

Elliptic integral evaluations of Bessel moments and applications

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Abstract

We record and substantially extend what is known about the closed forms for various Bessel function moments arising in quantum field theory, condensed matter theory and other parts of mathematical physics. In particular, we develop formulae for integrals of products of six or fewer Bessel functions. In consequence, we are able to discover and prove closed forms for $c_{n,k} := \int_0^\infty t^k K_0^n(t) dt$ with integers $n = 1, 2, 3, 4$ and $k \geq 0$, obtaining new results for the even moments $c_{3,2k}$ and $c_{4,2k}$. We also derive new closed forms for the odd moments $s_{n,2k+1} := \int_0^\infty t^{2k+1} I_0(t) K_0^{n-1}(t) dt$ with $n = 3, 4$ and for $t_{n,2k+1} := \int_0^\infty t^{2k+1} I_0^2(t) K_0^{n-2}(t) dt$ with $n = 5$, relating the latter to Green functions on hexagonal, diamond and cubic lattices. We conjecture the values of $s_{5,2k+1}$, make substantial progress on the evaluation of $c_{5,2k+1}$, $s_{6,2k+1}$ and $t_{6,2k+1}$ and report more limited progress regarding $c_{5,2k}$, $c_{6,2k+1}$ and $c_{6,2k}$.

In the process, we obtain 8 conjectural evaluations, each of which has been checked to 1200 decimal places. One of these lies deep in 4-dimensional quantum field theory and two are probably provable by delicate combinatorics. There remains a hard core of five conjectures whose proofs would be most instructive, to mathematicians and physicists alike.

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1 Introduction

As we shall show in this paper, integrals of products of Bessel functions play a significant role in various parts of physics. Such product integrals have a long history when four-or-fewer Bessel functions are engaged, and they become increasingly challenging to evaluate as the number increases. Moreover, these physically meaningful integrals have remarkable liaison with analytic number theory; this is largely because many can be evaluated in terms of elliptic integrals at singular values, as we discuss below. This interplay of physical and mathematical ideas provides a substantial test-bed for the techniques of experimental mathematics.

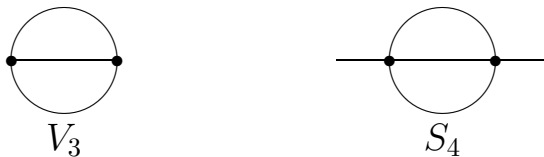
We present here a large collection of evaluations of these integrals, many of them explicitly in terms of well-known constants, and others given by intriguing expressions connecting disparate topics of modern mathematics and mathematical physics. Virtually all of this material is original. A few of these results were subsequently found, through diligent checking, in earlier published material; we have cited references in such instances.

What we study here are representations of the *vacuum* [35, 56] and *sunrise* [30, 40, 41] diagrams

$$V_n(a_1, \dots, a_n) := \int_0^\infty t \left(\prod_{j=1}^n K_0(a_j t) \right) dt \quad (1)$$

$$S_{n+1}(a_1, \dots, a_n, w) := \int_0^\infty t \left(\prod_{j=1}^n K_0(a_j t) \right) J_0(wt) dt, \quad (2)$$

where all the arguments of V_n and all but the last argument of S_{n+1} are real and positive. Here and below I_0 , J_0 and K_0 are the conventional *Bessel functions* of order zero as in [1, Chapter 15]. These integrals occur in quantum field theories in two spacetime dimensions, where we do not need to regularize ultraviolet divergences. Numbers generated by them are expected to occur in the finite parts of integrals from Feynman diagrams in four spacetime dimensions. To be concrete, we illustrate V_3 and S_4 as follows:



By casting Bessel's differential equation in the form

$$\left(\frac{1}{a} + \frac{d}{da} \right) \frac{d}{da} K_0(at) = t^2 K_0(at)$$

and applying the corresponding differential operator to (1), we may increase the exponent of t in the integrand by steps of 2. But to obtain even powers of t , we need to start with

$$\bar{V}_n(a_1, \dots, a_n) := \int_0^\infty \left(\prod_{j=1}^n K_0(a_j t) \right) dt, \quad (3)$$

which plays no obvious role in quantum field theory. To evaluate the latter form, we found it useful to regard the Fourier transform

$$\bar{S}_{n+1}(a_1, \dots, a_n, w) := \frac{1}{\pi} \int_0^\infty \left(\prod_{j=1}^n K_0(a_j t) \right) \cos(wt) dt, \quad (4)$$

as an analogue of (2).

We shall be especially interested in the moments

$$c_{n,k} := \int_0^\infty t^k K_0^n(t) dt \quad (5)$$

for integers $n \geq 1$ and $k \geq 0$, as studied in [8, 10] and [26, 60].

In [10] these moments arose in the study of Ising-type integrals

$$C_{n,k} = \frac{1}{n!} \int_0^\infty \cdots \int_0^\infty \frac{dx_1 dx_2 \cdots dx_n}{(\cosh x_1 + \cdots + \cosh x_n)^{k+1}},$$

which are linked by

$$C_{n,k} = \frac{2^n}{n! k!} c_{n,k}. \quad (6)$$

In [26, 60] it is proven that for fixed n these moments satisfy a linear recursion for which a simple algorithm exists with coefficients polynomial in k . For example, for $n = 1$ and 2 one easily obtains the closed forms

$$c_{1,k} = 2^{k-1} \Gamma^2\left(\frac{k+1}{2}\right) \quad \text{and} \quad c_{2,k} = \frac{\sqrt{\pi} \Gamma^3\left(\frac{k+1}{2}\right)}{4 \Gamma\left(\frac{k}{2} + 1\right)}, \quad (7)$$

and for $n = 3$ and 4 one obtains the recursions

$$(k+1)^4 c_{3,k} - 2(5k^2 + 20k + 21)c_{3,k+2} + 9c_{3,k+4} = 0 \quad (8)$$

$$(k+1)^5 c_{4,k} - 4(k+2)(5k^2 + 20k + 23)c_{4,k+2} + 64(k+3)c_{4,k+4} = 0. \quad (9)$$

These recursion formulae may be written quite compactly as

$$\sum_{i=0}^M (-1)^i p_{n,i}(k+i+1) c_{n,k+2i} = 0, \quad (10)$$

where $M = \lfloor (n+1)/2 \rfloor$. For instance, for $n = 5$ and 6, we have

$$\begin{array}{ll} p_{5,0}(x) = x^6 & p_{6,0}(x) = x^7 \\ p_{5,1}(x) = 35x^4 + 42x^2 + 3 & p_{6,1}(x) = x(56x^4 + 112x^2 + 24) \\ p_{5,2}(x) = 259x^2 + 104 & p_{6,2}(x) = x(784x^2 + 944) \\ p_{5,3}(x) = 225 & p_{6,3}(x) = 2304x. \end{array} \quad (11)$$

The same recursions apply to the moments

$$s_{n,k} := \int_0^\infty t^k I_0(t) K_0^{n-1}(t) dt \quad (12)$$

for integers $n \geq 3$ and $k \geq 0$, and to

$$t_{n,k} := \int_0^\infty t^k I_0^2(t) K_0^{n-2}(t) dt \quad (13)$$

for integers $n \geq 5$ and $k \geq 0$.

2 Two Bessel functions

The transforms

$$S_2(a, w) = \int_0^\infty t K_0(at) J_0(wt) dt = \frac{1}{a^2 + w^2} \quad (14)$$

$$\bar{S}_2(a, w) = \frac{1}{\pi} \int_0^\infty K_0(at) \cos(wt) dt = \frac{1}{2\sqrt{a^2 + w^2}} \quad (15)$$

give $V_1(a) = 1/a^2$ and $\bar{V}_1(a)/\pi = 1/(2a)$ at $w = 0$. The distributions

$$\int_0^\infty v J_0(vt_1) J_0(vt_2) dv = 2\delta(t_1^2 - t_2^2) \quad (16)$$

$$\frac{2}{\pi} \int_0^\infty \cos(vt_1) \cos(vt_2) dv = \delta(t_1 + t_2) + \delta(t_1 - t_2) \quad (17)$$

(where δ is the Dirac delta distribution) then lead to the evaluations

$$\begin{aligned} V_2(a, b) &= \int_0^\infty t K_0(at) K_0(bt) dt = \int_0^\infty w S_2(a, w) S_2(b, w) dw \\ &= \frac{\log(a/b)}{a^2 - b^2} \end{aligned} \quad (18)$$

$$\begin{aligned} \bar{V}_2(a, b) &= \int_0^\infty K_0(at) K_0(bt) dt = 2\pi \int_0^\infty \bar{S}_2(a, w) \bar{S}_2(b, w) dw \\ &= \frac{\pi}{a+b} \mathbf{K} \left(\frac{a-b}{a+b} \right), \end{aligned} \quad (19)$$

with a *complete elliptic integral* of the first kind,

$$\mathbf{K}(k) := \int_0^{\pi/2} \frac{1}{\sqrt{1 - k^2 \sin^2 \phi}} d\phi, \quad (20)$$

appearing in (19) and a limit intended in (18) when $a = b$. We shall need to refer to the *complementary* integral $\mathbf{K}'(k) := \mathbf{K}(k')$, with $k' := \sqrt{1 - k^2}$. In the case $a \geq b$, this provides a compact alternative form of (19),

$$\bar{V}_2(a, b) = \frac{\pi}{2a} \mathbf{K}'(b/a), \quad (21)$$

obtained by the Landen [3] transformation in [1, 17.3.29].

3 Three Bessel functions

We follow Källén [51, 52] by constructing $S_3(a, b, w)$ from its discontinuity across the cut in the w^2 plane with branch point at $w^2 = -(a+b)^2$, obtaining

$$S_3(a, b, w) = \int_0^\infty t K_0(at) K_0(bt) J_0(wt) dt = \int_{a+b}^\infty \frac{2v D_3(a, b, v)}{v^2 + w^2} dv,$$

with a discontinuity

$$D_3(a, b, c) = \frac{1}{\sqrt{(a+b+c)(a-b+c)(a+b-c)(a-b-c)}}$$

that is completely symmetric in its 3 arguments. The v -integral is easily performed, to give

$$S_3(a, b, w) = 2 \operatorname{arctanh} \left(\sqrt{\frac{w^2 + (a-b)^2}{w^2 + (a+b)^2}} \right) D_3(a, b, iw), \quad (22)$$

and, in particular, the *on-shell* value [40]

$$s_{3,1} = S_3(1, 1, i) := \int_0^\infty t I_0(t) K_0^2(t) dt = L_{-3}(1) = \frac{\pi}{3\sqrt{3}},$$

where

$$L_{-3}(s) := \sum_{n=1}^{\infty} \frac{\chi_{-3}(n)}{n^s} = \sum_{k=0}^{\infty} \left(\frac{1}{(3k+1)^s} - \frac{1}{(3k+2)^s} \right)$$

is the Dirichlet L -function with the real character $\chi_{-3}(n)$ given by the Legendre–Jacobi–Kronecker symbol $(D|n)$ for discriminant $D = -3$.

Nomenclature. We shall refer to the construction of a Feynman amplitude from its discontinuity across a cut as a *dispersive* calculation. Kramers [53] and Kronig [54] founded this approach in studies of the dispersion of light, in the 1920’s. In the 1950’s, the utility of dispersive methods was recognized in particle physics [45, 52, 69]. Cutkosky [31] turned them into a calculus that became a routine part of the machinery of quantum field theory. Barton [20] has given a scholarly and instructive introduction to these techniques.

3.1 The odd moments $s_{3,2k+1}$

By differentiating

$$S_3(1, 1, ix) = \frac{2 \arcsin(x/2)}{x\sqrt{4-x^2}}$$

before setting $x = 1$, we evaluate

$$s_{3,3} = \int_0^\infty t^3 I_0(t) K_0^2(t) dt = \left(\frac{1}{x} + \frac{d}{dx} \right) \frac{dS_3(1, 1, ix)}{dx} \Big|_{x=1} = \frac{4}{3} s_{3,1}$$

and are then able to solve the recursion relation [26, 60] for $s_{3,2k+1}$ by the *closed form*

$$s_{3,2k+1} = \frac{\pi}{3\sqrt{3}} \left(\frac{2^k k!}{3^k} \right)^2 a_k \quad (23)$$

with integers

$$a_k = \sum_{j=0}^k \binom{k}{j}^2 \binom{2j}{j}. \quad (24)$$

Integer sequence (24) begins

$$1, 3, 15, 93, 639, 4653, 35169, 272835, 2157759, 17319837, 140668065, 1153462995 \quad (25)$$

and is recorded¹ as entry A2893 of the on-line version of [66], which gives the recursion

$$(k+1)^2 a_{k+1} - (10k^2 + 10k + 3) a_k + 9k^2 a_{k-1} = 0 \quad (26)$$

¹See <http://www.research.att.com/~njas/sequences/A002893>.

and the generating function

$$I_0^3(2t) = \sum_{k=0}^{\infty} a_k \left(\frac{t^k}{k!}\right)^2. \quad (27)$$

We have verified that recursion (26) reproduces the recursion for (23), which has the same form as for the odd moments in (8). We note that integers a_k were encountered in studies of cooperative phenomena in crystals [36] and also in studies of matrices [43] with entries 0 or 1. In [32, Prop. 2], they are related to enumeration of closed walks in a two-dimensional hexagonal lattice. They also appear in an enumeration of Feynman diagrams [61, Table 2] in quantum chromodynamics, via the constrained sum [18]

$$a_k = \sum_{p+q+r=k} \left(\frac{k!}{p!q!r!}\right)^2$$

that results from the Taylor expansion of I_0^3 .

It is notable that I_0^3 provides a generating function for moments of $I_0K_0^2$. In Section 4 we shall show that I_0^4 generates moments of $I_0K_0^3$.

3.2 The odd moments $c_{3,2k+1}$

Next, we construct

$$\begin{aligned} V_3(a, b, c) &:= \int_0^\infty t K_0(at)K_0(bt)K_0(ct) dt = \int_0^\infty w S_3(a, b, w)S_2(c, w) dw \\ &= \frac{L_3(a, b, c) + L_3(b, c, a) + L_3(c, a, b)}{4} D_3(a, b, c), \end{aligned} \quad (28)$$

with a dilogarithmic function

$$L_3(a, b, c) := \text{Li}_2\left(\frac{(a^2 + b^2 - c^2)D_3(a, b, c) + 1}{(a^2 + b^2 - c^2)D_3(a, b, c) - 1}\right) - \text{Li}_2\left(\frac{(a^2 + b^2 - c^2)D_3(a, b, c) - 1}{(a^2 + b^2 - c^2)D_3(a, b, c) + 1}\right)$$

computed by Davydychev and Tausk [35]. The representation has a removable singularity when $a + b = c$ with the parameters ordered so $0 < a \leq b \leq c$. As we were alerted to by John Zucker (private communication), L'Hospital's rule produces

$$V_3(a, b, a + b) = \frac{a \log(1 + b/a) + b \log(1 + a/b)}{ab(a + b)}.$$

Setting $a = b = c = 1$ in (28), we obtain

$$c_{3,1} = V_3(1, 1, 1) = \frac{3}{4} L_{-3}(2) = \frac{1}{9} \sum_{n=0}^{\infty} \left(\frac{-1}{27}\right)^n \sum_{k=1}^5 \frac{v_k}{(6n + k)^2},$$

where the vector of coefficients $v = [9, -9, -12, -3, 1]$ was discovered (and proven) in the course of investigation of 3-loop vacuum diagrams in 4 dimensions [29].

Similarly,

$$c_{3,3} = L_{-3}(2) - \frac{2}{3}$$

may be obtained by suitable differentiations of (28). Then higher moments $c_{3,2k+1}$ with $k > 1$ may be obtained by using (8). Because of the mixing of $L_{-3}(2)$ with unity, we were unable to write a closed form for their rational coefficients in $c_{3,2k+1}$.

3.3 The even moments $c_{3,2k}$

For even moments, we lack the dispersion relations [20] of quantum field theory and so fall back on the general *Aufbau*

$$\bar{S}_{m+n+1}(a_1, \dots, a_m, b_1, \dots, b_n, w) = \int_{-\infty}^{\infty} \bar{S}_{m+1}(a_1, \dots, a_m, v) \bar{S}_{n+1}(b_1, \dots, b_n, v+w) dv, \quad (29)$$

which follows from the distribution

$$\frac{1}{\pi} \int_{-\infty}^{\infty} \cos(vt_1) \cos((v+w)t_2) dv = \delta(t_1 + t_2) \cos(wt_2) + \delta(t_1 - t_2) \cos(wt_2)$$

obtained from (17) and the expansion $\cos((v+w)t_2) = \cos(vt_2) \cos(wt_2) - \sin(vt_2) \sin(wt_2)$.

In particular, by setting $m = n = 1$ in (29), we evaluate

$$\bar{S}_3(a, b, w) = \frac{1}{\pi} \int_0^{\infty} K_0(at) K_0(bt) \cos(wt) dt = \int_{-\infty}^{\infty} \bar{S}_2(a, v) \bar{S}_2(b, v+w) dv$$

as the complete elliptic integral

$$\bar{S}_3(a, b, w) = \frac{1}{4} \int_{-\infty}^{\infty} \frac{dv}{\sqrt{(a^2 + v^2)(b^2 + (v+w)^2)}} = \frac{\mathbf{K}\left(\sqrt{\frac{w^2 + (a-b)^2}{w^2 + (a+b)^2}}\right)}{\sqrt{w^2 + (a+b)^2}}, \quad (30)$$

and recover the previous result (19) for $\bar{V}_2(a, b) = \pi \bar{S}_3(a, b, 0)$ by setting $w = 0$.

Next, by setting $m = 2$ and $n = 1$ in (29), we write

$$\bar{S}_4(a, b, c, w) = \frac{1}{\pi} \int_0^{\infty} K_0(at) K_0(bt) K_0(ct) \cos(wt) dt = \int_{-\infty}^{\infty} \bar{S}_3(a, b, v) \bar{S}_2(c, v+w) dv$$

as an integral over an elliptic integral

$$\bar{S}_4(a, b, c, w) = \frac{1}{2} \int_{-\infty}^{\infty} \frac{\mathbf{K}\left(\sqrt{\frac{v^2 + (a-b)^2}{v^2 + (a+b)^2}}\right)}{\sqrt{(v^2 + (a+b)^2)((v+w)^2 + c^2)}} dv, \quad (31)$$

and at $w = 0$ obtain

$$\bar{V}_3(a, b, c) := \int_0^{\infty} K_0(at) K_0(bt) K_0(ct) dt = \pi \int_0^{\infty} \frac{\mathbf{K}\left(\sqrt{\frac{v^2 + (a-b)^2}{v^2 + (a+b)^2}}\right)}{\sqrt{(v^2 + (a+b)^2)(v^2 + c^2)}} dv. \quad (32)$$

Remarkably, the integral (32) may be evaluated by exploiting a more general identity given in W.N. Bailey's second paper on infinite integrals involving Bessel functions [17]. Without loss of generality, we assume that $c \geq b \geq a > 0$ and define

$$k_{\pm} := \frac{\sqrt{(c+a)^2 - b^2} \pm \sqrt{(c-a)^2 - b^2}}{2c}, \quad k'_{\pm} := \sqrt{1 - k_{\pm}^2}.$$

Then our result may be written as

$$\frac{2c}{\pi} \bar{V}_3(a, b, c) = \mathbf{K}(k_-) \mathbf{K}(k'_+) + \mathbf{K}(k_+) \mathbf{K}(k'_-). \quad (33)$$

We remark that when $c > a + b$ each term in (33) is real; otherwise, each is the complex conjugate of the other. The form of k_{\pm} comes from Bailey's conditions $k_+k_- = a/c$ and $k'_+k'_- = b/c$.

We proved (33) by setting $\nu = \rho = 0$ in Bailey's equation (3.3), to obtain

$$\int_0^{\infty} I_{\mu}(at)K_0(bt)K_0(ct) dt = \frac{1}{4c}W_{\mu}(k_+)W_{\mu}(k_-)$$

with a hypergeometric series

$$W_{\mu}(k) := \sum_{n=0}^{\infty} \frac{\Gamma^2\left(n + \frac{1+\mu}{2}\right) k^{2n+\mu}}{\Gamma(n+1+\mu)n!} = \frac{\sqrt{\pi}\Gamma\left(\frac{1+\mu}{2}\right)}{(1-k^2)^{1/4}} P^{-\mu/2}\left(\frac{2-k^2}{2\sqrt{1-k^2}}\right),$$

where P is the Legendre function defined in [1, 8.1.2]. Then (33) follows from the expansions

$$\begin{aligned} I_{\mu}(x) &= I_0(x) - \mu K_0(x) + O(\mu^2) \\ W_{\mu}(k) &= 2\mathbf{K}(k) - \mu\pi\mathbf{K}\left(\sqrt{1-k^2}\right) + O(\mu^2), \end{aligned}$$

where the derivative of $W_{\mu}(k)$ at $\mu = 0$ is obtained by setting $a = b = \frac{1}{2}$ and $z = 1 - k^2$ in [1, 15.3.10].

Specializing (33) to the case $a = b = 1$ we obtain

$$\frac{2c}{\pi} \int_0^{\infty} K_0^2(t)K_0(ct) dt = A(2/c) = B(c/2) \quad (34)$$

with the choice of a sum of squares or a product in the functions

$$A(x) := \mathbf{K}^2\left(\frac{\sqrt{1+x}-\sqrt{1-x}}{2}\right) + \mathbf{K}^2\left(\frac{\sqrt{1+x}+\sqrt{1-x}}{2}\right) \quad (35)$$

$$B(x) := 2x\mathbf{K}\left(\frac{\sqrt{1+x}-\sqrt{1-x}}{2}\right)\mathbf{K}\left(\frac{\sqrt{1+x}+\sqrt{1-x}}{2}\right), \quad (36)$$

with (35) coming directly from (33). The identity $A(x) = B(1/x)$ may be proven by showing that $A(1-y)$ and $B(1/(1-y))$ satisfy the same third-order differential equation and have Taylor series about $y = 0$ that agree in their first 3 terms.

Alternative one may use transformations of the *Meijer G-functions*

$$2\sqrt{\pi}A(x) = G_{33}^{23}\left(\frac{1}{x^2} \left| \begin{matrix} 1 \\ \frac{1}{2} & \frac{1}{2} & \frac{1}{2} \end{matrix} \right.\right) = G_{33}^{32}\left(x^2 \left| \begin{matrix} \frac{1}{2} & \frac{1}{2} & \frac{1}{2} \\ 0 & 0 & 0 \end{matrix} \right.\right) \quad (37)$$

$$2\sqrt{\pi}B(x) = G_{33}^{23}\left(x^2 \left| \begin{matrix} 1 \\ \frac{1}{2} & \frac{1}{2} & \frac{1}{2} \end{matrix} \right.\right) = x G_{33}^{23}\left(x^2 \left| \begin{matrix} \frac{1}{2} & \frac{1}{2} & \frac{1}{2} \\ 0 & 0 & 0 \end{matrix} \right.\right) \quad (38)$$

in the notation of [63, Vol. 3]. This provides an inversion formula, 8.2.1.14, used in (37) and a multiplication formula, 8.2.1.15, used in (38).

Remark. Our forms, (35) and (36), for the Bessel integral (34), were tabulated, without proof, in identities 2.16.46.4 and 2.16.46.5 of [63, Vol. 2]. Our proof of the more general identity (33) came from following a reference to Bailey's work, given in Section 7.14.2.43 of the Bateman project [37, Vol. 2].

Setting $c = 1$ in (34), we obtain

$$c_{3,0} = \frac{\pi}{2} K_3 K'_3 = \frac{3\Gamma^6\left(\frac{1}{3}\right)}{32\pi 2^{2/3}}, \quad (39)$$

with the product of $K_3 = \mathbf{K}(k_3)$ and $K'_3 = \sqrt{3}K_3$ obtained from (36) at $x = \frac{1}{2}$, where the third *singular value* [24]

$$k_3 = \frac{\sqrt{3}-1}{2\sqrt{2}} = \sin(\pi/12)$$

results. Moreover, Bessel's differential equation yields

$$c_{3,2} = \frac{\pi}{2} \left(\frac{1}{c} + \frac{d}{dc} \right) \frac{d}{dc} \frac{B(c/2)}{c} \Big|_{c=1} = \frac{\Gamma^6\left(\frac{1}{3}\right)}{96\pi 2^{2/3}} - \frac{4\pi^5 2^{2/3}}{9\Gamma^6\left(\frac{1}{3}\right)}, \quad (40)$$

upon use of the evaluations

$$\begin{aligned} \mathbf{E}(\sin(\pi/12)) &= \frac{K'_3 + 3K_3}{6} + \frac{\pi}{4K'_3} \\ \mathbf{E}(\cos(\pi/12)) &= \frac{K'_3 - K_3}{2} + \frac{\pi}{4K_3} \end{aligned}$$

of complete elliptic integrals of the second kind, recorded in [24, p. 28] and first found by Legendre. Prior to finding this proof, we discovered (40) in the more palatable form

$$c_{3,2} = \frac{1}{9} c_{3,0} - \frac{\pi^4}{24} c_{3,0}^{-1} \quad (41)$$

by using PSLQ [5, 12, 22] in a manner suggested by previous discoveries in quantum field theory, as described in Section 5.

3.4 Continued fraction

We recall that

$$9 \frac{c_{3,2}}{c_{3,0}} = \frac{9 \cdot 1^4}{d(1) - \frac{9 \cdot 3^4}{\dots - \frac{9 \cdot (2N-1)^4}{d(N) - \dots}}}, \quad (42)$$

where $d(N) := 40N^2 + 2$ was derived in [10]. Hence, dividing (41) by $c_{3,0}$, we obtain a neat continued fraction for

$$1 - 2^{7/3} 9 \left(\frac{\Gamma\left(\frac{2}{3}\right)}{\Gamma\left(\frac{1}{3}\right)} \right)^6 = 9 \frac{c_{3,2}}{c_{3,0}}. \quad (43)$$

3.5 Double integrals

Inspection of [10] also reveals that we now have evaluated the integrals

$$\int_0^\infty \int_0^\infty \frac{dx dy}{\sqrt{(1+x^2)(1+y^2)(1+(x+y)^2)}} = \frac{2}{3} K_3 K'_3 \quad (44)$$

$$\int_0^\infty \int_0^\infty \frac{dx dy}{\sqrt{(1+x^2)(1+y^2)(1+(x-y)^2)}} = \frac{4}{3} K_3 K'_3. \quad (45)$$

The first integral occurs in a formula for $4c_{3,0}/(3\pi)$ in [10]. To evaluate the second integral, we note that it is twice the value obtained from the simplex $x > y > 0$. The transformation $x = y + z$ then proves that (45) is twice (44).

In Section 5, we give evaluations of double integrals arising in quantum field theory.

3.6 Hypergeometric series

We may also obtain a simple hypergeometric series for $c_{3,0}$ from the Clausen product formula [24, p. 178] in the form

$$\frac{4}{\pi^2} \mathbf{K}^2(\sin(\alpha/2)) = {}_3F_2 \left(\begin{matrix} \frac{1}{2}, \frac{1}{2}, \frac{1}{2} \\ 1, 1 \end{matrix} \middle| \sin^2 \alpha \right), \quad (46)$$

which is valid for $\pi/2 \geq \alpha \geq 0$. Setting $\alpha = \pi/6$, so that $\sin(\alpha) = 1/2$, we recast (39) as

$$c_{3,0} = \frac{\sqrt{3}\pi^3}{8} \sum_{n=0}^{\infty} \frac{\binom{2n}{n}^3}{2^{8n}} = \frac{\sqrt{3}\pi^3}{8} {}_3F_2 \left(\begin{matrix} \frac{1}{2}, \frac{1}{2}, \frac{1}{2} \\ 1, 1 \end{matrix} \middle| \frac{1}{4} \right). \quad (47)$$

Moreover, we conjectured the compact formula

$$c_{3,2} = \frac{\sqrt{3}\pi^3}{288} \sum_{n=0}^{\infty} \frac{\binom{2n}{n}^3}{2^{8n}} \frac{1}{(n+1)^2} = \frac{\sqrt{3}\pi^3}{288} {}_3F_2 \left(\begin{matrix} \frac{1}{2}, \frac{1}{2}, \frac{1}{2} \\ 2, 2 \end{matrix} \middle| \frac{1}{4} \right) \quad (48)$$

as an alternative to (41). A proof was provided by *Maple*, which evaluates this sum in terms of K_3 and E_3 . Our evaluation of the latter then shows that (48) follows from (40).

3.7 Integrals of elliptic integrals

Setting $a = b = 1$, $w = 2 \tan \theta$ and $c = 2 \sin \alpha$ in (32), we obtain from (34) the evaluation

$$\int_0^{\pi/2} \frac{\mathbf{K}(\sin \theta)}{\cos \theta \sqrt{\tan^2 \theta + \sin^2 \alpha}} d\theta = \frac{B(\sin \alpha)}{2 \sin \alpha}$$

and hence, by trigonometric simplification, we prove the identity

$$\int_0^{\pi/2} \frac{\mathbf{K}(\sin \theta)}{\sqrt{1 - \cos^2 \alpha \cos^2 \theta}} d\theta = \mathbf{K}(\sin(\alpha/2)) \mathbf{K}(\cos(\alpha/2)), \quad (49)$$

which we had conjectured empirically from interpolating known results, using *Maple's* `MinimalPolynomial`. At $\alpha = \pi/2$, identity (49) reduces to the evaluation

$$\int_0^1 \frac{\mathbf{K}(k)}{\sqrt{1 - k^2}} dk = \mathbf{K}^2 \left(\frac{1}{\sqrt{2}} \right) = \frac{\Gamma^4 \left(\frac{1}{4} \right)}{16\pi}$$

given in [24, p. 188]. At $\alpha = \pi/6$, we obtain

$$2 \int_0^{\pi/2} \frac{\mathbf{K}(\sin \theta)}{\sqrt{1 + 3 \sin^2 \theta}} d\theta = K_3 K_3'. \quad (50)$$

We did not find identity (49) in the literature. However, John Zucker remarked to us that the left-hand side may be transformed to a double integral using (20). If we then exchange the order of integration and set $C = \cos^2 \alpha$ and $S = \sin^2 \phi$ in the evaluation

$$\int_0^{\pi/2} \frac{1}{\sqrt{(1-C \cos^2 \theta)(1-S \sin^2 \theta)}} d\theta = \mathbf{K}(\sqrt{C+S-CS})$$

given in [58], we obtain an identity first derived by Glasser [38], namely

$$\int_0^{\pi/2} \mathbf{K}(\sqrt{1-\sin^2 \alpha \cos^2 \phi}) d\phi = \mathbf{K}(\sin(\alpha/2)) \mathbf{K}(\cos(\alpha/2)), \quad (51)$$

which was re-derived by Joyce and Zucker and recorded in [23, Eq. 2.3.5].

3.8 Sum rule

Using the analysis of $c_{3,0}$ above and in [10] we obtain a sum rule

$$\sum_{n=0}^{\infty} \frac{\binom{2n}{n}^3}{2^{8n}} \left(\frac{8}{3} \log 2 - \sum_{k=1}^n \frac{1}{k(2k-1)} - \frac{\pi}{\sqrt{3}} \right) = 0. \quad (52)$$

In Section 5 we conjecture an integral counterpart to this sum rule.

4 Four Bessel functions

We may construct S_4 by folding one instance of S_3 , in (22), with the discontinuity of another, to obtain

$$S_4(a, b, c, w) = \int_{a+b}^{\infty} 2uD_3(a, b, u)S_3(u, c, w) du, \quad (53)$$

from which we obtain an evaluation of the *on-shell* value

$$s_{4,1} = S_4(1, 1, 1, i) = \int_2^{\infty} \frac{4 \operatorname{arctanh}\left(\sqrt{\frac{u-2}{u+2}}\right)}{u(u^2-4)} du = \int_0^1 \frac{2y \log(y)}{y^4-1} dy = \frac{\pi^2}{16} \quad (54)$$

by the substitution $u = y + 1/y$.

4.1 The odd moments $s_{4,2k+1}$

By differentiation of

$$S_4(1, 1, 1, ix) = \int_2^{\infty} \frac{4 \operatorname{arctanh}\left(\sqrt{\frac{(u-1)^2-x^2}{(u+1)^2-x^2}}\right)}{\sqrt{(u^2-4)((u-1)^2-x^2)((u+1)^2-x^2)}} du$$

we evaluate

$$s_{4,3} = \left(\frac{1}{x} + \frac{d}{dx} \right) \frac{dS_4(1, 1, 1, ix)}{dx} \Big|_{x=1} = \frac{\pi^2}{64}$$

and are then able to solve the recursion relation [26, 60] for $s_{4,2k+1}$ by the *closed form*

$$s_{4,2k+1} = \frac{\pi^2}{16} \left(\frac{k!}{4^k}\right)^2 b_k \quad (55)$$

with integers

$$b_k = \sum_{j=0}^k \binom{k}{j}^2 \binom{2k-2j}{k-j} \binom{2j}{j}. \quad (56)$$

Integer sequence (56) begins

$$1, 4, 28, 256, 2716, 31504, 387136, 4951552, 65218204, 878536624, 12046924528 \quad (57)$$

and is recorded² as entry A2895 of the on-line version of [66], which gives the recursion

$$k^3 b_k - 2(2k-1)(5k^2 - 5k + 2)b_{k-1} + 64(k-1)^3 b_{k-2} = 0 \quad (58)$$

and the generating function

$$I_0^4(2t) = \sum_{k=0}^{\infty} b_k \left(\frac{t^k}{k!}\right)^2. \quad (59)$$

We have verified that recursion (58) reproduces the recursion for (55), which has the same form as for the odd moments in (9). We note that in [36, 43] the integers b_k were related to enumeration of paths in three-dimensional diamond lattices. They also appear in a study [21, Eq. 6.10] of lattice magnetic walks. From the generating function I_0^4 we see that they result from the constrained sum

$$b_k = \sum_{p+q+r+s=k} \left(\frac{k!}{p!q!r!s!}\right)^2.$$

The economical recursion in (58) will be used in Section 5.

4.2 Dispersion relation

We adapt the dispersive method of [20, 28, 65] to two spacetime dimensions and take the discontinuity of (53) across the cut with branch point $w^2 = -(a+b+c)^2$, obtaining the dispersion relation

$$S_4(a, b, c, w) = \int_{a+b+c}^{\infty} \frac{2v D_4(a, b, c, v)}{v^2 + w^2} dv, \quad (60)$$

with a discontinuity given by a complete elliptic integral \mathbf{K} of the first kind, and hence by an arithmetic-geometric mean [3, 24], namely

$$D_4(a, b, c, d) = \int_{a+b}^{d-c} 2u D_3(a, b, u) D_3(u, c, d) du \quad (61)$$

$$= \frac{2\mathbf{K}\left(\frac{Q(a,b,c,-d)}{Q(a,b,c,d)}\right)}{Q(a,b,c,d)} = \frac{\pi}{\text{AGM}\left(Q(a,b,c,d), 4\sqrt{abcd}\right)}, \quad (62)$$

²See <http://www.research.att.com/~njas/sequences/A002895>.

where

$$Q(a, b, c, d) := \sqrt{(a+b+c+d)(a+b-c-d)(a-b+c-d)(a-b-c+d)}$$

is completely symmetric in its 4 arguments.

In physical terms, $D_4(a, b, c, d)$ gives the volume of phase space for the decay of a particle of mass $d > a + b + c$ into 3 particles with masses a , b and c in two spacetime dimensions. In 4 spacetime dimensions, one would obtain an incomplete elliptic integral for the area of the Dalitz plot, in the generic mass case; in two spacetime dimensions we obtain a simple arithmetic-geometric mean for the length of a Dalitz line [33].

Using this elliptic representation for $S_4(1, 1, 1, 0) = V_3(1, 1, 1) = c_{3,1}$, we obtain an evaluation of the integral

$$\int_0^{\frac{1}{3}} D(y) dy = c_{3,1} = \frac{3}{4} L_{-3}(2), \quad (63)$$

with $D(y) := 2D_4(1, 1, 1, 1/y)/y$ given by

$$D(y) = \frac{4y \mathbf{K} \left(\sqrt{\frac{(1-3y)(1+y)^3}{(1+3y)(1-y)^3}} \right)}{\sqrt{(1+3y)(1-y)^3}} = \frac{3\sqrt{3}\pi y}{2} \text{HeunG}(-8, -2; 1, 1, 1, 1; 1-9y^2), \quad (64)$$

where the *general Heun* function, HeunG , satisfies *Heun's differential equation* as specified in *Maple*, see [64]. Similarly,

$$\int_0^{\frac{1}{3}} D(y) y^2 dy = \frac{1}{4} c_{3,3} = \frac{1}{4} L_{-3}(2) - \frac{1}{6}.$$

In Section 5 we shall show that the HeunG representation of the elliptic integral (64), from quantum field theory, may be related to the hexagonal lattice sequence (24) of crystal theory. For the present, we note that (54) and (60) provide the evaluation

$$\int_0^{\frac{1}{3}} \frac{D(y)}{1-y^2} dy = s_{4,1} = \frac{\pi^2}{16}. \quad (65)$$

4.3 The odd moments $c_{4,2k+1}$

For V_4 we have two representations. First, from the elementary arctanh function in (22), we may compute

$$V_4(a, b, c, d) = \int_0^\infty w S_3(a, b, w) S_3(c, d, w) dw \quad (66)$$

and easily evaluate

$$c_{4,1} = \int_0^\infty \frac{4 \text{arctanh}^2 \left(\frac{w}{\sqrt{w^2+4}} \right)}{w(w^2+4)} dw = \int_0^1 \frac{4y \log^2(y)}{1-y^4} dy = \frac{7}{8} \zeta(3)$$

by the substitution $w = 1/y - y$. Similarly, by differentiation of (66), we obtain

$$c_{4,3} = \frac{7}{32} \zeta(3) - \frac{3}{16}.$$

In general, all the odd moments $c_{4,2k+1}$ are given by rational linear combinations of $\zeta(3)$ and unity, as shown in [10, 26, 60]. Because of the mixing of $\zeta(3)$ with unity, we were unable to write a closed form for their rational coefficients in $c_{4,2k+1}$.³

The alternative folding, using (62), is

$$\begin{aligned} V_4(a, b, c, d) &= \int_0^\infty w S_4(a, b, c, w) S_2(d, w) dw \\ &= \int_{a+b+c}^\infty 2v D_4(a, b, c, v) V_2(v, d) dv, \end{aligned}$$

which yields a novel formula for $\zeta(3)$, namely

$$\int_0^{\frac{1}{3}} \frac{D(y) \log(y)}{y^2 - 1} dy = c_{4,1} = \frac{7}{8} \zeta(3) \quad (67)$$

by the substitution $v = 1/y$.

4.4 The even moment $c_{4,0}$

The analogue to (66), for even moments, is

$$\bar{V}_4(a, b, c, d) = 2\pi \int_0^\infty \bar{S}_3(a, b, w) \bar{S}_3(c, d, w) dw, \quad (68)$$

with a product of elliptic integrals coming from (30). Setting $c = a$ and $d = b$, we obtain the intriguing case

$$\int_0^\infty K_0^2(at) K_0^2(bt) dt = 2\pi \int_0^\infty \frac{\mathbf{K}^2\left(\sqrt{\frac{w^2+(a-b)^2}{w^2+(a+b)^2}}\right)}{w^2 + (a+b)^2} dw, \quad (69)$$

where the square of \mathbf{K} may be replaced by a ${}_3F_2$ series [15] for only part of the range of the integration, because of the restricted validity of the Clausen product (46). In particular, it was not at first clear how to evaluate the integral in

$$c_{4,0} = \pi \int_0^{\pi/2} \mathbf{K}^2(\sin \theta) d\theta \quad (70)$$

obtained by setting $a = b = 1$ and $w = 2 \tan \theta$.

The key to unlock this puzzle was provided by the trigonometric series

$$\mathbf{K}(\sin \theta) = \sum_{n=0}^{\infty} \gamma_n \sin((4n+1)\theta) \quad (71)$$

with coefficients

$$\gamma_n := \left(\frac{\Gamma\left(n + \frac{1}{2}\right)}{\Gamma(n+1)} \right)^2 = \frac{4}{4n+1} + O\left(\frac{1}{n^3}\right) \quad (72)$$

³Closed forms are given in [10] for the rational coefficients of $\zeta(3)$ in the evaluation of $c_{4,2k+1}$, and for the rational coefficients of $L_{-3}(2)$ in the evaluation of $c_{3,2k+1}$.

given by F.G. Tricomi [68] and recorded in [37, Section 13.8, Eqn. (8)]. The identity (71) is valid for $\pi/2 > \theta > 0$. Thus, the integral in (70) is easily transformed to a hypergeometric sum in

$$c_{4,0} = \frac{\pi^2}{4} \sum_{n=0}^{\infty} \gamma_n^2 = \frac{\pi^4}{4} \sum_{n=0}^{\infty} \frac{\binom{2n}{n}^4}{2^{8n}} = \frac{\pi^4}{4} {}_4F_3 \left(\begin{matrix} \frac{1}{2}, \frac{1}{2}, \frac{1}{2}, \frac{1}{2} \\ 1, 1, 1 \end{matrix} \middle| 1 \right) \quad (73)$$

by using the orthogonality relation

$$\int_0^{\pi/2} \sin((4m+1)\theta) \sin((4n+1)\theta) d\theta = \frac{\pi}{4} \delta_{m,n}.$$

It is instructive to split $c_{4,0} = \mathcal{A}_1 + \mathcal{A}_2$ into the contributions

$$\mathcal{A}_1 = \pi \int_0^{\pi/4} \mathbf{K}^2(\sin \theta) d\theta, \quad \mathcal{A}_2 = \pi \int_0^{\pi/4} \mathbf{K}^2(\cos \theta) d\theta,$$

and use the Clausen product (46) for the former. The result is $\mathcal{A}_1 = \frac{1}{4}c_{4,0}$ which proves that $\mathcal{A}_2/\mathcal{A}_1 = 3$, as we had noticed numerically. A more direct derivation of this proven factor of 3 would probably be enlightening.

We also note that $\mathcal{A}_1 = \frac{1}{4}c_{4,0}$ may be obtained by setting $\phi = 0$ in the double series

$$\pi \int_{\phi/2}^{\pi/4} \mathbf{K}^2(\sin \theta) d\theta = \frac{\pi^3}{8} \cos \phi \sum_{n=0}^{\infty} \frac{\binom{2n}{n}^3}{2^{6n}} {}_2F_1 \left(\begin{matrix} \frac{1}{2}, \frac{1}{2} - n \\ \frac{3}{2} \end{matrix} \middle| \cos^2 \phi \right),$$

which is valid $\pi/2 \geq \phi \geq 0$.

4.5 Sum rule

Combining (73) with a more complicated sum in [10, Eq. 3-5], we get the discrete sum rule

$$\sum_{n=0}^{\infty} \frac{\binom{2n}{n}^4}{2^{8n}} \left\{ 8 \left(-\log 2 + \sum_{k=1}^n \frac{1}{2k(2k-1)} \right)^2 - \sum_{k=1}^n \frac{4k-1}{2k^2(2k-1)^2} - \frac{\pi^2}{3} \right\} = 0, \quad (74)$$

with one more central binomial coefficient and one more power of $\pi/\sqrt{3}$ than (52).

4.6 The even moment $c_{4,2}$

Integer relation algorithms (see [5, 7, 12] for extended discussion) led us to conjecture that

$$c_{4,2} = \frac{\pi^2}{256} \sum_{n=0}^{\infty} \gamma_n^2 \left(\frac{12}{n+1} - \frac{3}{(n+1)^2} - 8 \right), \quad (75)$$

which we shall now prove.

As before, we use Bessel's differential equation and operate on our master formula, in this case (68), before setting parameters to unity, obtaining

$$c_{4,2} = \pi \int_0^{\pi/2} \left(\frac{\cos 4\theta - 1}{16} + \frac{4 \cot \theta + \sin 4\theta}{32} \frac{d}{d\theta} \right) \mathbf{K}^2(\sin \theta) d\theta.$$

Then, using Tricomi's expansion (71), we easily reduce

$$\pi \int_0^{\pi/2} \mathbf{K}^2(\sin \theta) \cos 4\theta \, d\theta = \frac{\pi^2}{16} \sum_{n=0}^{\infty} \gamma_n^2 \left(2 - \frac{1}{n+1}\right)^2$$

to single sums of the form in (75). The term involving $\sin 4\theta$ gives a multiple of the same sum, using integration by parts.

However, the term involving $\cot \theta$ is more demanding. Integrating it by parts, we conclude that (75) is equivalent to the evaluation

$$\mathcal{B} := \int_0^{\pi/2} \frac{4\pi \mathbf{K}^2(\sin \theta) - \pi^3}{\sin^2 \theta} \, d\theta = \frac{\pi^2}{4} \sum_{n=0}^{\infty} \gamma_n^2 \frac{4n+3}{(n+1)^2}, \quad (76)$$

which we now prove by using a subtracted form for the differential of (71).

Defining $\delta_n := 4 - (4n+1)\gamma_n$, we prove by induction that

$$\sum_{m=0}^{n-1} \delta_m = 4n - 4n^2 \gamma_n = 1 - \sum_{m=n}^{\infty} \delta_m. \quad (77)$$

Then from this we derive a subtracted series for

$$\frac{d\mathbf{K}(\sin \theta)}{d\theta} - \frac{\sin^2 \theta}{\cos \theta} = \sum_{m=1}^{\infty} \delta_m (\cos \theta - \cos((4m+1)\theta)), \quad (78)$$

by subtracting the trigonometric series [59]

$$4 \sum_{m=0}^{\infty} \frac{\sin((4m+1)\theta)}{4m+1} = \frac{\pi}{2} + \log(\sec \theta + \tan \theta) \quad (79)$$

from (71) and then differentiating, to obtain

$$\frac{d\mathbf{K}(\sin \theta)}{d\theta} - \sec \theta = - \sum_{m=1}^{\infty} \delta_m \cos((4m+1)\theta).$$

Adding $\cos \theta$ to each side and using $\sum_{m=0}^{\infty} \delta_m = 1$, as a consequence of (77), we obtain (78).

By combining (71) and (78), we obtain the double series

$$\frac{\mathcal{B}}{2\pi^2} - \gamma_0 = \sum_{m,n \geq 0} \delta_m (M_{0,n} - M_{m,n}) \gamma_n,$$

using the triangular array M with entries

$$M_{m,n} := \frac{4}{\pi} \int_0^{\pi/2} \cot \theta \cos((4m+1)\theta) \sin((4n+1)\theta) \, d\theta$$

for non-negative integers m and n . These entries are very simple: $M_{m,n} = 2$, for $m < n$, $M_{m,n} = 0$, for $m > n$, and $M_{n,n} = 1$, resulting in

$$\frac{\mathcal{B}}{2\pi^2} = \gamma_0 + \sum_{m=0}^{\infty} \delta_m \left(-\gamma_m - \gamma_0 + 2 \sum_{n=0}^m \gamma_n \right) = \sum_{n=0}^{\infty} \gamma_n \varepsilon_n$$

with the γ_0 terms cancelling, since $\sum_{m=0}^{\infty} \delta_m = 1$. Here,

$$\varepsilon_n := -\delta_n + 2 \sum_{m=n}^{\infty} \delta_m = (8n^2 + 4n + 1)\gamma_n - 2(4n + 1)$$

appears by a change of the order of summation and is easily evaluated, by using (77).

Looking back to what needs to be proved, in (76), we see that we now need to establish the vanishing of

$$\sum_{n=0}^{\infty} \gamma_n \left(\frac{4n+3}{8(n+1)^2} \gamma_n - \varepsilon_n \right) = 0.$$

This is achieved by taking the $N \rightarrow \infty$ limit of the explicit evaluation

$$\sum_{n=0}^{N-1} \gamma_n \left(\frac{4n+3}{8(n+1)^2} \gamma_n - \varepsilon_n \right) = 2N^2 \gamma_N \delta_N = O\left(\frac{1}{N}\right) \quad (80)$$

of a truncated sum, which is easily proven by induction. We note that the **Gosper** algorithm [62] in *Maple* failed to evaluate (80), as written, since δ_n and ε_n mix binomial and polynomial terms. If one separates these by hand then our compact result is verified.

4.7 Further evaluation of integrals

We also succeeded in separating $\mathcal{B} = \mathcal{B}_1 + \mathcal{B}_2$ into the contributions

$$\mathcal{B}_1 := \int_0^{\pi/4} \frac{4\pi \mathbf{K}^2(\sin \theta) - \pi^3}{\sin^2 \theta} d\theta = -2\pi^2 + \mathcal{H} + \frac{\pi^2}{4} \sum_{n=0}^{\infty} \gamma_n^2 \frac{2n+1}{n+1} \quad (81)$$

$$\mathcal{B}_2 := \int_0^{\pi/4} \frac{4\pi \mathbf{K}^2(\cos \theta) - \pi^3}{\cos^2 \theta} d\theta = -2\pi^2 - \mathcal{H} + \frac{3\pi^2}{4} \sum_{n=0}^{\infty} \gamma_n^2 \frac{2n+1}{n+1}, \quad (82)$$

with a familiar factor of 3 multiplying the ${}_4F_3$ series in the latter and a new constant from the singular value $k_1 = \sin(\pi/4)$, namely

$$\begin{aligned} \mathcal{H} &:= \pi^3 \left(1 - {}_3F_2 \left(\begin{matrix} -\frac{1}{2}, \frac{1}{2}, \frac{1}{2} \\ 1, 1 \end{matrix} \middle| 1 \right) \right) \\ &= \pi^3 - \frac{\Gamma^4\left(\frac{1}{4}\right) + 16\Gamma^4\left(\frac{3}{4}\right)}{8}. \end{aligned}$$

The π^3 terms in \mathcal{H} and the integrand of (82) match, since $\int_0^{\pi/4} \sec^2 \theta d\theta = 1$.

4.8 Further evaluations of sums

Evaluations (81) and (82) were discovered using PSLQ. To prove (81), we may again use a Clausen product, with its first term subtracted. We then encounter the integrals

$$2 \int_0^{\pi/4} \frac{\sin^{2n} 2\theta}{\sin^2 \theta} d\theta = B\left(n - \frac{1}{2}, \frac{1}{2}\right) + \frac{2}{2n-1}$$

with $n > 0$. Here B is Euler's Beta function and yields yet another ${}_4F_3$ series, which we eliminate by using the $N \rightarrow \infty$ limit of the summation

$$\sum_{n=0}^{N-1} \gamma_n^2 \left(\frac{2}{1-2n} - \frac{1}{n+1} \right) = \frac{16N^3}{2N-1} \gamma_N^2 = 8 + O\left(\frac{1}{N}\right),$$

which was also proven by induction. To prove (82), we then subtract (81) from (76) and use the $N \rightarrow \infty$ limit of the summation

$$\sum_{n=0}^{N-1} \gamma_n^2 \left(8 - \frac{8}{n+1} + \frac{1}{(n+1)^2} \right) = 16N^2 \gamma_N^2 = 16 + O\left(\frac{1}{N}\right),$$

which was proven in the same manner.

Thus one may undo the explicit evaluations of parts of (82), in terms of π and Γ values, and instead write

$$\pi \int_0^{\pi/4} \frac{\mathbf{K}^2(\cos \theta)}{\cos^2 \theta} d\theta = \frac{\pi^3}{8} \sum_{n=0}^{\infty} \frac{\binom{2n}{n}^3}{2^{6n}} \frac{2n+1}{n+1} + \frac{\pi^4}{32} \sum_{n=0}^{\infty} \frac{\binom{2n}{n}^4}{2^{8n}} \frac{4n^2 + 10n + 5}{(n+1)^2}$$

in terms of undigested hypergeometric series.

More productively, we may use the explicit summations so far achieved to reduce

$$\frac{16c_{4,0} - 64c_{4,2}}{3\pi^4} - \frac{4}{\pi^2} = {}_4F_3 \left(\begin{matrix} \frac{1}{2}, \frac{1}{2}, \frac{1}{2}, \frac{1}{2} \\ 2, 1, 1 \end{matrix} \middle| 1 \right) \quad (83)$$

to a single ${}_4F_3$ series. Comparing this last result with (73), we conclude that all moments $c_{4,2k}$ can be expressed in terms π and a pair of contiguous ${}_4F_3$ series. An equivalent hypergeometric expression is

$$c_{4,2} = \frac{\pi^4}{64} \left\{ 4 {}_4F_3 \left(\begin{matrix} \frac{1}{2}, \frac{1}{2}, \frac{1}{2}, \frac{1}{2} \\ 1, 1, 1 \end{matrix} \middle| 1 \right) - 3 {}_4F_3 \left(\begin{matrix} \frac{1}{2}, \frac{1}{2}, \frac{1}{2}, \frac{1}{2} \\ 2, 1, 1 \end{matrix} \middle| 1 \right) \right\} - \frac{3\pi^2}{16}. \quad (84)$$

For comparison, we repeat

$$c_{4,0} = \frac{\pi^4}{4} {}_4F_3 \left(\begin{matrix} \frac{1}{2}, \frac{1}{2}, \frac{1}{2}, \frac{1}{2} \\ 1, 1, 1 \end{matrix} \middle| 1 \right). \quad (85)$$

4.9 Relation to Meijer's G-function

A generalization of (69) is derivable in terms of the *Meijer-G function* [63, Vol. 3]. For example, we have

$$I(a, b, k) := \int_0^\infty t^k K_0^2(at) K_0^2(bt) dt = \frac{\pi}{8a^{k+1}} G_{44}^{33} \left(\begin{matrix} b^2 \\ a^2 \end{matrix} \middle| \begin{matrix} \frac{1-k}{2} & \frac{1-k}{2} & \frac{1-k}{2} & \frac{1}{2} \\ 0 & 0 & 0 & -\frac{k}{2} \end{matrix} \right), \quad (86)$$

which may be proven by making two copies of the representation

$$t^\mu K_0^2(at) = \frac{\sqrt{\pi}}{2a^\mu} G_{13}^{30} \left(a^2 t^2 \middle| \begin{matrix} \frac{\mu+1}{2} \\ \frac{\mu}{2} & \frac{\mu}{2} \end{matrix} \right)$$

and integrating them with weight t to obtain

$$I(a, b, \mu + \nu + 1) = \frac{\pi}{4a^\mu b^\nu} \int_0^\infty t G_{13}^{30} \left(a^2 t^2 \middle| \begin{matrix} \frac{\mu+1}{2} \\ \frac{\mu}{2} & \frac{\mu}{2} \end{matrix} \right) G_{13}^{30} \left(b^2 t^2 \middle| \begin{matrix} \frac{\nu+1}{2} \\ \frac{\nu}{2} & \frac{\nu}{2} \end{matrix} \right) dt.$$

Then we use Meijer's result for the integral of the product of two G-functions to obtain

$$I(a, b, \mu + \nu + 1) = \frac{\pi}{8a^{\mu+2}b^\nu} G_{44}^{33} \left(\frac{b^2}{a^2} \left| \begin{array}{cccc} -\frac{\mu}{2} & -\frac{\mu}{2} & -\frac{\mu}{2} & \frac{\nu+1}{2} \\ \frac{\nu}{2} & \frac{\nu}{2} & \frac{\nu}{2} & -\frac{\mu+1}{2} \end{array} \right. \right).$$

The apparent freedom in the choice of parameters μ and ν is demystified by formula 8.2.1.15 in [63, Vol. 3], which shows that multiplication by a power of the argument of a G-function is equivalent to adding a constant to all its parameters, as in the example (38). We resolve this redundancy by setting $\mu = k - 1$ and $\nu = 0$ and hence prove (86). Similarly, we obtained

$$\int_0^\infty t^k K_0(at) K_0^2(bt) dt = \frac{2^{k-2} \sqrt{\pi}}{a^{k+1}} G_{33}^{32} \left(\frac{4b^2}{a^2} \left| \begin{array}{ccc} \frac{1-k}{2} & \frac{1-k}{2} & \frac{1}{2} \\ 0 & 0 & 0 \end{array} \right. \right). \quad (87)$$

In [10] the special cases of (86) and (87) with $a = b = 1$ were studied numerically, using Adamchik's algorithm [2]. This algorithm converges quickly in the case of $c_{3,k}$, obtained from (87) with an argument of 4. But in *Maple* it is painfully slow in the case of $c_{4,k}$, obtained from (86) with unit argument. Numerical evaluation of our new hypergeometric results (84) and (85) goes far faster, with *Maple*.

4.10 Another continued fraction

Again we may derive from [10] that

$$8 \frac{c_{4,2}}{c_{4,0}} = \frac{1^6}{e(1) - \frac{3^6}{\dots - \frac{(2N-1)^6}{e(N) - \dots}}}, \quad (88)$$

where $e(N) := N(20N^2 + 3)$ and the ratio $8c_{4,2}/c_{4,0}$ may be made explicit from (84,85).

4.11 The even moment $s_{4,0}$

The odd moment $s_{4,1}$ relates directly to quantum field theory; it is the two-loop on-shell equal-mass sunshine diagram in two spacetime dimensions. No such meaning attaches to $s_{4,0}$; it is hard to think of a physical application for this moment. However, we found a rather pretty formula for it, which we record as

$$s_{4,0} = \int_0^\infty I_0(t) K_0^3(t) dt = \int_0^{\pi/2} \mathbf{K}(\sin \theta) \mathbf{K}(\cos \theta) d\theta. \quad (89)$$

This amusing twist of the integral (70) for $c_{4,0}$ follows from Nicholson's integral representation [72, 13.72, Eq. 3] of the product

$$I_0(t) K_0(t) = \frac{2}{\pi} \int_0^{\pi/2} K_0(2t \sin \alpha) d\alpha.$$

Substituting $c = 2 \sin \alpha$ in (34) and using the appropriate reduction (36) to a product of \mathbf{K} values, we obtain

$$\int_0^\infty I_0(t) K_0^3(t) dt = \int_0^{\pi/2} \frac{B(\sin \alpha)}{2 \sin \alpha} d\alpha = \int_0^{\pi/2} \mathbf{K}(\sin(\alpha/2)) \mathbf{K}(\cos(\alpha/2)) d\alpha.$$

Setting $\alpha = 2\theta$, we prove (89). Then *Pari-GP* gives, in a tenth of a second, 64 digits of

$$s_{4,0} = 6.997563016680632359556757826853096005697754284353362908336255807\dots$$

A corresponding twist of the sum (73) for $c_{4,0}$ comes from Tricomi's expansion (71) and

$$\int_0^{\pi/2} \sin((4m+1)\theta) \cos((4n+1)\theta) d\theta = \frac{1}{4m+4n+2}.$$

This yields the double sum

$$s_{4,0} = \sum_{m,n \geq 0} \frac{\gamma_m \gamma_n}{4m+4n+2} = \sum_{n=0}^{\infty} \gamma_n^2 \left(\lambda_n - \frac{1}{8n+2} \right)$$

with γ_n in (72) and

$$\lambda_n := \frac{2}{\gamma_n} \sum_{m=0}^n \frac{\gamma_m}{4m+4n+2} = 1 + \sum_{m=1}^n \frac{8m}{16m^2-1},$$

where the latter form was proven by *Maple*. Hence we obtain

$$s_{4,0} = \int_0^{\infty} I_0(t) K_0^3(t) dt = \frac{\pi^2}{2} \sum_{n=0}^{\infty} \frac{\binom{2n}{n}^4}{2^{8n}} \left(\frac{1}{4n+1} + \sum_{k=0}^{2n-1} \frac{2}{2k+1} \right). \quad (90)$$

By way of comparison, we note the simpler evaluation

$$\int_0^{\infty} I_0^2(t) K_0^2(t) dt = \sum_{k=0}^{\infty} \binom{2k}{k} \frac{c_{2,2k}}{(2^k k!)^2} = \frac{\pi^2}{4} \sum_{k=0}^{\infty} \frac{\binom{2k}{k}^4}{2^{8k}} = \frac{1}{\pi^2} \int_0^{\infty} K_0^4(t) dt \quad (91)$$

from the closed form for $c_{2,2k}$ in (7) and the expansion

$$I_0^2(t) = \sum_{k=0}^{\infty} \binom{2k}{k} \left(\frac{t^k}{2^k k!} \right)^2. \quad (92)$$

4.12 Tabular summary

In Table 1 we recapitulate the key discoveries for the moments $c_{n,k} := \int_0^{\infty} t^k K_0^n(t) dt$ with $n = 3, 4$. The results for the even moments $c_{3,2k}$ and $c_{4,2k}$ are new. The table may be extended by using the recursions (8) and (9).

5 Five Bessel functions

Little is known for certain about integrals involving 5 Bessel functions. However, there are some remarkable conjectures arising from studies in quantum field theory [55, 56].

$c_{3,0}$	$= \frac{3\Gamma^6\left(\frac{1}{3}\right)}{32\pi 2^{2/3}} = \frac{\sqrt{3}\pi^3}{8} {}_3F_2\left(\begin{matrix} \frac{1}{2}, \frac{1}{2}, \frac{1}{2} \\ 1, 1 \end{matrix} \middle \frac{1}{4}\right)$
$c_{3,1}$	$= \frac{3}{4}L_{-3}(2)$
$c_{3,2}$	$= \frac{\Gamma^6\left(\frac{1}{3}\right)}{96\pi 2^{2/3}} - \frac{4\pi^5 2^{2/3}}{9\Gamma^6\left(\frac{1}{3}\right)} = \frac{\sqrt{3}\pi^3}{288} {}_3F_2\left(\begin{matrix} \frac{1}{2}, \frac{1}{2}, \frac{1}{2} \\ 2, 2 \end{matrix} \middle \frac{1}{4}\right)$
$c_{3,3}$	$= L_{-3}(2) - \frac{2}{3}$
$c_{4,0}$	$= \frac{\pi^4}{4} \sum_{n=0}^{\infty} \frac{\binom{2n}{n}^4}{2^{8n}} = \frac{\pi^4}{4} {}_4F_3\left(\begin{matrix} \frac{1}{2}, \frac{1}{2}, \frac{1}{2}, \frac{1}{2} \\ 1, 1, 1 \end{matrix} \middle 1\right)$
$c_{4,1}$	$= \frac{7}{8}\zeta(3)$
$c_{4,2}$	$= \frac{\pi^4}{16} {}_4F_3\left(\begin{matrix} \frac{1}{2}, \frac{1}{2}, \frac{1}{2}, \frac{1}{2} \\ 1, 1, 1 \end{matrix} \middle 1\right) - \frac{3\pi^4}{64} {}_4F_3\left(\begin{matrix} \frac{1}{2}, \frac{1}{2}, \frac{1}{2}, \frac{1}{2} \\ 2, 1, 1 \end{matrix} \middle 1\right) - \frac{3\pi^2}{16}$
$c_{4,3}$	$= \frac{7}{32}\zeta(3) - \frac{3}{16}$

Table 1: Evaluations for $c_{n,k}$ with $n = 3, 4$.

5.1 Conjectural evaluations of Feynman diagrams

In [55], Stefano Laporta developed an impressive technique for numerical evaluation of the coefficients of the Laurent expansion in ε of Feynman diagrams in $D = 4 - 2\varepsilon$ spacetime dimensions. Here we are concerned with just one of the many diagrams that he considered, namely the dimensionally regularized 3-loop sunrise diagram with 4 internal lines:

$$\mathcal{S}_5(w^2, D) := \int \int \int \frac{d^D p_1 d^D p_2 d^D p_3}{N(p_1)N(p_2)N(p_3)N(q-p_1-p_2-p_3)} \Big|_{q=q=w^2},$$

where $N(p) := p \cdot p + 1$ is the inverse propagator of a scalar particle with unit mass and momentum p . In the on-shell case, the Laurent expansion found by Laporta has the form

$$\frac{\mathcal{S}_5(-1, 4 - 2\varepsilon)}{(\pi^{2-\varepsilon}\Gamma(1+\varepsilon))^3} = \frac{2}{\varepsilon^3} + \frac{22}{3\varepsilon^2} + \frac{577}{36\varepsilon} + S_{205} + \mathcal{O}(\varepsilon)$$

with a numerical value $S_{205} \approx 21.92956264368$, for the finite part, given in equation (205) of [55]. Subsequently, in equation (21) of [56], this constant was conjecturally related to products of elliptic integrals of the first and second kind, with a numerical check to 1200 decimal places.

In a talk⁴ entitled “Reciprocal PSLQ and the Tiny Nome of Bologna”, Broadhurst

⁴Zentrum für interdisziplinäre Forschung in Bielefeld, 14th of June, 2007. Displays available from <http://www.physik.uni-bielefeld.de/igs/schools/ZiF2007/Broadhurst.pdf> leading to 200,000 decimal places for $c_{5,1}$ and $c_{5,3}$ in <http://paftp.open.ac.uk/pub/staff/ftp/dbroadhu/newconst/V5AB.txt>.

observed that Laporta's conjecture may be written rather intriguingly using the constant

$$C := \frac{\pi}{16} \left(1 - \frac{1}{\sqrt{5}}\right) \left(1 + 2 \sum_{n=1}^{\infty} \exp\left(-n^2 \pi \sqrt{15}\right)\right)^4 \quad (93)$$

and its *reciprocal* $1/C$, in terms of which he wrote Laporta's conjecture as

$$S_{205} \stackrel{?[1]}{=} \frac{6191}{216} - \frac{\pi^2}{3} \left(4C + \frac{7}{40C}\right). \quad (94)$$

Broadhurst further conjectured that the odd moments

$$s_{5,2k+1} = \int_0^{\infty} t^{2k+1} I_0(t) K_0^4(t) dt$$

are linear combinations of $\pi^2 C$ and π^2/C , with rational coefficients, and in particular that

$$\frac{s_{5,1}}{\pi^2} \stackrel{?[2]}{=} C \quad (95)$$

$$\frac{s_{5,3}}{\pi^2} \stackrel{?[3]}{=} \left(\frac{2}{15}\right)^2 \left(13C - \frac{1}{10C}\right) \quad (96)$$

$$\frac{s_{5,5}}{\pi^2} \stackrel{?[4]}{=} \left(\frac{4}{15}\right)^3 \left(43C - \frac{19}{40C}\right), \quad (97)$$

with higher moments obtained by a recursion of the form (10) with polynomials $p_{5,i}$ given in (11). We have checked these 3 conjectures to 1200 decimal places.

In the course of this work, we discovered that the moments

$$t_{5,2k+1} = \int_0^{\infty} t^{2k+1} I_0^2(t) K_0^3(t) dt$$

follow an uncannily similar pattern. If q_k and r_k are the rational numbers that give $s_{5,2k+1}/\pi^2$, conjecturally, as $q_k C - r_k/C$, then we found that $q_k C + r_k/C$ gives the value of $2t_{5,2k+1}/(\sqrt{15}\pi)$. We checked 60,000 decimal places of the resultant evaluations

$$\frac{2t_{5,1}}{\sqrt{15}\pi} \stackrel{\sqrt{[5]}}{=} C \quad (98)$$

$$\frac{2t_{5,3}}{\sqrt{15}\pi} \stackrel{\sqrt{[6]}}{=} \left(\frac{2}{15}\right)^2 \left(13C + \frac{1}{10C}\right) \quad (99)$$

$$\frac{2t_{5,5}}{\sqrt{15}\pi} \stackrel{\sqrt{[7]}}{=} \left(\frac{4}{15}\right)^3 \left(43C + \frac{19}{40C}\right), \quad (100)$$

for which we eventually found a proof, presented in subsection 5.10.

Finally, by doubling one of the masses in the Feynman diagram corresponding to $t_{5,1}$, we arrived at the conjectural evaluation

$$\int_0^{\infty} t I_0^2(t) K_0^2(t) K_0(2t) dt \stackrel{?[8]}{=} \frac{1}{12} K_3 K_3', \quad (101)$$

which has been checked to 1200 decimal places.

Notation. In the 8 evaluations (94) to (101) we have used the device $\frac{?[n]}{\underline{\underline{\quad}}}$ or $\frac{\sqrt{[n]}}{\underline{\underline{\quad}}}$ to distinguish the cases that remain unproven from the 3 cases in (98) to (100), which we were eventually able to prove. Some of the labels $n = 1 \dots 8$ will recur, as we give equivalent forms of these conjectured or proven evaluations.

5.2 The odd moments $t_{5,2k+1}$

Evaluations (98,99,100) were easy to check to high precision, thanks to our closed form (55) for the odd moments $s_{4,2k+1}$. By expanding one of the functions

$$I_0(t) = \sum_{n=0}^{\infty} \left(\frac{t^n}{2^n n!} \right)^2$$

in the integrand, $t^{2k+1} I_0^2(t) K_0^3(t)$, of $t_{5,2k+1}$, we obtain a rapidly converging sum in

$$t_{5,2k+1} = 4^{k-2} \pi^2 \sum_{n=k}^{\infty} b_n \left(\frac{n!}{8^n (n-k)!} \right)^2 \quad (102)$$

in terms of the diamond lattice integers (56). To relate $t_{5,1}$ to a product of complete elliptic integrals we use Jacobi's identity

$$\sqrt{\frac{2\mathbf{K}(k)}{\pi}} = \theta_3(q) := \sum_{n=-\infty}^{\infty} q^{n^2} \quad (103)$$

with a *nome* related to k by $q = \exp(-\pi \mathbf{K}'(k)/\mathbf{K}(k))$. Specializing to the *singular value* [24]

$$k_{15} = \frac{(2 - \sqrt{3})(\sqrt{5} - \sqrt{3})(3 - \sqrt{5})}{8\sqrt{2}}$$

with the "tiny nome" $q_{15} := \exp(-\pi\sqrt{15}) \approx 0.000005197$, we obtain from (93)

$$C = \frac{\sqrt{5}-1}{4\sqrt{5}\pi} K_{15}^2 = \frac{1}{2\sqrt{15}\pi} K_{15} K_{5/3}$$

with $K_{15} := \mathbf{K}(k_{15})$ and $K_{5/3} := \mathbf{K}(k_{5/3})$, where

$$k_{5/3} = \frac{(2 - \sqrt{3})(\sqrt{5} + \sqrt{3})(3 + \sqrt{5})}{8\sqrt{2}}$$

yields the larger nome $q_{5/3} := \exp(-\pi\sqrt{5/3}) = q_{15}^{1/3}$. Thus evaluation (98) amounts to

$$t_{5,1} = \frac{\pi^2}{16} \sum_{n=0}^{\infty} \frac{b_n}{64^n} \frac{\sqrt{[5]}}{\underline{\underline{\quad}}}}{4} K_{15} K_{5/3} \quad (104)$$

with a summand $b_n/64^n = O(n^{-3/2}/4^n)$, from (56), giving rapid convergence. By taking 10^5 terms, we checked (98) to 60,000 decimal places, using the recursion (58) for the diamond lattice sequence b_n . Our closed form in (104) resulted from paying diligent attention to a footnote in [56, p. 121], which led us, eventually, to discover and prove the connection between quantum field theory and these diamond lattice integers.

We remark that our evaluations of $s_{5,2k+1}$ and $t_{5,2k+1}$ may be expressed in terms of Γ values, using the corresponding evaluation of K_{15}^2 in [7], as was remarked by Laporta after Broadhurst's talk (see footnote 3). For example, we may re-write the conjectural evaluation for $s_{5,3}$ in (96) as

$$\frac{\sqrt{5}}{2} \int_0^\infty t^3 I_0(t) K_0^4(t) dt \stackrel{?[3]}{=} \frac{13 \Gamma\left(\frac{1}{15}\right) \Gamma\left(\frac{2}{15}\right) \Gamma\left(\frac{4}{15}\right) \Gamma\left(\frac{8}{15}\right)}{30^3} - \frac{\Gamma\left(\frac{7}{15}\right) \Gamma\left(\frac{11}{15}\right) \Gamma\left(\frac{13}{15}\right) \Gamma\left(\frac{14}{15}\right)}{15}, \quad (105)$$

which contains all 8 values of $\Gamma(n/15)$ with $n \in [1, 14]$ and coprime to 15. Then the counterpart for $t_{5,3}$ in (99) may be written as

$$\frac{\pi^3}{4\sqrt{3}} \sum_{n=1}^\infty \frac{n^2 b_n}{64^n} \stackrel{\surd[6]}{=} \frac{13 \Gamma\left(\frac{1}{15}\right) \Gamma\left(\frac{2}{15}\right) \Gamma\left(\frac{4}{15}\right) \Gamma\left(\frac{8}{15}\right)}{30^3} + \frac{\Gamma\left(\frac{7}{15}\right) \Gamma\left(\frac{11}{15}\right) \Gamma\left(\frac{13}{15}\right) \Gamma\left(\frac{14}{15}\right)}{15} \quad (106)$$

by the remarkable sign change discovered in our present work and the relation to diamond lattice numbers in (102).

5.3 Double integrals

The moments $c_{5,1}$, $s_{5,1}$ and $t_{5,1}$ are easily expressible as double integrals of elementary functions.

For the 4-loop *vacuum* [56] diagram

$$V_5(a, b, c, d, e) = \int_0^\infty t K_0(at) K_0(bt) K_0(ct) K_0(dt) K_0(et) dt$$

in two spacetime dimensions, we obtain the double integral

$$V_5(a, b, c, d, e) = \int_0^\infty \int_0^\infty xy S_3(a, b, x) D_3(x, y, ic) S_3(d, e, y) dx dy,$$

by grouping the internal lines with masses a and b to give a total momentum with norm x^2 and those with masses d and e to give a total momentum with norm y^2 . Then the coupling term

$$\frac{1}{\pi} \int_0^\pi \frac{d\theta}{x^2 + 2xy \cos \theta + y^2 + c^2} = \frac{1}{\sqrt{(x+y)^2 + c^2} \sqrt{(x-y)^2 + c^2}} = D_3(x, y, ic)$$

comes from an angular average in two Euclidean dimensions. Setting the five masses to unity, we obtain

$$c_{5,1} = \int_0^\infty \int_0^\infty \frac{4 \operatorname{arcsinh}(x/2) \operatorname{arcsinh}(y/2) dx dy}{\sqrt{(4+x^2)(4+y^2)(1+(x+y)^2)(1+(x-y)^2)}}, \quad (107)$$

where we have converted the $\operatorname{arctanh}$ function of (22) to a more convenient $\operatorname{arcsinh}$ function, in the equal-mass case.

Similarly, the 3-loop *sunrise* [40] diagram

$$S_5(a, b, c, d, z) = \int_0^\infty t K_0(at) K_0(bt) K_0(ct) K_0(dt) J_0(zt) dt$$

yields the double integral

$$S_5(a, b, c, d, z) = \int_0^\infty \int_0^\infty xy S_3(a, b, x) D_3(x, y, ic) D_3(y, z, id) dx dy,$$

by cutting one line in V_5 and setting the norm of its Euclidean momentum to z^2 . Setting the 4 masses to unity and analytically continuing to the on-shell point $z^2 = -1$, we obtain

$$s_{5,1} = \int_0^\infty \int_0^\infty \frac{2 \operatorname{arcsinh}(x/2) dx dy}{\sqrt{(4+x^2)(4+y^2)(1+(x+y)^2)(1+(x-y)^2)}} \stackrel{?[2]}{=} \frac{\pi}{2\sqrt{15}} K_{15} K_{5/3}, \quad (108)$$

whose conjectural evaluation is given by (95).

We then define

$$T_5(w, a, b, c, z) := \int_0^\infty t J_0(wt) K_0(at) K_0(bt) K_0(ct) J_0(zt) dt$$

as the angular average of the diagram obtained by cutting two lines in V_5 and setting the norms of their momenta to w^2 and z^2 . Hence we obtain the double integral

$$T_5(w, a, b, c, z) = \int_0^\infty \int_0^\infty xy D_3(w, x, ia) D_3(x, y, ib) D_3(y, z, ic) dx dy,$$

which leads to

$$t_{5,1} = \int_0^\infty \int_0^\infty \frac{dx dy}{\sqrt{(4+x^2)(4+y^2)(1+(x+y)^2)(1+(x-y)^2)}} \stackrel{\surd[5]}{=} \frac{1}{4} K_{15} K_{5/3}, \quad (109)$$

whose evaluation is given by (98). If we multiply (109) by 4, we recover the double-integral discovery reported by Laporta in Eqs. 17, 18 and 19 of [56].

Finally, by doubling one of the internal masses, we obtain

$$\int_0^\infty t I_0^2(t) K_0^2(t) K_0(2t) dt = \int_0^\infty \int_0^\infty \frac{dx dy}{\sqrt{(4+x^2)(4+y^2)(4+(x+y)^2)(4+(x-y)^2)}}$$

and hence the conjectural evaluation

$$\int_0^\infty \int_0^\infty \frac{dx dy}{\sqrt{(1+x^2)(1+y^2)(1+(x+y)^2)(1+(x-y)^2)}} \stackrel{?[8]}{=} \frac{1}{3} K_3 K_3', \quad (110)$$

after rescaling x and y by a factor of 2 and invoking (101).

Evaluation (110) resonates with the proven evaluations (44) and (45) in Section 3, where we found that removing $(1+(x-y)^2)$ from the square root in (110) doubles the value of the integral and that removing $(1+(x+y)^2)$ multiplies it by 4.

We were unable find a transformation of variables for the double integrals in (109) and (110) that suggested their evaluations as products at the singular values k_{15} and k_3 , respectively. In the next 3 subsections we show how to express (109) as a single integral of a complete elliptic integral, in 3 rather different ways.

As observed in a footnote in [56, p. 120], entry 3.1.5.16 in [63, Vol. 1] is intriguing: for real parameters k_1 and k_2 , with $k_1^2 + k_2^2 < 1$, one has

$$\int_0^{\pi/2} \int_0^{\pi/2} \frac{d\theta d\phi}{\sqrt{1 - k_1^2 \sin^2 \theta - k_2^2 \sin^2 \phi}} = \frac{2 \mathbf{K}(\alpha) \mathbf{K}'(\beta)}{1 + \sqrt{1 - k_2^2}}, \quad (111)$$

where

$$\alpha := \frac{\sqrt{1-k_1^2} - \sqrt{1-k_1^2-k_2^2}}{1 + \sqrt{1-k_2^2}} \quad \text{and} \quad \beta := \frac{\sqrt{1-k_1^2} + \sqrt{1-k_1^2-k_2^2}}{1 + \sqrt{1-k_2^2}}.$$

Perhaps there are implications for (110) from this general form. As discussed in [19, 39], one can establish a more recondite counterpart for

$$\int_0^{\pi/2} \int_0^{\pi/2} \sqrt{1 - k_1^2 \sin^2 \theta - k_2^2 \sin^2 \phi} \, d\theta \, d\phi.$$

5.4 Single integrals from polar coordinates

We may recast evaluations (109) and (110) by transforming the more general double integral

$$J(c) := \int_0^\infty \int_0^\infty \frac{dx \, dy}{\sqrt{(c+x^2)(c+y^2)(1+(x+y)^2)(1+(x-y)^2)}}$$

to polar coordinates. With $x = r \cos \theta$ and $y = r \sin \theta$, the product of the first two factors in the square root gives a term linear in $w := \cos 4\theta$, as does the remaining product. An angular integral of the form

$$\int_{-1}^1 \frac{dw}{\sqrt{(1-w^2)(2A^2-1-w)(2B^2-1+w)}} = \frac{1}{AB} \mathbf{K} \left(\frac{\sqrt{A^2+B^2-1}}{AB} \right)$$

results, with $A = 1 + 2c/r^2$ and $B = 1 + 1/r^2$. Transforming to $z = r^2/(1+r^2)$, we obtain the single integral

$$J(c) = \int_0^1 \mathbf{K} \left(\frac{z\sqrt{1+4c(1-z)(z+c(1-z))}}{z+2c(1-z)} \right) \frac{dz}{z+2c(1-z)}. \quad (112)$$

Setting $c = 4$, we transform evaluation (109) to

$$\int_0^1 \mathbf{K} \left(\frac{z\sqrt{(13-12z)(5-4z)}}{8-7z} \right) \frac{dz}{8-7z} \stackrel{[5]}{=} \frac{1}{4} K_{15} K_{5/3}. \quad (113)$$

Setting $c = 1$, we transform conjecture (110) to

$$\int_0^1 \mathbf{K} \left(\frac{z\sqrt{5-4z}}{2-z} \right) \frac{dz}{2-z} \stackrel{[8]}{=} \frac{1}{3} K_3 K_{1/3} \quad (114)$$

since, by definition of a singular value, $K_{1/3} = K'_3$. A hypergeometric version of (114) may be obtained by writing its left-hand side as the ornate triple sum

$$\frac{\pi}{4} \sum_{n=0}^{\infty} \left(\frac{(2n)!}{2^{2n} n!} \right)^3 \sum_{m=0}^n 2^{2m} \frac{{}_2F_1 \left(\begin{matrix} 2n+1, 2n+1 \\ 2n+2+m \end{matrix} \middle| \frac{1}{2} \right)}{(n-m)!(2n+1+m)!} \stackrel{[8]}{=} \frac{\pi^2}{4\sqrt{3}} {}_3F_2 \left(\begin{matrix} \frac{1}{2}, \frac{1}{2}, \frac{1}{2} \\ 1, 1 \end{matrix} \middle| \frac{1}{4} \right).$$

We computed the single integrals in (113) and (114) using *Pari-GP*, which provides an efficient `agm` procedure, for evaluating the complete elliptic integral \mathbf{K} , and an efficient `intnum` procedure, for the numerical quadrature. In each case, we confirmed the evaluation to 1200 decimal places but were none the wiser as to its origin.

5.5 Single integrals over discontinuities

Seeking illumination, we turned to integrals over the elliptic integral (62) in the discontinuity D_4 , coming from the Dalitz-plot integration in (61).

For the 4-loop vacuum diagram V_5 we may fold D_4 from (62) with V_3 from (28), to obtain

$$V_5(a, b, c, d, e) = \int_{a+b+c}^{\infty} 2v D_4(a, b, c, v) V_3(v, d, e) dv. \quad (115)$$

With unit masses and $y = 1/v$, this gives the moments

$$c_{5,1} = \int_0^{\frac{1}{3}} \frac{D(y)L(y)}{\sqrt{1-4y^2}} dy \quad (116)$$

$$c_{5,3} = \int_0^{\frac{1}{3}} \frac{y^2 D(y)}{(1-4y^2)^2} \left(\frac{4(1-2y^2+4y^4)L(y)}{\sqrt{1-4y^2}} + 2 - 8y^2 + 8(1-y^2)\log(y) \right) dy, \quad (117)$$

with a complete elliptic integral in $D(y)$, from (64), and a dilogarithmic function

$$L(y) := \frac{1}{2} \text{Li}_2 \left(\frac{\sqrt{1-4y^2}-1}{\sqrt{1-4y^2}+1} \right) - \frac{1}{2} \text{Li}_2 \left(\frac{\sqrt{1-4y^2}+1}{\sqrt{1-4y^2}-1} \right) \quad (118)$$

$$= -\text{Li}_2 \left(\frac{1-\sqrt{1-4y^2}}{2} \right) + \frac{1}{2} \log^2 \left(\frac{1-\sqrt{1-4y^2}}{2} \right) - \log^2(y) + \frac{\pi^2}{12}, \quad (119)$$

with (118) coming from (28) and the reduction to a single convenient Li_2 value in (119) obtained by transformations in [57, A.2.1] and noted in [34, Eq. 3.21]. Further differentiations yield an even lengthier integrand for $c_{5,5}$. However, we expected the odd moments $c_{5,2k+1}$ with $k > 1$ to be expressible as Q-linear combinations of $c_{5,3}$, $c_{5,1}$ and unity. Hence we lazily used PSLQ to arrive at our ninth conjecture

$$c_{5,5} \stackrel{?[9]}{=} \frac{76}{15} c_{5,3} - \frac{16}{45} c_{5,1} + \frac{8}{15} \quad (120)$$

with a final rational term originating, presumably, from the analytically trivial input

$$\int_0^{\infty} t^5 K_0(t) K_1^4(t) dt = \lim_{t \rightarrow 0} \frac{t^5 K_1^5(t)}{5} = \frac{1}{5} \quad (121)$$

to the richer (and more challenging) recursions considered in the talk of footnote 3, which dealt with integrals of products of powers of t , $K_0(t)$ and the derivative $K_0'(t) = -K_1(t)$. From (116), (117) and the eminently believable conjecture (120), higher odd moments are obtainable from (10) and (11). Unfortunately we lack a more explicit evaluation of the single integrals for $c_{5,1}$ and $c_{5,3}$.

For the 3-loop sunrise diagram, the corresponding folding is

$$S_5(a, b, c, d, w) = \int_{a+b+c}^{\infty} 2v D_4(a, b, c, v) S_3(v, d, w) dv, \quad (122)$$

from which we obtain the on-shell value

$$s_{5,1} = \int_0^{\frac{1}{3}} \frac{2D(y)}{\sqrt{1-4y^2}} \operatorname{arctanh} \left(\sqrt{\frac{1-2y}{1+2y}} \right) dy \stackrel{?[2]}{=} \frac{\pi}{2\sqrt{15}} K_{15} K_{5/3} \quad (123)$$

and, by use of Bessel's equation, the more complicated integral

$$s_{5,3} = \int_0^{\frac{1}{3}} \frac{4y^2 D(y)}{(1-4y^2)^2} \left(\frac{2(1-2y^2+4y^4) \operatorname{arctanh} \left(\sqrt{\frac{1-2y}{1+2y}} \right)}{\sqrt{1-4y^2}} - 1 + y^2 \right) dy \quad (124)$$

for the next odd moment, conjecturally given by (96). Then PSLQ gives

$$s_{5,5} \stackrel{?[2,3,4]}{=} \frac{76}{15} s_{5,3} - \frac{16}{45} s_{5,1}, \quad (125)$$

which presumably results from a partial integration in the even richer (and even more challenging) recursions for integrals of products of powers of t , $I_0(t)$, $I_1(t)$, $K_0(t)$ and $K_1(t)$. We used *Pari-GP* to evaluate the dispersive single integrals for the first 3 odd moments $s_{5,2k+1}$, with $k = 0, 1, 2$, to 1200 decimal places, and hence checked the conjectured evaluations (95), (96) and (97) and their consequent integer relation (125), to this high precision.

Similarly, the folding

$$T_5(u, a, b, c, w) = \int_{a+b+c}^{\infty} 2v D_4(a, b, c, v) D_3(u, iv, w) dv \quad (126)$$

gives, with $y = 1/v$, the on-shell, unit-mass result

$$t_{5,1} = \int_0^{\frac{1}{3}} \frac{D(y)}{\sqrt{1-4y^2}} dy \stackrel{\sqrt{[5]}}{=} \frac{1}{4} K_{15} K_{5/3} \quad (127)$$

and, by use of Bessel's equation,

$$t_{5,3} = \int_0^{\frac{1}{3}} \frac{4y^2(1-2y^2+4y^4)D(y)}{(1-4y^2)^{5/2}} dy \quad (128)$$

for the next odd moment, given by (99). Then PSLQ gives

$$t_{5,5} \stackrel{\sqrt{[7]}}{=} \frac{76}{15} t_{5,3} - \frac{16}{45} t_{5,1}, \quad (129)$$

which was checked to 60,000 decimal places, in the more convenient sum

$$\sum_{n=0}^{\infty} \frac{b_n}{64^n} \left(16n^2(n-1)^2 - \frac{76}{15} 4n^2 + \frac{16}{45} \right) \stackrel{\sqrt{[7]}}{=} 0 \quad (130)$$

over the diamond lattice integers in (102).

By setting $u = w = i$, $a = b = 1$ and $c = 2$ in (126) and transforming to $y = 4/v$, we obtain the representation

$$\int_0^1 \frac{4y \mathbf{K} \left(\frac{2+y}{2-y} \sqrt{\frac{1-y}{1+y}} \right)}{\sqrt{(2-y)^3(2+y)(1+y)}} dy \stackrel{?[8]}{=} \frac{1}{3} K_3 K_{1/3} \quad (131)$$

as the dispersive counterpart to (114), but still have no better idea as to why the third singular value occurs.

5.6 Relations between elliptic integrals

We found a third way of stating our conjectures in terms of integrals over \mathbf{K} . This arose from the double-integral representation

$$s_{5,1} = \int_0^\infty \int_0^\infty \frac{2 \operatorname{arcsinh}(x/2) dx dy}{\sqrt{(4+x^2)(4+y^2)R(x,y)}} \stackrel{?[2]}{=} \frac{\pi}{2\sqrt{15}} K_{15} K_{5/3} \quad (132)$$

with the product $(1+(x+y)^2)(1+(x-y)^2)$ in (108) replaced by the non-factorizable term

$$R(x,y) = \left| \frac{(x+i)^2 + 4 + y^2}{2} \right|^2 = x^2 + \left(\frac{3+x^2+y^2}{2} \right)^2.$$

We obtained (132) by introducing a Feynman parameter, z , to combine two unit-mass propagators, with momenta $q-p$ and $r-q$, in the integral

$$\frac{1}{AB} = \int_0^1 \frac{dz}{(zA + (1-z)B)^2}$$

with $A := N(q-p)$ and $B := N(r-q)$. Here, p is the combined momentum of the other two internal lines and r is the external momentum of the 3-loop sunrise diagram. Integration over the two-dimensional vector q leaves an integral over z with a denominator $z(1-z)(r-p) \cdot (r-p) + 1$ that is symmetric about the mid-point $z = \frac{1}{2}$. Integrating over the angle between p and r , setting $p \cdot p = x^2$ and analytically continuing to the on-shell point $r \cdot r = -1$, we obtain (132) by making the transformation $z(1-z) = 1/(4+y^2)$ which maps $z=0$ to $y=\infty$ and the mid-point $z = \frac{1}{2}$ to $y=0$.

This method provided an analytical advance, since it proved the equality $E_1(u) = E_2(u)$ between the elliptic integrals

$$E_1(u) := \frac{1}{2} \int_0^\infty \frac{dv}{\sqrt{v(4+v)(1+2u+2v+(u-v)^2)}} \quad (133)$$

$$E_2(u) := \int_0^\infty \frac{dv}{\sqrt{v(4+v)(4u+(3+u+v)^2)}}, \quad (134)$$

where we have transformed to $u = x^2$ and $v = y^2$. When *Maple* was asked to evaluate E_1 and E_2 it printed different expressions, each containing an incomplete elliptic integral

$$F(\sin \phi, k) := \int_0^\phi \frac{1}{\sqrt{1-k^2 \sin^2 \theta}} d\theta$$

with a relation between k and ϕ which we reduced to the form

$$k = \frac{\sqrt{1-2\cos\phi}}{(1-\cos\phi)\sin\phi}. \quad (135)$$

The incomplete integral was eliminated by computing $(2E_1 + E_2)/3$, for which *Maple* gave an expression involving only the complete elliptic integral $\mathbf{K}(k)$. By this means, we proved that

$$F(\sin \phi, k) = \frac{2}{3} \mathbf{K}(k) \quad (136)$$

whenever k and ϕ are related by condition (135). Moreover, by using [1, 17.4.13], we proved that this condition also gives the evaluation

$$F(1 - \cos \phi, k) = \frac{1}{3} \mathbf{K}(k), \quad (137)$$

which we shall use in the next subsection.

Our result for $E(x) := E_1(x^2) = E_2(x^2)$ is

$$E(x) = \sqrt{\frac{\sin(2\alpha(x))}{2x} \frac{\mathbf{K}(\sin \alpha(x))}{3}} = \frac{\pi}{3\sqrt{3}} \text{HeunG}(9, 3; 1, 1, 1, 1; -x^2) \quad (138)$$

with

$$\alpha(x) = \frac{3 \arctan(x) - \arctan(x/3)}{2}. \quad (139)$$

This then gives

$$s_{5,1} = \int_0^\infty \frac{2E(x)}{\sqrt{4+x^2}} \operatorname{arcsinh}\left(\frac{x}{2}\right) dx \stackrel{?[2]}{=} \frac{\pi}{2\sqrt{15}} K_{15} K_{5/3} \quad (140)$$

$$t_{5,1} = \int_0^\infty \frac{E(x)}{\sqrt{4+x^2}} dx \stackrel{\surd[5]}{=} \frac{1}{4} K_{15} K_{5/3} \quad (141)$$

as the non-dispersive counterparts to the integrals (123) and (127) over the different complete elliptic integral in $D(y)$, with a closely related **HeunG** function in (64).

We note that $E(x)$ contains a factor of $1/3$ from evaluating $(2E_1 + E_2)/3$. This ensures that we correctly reproduce

$$s_{3,1} = E(0) = \frac{\pi}{3\sqrt{3}} = L_{-3}(1)$$

using $\alpha(x) = 4x/3 + O(x^3)$. The relationship

$$\tan(2\alpha(x)) = \frac{8x}{3 - 6x^2 - x^4} \quad (142)$$

gives $E(x) = \log(x^2)/x^2 + O(\log(x)/x^4)$, as expected at large momentum.

5.7 Expansions near singularities

The **HeunG** forms for $D(y)$ and $E(x)$, in (64) and (138), yield expansions near the regular points $y = \frac{1}{3}$ and $x = 0$, respectively. However, these regular expansions were not needed in our numerical integrations, since the **agm** procedure of *Pari-GP* is highly efficient for the evaluation of $\mathbf{K}(k)$ when k is not close to the singular point at $k = 1$. What we really need, and eventually found, are the expansions

$$\frac{D(y)}{3y} = - \sum_{k=0}^{\infty} (h_k + a_k \log(y^2)) y^{2k} \quad (143)$$

$$x^2 E(x) = - \sum_{k=0}^{\infty} \frac{h_k - a_k \log(x^2)}{(-x^2)^k} \quad (144)$$

that isolate the logarithmic singularities as $y \rightarrow 0$ and $x \rightarrow \infty$, respectively. Here a_k is the hexagonal lattice integer of (24) and h_k is determined by the differential equation for $D(y)$, or equivalently $E(x)$, which yields the recursion

$$(k+1)^2 h_{k+1} - (10k^2 + 10k + 3)h_k + 9k^2 h_{k-1} = -2(k+1)a_{k+1} + 10(2k+1)a_k - 18ka_{k-1} \quad (145)$$

with a starting value $h_0 = 0$. We note that (143) converges for $0 < y < \frac{1}{3}$ and (144) converges for $x > 3$. We were alerted to role of the hexagonal lattice integers by the regular expansion

$$E(x) = \frac{\pi}{3\sqrt{3}} \sum_{k=0}^{\infty} a_k \left(\frac{-x^2}{9} \right)^k, \quad (146)$$

which is valid for $|x| < 1$, since $a_k = O(9^k/k)$ for large k .

We were able to solve the recursion (145) in closed form, by considering the moment

$$T_4(u, a, b, v) := \int_0^{\infty} t J_0(ut) K_0(at) K_0(bt) J_0(vt) dt = \int_{a+b}^{\infty} 2w D_3(a, b, w) D_3(u, v, iw) dw$$

which yields, in general, an incomplete elliptic integral

$$T_4(u, a, b, v) = \int_{(a+b)^2}^{\infty} \frac{dx}{\sqrt{(x - (a+b)^2)(x - (a-b)^2)(x + (u+v)^2)(x + (u-v)^2)}} \quad (147)$$

by transforming to $x = w^2$. In the special case with $a = 1$, $b = 1/y > 1$ and $u = v = i$, *Maple* gave the evaluation

$$T_4(i, 1, 1/y, i) = \frac{2y^2 F(1 - \cos \phi, k)}{\sqrt{(1+3y)(1-y)^3}}$$

with

$$\phi = \arccos \left(\frac{2y}{1+y} \right), \quad k = \sqrt{\frac{(1-3y)(1+y)^3}{(1+3y)(1-y)^3}}. \quad (148)$$

This relation between k and ϕ is precisely as in (135). Hence, using (137), we obtain

$$\frac{y D(y)}{6} = T_4(i, 1, 1/y, i) := \int_0^{\infty} t I_0^2(t) K_0(t) K_0(t/y) dt \quad (149)$$

since $D(y)$ in (64) contains the complete elliptic integral $\mathbf{K}(k)$ with k given in (148). Then we used the expansion of $I_0^2(t)$, in (92), and of [1, 9.6.13]

$$K_0(t) = -(\log(t/2) + \gamma) I_0(t) + \sum_{k=1}^{\infty} \left(\frac{t^k}{2^k k!} \right)^2 \sum_{n=1}^k \frac{1}{n}, \quad (150)$$

where γ is Euler's constant, to obtain from (143) and (149) the closed form

$$h_k = \sum_{j=1}^k \binom{k}{j}^2 \binom{2j}{j} \sum_{n=0}^{j-1} \frac{2}{k-n}, \quad (151)$$

which is a harmonic twist of the closed form (24) for the hexagonal lattice integers a_k . Hence we obtain an integer sequence for $H_k := k! h_k / 4$, with $k > 0$, beginning with

$$1, 13, 263, 7518, 280074, 12895572, 707902740, 45152821872, 3282497058384 \dots$$

Thanks to this sequence, we were able to evaluate all the single integrals over $D(y)$ and $E(x)$ in this work to 1200 decimal places, since we had very good control of logarithmic singularities near the endpoints, as $y \rightarrow 0$ and $x \rightarrow \infty$, respectively.

5.8 A modular identity from quantum field theory

A careful analysis [33] of the Dalitz plot shows that the relation (135) between k and ϕ implies that [33, Eq. 5.17]

$$Z(F(\sin \phi, k), k) = \frac{1}{3}k^2 \sin^3 \phi, \quad (152)$$

where Z is *Maple's* `JacobiZeta` function. Combining our new finding (136) with this, we obtain from [1, 17.4.38] an elementary evaluation of

$$\frac{\sqrt{3}\pi}{4\mathbf{K}(k)} \sum_{n=0}^{\infty} \left(\frac{4}{(q^{-3n-1} - q^{3n+1})} - \frac{4}{(q^{-3n-2} - q^{3n+2})} \right) = \frac{1}{2}t^{-1} - \frac{1}{6}t^{-3}, \quad (153)$$

where q is the *nome* associated with k and $t = \tan(\phi/2)$ is determined algebraically by

$$\begin{aligned} r &= (4k^2(1-k^2))^{\frac{1}{3}}, \quad s = 2k\sqrt{r+k^2} + 2k^2 + \frac{2(1-2k^2)r}{\sqrt{1+r+r^2}} - r, \\ t &= \left(\frac{k - \sqrt{r+k^2} + \sqrt{s}}{3k + \sqrt{r+k^2} - \sqrt{s}} \right)^{\frac{1}{2}}. \end{aligned}$$

In particular, for $k = 1/\sqrt{2}$ we obtain $t = (2/\sqrt{3} - 1)^{1/4}$.

A modular setting for this result is provided by Jacobi's identity

$$\sqrt{k} \theta_3(q) = \theta_2(q) := \sum_{n=-\infty}^{\infty} q^{(n+\frac{1}{2})^2} \quad (154)$$

with $\theta_3(q)$ related to $\mathbf{K}(k)$ by (103). Summation of the Lambert series in (153) gives $\theta_2^3(q^{3/2})/\theta_2(q^{1/2})$, which is a result known to Ramanujan. Thus we have proven the *modular identity*

$$\sqrt{3} \frac{\theta_2^3(q^{3/2})}{\theta_3^2(q)\theta_2(q^{1/2})} = t^{-1} - \frac{1}{3}t^{-3}, \quad (155)$$

where $c := t^{-2}$ is the unique positive root of the polynomial

$$S(x) = 3 + 8 \left(1 - 2 \frac{\theta_2^4(q)}{\theta_3^4(q)} \right) x + 6x^2 - x^4 \quad (156)$$

and indeed $1 \leq c \leq 3$. The real roots are $-\theta_2^2(q^{1/3})/\theta_3^2(q)$ and $3\theta_2^2(q^3)/\theta_3^2(q)$, as has been known since Joubert and Cayley [24, (4.6.14)]. Hence (155) devolves to

$$\frac{\theta_2^3(q^{3/2})}{\theta_2(q^{1/2})} = \theta_3^2(q) \left\{ \frac{\theta_3(q^3)}{\theta_3(q)} - \frac{\theta_3^3(q^3)}{\theta_3^3(q)} \right\}. \quad (157)$$

Such modular identities are machine-provable—in principle and in practice—by computing that sufficiently many terms of the Taylor series agree. This is the so-called “modular machine” [25, §3]. In this case confirming 1000-term agreement is more than adequate to prove (157); as takes seconds in *Maple*. A conventional proof can be pieced together from [24, Thm. 4.11]. Our proof came from quite another source: the Lorentz invariance of quantum field theory in two spacetime dimensions, which enabled us to prove that (133) and (134) are identical.

5.9 A discrete sum rule

It seemed reasonable to try to prove the evaluation for $t_{5,1}$ in one of its forms

$$t_{5,1} = \int_0^{\frac{1}{3}} \frac{D(y) dy}{\sqrt{1-4y^2}} \stackrel{\sqrt{[5]}}{=} \frac{1}{4} K_{15} K_{5/3} \quad (158)$$

$$t_{5,1} = \int_0^\infty \frac{E(x) dx}{\sqrt{4+x^2}} \stackrel{\sqrt{[5]}}{=} \frac{1}{4} K_{15} K_{5/3} \quad (159)$$

with $D(y)$ given by (64) and $E(x)$ by (138).

For example, by using [23, (2.35), p. 119] one may deduce that

$$\int_0^{\pi/2} \int_0^{\pi/2} \frac{d\theta d\phi}{\sqrt{64 - (16 - \sin^2 \phi) \sin^2 \theta}} = \frac{1}{8} K_{15} K_{5/3} \quad (160)$$

and then hope to relate some such recognizable double integral to the single integrals in (158) and (159).

In fact, the integral forms (158) and (159) resisted prolonged and intense efforts to find a proof. A break-through came from the sum in (104), which we rewrite as

$$\sum_{k=1}^{\infty} \frac{b_{k-1}}{64^k} \stackrel{\sqrt{[5]}}{=} \frac{1}{16\pi^2} K_{15} K_{5/3}, \quad (161)$$

whose right-hand side we shall relate to the first of the generalized Watson integrals [49, 50]

$$W_j(z) := \frac{1}{\pi^3} \int_0^\pi \int_0^\pi \int_0^\pi \frac{d\theta_1 d\theta_2 d\theta_3}{1 - z w_j(\theta_1, \theta_2, \theta_3)} \quad (162)$$

with

$$w_1(\theta_1, \theta_2, \theta_3) = \frac{\cos \theta_1 \cos \theta_2 + \cos \theta_2 \cos \theta_3 + \cos \theta_3 \cos \theta_1}{3} \quad (163)$$

in the case of a *face-centred cubic* (f.c.c.) lattice [46],

$$w_2(\theta_1, \theta_2, \theta_3) = \frac{\cos \theta_1 + \cos \theta_2 + \cos \theta_3}{3} \quad (164)$$

in the case of a *simple cubic* (s.c.) lattice [48],

$$w_3(\theta_1, \theta_2, \theta_3) = \cos \theta_1 \cos \theta_2 \cos \theta_3 \quad (165)$$

in the case of a *body-centred cubic* (b.c.c.) lattice [47] and

$$w_4(\theta_1, \theta_2, \theta_3) = \frac{1 + \cos \theta_1 \cos \theta_2 + \cos \theta_2 \cos \theta_3 + \cos \theta_3 \cos \theta_1}{4} \quad (166)$$

in the case of a *diamond* lattice [44].

In 1971, Joyce gave the notable f.c.c. evaluation [46, Eq. 4]

$$W_1(z) = \frac{12}{\pi^2} \frac{\mathbf{K}(k_+(z)) \mathbf{K}(k_-(z))}{3+z} \quad (167)$$

with

$$k_\pm^2(z) = \frac{1}{2} \pm \frac{2\sqrt{3}z}{(3+z)^{3/2}} - \frac{\sqrt{3}(3-z)(1-z)^{1/2}}{(3+z)^{3/2}}. \quad (168)$$

Our progress resulted from the intriguing observation that at $z = \frac{1}{5}$ this gives $k_-(1/5) = k_{15}$ and $k_+(1/5) = k_{5/3}$. Hence we obtain

$$W_1\left(\frac{1}{5}\right) = \frac{15}{4\pi^2} K_{15} K_{5/3}, \quad (169)$$

which reduces (161) to the discrete sum rule

$$\sum_{k=1}^{\infty} \frac{b_{k-1}}{64^k} \stackrel{\sqrt{[5]}}{=} \sum_{k=1}^{\infty} \frac{f_{k-1}}{60^k} \quad (170)$$

where the f.c.c. lattice integers

$$f_k := \frac{4^k}{\pi^3} \int_0^\pi \int_0^\pi \int_0^\pi (\cos \theta_1 \cos \theta_2 + \cos \theta_2 \cos \theta_3 + \cos \theta_3 \cos \theta_1)^k d\theta_1 d\theta_2 d\theta_3 \quad (171)$$

give the Taylor coefficients of the expansion

$$W_1(z) = \sum_{k=0}^{\infty} f_k \left(\frac{z}{12}\right)^k \quad (172)$$

for $|z| \leq 1$. In the next subsection, we show that (170) derives from a more general set of sum rules. Then, in subsection 5.11, we shall expose a cubic modular equation, implicit in (168).

5.10 Sum rules for diamond and cubic lattice integers

The first few terms in the sequence for the f.c.c. lattice integers (171) are

$$1, 0, 12, 48, 540, 4320, 42240, 403200, 4038300, 40958400, 423550512, 4434978240 \quad (173)$$

for $n = 0 \dots 11$. The values up to $f_8 = 4038300$ are recorded in [70, Table 1] and the next integer, $f_9 = 40958400$, was given by Domb [36] and recorded⁵ in entry A2899 of the on-line version of [66], which provided us with no closed formula for f_k . By way of contrast, the s.c., b.c.c. and diamond lattice expansions

$$W_2(z) = \sum_{k=0}^{\infty} \binom{2k}{k} a_k \left(\frac{z}{6}\right)^{2n} \quad (174)$$

$$W_3(z) = \sum_{k=0}^{\infty} \binom{2k}{k}^3 \left(\frac{z}{8}\right)^{2n} \quad (175)$$

$$W_4(z) = \sum_{k=0}^{\infty} b_k \left(\frac{z}{16}\right)^n \quad (176)$$

lead to explicit expressions for the integer sequences in entries A2896, A2897 and A2895, respectively, of the on-line version of [66]. As in the f.c.c. case (172), expansions (174) to (176) are valid for $|z| \leq 1$. For convenience, we repeat here the closed forms

$$a_k = \sum_{j=0}^k \binom{k}{j}^2 \binom{2j}{j}, \quad b_k = \sum_{j=0}^k \binom{k}{j}^2 \binom{2k-2j}{k-j} \binom{2j}{j}, \quad (177)$$

⁵See <http://www.research.att.com/~njas/sequences/A002899>.

for the hexagonal and diamond lattice integers, previously given in (24) and (56). The hexagonal lattice integers a_k appear in the s.c. lattice integers $\binom{2k}{k}a_k$ of expansion (174). We also note the terminating hypergeometric series

$$b_k = \binom{2k}{k} {}_4F_3 \left(\begin{matrix} \frac{1}{2}, -k, -k, -k \\ 1, 1, -k + \frac{1}{2} \end{matrix} \middle| 1 \right)$$

for the diamond lattice integers. Likewise

$$a_k = {}_3F_2 \left(\begin{matrix} \frac{1}{2}, -k, -k \\ 1, 1 \end{matrix} \middle| 4 \right).$$

We were able to derive the closed form

$$f_k = \sum_{j=0}^k \binom{k}{j} (-4)^{k-j} b_j \quad (178)$$

for the f.c.c. lattice integers, by noting the similarity between (163) and (166), which leads to the functional relationship

$$\frac{1}{4N+4} W_4 \left(\frac{4}{N+1} \right) = \frac{1}{4N} W_1 \left(\frac{3}{N} \right) \quad (179)$$

between the Green functions for the diamond and f.c.c. lattices. Then for $N \geq 3$ we may expand each side, to obtain the sum rule

$$\sum_{k=1}^{\infty} \frac{b_{k-1}}{(4N+4)^k} = \sum_{k=1}^{\infty} \frac{f_{k-1}}{(4N)^k} \quad (180)$$

and derive the closed form (178) for the f.c.c. lattice integers defined in (171) by further expanding the left-hand side in powers of $1/N$.

Setting $N = 3$ in (180), we prove the sum rule

$$\sum_{k=1}^{\infty} \frac{b_{k-1}}{16^k} = \sum_{k=1}^{\infty} \frac{f_{k-1}}{12^k} = \frac{1}{12} W_1(1) = \frac{1}{4\pi^2} K_3 K_{1/3} \quad (181)$$

from Watson's evaluation [71] of $W_1(1)$, at the singular value k_3 .

Setting $N = 15$ in (180), we prove the sum rule

$$\sum_{k=1}^{\infty} \frac{b_{k-1}}{64^k} = \sum_{k=1}^{\infty} \frac{f_{k-1}}{60^k} = \frac{1}{60} W_1 \left(\frac{1}{5} \right) = \frac{1}{16\pi^2} K_{15} K_{5/3} \quad (182)$$

at the singular value k_{15} . Hence we have proven (170) and all the other forms of our initial conjecture (98) for the moment $t_{5,1}$. By taking up to 4 differentials of $W_1(3/N)$, before setting $N = 15$, one may also prove the evaluations of $t_{5,3}$ in (99) and $t_{5,5}$ in (100), using the evaluations of the elliptic integrals $\mathbf{E}(k_{15})$ and $\mathbf{E}(k_{5/3})$ given explicitly in the talk of footnote 3 and derivable from identities in [24].

These eventual proofs of our conjectures for the moments $t_{5,2k+1}$ came from noting a parenthetical remark in [48, p. 601] to the effect that the Green function for the diamond

lattice is given by a product of complete elliptic integrals. It will be useful to consider the generating function \tilde{D} which has the explicit form

$$\tilde{D}(y) := \frac{2\mathbf{K}\left(\sqrt{\frac{16y^3}{(1+3y)(1-y)^3}}\right)}{\pi\sqrt{(1+3y)(1-y)^3}} = \frac{1}{\text{AGM}(\sqrt{(1-3y)(1+y)^3}, \sqrt{(1+3y)(1-y)^3})} \quad (183)$$

with a complete elliptic integral that is complementary to that in (64) for $D(y)$. For $|y| < \frac{1}{3}$, we have the expansion

$$\tilde{D}(y) = \text{HeunG}(9, 3; 1, 1, 1, 1; 9y^2) = \sum_{k=0}^{\infty} a_k y^{2k} \quad (184)$$

in terms of the hexagonal lattice integers in (177).

The full story, for the f.c.c., s.c., b.c.c. and diamond lattices, is then provided by the four identities

$$\tilde{D}^2(\sqrt{-x}) = \left(\sum_{k=0}^{\infty} a_k (-x)^k\right)^2 = \sum_{k=0}^{\infty} f_k \frac{x^k}{(1+3x)^{2k+2}} \quad (185)$$

$$= \sum_{k=0}^{\infty} a_k \frac{\binom{2k}{k} (-x(1+x)(1+9x))^k}{((1-3x)(1+3x))^{2k+1}} \quad (186)$$

$$= \sum_{k=0}^{\infty} \frac{\left(\binom{2k}{k} x^k\right)^3}{((1+x)^3(1+9x))^{k+\frac{1}{2}}} \quad (187)$$

$$= \sum_{k=0}^{\infty} b_k \frac{x^k}{((1+x)(1+9x))^{k+1}}, \quad (188)$$

which are valid for sufficiently small x and were obtained by simplification of formulae in [46, 47, 48].

At bottom, all 4 results (185) to (188) originate from the first paper [16] of Wilfrid Norman Bailey's adroit series on infinite integrals involving Bessel functions, in much the same way that our proof of (33) resulted from his second paper [17]. In [16, Eq. 8.1], Bailey showed that $\int_0^\infty J_\mu(at)J_\nu(bt)J_\rho(ct)dt$ is given by a product of ${}_2F_1$ hypergeometric functions. In [46, 47, 48], Joyce used this result to obtain diamond and cubic lattice Green functions, in three spatial dimensions, from the *square* of the Green function (183) for the hexagonal (or "honeycomb") lattice in two spatial dimensions, for which we have given a **HeunG** form in (184) equivalent to that given in [42, Eq. 4]. With $x \geq 0$, the explicit form of E in (138) provides an analytic continuation for

$$\tilde{D}(\sqrt{-x}) = \frac{3\sqrt{3}}{\pi} E(3\sqrt{x}). \quad (189)$$

The singular value k_{15} , obtained from the diamond and f.c.c. lattice sums in (182), also appears in the s.c. and b.c.c. lattice sums

$$\sum_{k=0}^{\infty} \frac{\binom{2k}{k}}{(-45)^k} a_k = \frac{3\sqrt{5}}{2\pi^2} K_{15} K_{5/3} \quad (190)$$

$$\sum_{k=0}^{\infty} \frac{\binom{2k}{k}^3}{2^{4k}(\sqrt{5}+1)^{8k}} = \frac{4}{\pi^2} K_{15}^2 \quad (191)$$

obtained by setting $x = x_{15} := 3 - \frac{4}{3}\sqrt{5} \approx 0.018576$ in (186) and (187). Setting $x = x_{15}$ in (189), we obtain the singular value $k_{5/3} = \sin(\alpha(3\sqrt{x_{15}}))$ from definition of the angle $\alpha(x)$ in (139). This is confirmed by the formula for $\tan(2\alpha(x))$ in (142). We remark that (190) follows from the functional relationship given in [50, Eq. 3.23] and that (191) follows from [24, Table 5.2a ($N = 15$)] and the Clausen product in [24, Th. 5.7(a)(i), p. 180]. We now show how to obtain other singular values from lattice Green functions, using a modular identity.

5.11 Cubic modular equations

The *cubic modular equation* [24, Th. 4.1, p. 110]

$$\theta_4(q)\theta_4(q^3) + \theta_2(q)\theta_2(q^3) = \theta_3(q)\theta_3(q^3) \quad (192)$$

relates instances of the Jacobi functions θ_2 , in (154), and θ_3 , in (103), with *nomes* q and q^3 , to corresponding instances of

$$\sqrt{k'}\theta_3(q) = \theta_4(q) := \sum_{n=-\infty}^{\infty} (-1)^n q^{n^2} \quad (193)$$

with $k' := \sqrt{1-k^2}$ and *nome* q associated with k . If we associate q^3 with the complete elliptic argument l , then (192) gives the identity [24, Eqn. 4.2.6] $\sqrt{k'l'} + \sqrt{k'l} = 1$. The results of the previous subsection follow from the notable circumstance that (168) gives

$$\sqrt{k'_+(z)k'_-(z)} + \sqrt{k_+(z)k_-(z)} - 1 = 0, \quad (194)$$

which may be proven symbolically, by setting $z = 1 - t^2$ and denoting the left-hand side of (194) by $y(t)$. Then $y(t)$ is analytic on the closed unit disk, $|t| \leq 1$, and *Maple* computes an algebraic equation of the form $y(t)P(y(t), t) = 0$ with $P(0, 0)$ non-zero. This proves that $y(t)$ vanishes in some neighbourhood of $t = 0$ and hence for $|t| \leq 1$.

The resulting modular identities for the Green functions of cubic lattices are most conveniently obtained from the Green function W_4 , for the diamond lattice, with a parametric solution

$$W_4(z_4) = \theta_3^2(q)\theta_3^2(q^3), \quad z_4 := \frac{1 - 4\eta^2}{1 - \eta^2}, \quad \eta := \frac{3\theta_3^4(q^3) - \theta_3^4(q)}{3\theta_3^4(q^3) + \theta_3^4(q)}, \quad (195)$$

corresponding to the series solution (188) at $x = (1 - 2\eta)/(3 + 6\eta)$. Then the Green functions for the f.c.c., s.c. and b.c.c. lattices are given by the functional relationships

$$\frac{4}{3}(1 - \eta^2)W_1(z_1) = \frac{2}{3\eta}(1 - \eta^2)W_2(z_2) = \sqrt{\frac{3 - 3\eta}{1 + \eta}}W_3(z_3) = W_4(z_4) \quad (196)$$

with the arguments

$$z_1 = 1 - 4\eta^2, \quad z_2 = \sqrt{z_1 \left(1 - \frac{1}{\eta^2}\right)}, \quad z_3 = \frac{1 - 2\eta}{2 + 2\eta} \sqrt{z_4}, \quad (197)$$

obtained from (185) to (187), respectively, by the substitution $x = (1 - 2\eta)/(3 + 6\eta)$ that gave (195). We note the alternative b.c.c. parameterization [24, Th. 5.7(a)(i), p. 180],

$$W_3(z_3) = {}_3F_2 \left(\begin{matrix} \frac{1}{2}, \frac{1}{2}, \frac{1}{2} \\ 1, 1 \end{matrix} \middle| z_3^2 \right) = \theta_3^4(q^3), \quad z_3 = 2l\sqrt{1 - l^2}, \quad l := \frac{\theta_2^2(q^3)}{\theta_3^2(q^3)}. \quad (198)$$

The equivalence of the forms for z_3 in (197) and (198) results from the modular identity

$$z_3^2 = \frac{(1-2\eta)^2}{(2+2\eta)^2} \frac{1-4\eta^2}{1-\eta^2} = 4l^2(1-l^2) = (2ll')^2 \quad (199)$$

with η defined in (195) and l in (198). To prove (199), we combined the cubic modular identity (192) with the Joubert–Cayley result [24, (4.6.14)] $S(3\theta_3^2(q^3)/\theta_3^2(q)) = 0$, where S is defined in (156). Alternatively, we may again apply the “modular machine” [25, §3].⁶

Noting that the lattices sums in (181) and (182) yield the singular values k_3 and k_{15} , from rational summands, we wondered if any other singular value might be obtained from a lattice Green function in such a neat manner. We know from Watson’s classic work [71] that $W_3(1)$ yields the singular value $k_1 = 1/\sqrt{2}$ while $W_2(1)$ yields the singular value $k_6 = (\sqrt{3} - \sqrt{2})(2 - \sqrt{3})$, as noted in [23]. Moreover, (198) is equivalent to $W_3(2k_N k'_N) = 4K_N^2/\pi^2$, for $q^3 = \exp(-\pi\sqrt{N})$. Hence $W_3(z_3)$ yields the singular values k_1, k_3, k_7 for the rational arguments $z_3 = 1, \frac{1}{2}, \frac{1}{8}$, respectively.

Prompted by the sum over s.c. lattice integers in (190), we sought further examples, in which a sum over rational numbers might lead to a singular value k_N . We found 5 new results for W_2 , which appear to exhaust the cases with rational summands. These occur with $N/3 = 7, 11, 19, 31, 59$, for which we obtained

$$\sum_{k=0}^{\infty} \frac{\binom{2k}{k}}{(-108)^k} a_k = \frac{6}{\pi^2} (3\sqrt{3} - \sqrt{21}) K_{21} K_{7/3} = \frac{3}{7} G(21) \quad (200)$$

$$\sum_{k=0}^{\infty} \frac{\binom{2k}{k}}{(-396)^k} a_k = \frac{6}{\pi^2} (3\sqrt{33} - 5\sqrt{11}) K_{33} K_{11/3} = \frac{\sqrt{3}}{\sqrt{11}} G(33) \quad (201)$$

$$\sum_{k=0}^{\infty} \frac{\binom{2k}{k}}{(-2700)^k} a_k = \frac{30}{\pi^2} (3\sqrt{57} - 13\sqrt{3}) K_{57} K_{19/3} = \frac{15}{19} G(57) \quad (202)$$

$$\sum_{k=0}^{\infty} \frac{\binom{2k}{k}}{(-24300)^k} a_k = \frac{90}{\pi^2} (39\sqrt{3} - 7\sqrt{93}) K_{93} K_{31/3} = \frac{45}{31} G(93) \quad (203)$$

$$\sum_{k=0}^{\infty} \frac{\binom{2k}{k}}{(-1123596)^k} a_k = \frac{69}{8\pi^2} (\sqrt{3} - 1)^9 \sqrt{59} K_{177} K_{59/3} = \frac{23\sqrt{3}}{\sqrt{59}} G(177), \quad (204)$$

with reductions to Γ values given by

$$G(N) = \frac{1}{2\sqrt{2}\pi} \prod_{n=1}^{4N-1} \left[\Gamma\left(\frac{n}{4N}\right) \right]^{\frac{1}{4}(-4N|n)}, \quad (205)$$

where $\Gamma(n/(4N))$ contributes to the product if n is coprime to $4N$ and then occurs with an exponent $\pm\frac{1}{4}$, according as the sign of the Legendre–Jacobi–Kronecker symbol $(-4N|n)$. We remark that $p = 7, 11, 19, 31, 59$ are the only primes for which $N = 3p$ is a *disjoint discriminant of type one*, as considered in [24, Eq. 9.2.8, p. 293].

⁶Striking cubic modular equations ($q \mapsto q^3$ or $N \mapsto 9N$), originating with Ramanujan, are explored in [24, §4.7]. In particular there are attractive cubic recursions for the *cubic multiplier* $M = \sqrt{(1+\eta)/(3-3\eta)} = \theta_3^2(q^3)/\theta_3^2(q)$, as occurs in (196).

We may obtain other singular values by choosing the argument of W_4 in (195) to be an appropriate *algebraic* number. For example, the sums

$$\sum_{k=0}^{\infty} \frac{b_k}{(12 + 4\sqrt{13})^{2k}} = \frac{4}{\pi^2} K_{39} K_{13/3} \quad (206)$$

$$\sum_{k=0}^{\infty} \frac{b_k}{(3\sqrt{3} + 5)^{2k} (6\sqrt{3} + 4\sqrt{7})^{2k}} = \frac{4}{\pi^2} K_{105} K_{35/3} \quad (207)$$

over the diamond lattice integers b_k in (177) have relatively simple surds in their summands, obtained by setting $q = \exp(-\pi\sqrt{13/3})$ and $q = \exp(-\pi\sqrt{35/3})$ in the parametric solution (195). We may also obtain quartic values of z_4 and evaluations like (207) at the even singular values k_N with $N/6 = 3, 5, 7, 13, 17$. We remark that $p = 5, 7, 13, 17$ are the only primes for which $N/2 = 3p$ is a *disjoint discriminant of type two*, as considered in [24, Eq. 9.2.9, p. 293].

5.12 Integral sum rules

Unfortunately, the discrete sum rule (181), at the singular value k_3 , does not prove conjecture (101) but instead converts it to the conjectural integral sum rule

$$\int_0^{\infty} t I_0(t) \left(I_0(t) K_0(2t) - \frac{1}{3} I_0(2t) K_0(t) \right) K_0^2(t) dt, \stackrel{?[8]}{=} 0, \quad (208)$$

where the term containing $I_0(2t)$ is now proven to yield the singular value k_3 , whose appearance in the term containing $K_0(2t)$ was conjectured in (101).

It looks to be an even tougher proposition to prove the sum rule

$$\int_0^{\infty} t I_0(t) \left(K_0(t) - \frac{2\pi}{\sqrt{15}} I_0(t) \right) K_0^3(t) dt \stackrel{?[2]}{=} 0, \quad (209)$$

for which we have now obtained two representations in terms of integrals of complete elliptic integrals, namely

$$\int_0^{\frac{1}{3}} \frac{D(y)}{\sqrt{1-4y^2}} \left(\operatorname{arctanh} \left(\sqrt{\frac{1-2y}{1+2y}} \right) - \frac{\pi}{\sqrt{15}} \right) dy \stackrel{?[2]}{=} 0 \quad (210)$$

$$\int_0^{\infty} \frac{E(x)}{\sqrt{4+x^2}} \left(\operatorname{arcsinh} \left(\frac{x}{2} \right) - \frac{\pi}{\sqrt{15}} \right) dx \stackrel{?[2]}{=} 0, \quad (211)$$

with $D(y)$ given in (64), $E(x)$ given in (138) and the 3-loop sunrise diagram $s_{5,1}$ appearing via the more demanding logarithmic terms in (123) and (140).

As a companion to the proven evaluation (50) and the discrete sum rule (52), we present

$$\int_0^{\pi/2} \frac{\mathbf{K}(\sin \theta)}{\sqrt{1+3\sin^2 \theta}} \left(\operatorname{arcsinh}(2 \tan \theta) - \frac{\pi}{\sqrt{3}} \right) d\theta \stackrel{?[10]}{=} 0 \quad (212)$$

as our penultimate conjecture, also checked to 1200 decimal places. If the mathematics of sum rule (212) might be elucidated at the singular value k_3 , then there might be some hope for a proof of the quantum field theory result (209), at the singular value k_{15} .

5.13 The even moment $c_{5,0}$

We were unable to derive single integrals of elliptic integrals for the even moments $c_{5,2k}$. A double-integral representation is readily available by setting $w = 0$ in the *Aufbau*

$$\begin{aligned}\overline{S}_6(a, b, c, d, e, w) &= \int_{-\infty}^{\infty} \overline{S}_4(a, b, c, v) \overline{S}_3(d, e, v + w) dv \\ &= \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \overline{S}_3(a, b, u) \overline{S}_2(c, u + v) \overline{S}_3(d, e, v + w) du dv\end{aligned}\quad (213)$$

to obtain

$$\overline{V}_5(a, b, c, d, e) = \frac{\pi}{2} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \frac{\overline{S}_3(a, b, u) \overline{S}_3(d, e, v)}{\sqrt{c^2 + (u + v)^2}} du dv \quad (214)$$

with \overline{S}_3 given by (30). Setting the 5 parameters to unity and making the transformations $u = 2 \tan \theta$ and $v = 2 \tan \phi$, we obtain

$$c_{5,0} = \frac{\pi}{2} \int_{-\pi/2}^{\pi/2} \int_{-\pi/2}^{\pi/2} \frac{\mathbf{K}(\sin \theta) \mathbf{K}(\sin \phi)}{\sqrt{\cos^2 \theta \cos^2 \phi + 4 \sin^2(\theta + \phi)}} d\theta d\phi. \quad (215)$$

The higher even moments are obtained by suitable differentiations of (214) with respect to c , before setting $c = 1$.

6 Six Bessel functions

We are now equipped to write the odd moments $t_{6,1}$, $s_{6,1}$ and $c_{6,1}$ as single or double integrals over complete elliptic integrals, with integrands that are computable with great efficiency, using the exponentially fast process of the arithmetic-geometric mean, discovered by Lagrange, around 1784, and independently by Gauss, at the age of 14, in 1791 [3, 24].

6.1 The odd moments $t_{6,2k+1}$

We begin by folding D_4 , in (62), with T_4 , in (147), to determine

$$\begin{aligned}T_6(u, a, b, c, d, v) &:= \int_0^{\infty} t J_0(ut) K_0(at) K_0(bt) K_0(ct) K_0(dt) J_0(vt) dt \\ &= \int_{a+b+c}^{\infty} 2w D_4(a, b, c, w) T_4(u, d, w, v) dw,\end{aligned}$$

where we group the 3 internal lines with masses a, b and c to have a total momentum with norm w^2 . Setting $a = b = c = d = 1$, $u = v = i$ and $w = 1/y$, we obtain one instance of $D(y)$, from its definition $D(y) := 2D_4(1, 1, 1, 1/y)/y$, and another, somewhat surprisingly, from the novel result $D(y) = 6T_4(i, 1, 1/y, i)/y$ in (149). Hence we obtain

$$t_{6,1} = \int_0^{\infty} t I_0^2(t) K_0^4(t) dt = \frac{1}{3} \int_0^{\frac{1}{3}} \frac{D^2(y)}{2y} dy \quad (216)$$

with an initial factor of $\frac{1}{3}$ arising from (137), in the special case (135). This is a rather efficient representation of $t_{6,1}$, which delivers 1200 decimal places in two minutes, using

Pari-GP. Similarly, we may derive a one-dimensional integral for higher odd moments by differentiations of $D_4(a, b, c, w)$ with respect to one of its masses, before going to the equal-mass point. More conveniently, one may use the summation

$$t_{6,2k+1} = \sum_{n=0}^{\infty} \binom{2n}{n} \frac{c_{4,2k+2n+1}}{(2^n n!)^2}$$

that follows from (92). By this means, we found that $\frac{85}{72}t_{6,3} - \frac{1}{36}t_{6,1}$ reproduces the value of $t_{6,5}$ to 1200 decimal places.

6.2 The odd moments $s_{6,2k+1}$

We were unable to derive a one-dimensional integral over **agm** functions for $s_{6,1}$, though we shall conjecture such an integral, in the next subsection. Here, the best that we can do comes from using the folding

$$S_6(a, b, c, d, e, w) = \int_{a+b+c}^{\infty} 2u D_4(a, b, c, u) S_4(d, e, u, w) du,$$

which leads to a choice of integrals for

$$S_4(d, e, u, w) = \int_{d+e+u}^{\infty} 2v D_4(d, e, u, v) S_2(v, w) dv = \int_{d+e}^{\infty} 2v D_3(d, e, v) S_3(v, u, w) dv,$$

with the first form involving an **agm** and the second an **arctanh** procedure. The latter is more convenient, since it yields the rectangular double integral

$$s_{6,1} = \int_0^{\frac{1}{3}} D(y) \int_0^{\frac{1}{2}} \frac{4z \operatorname{arctanh} \sqrt{A_-/A_+}}{\sqrt{(1-4z^2)A_+A_-}} dz dy, \quad (217)$$

with $A_{\pm} := (y \pm z)^2 - y^2 z^2$, obtained by transforming to $y = 1/u$ and $z = 1/v$, and $D(y)$ given in (64). We remark that A_+ is positive, within the rectangle of integration, and that when A_- is negative an analytic continuation of **arctanh** to **arctan** keeps the integrand real and positive. Higher odd moments may be obtained by differentiations with respect to w , before setting $w^2 = -1$. More conveniently, we may use the summation

$$s_{6,2k+1} = \sum_{n=0}^{\infty} \frac{c_{5,2k+2n+1}}{(2^n n!)^2}, \quad (218)$$

since $c_{5,1}$ and $c_{5,3}$ were computed by Broadhurst to 200,000 decimal places (see footnote 3) and higher moments are (conjecturally) determined by them, using (120) and the appropriate recursion from (10). By this means, we found that $\frac{85}{72}s_{6,3} - \frac{1}{36}s_{6,1}$ reproduces the value of $s_{6,5}$ to 1200 decimal places.

6.3 Sum rules

Our final conjecture is that there is a infinite tower of sum rules relating moments in which powers of K_0 are replaced by corresponding powers of πI_0 . We were alerted to this possibility by the sum rule

$$\int_0^{\infty} (\pi^2 I_0^2(t) - K_0^2(t)) K_0^2(t) dt = 0 \quad (219)$$

proven in (91). For each pair of integers (n, k) with $n \geq 2k \geq 2$ we conjecture that

$$Z_{2n, n-2k} := \sum_{m=0}^{\lfloor n/2 \rfloor} (-1)^m \binom{n}{2m} \int_0^\infty t^{n-2k} [\pi I_0(t)]^{n-2m} [K_0(t)]^{n+2m} dt \stackrel{?[11]}{=} 0, \quad (220)$$

with the vanishing of $Z_{4,0}$ proven in (219), in the case with $n = 2$ and $k = 1$.

With 6 Bessel functions in play, the sum rule

$$Z_{6,1} := \pi \int_0^\infty t I_0(t) (\pi^2 I_0^2(t) - 3K_0^2(t)) K_0^3(t) dt \stackrel{?[11]}{=} 0 \quad (221)$$

relates a pair of odd moments, giving the conjectural evaluation

$$s_{6,1} \stackrel{?[11]}{=} \frac{\pi^2}{3} \int_0^\infty t I_0^3(t) K_0^3(t) dt. \quad (222)$$

At first sight, this seems to be hard to check, at high precision, because it involves the slowly convergent moment

$$\int_0^\infty t I_0^3(t) K_0^3(t) dt = \sum_{k=0}^\infty a_k \frac{c_{3,2k+1}}{(2^k k!)^2},$$

with an integrand of order $1/t^2$, at large t , and a summand of order $1/k^2$, at large k , coming from the hexagonal lattice integers a_k in (24). However, we were able to exploit the integral representation

$$\frac{c_{3,2k+1}}{(2^k k!)^2} = \int_0^{\frac{1}{3}} D(y) y^{2k} dy$$

to obtain

$$\int_0^\infty t I_0^3(t) K_0^3(t) dt = \int_0^{\frac{1}{3}} D(y) \tilde{D}(y) dy \quad (223)$$

as an integral over a pair of **agm** functions, with $D(y)$ given by (64) and $\tilde{D}(y)$ by (183). Then conjecture (221) is equivalent to the evaluation

$$s_{6,1} = \int_0^\infty t I_0(t) K_0^5(t) dt \stackrel{?[11]}{=} \frac{\pi^2}{3} \int_0^{\frac{1}{3}} D(y) \tilde{D}(y) dy, \quad (224)$$

which was confirmed to 1200 decimal places, by setting $k = 0$ in (218) to compute $s_{6,1}$ and by using *Pari-GP* to evaluate the integral over y . We find it remarkable that the complicated double integral 4-loop sunrise diagram in (217) seems to be reducible to the attractive single integral in (224), by removing a factor $\frac{1}{3}\pi^2$.

With 8 Bessel functions in play, conjecture (220) gives a pair of sum rules. From the vanishing of $Z_{8,0}$ and $Z_{8,2}$, we obtain

$$c_{8,0} \stackrel{?[11]}{=} \pi^2 \int_0^\infty I_0^2(t) (6K_0^2(t) - \pi^2 I_0^2(t)) K_0^4(t) dt \quad (225)$$

$$c_{8,2} \stackrel{?[11]}{=} \pi^2 \int_0^\infty t^2 I_0^2(t) (6K_0^2(t) - \pi^2 I_0^2(t)) K_0^4(t) dt, \quad (226)$$

again noting the slow convergence of these integrals and of the equivalent sums

$$c_{8,0} \stackrel{?[11]}{=} \sum_{k=0}^{\infty} \left(\frac{\pi}{2^k k!} \right)^2 \left(\binom{2k}{k} 6c_{6,2k} - \pi^2 b_k c_{4,2k} \right) \quad (227)$$

$$c_{8,2} \stackrel{?[11]}{=} \sum_{k=0}^{\infty} \left(\frac{\pi}{2^k k!} \right)^2 \left(\binom{2k}{k} 6c_{6,2k+2} - \pi^2 b_k c_{4,2k+2} \right), \quad (228)$$

which involve the diamond lattice integers b_k in (56) or (177).

Conjecture (220) gives novel evaluations of $c_{4n,2k}$ and $s_{4n+2,2k+1}$, for $n > k \geq 0$. We remark, however, that (227) and (228) do not exhaust the integer relations for moments with 8 Bessel functions. We also found that the ratio

$$\frac{\int_0^\infty t I_0^2(t) K_0^6(t) dt}{\int_0^\infty t I_0^4(t) K_0^4(t) dt} = \frac{\sum_{k=0}^{\infty} \binom{2k}{k} \frac{c_{6,2k+1}}{(2^k k!)^2}}{\sum_{k=0}^{\infty} b_k \frac{c_{4,2k+1}}{(2^k k!)^2}}$$

coincides with $\frac{9}{14}\pi^2$, to 80 decimal places.

6.4 The odd moments $c_{6,2k+1}$

Grouping the 6 internal lines of the 5-loop *vacuum* diagram

$$V_6(a, b, c, d, e, f) = \int_{a+b+c}^{\infty} \int_{d+e+f}^{\infty} 4uv D_4(a, b, c, u) V_2(u, v) D_4(v, d, e, f) dv du$$

into two sets of 3 lines, we obtain

$$c_{6,1} = \int_0^{\frac{1}{3}} D(y) \int_0^{\frac{1}{3}} \frac{D(z) \log(z/y)}{z^2 - y^2} dz dy, \quad (229)$$

after setting the masses to unity and transforming to $y = 1/u$ and $z = 1/v$. We also note that Broadhurst conjectured that the value of $c_{6,5}$ is $\frac{85}{72}c_{6,3} - \frac{1}{36}c_{6,1} + \frac{5}{48}$. This was later checked to 500 decimal places, using data in [9].

6.5 The even moment $c_{6,0}$

Finally, we obtain 3 complete elliptic integrals in the integrand of

$$\bar{V}_6(a, b, c, d, e, f) = \pi \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \bar{S}_3(a, b, u) \bar{S}_3(c, d, u+v) \bar{S}_3(e, f, v) du dv \quad (230)$$

using the *Aufbau* (29). This then delivers

$$c_{6,0} = \frac{\pi}{2} \int_{-\pi/2}^{\pi/2} \int_{-\pi/2}^{\pi/2} \frac{\mathbf{K}(\sin \theta) \mathbf{K}(\sin \phi) \mathbf{K} \left(\frac{\sin(\theta+\phi)}{\sqrt{\cos^2 \theta \cos^2 \phi + \sin^2(\theta+\phi)}} \right)}{\sqrt{\cos^2 \theta \cos^2 \phi + \sin^2(\theta+\phi)}} d\theta d\phi \quad (231)$$

by the same transformations as for (215).

7 Computational notes

This paper contains several proofs of identities that we first conjectured on the basis of numerical investigation, hugely facilitated by access to Sloane’s wonderful sequence finder. For the many one-dimensional integrals that we have noted, we were greatly aided by the efficiency of the `agm` and `intnum` procedures of *Pari-GP*, for evaluations of integrands and integrals at precisions up to 1200 decimal places. Results were then fed to the implementation of the PSLQ algorithm in *Pari-GP*’s `linddep` procedure, with which we performed many unsuccessful searches for integer relations, as well as obtaining the positive results reported in the paper. By way of example, we remark that the integral

$$\mathcal{E} := \int_0^\infty \frac{E(x)}{\sqrt{4+x^2}} \operatorname{arcsinh}^2\left(\frac{x}{2}\right) dx$$

was evaluated to high precision in order to search for relations between $c_{5,1}$, $c_{5,3}$, \mathcal{E} and products of powers of π , C and $1/C$, with coefficients that might be \mathbb{Q} -linear combinations of 1 , $\sqrt{3}$, $\sqrt{5}$ and $\sqrt{15}$. No such relation was found.

Maple was especially useful for its `HeunG`, `MeijerG` and `Gosper` procedures and also for quick PSLQ searches with few terms, at relatively low precision.

But for two-dimensional numerical quadratures we found neither *Pari-GP* nor *Maple* to be remotely adequate for our demanding investigations. For these, we came to rely on Bailey’s multiprecision code for two-dimensional integrals [6, 11, 14], which confirmed, to more than 100 decimal places, the correctness of derivations of (215), (231) and other identities. Here we offer a brief description of this scheme.

7.1 Multi-dimensional quadrature

Bailey’s 1-D and 2-D schemes, as well as the one-dimensional `intnum` procedure in *Pari-GP*, employ the tanh-sinh quadrature algorithm, which was originally discovered by Takahasi and Mori [67]. It is rooted in the Euler-Maclaurin summation formula [4, p. 285], which implies that for certain bell-shaped integrands $f(x)$ on $[0, 1]$, where the function and all higher derivatives rapidly approach zero at the endpoints, approximating the integral of $f(x)$ by a simple step-function summation is remarkably accurate. This observation is combined with the transformation $x = \tanh((\pi/2) \sinh t)$, which converts most “reasonable” integrand functions on $(-1, 1)$ (including many functions with singularities or infinite derivatives at one or both endpoints) into bell-shaped functions with the desired property.

In particular, we can write, for an interval length $h > 0$,

$$\int_{-1}^1 f(x) dx = \int_{-\infty}^{\infty} f(g(t))g'(t) dt \approx h \sum_{j=-N}^N w_j f(x_j), \quad (232)$$

where $g(t) = \tanh((\pi/2) \sinh t)$, $x_j = g(hj)$, $w_j = g'(hj)$, and N is chosen large enough that $|w_j f(x_j)| < \epsilon$ for $|j| > N$. Here $\epsilon = 10^{-p}$, where p is the numeric precision level in digits. Note that the resulting quadrature formula (232) has the form similar to Gaussian quadrature, namely a simple summation with abscissas x_j and weights w_j , both sets of which can be pre-computed since they are independent of the integrand function. For many integrand functions, once h is sufficiently small, reducing h by half yields twice as many correct digits in the result (although all computations must be performed to at

least the level of precision desired for the final result, and perhaps double this level if the function is not well-behaved at endpoints). Additional details of efficient implementations are given in [6, 14].

One of the numerous applications of one-dimensional tanh-sinh quadrature in this study was the verification of our final conjecture given in (220). This was done using Bailey's implementation of the one-dimensional tanh-sinh algorithm, together with the ARPREC extreme-precision software package [13]. Evaluation of the Bessel function $I_0(t)$ was performed using a hybrid scheme where formula 9.6.12 of [1] was used for modest-sized values, and formula 9.7.1 for large values. Evaluation of $K_0(t)$ was performed using 9.6.13 of [1] for modest-sized values, and 9.7.2 for large values. Note however that formula 9.6.13 for $K_0(t)$ must be implemented using a working precision that is roughly twice the level desired for the final result, due to the sensitive subtraction operation in this formula. Also note that when $m = 0$ in (220), this combination of formulas is not satisfactory, because for large t the function $I_0(t)$ is exceedingly large, and $K_0(t)$ is exceedingly small, and even though the product is of modest size, overflows and underflows are possible in intermediate function evaluations, even when using high-precision software that has an enormously extended dynamic range. For such cases ($m = 0$ and t large), we employed formula 9.7.5 of [1], which gives an asymptotic series for the product $I_0(t)K_0(t)$. We had differently addressed this issue in the special case of (222).

Armed with an efficient implementation of these schemes, we were able to verify (220) for all (n, k) pairs, where $1 \leq k \leq \lfloor n/2 \rfloor$ and $4 \leq n \leq 12$ (there are 43 such pairs), in each case to over 340-digit accuracy. In addition, we verified (220) for a variety of larger (n, k) pairs, including (15, 7), (20, 10), (25, 11), (30, 12), (37, 13), and (41, 14), again to over 340-digit accuracy in each case.

The tanh-sinh quadrature algorithm can also be performed in two or more dimensions as an iterated version of the one-dimensional scheme. Such computations are many times more expensive than in one dimension. For example, if roughly 1,000 function evaluations are required in one dimension to achieve a desired precision level, then at least 1,000,000 function evaluations are typically required in two dimensions, and 1,000,000,000 in three dimensions. Additionally, the behaviour of multi-dimensional tanh-sinh quadrature on integrand functions with singularities or infinite derivatives on the boundaries of the region is not as predictable or well-understood as in one dimension.

Nonetheless, we were able to use 2-D tanh-sinh quadrature to successfully evaluate a number of the double integrals mentioned in this paper, after making some minor transformations. As one example, consider the integral mentioned above for $c_{5,0}$, namely

$$c_{5,0} = \frac{\pi}{2} \int_{-\pi/2}^{\pi/2} \int_{-\pi/2}^{\pi/2} \frac{\mathbf{K}(\sin \theta) \mathbf{K}(\sin \phi)}{\sqrt{\cos^2 \theta \cos^2 \phi + 4 \sin^2(\theta + \phi)}} d\theta d\phi. \quad (233)$$

Note that this function (see Figure 1) has singularities on all four sides of the region of integration, with particularly troublesome singularities at $(\pi/2, -\pi/2)$ and $(-\pi/2, \pi/2)$. However, after making the substitutions $s \leftarrow \pi/2 - s$, $t \leftarrow \pi/2 - t$ and $r \leftarrow s/t$, and taking advantage of the symmetry evident from Figure 1, we obtain

$$c_{5,0} = 2\pi \int_0^{\pi/2} \int_0^1 \frac{t \mathbf{K}(\cos(rt)) \mathbf{K}(\cos t) dr dt}{\sqrt{\sin^2(rt) \sin^2 t + 4 \sin^2(t(1+r))}} + 2\pi \int_0^{\pi/2} \int_0^1 \frac{t \mathbf{K}(\cos(rt)) \mathbf{K}(\cos t) dr dt}{\sqrt{\sin^2(rt) \sin^2 t + 4 \sin^2(t(1-r))}}, \quad (234)$$

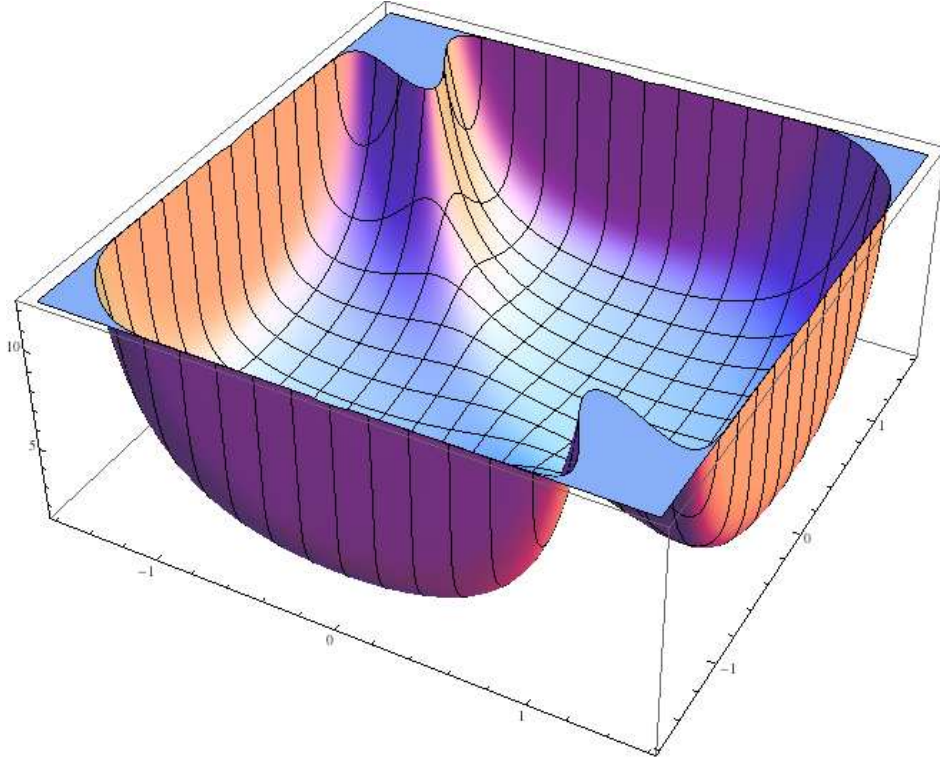


Figure 1: Plot of $c_{5,0}$ integrand function in (233)

which is significantly better behaved (although these integrands still have singularities on two of the four sides of the region). As a result, we were able to compute $c_{5,0}$ with this formula to 120-digit accuracy, using 240-digit working precision. This run required a parallel computation (using the MPI parallel programming library) of 43.2 minutes on 512 CPUs (1024 cores) of the “Franklin” system at the National Energy Research Scientific Computing Center at the Lawrence Berkeley National Laboratory. The final result matched the value that we had previously calculated using (5) (see [9]) to 120-digit accuracy.

This same strategy was successful for several other 2-D integrals. For example, we computed $c_{6,0}$ to 116-digit accuracy, which again matched the value we had previously computed, in 64.8 minutes on 1024 cores of the Franklin system. In the case of $c_{6,1}$, the transformation described above for $c_{5,0}$ converted the integrand function of (229) into a completely well-behaved function, without any singularities. As a result, we were able to compute $c_{6,1}$ to 120-digit accuracy using only an Apple Intel-based workstation with four computational cores, in 28 minutes. As before, the result matched the earlier calculation.

As already noted, complex numbers are avoided in integral (217) by writing it as

$$s_{6,1} = \int_0^{\frac{1}{3}} D(y) \int_0^{\frac{1}{2}} \frac{4z f(A_-/A_+)}{A_+ \sqrt{1-4z^2}} dz dy, \quad (235)$$

where

$$f(x) := \begin{cases} \operatorname{arctanh}(\sqrt{x})/\sqrt{x} & \text{for } x > 0 \\ 1 & \text{for } x = 0 \\ \operatorname{arctan}(\sqrt{-x})/\sqrt{-x} & \text{for } x < 0 \end{cases}$$

yields positive real numbers within the rectangle of integration. We were able to confirm that the double integral (235) yields the first 120 of the 1200 decimal places obtained, far more easily, from the single integral (224).

8 Conclusions

Despite notable progress in discovering and proving many new results, we are left with 8 outstanding conjectures.⁷ Of these, 5 have their first instances in Equations (94) to (97) and Equation (101) of Section 5.1, with 3 outliers, in Equations (120), (212) and (220).

Conjecture (94) lies deep in 4-dimensional quantum field theory, but it is reasonable to suppose that it might be derivable from the two-dimensional conjectures (95), (96) and (97), together with their proven sign-changed variants in (98), (99) and (100).

The conjectural integer relations (120) and (125) may be provable by adding rational data such as (121) to a set of recursions richer than those considered in [26, 60].

The real challenge is set by the remarkable sum rule (209), with a dispersive presentation (210), a non-dispersive presentation (211) and a kindergarten analogue (212).

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⁷Conjecture [8], as given in (101), has now been proven by contour integration (see [27]), and conjecture [11], as given in (220), has also now been resolved.

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