ \text{Cl}_2(2\psi_1 + 2\delta) - \text{Cl}_2(2\psi_1 - 2\delta) + \text{Cl}_2(2\psi_3 + 2\delta) - \text{Cl}_2(2\psi_3 - 2\delta) \\ - \text{Cl}_2(\pi - 2\psi_2 + 2\delta) + \text{Cl}_2(\pi - 2\psi_2 - 2\delta) + 2\text{Cl}_2(\pi - 2\delta) \}. \quad (20)$$

When $\{1-v, 1-w, 1-x^2, G\}$ are all positive, $\{\psi_1, \psi_2, \psi_3, \delta\}$ are all real and (20) is 4 times the volume of a bi-rectangular tetrahedron in hyperbolic space, since the full tetrahedron may be dissected into 4 congruent bi-rectangular parts [6].

In the case that $\{1-v, 1-w, 1-x^2, G\}$ are all negative, δ is imaginary, while $\{\psi_1, \psi_2, \psi_3\}$ are real. Then both the numerator and denominator of (19) are pure imaginary and we obtain a geometric interpretation that entails the volume of a tetrahedron in spherical space. For the residual sign possibilities, there is *no* interpretation in terms of real geometry. Indeed, unitarity often requires the amplitude to be complex. Thus vanishing of the Gram determinant of the external momenta, at $G = 0$, is emphatically *not* the signal for the geometry to change from one sign of curvature to the other. If one has a real geometry at some point $\{s, t, u\}$ near $G = 0$, then there is no real geometry at a neighbouring point, with the opposite sign of G , since there (17) forces $\{\psi_1, \psi_2, \psi_3\}$ to be imaginary.

By way of examples of geometric and non-geometric behaviour, we consider $B_0(s, t) := B(s, t, -s-t)$, with light-like external momenta. In the hyperbolic regime, we obtain

$$B_0(4, 4) = 4\text{Cl}_2(\frac{1}{2}\pi), \quad B_0(6, 6) = \frac{5\text{Cl}_2(\frac{1}{3}\pi)}{\sqrt{3}}, \quad B_0(\frac{16}{3}, \frac{16}{3}) = \frac{3\text{Cl}_2(2\alpha) + 6\text{Cl}_2(\frac{1}{2}\pi - \alpha)}{2\sqrt{2}} \quad (21)$$

with the first example giving 4 times Catalan's constant, while the second is a rational multiple of a constant found in the 2-loop 4-dimensional vacuum diagram with 3 equal masses [17], which enjoys a 'magic' connection [16] to a massless 1-loop triangle diagram. The final example entails $\alpha := \arcsin \frac{1}{3}$, though in a manner markedly different from (2).

Non-geometric results are obtainable from the instructive duality relation

$$B_0(s, t) - B_0(\lambda/s, \lambda/t) = \frac{2}{\sqrt{\lambda}} \arccos\left(\frac{s}{2} - 1\right) \text{arccosh}\left(\frac{\lambda}{2s} - 1\right) + \{s \leftrightarrow t\}, \quad (22)$$

with $\lambda := 4s + 4t - st$. It was proven by analytic continuation of (20), after the discovery by PSLQ that

$$B_0(\frac{8}{3}, \frac{8}{3}) - B_0(\frac{16}{3}, \frac{16}{3}) = \frac{3(\frac{1}{2}\pi - \alpha) \log 3}{2\sqrt{2}}, \quad (23)$$

with product terms familiar from [1, 4, 18]. When one box in (22) is geometric, the products of angles and logs show that its dual is not. Since (10) has no such product, it cannot be such a non-geometric box. We now consider whether it might be geometric.

3.2 Obstacles to a single 3-loop vacuum volume

Analytical considerations and numerical investigations, alike, suggest that no geometric interpretation as a single tetrahedral volume, and hence no relation to a single 1-loop diagram, is obtainable for the 3-loop 3-dimensional vacuum diagram $C(a, b)$.

The argument against a real tetrahedral volume in spherical space is compelling: the formula for such a volume involves the real parts of complex Li_2 values [6, 15]. In contrast, our result (5) entails purely real Li_2 values when $a^2 + b^2 > 4$. Thus the simplicity of the vacuum diagram seems to preclude a geometric interpretation in a space of positive curvature, since any such interpretation would be too complicated, analytically speaking.

We argue that there is no interpretation as a single volume in hyperbolic space, for $a^2 + b^2 < 4$. Here we are guided by the fact that all attempts to reduce the Clausen values in (10) from 8 to 7, as would be required by (20), met with abject failure.

Since no-go claims based on analysis are notoriously fallible, we also investigated the situation empirically, using PSLQ. The first step was clear: is there a simple integer relations between the 8 Clausen values in (10)? PSLQ replied with an emphatic *no*, by proving that any integer relation would entail a coefficient in excess of 10^{30} .

Then we considered relations between Clausen values generated by Abel's identity for 5 dilogarithms [9]. Since the imaginary part of a dilogarithm generates 3 Clausen values, the generic relation will entail 15 Clausen values. The symmetric form of the result is

$$0 = \sum_{6 \geq k \geq 1} \theta_k = \sum_{6 \geq k \geq 1} \sin \theta_k \implies 0 = \sum_{6 \geq j > k \geq 1} \text{Cl}_2(\theta_j + \theta_k), \quad (24)$$

with 6 angles, whose values and sines sum to zero, producing 15 Clausen values, which also sum to zero. From (12,24) we derived 3 relations between Clausen values whose arguments are linear combinations of $\{\phi, \phi_a, \phi_b\}$. A pair is formed by

$$\begin{aligned} 0 = & 2\text{Cl}_2(2\phi) - 4\text{Cl}_2(2\phi_b) + \text{Cl}_2(4\phi_b) + 2\text{Cl}_2(2\phi_b - 2\phi) - 2\text{Cl}_2(2\phi_a - 2\phi) \\ & + \text{Cl}_2(2\phi_a - 4\phi) + 2\text{Cl}_2(2\phi_a + 2\phi_b - 2\phi) - \text{Cl}_2(2\phi_a + 4\phi_b - 4\phi) \end{aligned} \quad (25)$$

and its $a \leftrightarrow b$ transform, while the third is symmetric:

$$\begin{aligned} 0 = & 2\text{Cl}_2(2\phi) - 2\text{Cl}_2(2\phi_a - 2\phi) - 2\text{Cl}_2(2\phi_b - 2\phi) + \text{Cl}_2(2\phi_a - 4\phi) + \text{Cl}_2(2\phi_b - 4\phi) \\ & - 2\text{Cl}_2(2\phi_a + 2\phi_b - 2\phi) + 2\text{Cl}_2(2\phi_a + 2\phi_b - 4\phi) - \text{Cl}_2(4\phi_a + 4\phi_b - 8\phi) \\ & + \text{Cl}_2(2\phi_a + 4\phi_b - 4\phi) + \text{Cl}_2(4\phi_a + 2\phi_b - 4\phi). \end{aligned} \quad (26)$$

The next step was to engage PSLQ to search for more relations. At the arbitrarily chosen transcendental point $a = \exp(-1)$, $b = 1/\pi$, we computed, to 360-digit precision, 44 Clausen values of the form $\text{Cl}_2(2j\phi_a + 2k\phi - 2n\phi)$, with non-negative integers bounded by $j < 3$, $k < 3$, $n < 5$, $j + k + n > 0$. PSLQ found only the 3 known relations. Moreover, it proved that any other relation would involve an integer in excess of 10^5 . Enlarging the search space to include angles in which the coefficients of ϕ_a and ϕ_b differ in sign, we found no new relation. It is easy to show that the 3 proven relations do not enable a reduction of (10) to less than 8 Clausen values. Hence, a reduction to 7 real Clausen values, as required for a single Schläfli function, would seem to require a non-linear transformation of angles, for which we have seen no precedent.

3.3 Reduction of diagrams to ideal tetrahedra

The difficulty in relating (10) to a geometric box is more apparent when one writes it in terms of *differences* of volumes of ideal hyperbolic tetrahedra. An ideal tetrahedron has all its vertices at infinity and is specified by 2 dihedral angles, θ_1 and θ_2 , at adjacent edges. The dihedral angle at the edge adjacent to these is $\theta_3 := \pi - \theta_1 - \theta_2$. Each remaining edge has a dihedral angle equal to that at its opposite edge. The volume of such a ideal tetrahedron is [6]

$$V(\theta_1, \theta_2) := \frac{1}{2} \sum_{k=1}^3 \text{Cl}_2(\theta_k) = \frac{1}{2} \{ \text{Cl}_2(2\theta_1) + \text{Cl}_2(2\theta_2) - \text{Cl}_2(2\theta_1 + 2\theta_2) \}. \quad (27)$$

Thus (10) may be written, rather neatly, as

$$\frac{1}{16} ab\gamma C(a, b) = V(\phi, \psi_a) + V(\phi, \psi_b) - V(\phi, \psi_a + \psi_b) - V(\phi, \phi), \quad (28)$$

where $\psi_{a,b} := \phi_{a,b} - \phi$ are confined to the interval $[\phi, \pi/2 - \phi]$, with ϕ confined to $[0, \pi/4]$. Similarly, the box volume (20) may be written as

$$\begin{aligned} N(\psi_1, \psi_2, \psi_3) &= V(\delta + \psi_1, \delta - \psi_1) + V(\delta + \psi_3, \delta - \psi_3) \\ &+ V(\frac{1}{2}\pi + \psi_2 - \delta, \frac{1}{2}\pi - \psi_2 - \delta) + V(\frac{1}{2}\pi - \delta, \frac{1}{2}\pi - \delta) \end{aligned} \quad (29)$$

with the auxiliary angle δ given by (18).

Both the vacuum result (28) and the box volume (29) are non-negative, in their hyperbolic regimes, where the angles are real. Now we consider their zeros and maximum values. The box volume (29) vanishes only for $\cos \psi_2 = \sin \psi_1 \sin \psi_3$, where the denominator (18) of the diagram vanishes, at the boundary of the hyperbolic regime. The maximum volume is $N(0, 0, 0) = 4\text{Cl}_2(\pi/2)$, achieved in the case of the box diagram $B_0(4, 4)$ in (21), with $D(0, 0, 0) = 1$. In contrast, the vacuum diagram yields a combination (28) of ideal tetrahedral volumes that vanishes at $b = 0$, where $\psi_a = \phi$ and $\psi_b = \frac{1}{2}\pi - \phi$, with the last term cancelling the first, and the third cancelling the second; and at $a = 0$, with the last cancelling the second, and the third cancelling the first; and at $\gamma = 0$, where all terms vanish separately. Its maximum value occurs at the totally symmetric point $a = b = 1$, where (15) gives a combination of volumes that is more than 200 times smaller than the maximum volume, $N(0, 0, 0) = 3.66386237$, achieved by the box.

From the above, the difficulty of relating the vacuum diagram to a box is glaring. The geometric insight of [6] led to the conclusion that every 4-dimensional 1-loop box diagram may be evaluated by dissecting¹ its associated volume into no more than 6 bi-rectangular parts, each given by a Schläfli function. We have shown that the addition and subtraction of ideal tetrahedra, entailed by the vacuum diagram in (28), leads to net volumes that are, typically, two orders of magnitude smaller than the volumes associated with a box diagram, via the additions in (29).

Yet there *is* a remarkably strong connection between 3-loop vacuum diagrams and 1-loop boxes: both entail *combinations* of volumes of ideal tetrahedra. We have show this

¹We discount the possibility that this dissection might entail subtraction of bi-rectangular volumes in the totally symmetric case (15).

for the vacuum diagram (27). In the more complicated case of an arbitrary box diagram, one may obtain up to 24 ideal tetrahedra, with each of the 6 bi-rectangular constituents [6] of a general tetrahedron yielding 4 ideal tetrahedra, via (29). Moreover every such ideal tetrahedron equates to a massless 1-loop triangle diagram [6, 16].

We conclude that 3-loop 3-dimensional vacuum diagrams and 1-loop 4-dimensional boxes do not equate, directly. Rather, they share a common reduction, via hyperbolic geometry, to 1-loop massless 4-dimensional triangle diagrams, i.e. ideal tetrahedra.

4 Hyperbolic manifolds from multi-loop diagrams

The box-diagram value $B_0(4, 4) = N(0, 0, 0) = 4\text{Cl}_2(\pi/2) = 3.66386237$ is familiar in an apparently quite different context: it is the hyperbolic volume complementary to Whitehead's 2-component link, with 5 crossings [19]. Like the majority of knots and links, this link is hyperbolic, which means that the 3-manifold complementary to it admits a metric of constant negative curvature. The volume of this hyperbolic manifold is then an invariant [20] associated with the link. The Borromean rings have a volume twice as large, namely 8 times Catalan's constant. Moreover, the numerator $N(\pi/4, 0, \pi/4) = \frac{5}{2}\text{Cl}_2(\pi/3)$ of the box diagram $B_0(6, 6)$ in (21) is a rational multiple of the volume, $2\text{Cl}_2(\pi/3) = 2.02988231$, of the figure-8 knot, which is the unique knot with 4 crossings.

The common analytical feature of such link invariants and the Feynman diagrams of this paper is the volume, (27), of an ideal tetrahedron. It may be regarded as a real-valued function of a single complex variable [21]:

$$\mathcal{V}(z) := \Im \{ \text{Li}_2(z) + \log |z| \log(1 - z) \} = V(\arg(z), -\arg(1 - z)) \quad (30)$$

with dihedral angles that are the arguments of $\{z, 1/(1 - z), 1 - 1/z\}$. The symmetries

$$\mathcal{V}(1 - z) = \mathcal{V}(1/z) = \mathcal{V}(\bar{z}) = -V(z), \quad (31)$$

where \bar{z} is the complex conjugate of z , imply that $\{z, 1/\bar{z}, 1/(1 - z), 1 - \bar{z}, 1 - 1/z, \bar{z}/(\bar{z} - 1)\}$ all give the same value for (30), while their conjugates give a result differing only in sign. The hyperbolic volume of a knot or link is expressible as a finite number of ideal terms of the form (30), with arguments that result from complex roots of polynomials [19, 20]. For example, the volume of the figure-8 knot is $2\mathcal{V}(z)$, with $z(1 - z) = 1$, while the volume of the Borromean rings is $8\mathcal{V}(z)$, with $z(1 - z) = \frac{1}{2}$. The sole hyperbolic 5-crossing knot, 5_2 , has a volume, 2.8281220, given by $3\mathcal{V}(z)$, with $z^3 = z - 1$. This cubic gives the relation $3\theta_1 + \theta_2 = \pi$ between the dihedral angles in (30). We shall meet it again, at 12 crossings, in the context of 8-loop quantum field theory.

4.1 Positive hyperbolic knots at 7 loops

In [7], Dirk Kreimer and I considered knots with up to 15 crossings, classifying the numerical content of field-theory counterterms up to 9 loops. An account of the wider issues

is provided by [22]. The knots in question are all positive, i.e. their minimal braidwords involve only positive powers of the generators, σ_k , of the braid group [23]. A consequence is that no hyperbolic knot is encountered in the analysis of diagrams with less than 7 loops, where only torus knots are encountered. At the 7-loop level one encounters two 10-crossing knots that are both positive and hyperbolic, with braidwords $10_{139} = \sigma_1\sigma_2^3\sigma_1^3\sigma_2^3$ and $10_{152} = \sigma_1^2\sigma_2^2\sigma_1^3\sigma_2^3$, offering the first possibility to study the reduction to ideal tetrahedra of knots implicated by counterterms. Numerical triangulations were obtained, at 12-digit accuracy, from Jeff Weeks' program SnapPea [24]. We then used PSLQ to identify the relevant polynomials, whose roots were extracted to 50 digits, giving

$$V_{10_{139}} = 4.85117075733273756705832705211531247884528302776999 \quad (32)$$

$$V_{10_{152}} = 8.53606534720560860314418192054932599496499139691401 \quad (33)$$

as the volumes of the positive 10-crossing knots. SnapPea identified the manifold complementary to 10_{139} as isometric to entry m389 in its census. Its volume coincides with that of m391, for the 8-crossing 2-component link labelled 8_2^2 in the appendices of [19] and [25]. The manifold complementary to 10_{152} has a volume greater than any in SnapPea's census of 6,075 cusped manifolds triangulated by not more than 7 tetrahedra.

We found that (32) results from a remarkably simple triangulation,

$$V_{10_{139}} = 4\mathcal{V}(z) + \mathcal{V}(z^2 + 1); \quad z^2 + 1 = z^2(z - 1)^2, \quad (34)$$

with a matching condition that makes the dihedral angles of the second term linear combinations of those of the first. This simplicity is in marked contrast to

$$V_{10_{152}} = \mathcal{V}(z) + 2\mathcal{V}(z + 1) + \mathcal{V}(2z - z^2) + \mathcal{V}(z^2(z - 1)^2) + 4\mathcal{V}\left(\frac{2z - 1}{2z - z^2}\right);$$

$$z(2z - z^2)^2 = (z + 1)^2(z - 1), \quad (35)$$

whose quintic produces 15 distinct Clausen values, with angles reducible to linear combinations of the arguments of $\{z^2, (z + 1)^2, (z - 1)^2, (2z - 1)^2\}$. The simpler form of (34), with only 2 distinct tetrahedra, and only 2 linearly independent angles, accords with the experience of [26], where it was found that 10_{139} is simpler than 10_{152} in the field-theory context, since it is more readily obtained from the skeining of link diagrams that encode the intertwining of momenta in 7-loop diagrams.

4.2 Positive hyperbolic knots at 8 loops

Observing the contrasting reductions (34,35) to ideal volumes, we proceeded to 12 crossings, relevant to 8-loop counterterms [7]. Work with John Gracey and Dirk Kreimer [8] had focussed on a pair of positive hyperbolic knots, $12_A := \sigma_1\sigma_2^7\sigma_1\sigma_2^3$ and $12_B := \sigma_1\sigma_2^5\sigma_1\sigma_2^5$, one of which is associated with the appearance of the irreducible [27, 28, 29] double Euler sum $\zeta_{9,3} := \sum_{j>k>0} j^{-9}k^{-3}$ in counterterms, while the other relates to a quadruple sum that cannot be reduced to simpler non-alternating sums, and was found in [29] to entail the alternating Euler sum $U_{9,3} := \sum_{j>k>0} (-1)^{j+k} j^{-9}k^{-3}$. In [8] we tentatively identified

12_A as the knot associated with $\zeta_{9,3}$, by study of counterterms in the large- N limit, at $O(1/N^3)$, where $\zeta_{9,3}$ occurs, but $U_{9,3}$ is absent. Thus we expect 12_A to have a simpler reduction to ideal tetrahedra than that for 12_B .

This expectation was notably confirmed by computation, which gave the volumes

$$V_{12_A} = 2.82812208833078316276389880927663494277098131730065 \quad (36)$$

$$V_{12_B} = 5.91674573518278869527226015189683245321707317046868 \quad (37)$$

with triangulations that SnapPea identified with the manifolds m016 and v2642. The result for $12_A := \sigma_1 \sigma_2^7 \sigma_1 \sigma_2^3$ is indeed rather special: the volume is equal to that of manifold m015, for the hyperbolic knot with 5 crossings²:

$$V_{12_A} = V_{5_2} = 3\mathcal{V}(z); \quad z^3 = z - 1. \quad (38)$$

Equalities between volumes of hyperbolic knots are rare, with none occurring at less than 10 crossings. It is intriguing that the knot 12_A , identified with $\zeta_{9,3}$ in [8], has a triangulation as simple as that for the knot 5_2 . By contrast the result for $12_B := \sigma_1 \sigma_2^5 \sigma_1 \sigma_2^5$,

$$\begin{aligned} V_{12_B} &= 4V(\psi_1, \psi_2) + V(2\psi_1, 2\psi_1 + 2\psi_2) + 2V(3\psi_1 + \psi_2, \psi_1 - \psi_2); \\ &\psi_1 = \arg(z); \quad \psi_2 = -\arg(1 - z); \quad 4z^4 = 2z^2 - 2z + 1, \end{aligned} \quad (39)$$

involves 9 distinct Clausen values, with angles coming from the solution to a quartic. As before, the relative ease with which positive hyperbolic knots are obtained from Feynman diagrams is reflected by the relative simplicity of their triangulations. As further confirmation of this trend, we cite the cases of the remaining 5 positive knots with 12 crossings, which were not obtained from skeining counterterms in [8], nor related to Euler sums in [7]. Their volumes exceed that of (37), ranging from 7.40 to 13.64, with commensurately complicated triangulations.

It thus appears that Feynman diagrams entail positive knots that are either not hyperbolic, as in the case of torus knots, which suffice through 6 loops, or ‘marginally’ hyperbolic, with a small volume, related to a relatively simple triangulation.

4.3 A simple hyperbolic volume at infinite loops

We now study the volume, V_{2n} , of the positive $2n$ -crossing knot $K_{2n} := \sigma_1 \sigma_2^{2n-5} \sigma_1 \sigma_2^3$, related to double Euler sums of weight $2n$ in counterterms at $n + 2 \geq 6$ loops [7, 8]. We found that this volume is bounded, as $n \rightarrow \infty$.

Since $K_8 = 8_{19}$ and $K_{10} = 10_{124}$ are the (4,3) and (5,3) torus knots, $V_8 = V_{10} = 0$. At 12 crossings, $V_{12} := V_{12_A}$ is given by (36,38); the appendix of [19] shows that no hyperbolic knot from 6 through 9 crossings has a volume as small as this. We found that K_{14} , with manifold m223, has the same volume, 4.12490325, as $8_{20} = \sigma_1 \sigma_2^{-3} \sigma_1 \sigma_2^3$, with manifold m222. In general, the volume of the $2n$ -crossing positive knot $K_{2n} := \sigma_1 \sigma_2^{2n-5} \sigma_1 \sigma_2^3$, with

²Section 5.3 of [19] gives an excellent introduction to hyperbolic knots. Unfortunately, Fig 5.29 is misdrawn, depicting $\sigma_1 \sigma_2^{-7} \sigma_1 \sigma_2^3$, with manifold v0960, instead of the positive knot $12_A := \sigma_1 \sigma_2^7 \sigma_1 \sigma_2^3$.

$2n \geq 12$, coincides with that of the non-positive knot $\sigma_1\sigma_2^{11-2n}\sigma_1\sigma_2^3$, formally obtained by $n \rightarrow 8 - n$, and hence having a crossing number that cannot exceed $2n - 6$.

The manifolds of K_{16} and K_{18} were identified as s384 and v0959, triangulated by 6 and 7 tetrahedra, respectively; their volumes are not much larger than that of K_{14} . Moreover, the trend of

$$\begin{array}{ll}
V_{14} = 4.124903252 & V_{30} = 5.227842810 \\
V_{16} = 4.611961374 & V_{32} = 5.244429225 \\
V_{18} = 4.854663387 & V_{34} = 5.257409836 \\
V_{20} = 4.993271973 & V_{36} = 5.267755714 \\
V_{22} = 5.079718733 & V_{38} = 5.276132543 \\
V_{24} = 5.137154054 & V_{40} = 5.283008797 \\
V_{26} = 5.177195133 & V_{42} = 5.288721773 \\
V_{28} = 5.206190226 & V_{44} = 5.293519248
\end{array} \tag{40}$$

suggests an asymptotic value

$$\begin{aligned}
V_\infty &= 3\text{Cl}_2(2\omega) - 3\text{Cl}_2(4\omega) + \text{Cl}_2(6\omega) \\
&= 5.33348956689811958159342492522130008819676777710528
\end{aligned} \tag{41}$$

with $\omega := \arctan \sqrt{7}$, which is equal to the volume

$$V_{(\sigma_1^2\sigma_2^{-1})^2} = 4\mathcal{V}(z) + 2\mathcal{V}(2z); \quad 2z^2 = 3z - 2 \tag{42}$$

of manifold s776, complementary to the 6-crossing 3-component link $6_1^3 := (\sigma_1^2\sigma_2^{-1})^2$. To test (41), we used SnapPea to evaluate volumes for a selection of crossing numbers from 50 up to 500, corresponding to counterterms with up to 252 loops. The tight bounds

$$\left(\frac{1}{4}n - 1\right)^2 \{V_\infty - V_{2n}\} \in [0.811, 0.816]; \quad 2n \in [50, 500], \tag{43}$$

make a compelling case for the asymptotic behaviour

$$V_{2n} = V_\infty - \frac{C}{\left(\frac{1}{4}n - 1\right)^2} + O(n^{-4}), \tag{44}$$

with an invariance under $n \rightarrow 8 - n$, noted above, and a constant $C = 0.8160 \pm 0.0001$.

Thus we come full circle, from an infinite number of loops back to a 1-loop result, since (41) relates directly to a 1-loop box, with

$$V_\infty = V_{(\sigma_1^2\sigma_2^{-1})^2} = 3N\left(\frac{1}{3}\pi, 0, \frac{1}{3}\pi\right) = \frac{3}{4}\sqrt{7}B_0(7, 7) \tag{45}$$

being 3 times the volume of the light-like equal-mass box diagram of Section 3.1, at $s = t = 7$. This complements the link invariants obtained at $s = t = 4$ and $s = t = 6$ in (21). Moreover, the 12-crossing 3-component link $(\sigma_1^2\sigma_2^{-2})^3$ has a volume

$$\begin{aligned}
V_{(\sigma_1^2\sigma_2^{-2})^3} &= 6N\left(\frac{1}{6}\pi, 0, \frac{1}{6}\pi\right) = \frac{3}{2}\sqrt{15}B_0(5, 5) \\
&= 18.83168336678760750554026296116895115755581340126291
\end{aligned} \tag{46}$$

which is 6 times the volume of the box diagram at $s = t = 5$. Thus we now have 4 relations between Feynman diagrams and link invariants.

1. The volume of the figure-8 knot, 4_1 , is $2\text{Cl}_2(\pi/3) = \frac{4}{5}N(\pi/4, 0, \pi/4)$. This Clausen value occurs in the 2-loop equal-mass vacuum diagram [17], the 1-loop massless triangle diagram at its symmetric point [16], and the equal-mass light-like box diagram of [6] at $s = t = 6$.
2. The volumes of the Whitehead link, 5_1^2 , and the Borromean rings, $6_2^3 := (\sigma_1\sigma_2^{-1})^3$, are multiples of Catalan's constant, $\text{Cl}_2(\pi/2) = \frac{1}{4}N(0, 0, 0)$. This Clausen value results at the simultaneous threshold values $s = t = 4$ of the box.
3. At $s = t = 5$ we obtain the volume of the link $(\sigma_1^2\sigma_2^{-2})^3$ in (46).
4. At $s = t = 7$ we obtain the volume of the link $6_1^3 := (\sigma_1^2\sigma_2^{-1})^2$ in (45). This is also the infinite-loop limit of the hyperbolic volumes of the knots $\sigma_1\sigma_2^{2n-5}\sigma_1\sigma_2^3$, associated in [7, 8] with the appearance in counterterms [22, 26], at $n + 2 \geq 6$ loops, of irreducible double Euler sums [29, 31] of weight $2n$.

There are further cases of knots and links whose volumes entail a single Schläfli function, and hence a single box diagram. Harnessing PSLQ to SnapPea, we obtained

$$\begin{aligned} V_{9_{41}} &= 10N\left(\frac{2}{5}\pi, \frac{1}{10}\pi, \frac{1}{5}\pi\right) = 10\text{Cl}_2\left(\frac{2}{5}\pi\right) + 5\text{Cl}_2\left(\frac{4}{5}\pi\right) \\ &= 12.09893602599078738356455696387624160295557377848341 \end{aligned} \quad (47)$$

$$\begin{aligned} V_{10_{123}} &= 10N\left(\frac{3}{10}\pi, \frac{1}{5}\pi, \frac{1}{10}\pi\right) = 15\text{Cl}_2\left(\frac{2}{5}\pi\right) + 5\text{Cl}_2\left(\frac{4}{5}\pi\right) \\ &= 17.08570948298286127690097484048365482503835960943063 \end{aligned} \quad (48)$$

for the volumes of the knots 9_{41} and 10_{123} , and

$$\begin{aligned} V_{(\sigma_1^2\sigma_2^{-1})^3} &= 6N\left(\frac{1}{4}\pi, \frac{1}{6}\pi, \frac{1}{4}\pi\right) \\ &= 12.04609204009437764726837862923359423099605804944500 \end{aligned} \quad (49)$$

$$\begin{aligned} V_{(\sigma_1\sigma_2^{-2}\sigma_3\sigma_2^{-2})^2} &= 6N\left(\frac{1}{6}\pi, \frac{1}{6}\pi, \frac{1}{6}\pi\right) \\ &= 16.59129969483175048405984013396780188163367504042159 \end{aligned} \quad (50)$$

for the 9-crossing 2-component link $9_{40}^2 := (\sigma_1^2\sigma_2^{-1})^3$ and the 12-crossing 4-component link $(\sigma_1\sigma_2^{-2}\sigma_3\sigma_2^{-2})^2$. At 8 crossings, we found that

$$\begin{aligned} V_{8_{18}} &= 3\text{Cl}_2(2\beta) + 12\text{Cl}_2\left(\frac{1}{2}\pi + \beta\right) \\ &= 12.35090620915820017473630443842615201419925670412000 \end{aligned} \quad (51)$$

$$\begin{aligned} V_{8_{21}} &= \frac{1}{2}V_\infty + \frac{1}{3}V_{8_{18}} \\ &= 6.783713519835126515708813942086034048831469456592638 \end{aligned} \quad (52)$$

with $\beta := \arcsin \frac{\sqrt{2}-1}{2}$. Integer relations between volumes, as in (52), appear to be fairly common; we cite $V_{7_6^2} = V_\infty + V_{5_1^2}$ as another example, with the infinite-loop limit of the knots of [7] here appearing as the difference in volume of a pair of 2-component links.

5 Conclusions

The volumes of ideal hyperbolic tetrahedra play (at least) 6 roles in field theory.

1. They result from the evaluation of 3-loop 3-dimensional vacuum diagrams, where their volumes tend to cancel, making the maximum [1] value (15) remarkably small.
2. They also result from 1-loop 4-dimensional box diagrams [6], where their volumes tend to add, giving $O(10^2)$ times the volume of 3-loop vacuum diagrams.
3. Each ideal volume corresponds to a massless 1-loop triangle diagram [6].
4. Each ideal volume also corresponds to a massive 2-loop vacuum diagram [16].
5. The ease with which the volume of a positive hyperbolic knot is reduced to ideal volumes is indicative of the ease with which the knot results from skeining momentum flow in counterterms [22, 26].
6. The family of knots $\sigma_1\sigma_2^{2n-5}\sigma_1\sigma_2^3$, associated with multiple zeta values [27, 29] in counterterms [7, 8] at $n + 2 \geq 6$ loops, yields a hyperbolic volume, at infinite loops, which is 3 times that for a simple 1-loop box.

Conclusion 1 was obtained via (5), for a 3-loop vacuum diagram, with 3 distinct masses, in 3 dimensions. Its analytic continuation to the hyperbolic regime, $a^2 + b^2 < 4$, is given by (10), which may be expressed, as in (28), in terms of 4 volumes of ideal tetrahedra, 2 of which enter with minus signs. Conclusions 2–4 result from the work in [6, 16], which we here extended by exposing the duality relation (22) and showing how the additions in (29), for box diagrams, tend to produce results two orders of magnitude greater than those from the cancellations in (28), for 3-loop vacuum diagrams. Conclusion 5 is based on contrasting (34) with (35), at 7 loops, and (38) with (39), at 8 loops. Conclusion 6 is based on the strong numerical evidence (43) for the asymptote (45), corresponding to the volume of the link $6_1^3 := (\sigma_1^2\sigma_2^{-1})^2$, which is 3 times that of the light-like equal-mass box diagram at $s = t = 7$.

The discovery (5), which sparked these hyperbolic connections, is now proven, though it was not derived, in the traditional sense; instead it was inferred by numerical investigation and then verified by routine differentiation w.r.t. masses. Similarly empirical methods led to (22,45). Such procedures prompt a question: what is served by mathematical proof? The result (2) was discovered in [1] at modest numerical precision, and then checked to 1,000 digits. There was no shadow of doubt that it was correct, though unproven. Now it is proven, yet by a method as thoroughly empirical as that which enabled its discovery. More important than the proof itself is the route to it, since discovery of (5), with 3 distinct masses, provides fertile ground for conjectures on behaviour with more mass scales, or in 4 dimensions. A comparable situation was apparent in [4, 18], where the results themselves, again from PSLQ, were more illuminating than the *post hoc* proofs found for some of them. As Michael Atiyah has remarked [32]: if possession is nine tenths of the law, discovery is nine tenths of the proof.

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