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Integrals of the Ising class

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Abstract: From an experimental-mathematics perspective we analyze some structurally interrelated n-dimensional integrals we call C_n, D_n, E_n, where D_n is a magnetic susceptibility integral relevant to the Ising theory of solid-state physics. With a view to closed-form results for such "Ising-class" integrals, we analyze in depth the most tractable of the collection, namely

$$C_n \quad := \quad \frac{4}{n!} \int_0^\infty \cdots \int_0^\infty \frac{1}{\left(\sum_{j=1}^n (u_j + 1/u_j) \right)^2} \frac{du_1}{u_1} \cdots \frac{du_n}{u_n}.$$

We first conjectured, on the basis of extreme-precision numerical quadrature, that C_n has a *finite* large-n limit, namely $C_\infty = 2e^{-2\gamma}$, with γ being the Euler constant. On such a numerological clue we are able to prove the conjecture. We also present results relevant to the more recondite integrals D_n and E_n; for example, both these integrals are now known to decay exponentially with n, in a certain rigorous sense. Also, both integrals now enjoy proven closed forms for $n = 1, 2, 3, 4$. And for E_5, we posit a closed form whose discovery involved three-dimensional integration of an intricate integrand, performed via highly parallel numerical quadrature.

Part I. Experimental-mathematics approaches

1 Background and nomenclature

This research began as a quest for a numerical scheme for high-precision values of *Ising susceptibility integrals*, in our preferred normalization being defined as

$$D_n \quad := \quad \frac{4}{n!} \int_0^\infty \cdots \int_0^\infty \frac{\prod_{i<j} \left(\frac{u_i - u_j}{u_i + u_j}\right)^2}{\left(\sum_{j=1}^n (u_j + 1/u_j)\right)^2} \frac{du_1}{u_1} \cdots \frac{du_n}{u_n}. \tag{1}$$

The integrals D_n appear in susceptibility expansions from Ising theory, as detailed in the literature [17, 18, 21, 22, 23, 24]. Very briefly, the importance of D_n in Ising physics runs as follows [20]. Magnetic susceptibility $\chi(T)$—essentially a spin-spin correlation in the 2D Ising model—depends asymptotically on temperature T as

$$\chi_\pm(T) \quad \sim \quad \mathcal{C}_{0\pm} \left(1 - \frac{T}{T_c}\right)^{-7/4},$$

where T_c is the critical temperature and the subscript $\pm$ indicates whether $T > T_c$ (plus) or $T < T_c$ (minus). The connection with our present analysis is that the so-called *susceptibility amplitudes*

$$\mathcal{C}_{0+} \quad = \quad \mathcal{C}_+ \sum_{n=0}^\infty I_{2n+1}$$

$$\mathcal{C}_{0-} \quad = \quad \mathcal{C}_- \sum_{n=1}^\infty I_{2n},$$

where $\mathcal{C}_\pm$ are explicitly known constants [21], involve integrals I_n proportional to our D_n; specifically

$$I_n \quad := \quad 2^{-n} \pi^{1-n} D_n.$$

We have taken the D_n integral, therefore, as a prime candidate for experimental-mathematics research; i.e. knowing a D_n in closed form traces immediately back to an important term from a susceptibility expansion.

It was suggested to us by C. Tracy [20] and emphasized by J-M. Maillard [14] that evaluation of the D_n susceptibility integrals—to sufficient precision—could well lead to experimental-mathematical capture for some $n > 4$. In fact, the appearance of Riemann-zeta evaluations is already a known phenomenon in related nonlinear physics [7]. Now, because closed forms for the D_n are difficult, as are numerical evaluations for large n, we elected to study first some related but simpler integrals. This was the initial motive for defining the entities

$$C_n \quad := \quad \frac{4}{n!} \int_0^\infty \cdots \int_0^\infty \frac{1}{\left(\sum_{j=1}^n (u_j + 1/u_j)\right)^2} \frac{du_1}{u_1} \cdots \frac{du_n}{u_n}, \tag{2}$$

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(not to be confused with the $\mathcal{C}$ amplitudes of Ising theory).

Because these C_n are relatively easy to resolve to extreme[1] precision, we remain hopeful that finding closed forms experimentally for some C_n will suggest, at least qualitatively, what fundamental constants might appear in the higher D_n. Indeed, a mere glance at similarities between closed forms at a given level n vindicates this expectation (see Table 1 in Section 2). In the sense that we are taking not a physics-oriented but an experimental-mathematics approach, the present work is reminiscent of [9, pg. 312–313] and [6, 5, 4]. Moreover, as enunciated in our Abstract, these C_n for large n appeared to approach a positive constant, in fact rather rapidly. The natural conjecture and proof of same are given in a later section.

While only D_n,being an Ising-susceptibility component, has immediate physical significance, we assert that the C_n, E_n are mathematically natural variants, with the C_n being numerically accessible (and asymptotically well behaved) while the E_n provide important bounds on the elusive D_n. In any case, we anticipate experimental-mathematical capture to provide "similar" fundamental constants for all these Ising-class integrals.

We have found the following symbolic machinations particularly useful. For either integral (1) or (2), consider the simplex $u_1 > u_2 > \cdots > u_n$. We may then use the change of variables $u_k := \prod_{i=1}^{k} t_i$, with $t_1 \in (0, \infty)$ and all other $t_i \in (0, 1)$, to transform the integration domain into a finite one. Define

$$w_k \;\; := \;\; \prod_{i=2}^{k} t_i, \quad v_k \;\; := \;\; \prod_{i=k}^{n} t_i.$$

and the functions

$$\mathcal{A}_n(t_2, t_3 \ldots, t_n) \;\; := \;\; \left(\prod_{n \geq k > j \geq 1} \frac{u_k/u_j - 1}{u_k/u_j + 1} \right)^2$$

$$\mathcal{B}_n(t_2, t_3 \ldots, t_n) \;\; := \;\; \frac{1}{(1 + \sum_{k=2}^{n} w_k)(1 + \sum_{k=2}^{n} v_k)}.$$

Then the relevant integrals can be cast like so:

$$D_n \;\; = \;\; 2 \int_0^1 \cdots \int_0^1 \mathcal{A}\mathcal{B} \, dt_2 \, dt_3 \cdots dt_n, \tag{3}$$

$$C_n \;\; = \;\; 2 \int_0^1 \cdots \int_0^1 \mathcal{B} \, dt_2 \, dt_3 \cdots dt_n, \tag{4}$$

Here, the $1/n!$ normalization has disappeared due to the $n!$ ways of ordering the simplex indices, and we have symbolically integrated over t_1. It will turn out

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[1]By "extreme precision" we mean, loosely, "precision sufficient for reasonable confidence in experimental detection," which in our experience is between 100 and 1000 digits.

to be useful to define also an integral

$$E_n \quad := \quad 2 \int_0^1 \cdots \int_0^1 \mathcal{A}\, dt_2\, dt_3 \cdots dt_n. \tag{5}$$

It transpires that, for all $n \geq 1$, we have

$$D_n \leq E_n \leq C_n. \tag{6}$$

The first inequality is trivial, and also trivial is the implicit relation $D_n \leq C_n$, since by their very definitions $\mathcal{A}, \mathcal{B} \in [0,1]$ on the domain of integration. Almost as obvious is the inequality $E_n \leq n^2 D_n$. But it will require more work to establish the hardest branch $E_n \leq C_n$ (see text after Theorem 3).

Beyond such inequalities, one can go yet further in the matter of asymptotic analysis. Using representations (3, 5) we shall be able to establish that $(D_n), (E_n)$ sequences are both strictly monotone decreasing and *genuinely exponentially decaying* in the sense that for positive constants a, b, A, B we have

$$\frac{a}{b^n} \quad \leq \quad D_n \leq E_n \leq \frac{A}{B^n}.$$

In Section 7 we shall not only prove this (Theorem 3) but also give effective a, b, A, B values.

2   Tabulation of results

Table 1 exhibits known evaluations of D_n and the structurally related Ising-class integrals C_n, E_n. The reader should beware of varying normalizations in the physics literature; yet every Ising-susceptibility integrand involves, as do our D_n from (1), some manner of combinatorial entity constructed over (i, j) index pairs. (For $n = 1$ we interpret the $(i < j)$ product in the definition (1) as unity.) Our particular normalization for D_n vs. $I_n := D_n/(2^n \pi^{n-1})$ means, in reference to our Table 1, that $I_1 = 1$, $I_2 = 1/(12\pi)$, and so on. For example, the *ferromagnetic constant* of solid-state physics is thus $I_3 = D_3/(8\pi^2) \approx 0.00081446$, as in the literature [22] [15]. The entity $I_4 = D_4/(16\pi^3) \approx 0.000025448$ is the *McCoy–Tracy–Wu constant* resolved in closed form c. 1977 [19], while D_5, though still algebraically elusive, was resolved to 30 decimal places by B. Nickel in 1999 [15]—these respective symbolic and numerical achievements being remarkable for their eras. (See Section 12 and Appendix 2 for our recent extreme-precision renditions of D_5, E_5.)

In the construction of Table 1, we have invoked a *Dirichlet L-function* that occurs frequently in mathematical physics (see [8, §2.6], [9, Chapter 3]) namely[2]

$$\mathrm{L}_{-3}(2) \quad := \quad \sum_{n \geq 0} \left(\frac{1}{(3n+1)^2} - \frac{1}{(3n+2)^2} \right),$$

---

[2]Note that some literature treatments (e.g. [19]) use the Clausen function [13] which is algebraically related to the stated L-function.

n	C_n	D_n	E_n
1	$= 2$	$= 2$	$= 2$
2	$= 1$	$= 1/3$	$= 6 - 8\log 2$
3	$= \mathrm{L}_{-3}(2)$	$= 8 + 4\pi^2/3 - 27\,\mathrm{L}_{-3}(2)$	$= 10 - 2\pi^2 - 8\log 2 + 32\log^2 2$
4	$= 7\zeta(3)/12$	$= 4\pi^2/9 - 1/6 - 7\zeta(3)/2$	$\begin{aligned} &= 22 - 82\zeta(3) - 24\log 2 \\ &+176\log^2 2 - 256(\log^3 2)/3 \\ &+16\pi^2\log 2 - 22\pi^2/3 \end{aligned}$
5	$0.6657598001\ldots$	$0.0024846057\ldots$	$\begin{aligned} &\overset{?}{=} 42 - 1984\,\mathrm{Li}_4(1/2) + 189\pi^4/10 \\ &-74\zeta(3) - 1272\zeta(3)\log 2 \\ &+40\pi^2\log^2 2 - 62\pi^2/3 \\ &+40(\pi^2\log 2)/3 + 88\log^4 2 \\ &+464\log^2 2 - 40\log 2 \end{aligned}$
6	$0.6486342090\ldots$	$0.0004891422\ldots$	$0.00068783287\ldots$
$\ldots$			
n	$\sim 2e^{-2\gamma}$	$\Omega\left(\frac{1}{b^n}\right), O\left(\frac{1}{B^n}\right)$	$\Omega\left(\frac{1}{b^n}\right), O\left(\frac{1}{B^n}\right)$

Table 1: What is known of Ising-class integrals: '$=$' connotes proven and '$\overset{?}{=}$' detected experimentally.

and also the standard *polylogarithm*

$$\mathrm{Li}_s(z) \quad := \quad \sum_{k \geq 1} \frac{z^k}{k^s}.$$

All the closed forms in Table 1 are proven, except for the one shown for E_5—an experimental result based on a 240-digit computation. This E_5 relation was found using PSLQ at a confidence level of 190 digits beyond the level that could reasonably be ascribed to numerical round-off error (we will describe the computation of E_5 in Section 12). As for large-n behavior implied in Table 1, we know C_∞ rigorously as an exotic constant, while the Ω, O notation means both D_n, E_n decay exponentially but no faster than that (see Theorem 3). Numerical entries here are known to higher precision than is displayed—in fact we know many C_n, as well as D_5, E_5, to extreme precision (see Section 12 and Appendix 1).

3 Bessel-kernel representations for C_n

Let us first use the transformation $u_k \to e^{x_k}$ in (1), (2) to achieve the representations

$$D_n \quad = \quad \frac{1}{n!} \int \mathcal{D}\vec{x} \frac{\prod_{i<j} \tanh^2 \left(\frac{x_i - x_j}{2} \right)}{(\cosh x_1 + \cdots + \cosh x_n)^2}, \tag{7}$$

$$C_n \quad := \quad \frac{1}{n!} \int \frac{\mathcal{D}\vec{x}}{(\cosh x_1 + \cdots + \cosh x_n)^2}. \tag{8}$$

where here and elsewhere $\int \mathcal{D}\vec{x}$ is interpreted symbolically as the full-space operation $\int_{-\infty}^{\infty} \cdots \int_{-\infty}^{\infty} dx_1 \cdots dx_n$.[3]

Now C_n can be put in the form

$$C_n \quad = \quad \frac{1}{n!} \int_0^{\infty} p \int \mathcal{D}\vec{x} \, e^{-p \sum \cosh x_k} \, dp.$$

which leads to an attractive, 1-dimensional integral

$$C_n \quad = \quad \frac{2^n}{n!} \int_0^{\infty} p K_0^n(p) \, dp, \tag{9}$$

where K_0 is the standard, *modified Bessel function* [1]

$$K_0(p) \quad := \quad \int_0^{\infty} e^{-p \cosh t} dt. \tag{10}$$

In anticipation of experiments and theorems to follow, we state ascending and asymptotic expansions of K_0, respectively:

$$K_0^{(asc)}(t) \quad = \quad \sum_{k \geq 0} \frac{t^{2k}}{4^k k!^2} \left(H_k - \left(\gamma + \log \frac{t}{2} \right) \right) \tag{11}$$

$$K_0^{(asy)}(t) \quad \sim \quad \sqrt{\frac{\pi}{2t}} e^{-t} \sum_{m=0}^{\infty} \frac{(-1)^m ((2m)!)^2}{m!^3 (32t)^m}, \tag{12}$$

where γ denotes the *Euler constant* and the $H_k := \sum_{m \leq k} 1/m$ are the *harmonic numbers*, with $H_0 := 0$. It is known [1] that the error accrued in taking terms through index $m = M$ in (12) is no larger than the first dropped term (and with sign of that dropped term). We also make use of the representation

$$K_\nu(x) \quad = \quad \frac{2^\nu \Gamma(\nu + 1/2)}{x^v \sqrt{\pi}} \int_0^{\infty} \frac{\cos(xt) \, dt}{(1 + t^2)^{\nu + 1/2}}, \tag{13}$$

---

[3]It is a both a convenience and a pleasure to invoke thus the "curly-D" of Feynman path-integral lore, as the present research traces back to solid-state physics, not to mention that we contemplate at one juncture an infinite-dimensional limit.

valid for real $x > 0$ and $\text{Re}(\nu) > -1/2$ [1]. Observe that in the ascending series (11) the leading term is $-\gamma - \log(t/2)$, revealing a logarithmic singularity at the origin. It will turn out to be lucrative to define a "pivot point"

$$p_0 \;\; := \;\; 2\,e^{-\gamma},$$

such that said leading term vanishes at $t = p_0$. To simplify our derivations to follow, we also adopt an "effective big-O" notation, as

$$\Theta(f) \;\; = \;\; g,$$

meaning $|f/g| \leq 1$, equivalent to $O(\ )$ notation but with implied big-O multiplier of unity.

Again in anticipation of experiment and theory, we state the next result.

Lemma 1 *For the modified Bessel function $K_\nu(x)$ with real $\nu \geq 0$ and real $x > 0$, with pivot point p_0, we have*

$$0 < K_\nu(p) < \Gamma(\nu)\frac{2^{\nu-1}}{p^\nu} \;\; ; \;\; \nu > 0, \tag{14}$$

$$K_0' \;\; = \;\; -K_1, \tag{15}$$

$$K_0(p) \;\; = \;\; -\gamma - \log(p/2) + \Theta(p/3) \;\; ; \;\; p \in (0, p_0), \tag{16}$$

$$K_0(p) \;\; < \;\; \sqrt{\frac{\pi}{2p}}\, e^{-p}. \tag{17}$$

Proof. Relation (14) follows easily from integral (13), since $|\cos| \leq 1$. Relation (15) is standard [1]. Relation (16) follows from inspection of the ascending series (11) over the finite interval $(0, p_0)$. (Note that $\Theta(p/3)$ is simply some function bounded by $p/3$ on said interval, and could also be written $p\,\Theta(1/3)$.) Relation (17) either follows from general asymptotic theory [1], or from the observation that $\int_0^\infty e^{-p\cosh x}\,dx < e^{-p}\int_0^\infty e^{-px^2/2}\,dx$. **QED**

4 Experiment leads to theory

Later in Section 8 we discuss numerical evaluation of C_n for large n. Even a cursory examination of the high-precision numerical results displayed in Appendix 1 suggests that C_n appears to approach a definite limit, namely

$$C_\infty \;\; = \;\; 0.63047350337438679612204019271087890435458707871273234\ldots$$

After inserting the numerical value we obtained for C_{1024} into the smart lookup facility of the CECM *Inverse Symbolic Calculator* at
`http://oldweb.cecm.sfu.ca/cgi-bin/isc/`
we obtained the output:

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```
Mixed constants, 2 with elementary transforms.
  6304735033743867 = sr(2)^2/exp(gamma)^2
```

In fact, according to our calculations,

$$0 < C_{1024} - 2e^{-2\gamma} < 10^{-300}.$$

On the basis of this and other observations, we were convinced of the truth of the following, experimentally motivated conjecture:

Conjecture 1 *The sequence of integrals* $(C_n : n = 1, 2, 3, \dots)$ *is strictly decreasing. Moreover, we have the finite limit*

$$\lim_{n\to\infty} C_n \overset{?}{=} 2e^{-2\gamma}.$$

Indeed, armed with confidence in the above conjecture, we may proceed to prove all aspects of the conjecture, starting with

Theorem 1 $(C_n : n = 1, 2, 3, \dots)$ *is strictly decreasing.*

Proof. We may integrate by parts, starting with equation (9), to arrive, via Lemma 1 (15), at

$$C_n = \frac{2^{n-1}}{(n-1)!} \int_0^\infty p^2 K_1(p) K_0^{n-1}(p) \; dp. \qquad (18)$$

We may therefore express a difference

$$C_{n-1} - C_n = \frac{2^{n-1}}{(n-1)!} \int_0^\infty p(1 - pK_1(p)) K_0^{n-1}(p) \; dp \qquad (19)$$

But, by Lemma 1 (14), the integrand in (19) is nonnegative on $p \in (0, \infty)$, whence $C_{n-1} - C_n > 0$. **QED**

Our next observation is that certain generating functions can be used to extract limits of monotonic sequences. We have

Lemma 2 *Let* $(r_n : n = 1, 2, 3 \dots)$ *be a positive, strictly monotone-decreasing sequence. Denote, then,* $r = \lim_n r_n$, *and define a generating function*

$$R(z) := \sum_{n=1}^\infty r_n z^n. \qquad (20)$$

Then $r = \lim_{z\to 1^-} (1 - z)R(z)$.

Proof. For $z \in (0,1)$, we have

$$(1-z)\,R(z) \quad := \quad rz + T(z) \quad \text{where } T(z) := (1-z) \sum_{n=1}^{\infty} (r_n - r)z^n.$$

Now fix $\epsilon > 0$, and observe that

$$T(z) \quad \leq \quad r_1 N(1-z) + \frac{\epsilon}{2} z^{N+1},$$

when N is chosen such that $r_M - r < \epsilon/2$ for $M \geq N$.

Set $\delta := \min\{\epsilon/(2(r + r_1 N)), \epsilon/2\}$. It follows that $|(1-z)R(z) - r| < \epsilon$ for $1 - z \leq \delta$. **QED**

Remark 1 Deeper such results obtain in Abelian–Tauberian theory, yet this lemma is quite sufficient for our present purpose.

Now we contemplate the generating function

$$C(z) \quad : \quad \sum_{n=1}^{\infty} C_n z^n, \tag{21}$$

and we use this construct to establish the large-n limit of our C_n:

Theorem 2 *The sequence* $(C_n : n = 1, 2, 3 \dots)$ *has*

$$\lim_{n \to \infty} C_n \quad = \quad 2\,e^{-2\gamma}.$$

Proof. The generating function (21) at hand may be developed, via the representation (9) and then (16), (17) of Lemma 1, like so:

$$\begin{aligned}
C(z) &= \int_0^{\infty} p\left(e^{2zK_0(p)} - 1\right)\,dp \\
&= \int_0^{p_0} pe^{2z(-\gamma - \log(p/2) + p\Theta(1/3))}\,dp + \Theta(c), \\
&= e^{-2z\gamma} \int_0^{p_0} \frac{p}{(p/2)^{2z}} e^{p\Theta(1/3)}\,dp + \Theta(c),
\end{aligned}$$

where c is a constant independent of z. Using the fact that for $x \in [0,1]$ we have $e^x = 1 + \Theta(x + x^2)$, we obtain

$$C(z) \quad = \quad e^{-2\gamma z} \frac{2^{2z} p_0^{2-2z}}{2 - 2z} + \Theta\left(c + \frac{c_1}{3 - 2z} + \frac{c_2}{4 - 2z}\right),$$

where c_1, c_2 are again z-independent constants. It follows that

$$\lim_{z \to 1^-} (1-z)\,C(z) \quad = \quad 2\,e^{-2\gamma},$$

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and via Lemma 2 the theorem follows. **QED**

It has become evident—largely on hindsight—that integration of (9) up to only the pivot point p_0 generally leaves an extremely small residual integral. Indeed, if we interpret the representation (9) as

$$C_n = \frac{2^n}{n!} \left(\int_0^{p_0} + \int_{p_0}^{\infty} \right) p K_0^n(p) \, dp$$

then the second integral is easily seen—via Lemma 1 (17)—to be factorially minuscule, in the sense that for any $n > 1$,

$$C_n = \frac{2^n}{n!} \int_0^{p_0} p \, K_0^n(p) \, dp + \Theta\left(\frac{1}{n!}\right).$$

By inserting the ascending series (11) into this pivot integral over $p \in (0, p_0)$, we obtain—after various manipulations—the asymptotic expansion

$$C_n \sim \frac{2}{n!} \sum_{J=1}^{\infty} \frac{e^{-2J\gamma}}{J} \sum_{k_1 + \cdots + k_n = J-1} \int_0^{\infty} e^{-y} \, dy \prod_{i=1}^{n} \frac{2H_{k_i} + y/J}{k_i!^2},$$

where the partitions are over nonnegative integers k_i. This attractive expansion is in the spirit of mathematical physics—it is essentially a perturbation expansion with coupling parameter $e^{-2\gamma}$. Indeed, the first few terms go

$$C_n \sim 2 e^{-2\gamma} + \frac{n+4}{2^n} e^{-4\gamma} + \frac{2n^2 + 23n + 57}{3^n \cdot 6} e^{-6\gamma} + \ldots \qquad (22)$$

Remarkably, just these displayed terms with $n = 32$ yield a C_{32} value to 17 good decimals—an efficient way to effect quadrature to reasonable precision on a 32-dimensional integral!

5   Further dimensional reduction for C_n

One way to proceed analytically is to invoke a scaled-coordinate system. Using the representation

$$C_n = \frac{4}{n!} \int_0^{\infty} \cdots \int_0^{\infty} \frac{1}{\left(\sum_{j=1}^{n} (u_j + 1/u_j) \right)^2} \frac{du_1}{u_1} \cdots \frac{du_n}{u_n}, \qquad (23)$$

we let the first coordinate u_1 be an overall scale. This is much the same as using n-dimensional "spherical coordinates" involving the scale (radius) r and $(n-1)$ angular coordinates. Let us posit, for (5.1),

$$u_1 = r, \quad u_2 = rx_0, \quad u_3 = rx_1, \quad \ldots, \quad u_n = rx_{n-2}.$$

It turns out that this scaled-coordinate transformation generally reduces the integral (23) by *two* dimensions, since one may easily integrate symbolically over r, then almost as easily over x_0. Inter alia we find, trivially, that

$$C_1 = 2 \quad \text{and} \quad C_2 = 1,$$

as start out our Table 1 entries for C_n. Beyond this, the general procedure yields an $(n-2)$-dimensional form

$$C_n = \frac{4}{n!} \int_0^\infty \cdots \int_0^\infty \frac{\log P}{Q-1} \frac{dx_1}{x_1} \cdots \frac{dx_{n-2}}{x_{n-2}}, \tag{24}$$

for $n \geq 3$, where P, Q are the interesting constructs (here and in what follows, P, Q are to be written in terms of the available integration variables $x_1, \dots$):

$$P := 1 + x_1 + \cdots + x_{n-2}, \tag{25}$$
$$Q := P \cdot (1 + 1/x_1 + \cdots + 1/x_{n-2}). \tag{26}$$

Thus, for $n = 3$ we only need evaluate a one-dimensional integral:

$$C_3 = \frac{2}{3} \int_0^\infty \frac{\log(1+x)}{x^2 + x + 1} \, dx,$$

which, via the transformation $x \to 1/t - 1$ becomes

$$= -\frac{2}{3} \int_0^1 \frac{(1+t)\log t}{1 + t^3} \, dt$$
$$= \frac{2}{3} \sum_{n \geq 0} (-1)^n \left(\frac{1}{(3n+1)^2} + \frac{1}{(3n+2)^2} \right)$$
$$= \mathrm{L}_{-3}(2),$$

where the factor '2/3' is removed from the final line on the observation that $1/1^2 + 1/2^2 - 1/4^2 - 1/5^2 + \cdots = (1 + 1/2)(1/1^2 - 1/2^2 + 1/4^2 - 1/5^2 + \dots)$.

For $n = 4$ we had conjectured, on the basis of numerical values, such as those in Appendix 1, and PSLQ integer relation finding facilities [8], that

$$C_4 \stackrel{?}{=} \frac{7}{12} \zeta(3).$$

This turns out to be *true*, derivable via the 2-dimensional reduced integral

$$C_4 = \frac{1}{6} \int_0^\infty \int_0^\infty \frac{\log(1+x+y)}{(1+x+y)(1+1/x+1/y) - 1} \frac{dx \, dy}{x \, y}.$$

Indeed performing the internal integration leads to

$$C_4 = \frac{1}{6} \int_0^\infty \frac{\mathrm{Li}_2\left(x^{-1}\right) - \mathrm{Li}_2\left(x\right)}{x^2 - 1} dx$$
$$= \frac{1}{3} \int_0^1 \frac{\mathrm{Li}_2\left(x^{-1}\right) - \mathrm{Li}_2\left(x\right)}{x^2 - 1} dx,$$

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by transforming $x \to 1/x$. Here $\mathrm{Li}_2(x) := \sum x^n/n^2$, is the *dilogarithm*, [8], analytically continued. Now, integrating by parts leads to

$$
\begin{aligned}
24\,C_4 \;=\;& 8\int_0^1 \frac{\ln^2(x+1)}{x}\,dx - 8\int_0^1 \frac{\ln(1+x)\log(1-x)}{x}\,dx \\
& -4\int_0^1 \frac{\log(x)\log(1+x)}{x}\,dx + 4\int_0^1 \frac{\log(x)\log(1-x)}{x}\,dx \\
\;=\;& 2\zeta(3) + 5\zeta(3) + 3\zeta(3) + 4\zeta(3) \;=\; 14\zeta(3),
\end{aligned}
$$

where each integral is an integral multiple of $\zeta(3)$, as can be obtained from the analysis of the *trilogarithm* $\mathrm{Li}_3(x) := \sum x^n/n^3$, in [13, §6.4 and Appendix A3.5].

For $n \geq 5$ we may continue the procedure at least once more and write an $(n-3)$-dimensional integral. One expresses the coordinates $(x_1, \ldots, x_{n-2})$ using x_1 as scale, to arrive at

$$
C_n \;=\; \frac{4}{n!}\int_0^\infty \cdots \int_0^\infty \mathcal{M}(Q)\,\frac{dt_1}{t_1}\cdots\frac{dt_{n-3}}{t_{n-3}}, \tag{27}
$$

where, here, $Q := Q(t_1, \ldots, t_{n-3})$ is the Q-form (25) for $(n-3)$ dimensions, and

$$
\mathcal{M}(Q) \;:=\; \int_0^\infty \frac{\log(1+u)}{u^2 + Qu + Q}\,du.
$$

Moreover, $\mathcal{M}(Q)$ is directly expressible in terms of logarithms and dilogarithms. In fact, with $\alpha := \frac{Q}{2} - 1 - \left(\left(\frac{Q}{2}-1\right)^2 - 1\right)^{1/2} > 0$ so that the larger quantity $1/\alpha = \frac{Q}{2} - 1 + \left(\left(\frac{Q}{2}-1\right)^2 - 1\right)^{1/2}$ we have

$$
\begin{aligned}
(Q^2 - 4Q)^{1/2}\,\mathcal{M}(Q) \;=\;& \mathrm{Li}_2(-\alpha) - \mathrm{Li}_2(-1/\alpha) \\
\;=\;& 2\,\mathrm{Li}_2(-\alpha) + \zeta(2) + \frac{1}{2}\log^2(\alpha)
\end{aligned}
$$

where the last equality follows from [13, A.2.1. (5)]. This development, for example, represents C_5 as a double integral, namely

$$
C_5 \;=\; \frac{1}{30}\int_0^\infty \int_0^\infty \mathcal{M}(Q)\,\frac{dx}{x}\frac{dy}{y} \tag{28}
$$

$$
\;=\; \frac{1}{10}\int_0^1 \int_0^1 \mathcal{M}(Q)\,\frac{dx}{x}\frac{dy}{y}, \tag{29}
$$

where $Q := (1+x+y)(1+1/x+1/y)$.

While the details are a bit foreboding, all of this suggests that in general C_n may well be a combination of polylogarithmic constants of order at most $n-1$. In this language the results we have obtained are $C_3 = (4/3)\,\mathrm{Im}\,\mathrm{Li}_2((-1)^{1/3})/\sqrt{3}$ and $C_4 = -(56/3)\,\mathrm{Re}\,\mathrm{Li}_3((-1)^{1/2})/3$.

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On the other hand, there is some theoretical evidence in support of a possible "blockade" against closed forms for C_5 and beyond. Namely, the Adamchik algorithm [2] for evaluating integrals of argument powers with Bessel-function powers does not extend beyond 4th powers of the Bessel terms [3]. Thus C_4 can be derived via the Adamchik method, but evidently C_5 cannot.

To summarize: We have rigorously established closed forms as in Table 1 for C_1 through C_4. However, the higher C_n's remain elusive. It is pleasing—and justifies our original research motivation—that the above closed forms for the C_n involve, at least for these small n, similar fundamental constants as appear for the few known D_n appearing in Table 1.

6 Symbolics for the susceptibility integrals D_n

A first approach to closed forms for D_n is to exploit various advantages of integral representation (3). We have, with $\mathcal{A}_n \mathcal{B}_n$ denoting the integrand with the $(n-1)$ variables $t_2, t_3, \ldots, t_n$, $\mathcal{A}_1 \mathcal{B}_1 := 1$ and $\mathcal{A}_2 \mathcal{B}_2 = (t_2 - 1)^2 / (t_2 + 1)^4$, while

$$\mathcal{A}_3 \mathcal{B}_3 = \frac{(t_2 - 1)^2 (t_2 t_3 - 1)^2 (t_3 - 1)^2}{(t_2 + 1)^2 (t_2 t_3 + 1)^2 (t_3 + 1)^2 (t_2 + t_2 t_3 + 1)(t_2 t_3 + t_3 + 1)}$$

Hence, $D_1 = 2$ while

$$D_2 = 2 \int_0^1 \frac{(x-1)^2}{(x+1)^4} \, dx = \frac{1}{3}$$

$$D_3 = \frac{1}{3} \int_0^1 \int_0^1 \mathcal{A}_3 \mathcal{B}_3(x, y) \, dx \, dy$$

$$= \frac{2}{3} \int_0^1 \int_0^x \mathcal{A}_3 \mathcal{B}_3(x, y) \, dx \, dy,$$

which integral *Maple* can reduce[4] to the exact value for D_3 given in our introduction, at least in the form

$$18 \, i \, \mathrm{Li}_2 \left(1/2 - 1/2 \, i \sqrt{3} \right) \sqrt{3} - 18 \, i \, \mathrm{Li}_2 \left(1/2 + 1/2 \, i \sqrt{3} \right) \sqrt{3} + 24 + 4 \, \pi^2.$$

As noted in our introduction, a closed form for D_4 is known (see the caption to our Table 1, with reference to the McCoy–Tracy–Wu constant), yet the status of higher values is open. The representation above for D_4 via $\mathcal{A}_4 \mathcal{B}_4$ was sufficient to compute 14 decimal places in *Maple* and so to recover this constant with PSLQ. In principle, these methods and especially those of Section Seven allow for a complete symbolic resolution of D_4 but the details are somewhat daunting.

---

[4] Adequate *Maple* code is
```
p := (x − 1)^2 * (x − y)^2 * (y − 1)^2/(x + 1)^2/(x + y)^2/(y + 1)^2/(1 + y + x)/(y + x + x * y) :
d := Int(Int(p, x = 0..infinity), y = 0..infinity) : evalc(value(d));
```

For a second analytical foray, one may envision possible roles of the C_n in D_n analysis. Looking longingly at (7), one may write

$$D_n \;=\; \frac{1}{n!} \int \mathcal{D}\vec{x}\; \frac{\prod_{i<j}\left(1 - \operatorname{sech}^2\left(\frac{x_i - x_j}{2}\right)\right)}{(\cosh x_1 + \cdots + \cosh x_n)^2}. \tag{30}$$

This form reveals that in a specific sense, C_n amounts to a first term in a finite sum of integrals. Indeed, one might expand the product into partial products of sech^2 terms, and furthermore employ the attractive Fourier identity

$$\operatorname{sech}^2\left(\frac{z}{2}\right) \;=\; 2\int_{-\infty}^{\infty} \frac{k}{\sinh(\pi k)} e^{ikz}\; dk. \tag{31}$$

We also have the convenient integral representation

$$\int_{-\infty}^{\infty} e^{-p\cosh x + ikx}\; dx \;=\; 2K_{ik}(p).$$

Now for small n one may extract closed forms for D_n using a (p,k)-transform apparatus. For example, we have

$$
\begin{aligned}
D_2 \;&=\; C_2 - 4\int_{-\infty}^{\infty} \frac{k\; dk}{\sinh \pi k} \int_0^{\infty} pK_{ik}^2(p)\; dp \\
&=\; C_2 - 2\pi \int_{-\infty}^{\infty} \frac{k^2\; dk}{\sinh^2 \pi k} = \frac{1}{3}.
\end{aligned}
$$

Notice the direct involvement of the C_2 value as a 1st-order term.

For higher n, one can still evaluate the Bessel-K integrals in terms of hypergeometric functions, but it is not clear how to handle the rapidly growing number of k variables. Still, these (p,k)-transforms may conceivably give rise to high-precision numerical schemes.

The problem with growing k-variable counts is that an appropriate term from the natural expansion of representation (30), say

$$\int_0^{\infty} p\; dp \int \mathcal{D}\vec{x}\; e^{-p\sum \cosh x_k} \prod_{(a,b)\in\mathcal{P}} \operatorname{sech}^2((x_a - x_b)/2),$$

where $\mathcal{P}$ is some set of index pairs, has expansion

$$\int_0^{\infty} p\; dp \int \mathcal{D}\vec{k} \prod_{q=1}^{c} \frac{k_q}{\sinh(\pi k_q)} K_{i\nu_q}(p),$$

where $c = \operatorname{card}(\mathcal{P})$. Unfortunately, c can be $O(n^2)$.

Still it may somehow be possible to somehow employ a higher-order sech-Fourier transform, namely a generalization of (31) [16]:

$$\operatorname{sech}^{2m}(x/2) \;=\; \frac{2^{2m-1}}{(2m-1)!} \int_{-\infty}^{\infty} \frac{k}{\sinh(\pi k)} e^{ikx} \prod_{h=1}^{m-1} \left(k^2 + h^2\right)\; dk.$$

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Likewise, it would be good to know the Fourier transform of

$$\prod_{(a,b)\in\mathcal{P}} \operatorname{sech}^2((x_a - x_b)/2)$$

in terms of *at most* n spectral variables k_q, rather than $c = \operatorname{card}(\mathcal{P}) = O(n^2)$ such variables. In any case, it may well be that an appropriate (k, p) transform would lead us back to the highly successful numerical approach that yielded results for the C_n. As interesting as these (k, p) transforms may be, such an approach may be misdirected in the sense that a "perturbation series" for D_n starting with leading term C_n is unrealistic, due to the different asymptotic character of D_n, as we next discuss.

7   Asymptotic character of D_n and E_n

With a view to proving that D_n, E_n are genuinely exponentially decaying in a certain sense, we first note the examples

$$
\begin{aligned}
E_1 &:= 2, \\
E_2 &= 2\int_0^1 \mathcal{A}\, dt_2 = 2\int_0^1 \left(\frac{1-x}{1+x}\right)^2 dx = 6 - 8\log 2 \approx 0.454823, \\
E_3 &= 2\int_0^1\int_0^1 \left(\frac{(1-x)(1-xy)(1-y)}{(1+x)(1+xy)(1+y)}\right)^2 dx\, dy \\
&= 10 - 2\pi^2 - 8\log 2 + 32\log^2 2 \approx 0.0901102,
\end{aligned}
$$

with E_4 and E_5 also enjoying a more extended but similar closed form (see Table 1). Just these few examples suggest exponential decay of the E_n integrals, with a decay constant about 5 (see Table 2 and Section 11).

For convenience in the theorem to follow, we define

$$R(x) := \left(\frac{1-x}{1+x}\right)^2,$$

and let $m := n - 1$, so that E_n is the integral over the unit m-cube of the product of (a triangular number) $m(m+1)/2$ instances of R. Specifically, for $n > 1$,

$$E_n = 2\int_{[0,1]^m} \mathcal{D}\vec{x} \prod_{k=1}^m R(x_k)\, R(x_k x_{k+1})\cdots R(x_k\cdots x_m).$$

Observe also that the reduced D_n integrand is the same R-product multiplied by the extra factor $\mathcal{B}_n(x_1,\ldots,x_m) := (1 + x_1 S)^{-1}(T + U x_1)^{-1}$, where

$$
\begin{aligned}
S &:= 1 + x_2 + x_2 x_3 + \cdots + x_2\cdots x_m, \\
T &:= 1 + x_m + x_m x_{m-1} + \cdots + x_m\cdots x_2,
\end{aligned}
$$

and $U := x_m\cdots x_2$.

Theorem 3 *The sequences (D_n) and (E_n) are both strictly monotone decreasing for $n \geq 1$. Moreover, D_n and E_n enjoy genuine exponential decay; that is, there exist positive constants a, b, A, B such that for all positive integers n*

$$\frac{a}{b^n} \leq D_n \leq E_n \leq \frac{A}{B^n},$$

where effective values are $\{a, b\} = \{19, 14\}$ and $\{A, B\} = \{12, 4\}$.

Proof. *First, monotonicity.* By bounding the integral over the first coordinate x_1 we see that

$$E_n \;\; \leq \;\; \left(\int_0^1 R(x_1) \; dx_1 \right) E_{n-1} \;\; = \;\; \frac{E_2}{2} \, E_{n-1} \;\; < \;\; 0.26 \, E_{n-1}.$$

This establishes strict monotonicity for the sequence (E_n); below we shall tighten this approach to yield better effective constant. As for monotonicity of the D_n, note that for $m := n - 1$ the R-product involving the first coordinate x_1 can be bounded as

$$R(x_1) R(x_1 x_2) \cdots R(x_1 \cdots x_m) \;\; \leq \;\; e^{-2x_1 S},$$

where S is given in the text prior to this theorem. This bound on the x_1-dependent part can be quickly obtained by taking the logarithm of the R-product, noting $\log R(z) = -2(z + z^3/3 + z^5/5 + \cdots) \leq -2z$. Now we obtain an upper bound for the integral over x_1, as

$$\int_0^1 \frac{e^{-2x_1 S}}{(1 + x_1 S)(T + U x_1)} \; dx_1 \;\; < \;\; \frac{0.37}{ST},$$

where we have used $\int_0^\infty e^{-2z}/(1 + z) \; dz = e^2 \mathrm{Ei}(1, 2) \approx 0.361$, an *exponential integral*, [1]. But $1/(ST)$ is precisely the $\mathcal{B}_{n-1}$ factor in the integrand for $D_{n-1} = 2 \int_{[0,1]^{n-2}} \mathcal{A}_{n-1} \mathcal{B}_{n-1} \; \mathcal{D}\vec{x}$, thus we establish monotonicity in the form $D_n < 0.37 D_{n-1}$.

Next, for a fundamentally tighter effective upper bound on E_n (and perforce D_n—recall the trivial inequality $D_n \leq E_n$). For a given n, the integrand for $E_n/2$ has at least $\lfloor (n - 1)/2 \rfloor$ disjoint triples of the form $R(x_i) R(x_i x_j) R(x_j)$, as inspection of a few cases suggests. For example, the integrand for $E_5/2$ with variables w, x, y, z is

$$\underline{R}(w) \, \underline{R}(wx) \, R(wxy) \, R(wxyz) \underline{R}(x) \, R(xy) \, R(xyz) \, \underline{R}(y) \, \underline{R}(yz) \, \underline{R}(z),$$

from which one may read off six (underlined) R's amounting to $\lfloor (5 - 1)/2 \rfloor = 2$ disjoint triples. Thus the integral for $E_n/2$ is bounded above by the product of $\lfloor (n - 1)/2 \rfloor$ copies of $E_3/2$ and so

$$\frac{1}{2} E_n \;\; \leq \;\; \left(\frac{2}{E_3} \right)^{-\lfloor (n-1)/2 \rfloor}$$

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and the upper bound follows.

Now for the lower bound. The reduced D_n integrand is a product of $m(m+1)/2$ evaluations of R (where $m := n - 1$) times the factor $\mathcal{B}_n$. Said integrand is *monotone decreasing* in all variables $x_1, \ldots, x_m$. That is, the integrand ι satisfies $\iota(\vec{x}) \leq \iota(\vec{y})$ whenever $x_k \leq y_k$ for all coordinate indices k. But this means that for any $\alpha \in [0, 1]$ the integral is bounded below by a natural approximation of the integral over the sub-cube $[0, \alpha]^m$. Namely, we evaluate all the R terms at the corner vector $\vec{\alpha} := (\alpha, \alpha, \ldots, \alpha)$, observing also $\mathcal{B}_n(\vec{\alpha}) \geq (1 - \alpha)^2$, and deduce

$$
\begin{aligned}
D_n \quad \geq \quad & 2(1 - \alpha)^2 \, \alpha^m \left(\frac{1 - \alpha}{1 + \alpha} \right)^{2m} \left(\frac{1 - \alpha^2}{1 + \alpha^2} \right)^{2m-2} \left(\frac{1 - \alpha^3}{1 + \alpha^3} \right)^{2m-4} \\
& \cdots \left(\frac{1 - \alpha^m}{1 + \alpha^m} \right)^2
\end{aligned}
\tag{32}
$$

since α^m is the volume of the reduced hyper-cube.

Interestingly, this expression in α may be bounded below by a theta-function term, as we may estimate

$$
\begin{aligned}
D_n \quad \geq \quad & 2(1 - \alpha)^2 \, \alpha^m \prod_{k=1}^{\infty} \left(\frac{1 - \alpha^k}{1 + \alpha^k} \right)^{2m} \\
= \quad & 2(1 - \alpha)^2 \left(\alpha \theta_4(\alpha)^2 \right)^m,
\end{aligned}
$$

where $\theta_4(q) := \sum_{n \in Z} (-q)^{n^2}$ is a *Jacobi theta function*, see [9]. Now $\alpha \theta_4(\alpha)^2$ has a maximum greater than 0.074 at $\alpha = \alpha_0 > 0.169$ and we conclude that $D_n \geq 2(1 - \alpha_0)^2 (0.074)^{n-1}$, leading immediately to the desired lower bound as well as effective constants.   **QED**

Remark 2 The effective values may be further improved with more aggressive application of the following techniques. For example, B can be $(2/E_p)^{1/(p-1)}$ for any $p > 1$, and so the approximate (nonrigorous) value for E_8 in Table 2 yields effective constant $B \approx 4.97$. Likewise, more effort to enhance (32) will presumably improve the lower bound b, the remaining inequalities being quite tight.

Corollary 1 *For all positive integers n, we have $E_n \leq C_n$.*

Proof. This follows directly from the observation that even for $n = 2$, Theorem 3 with $A := 12, B := 4.71$ gives us $E_{(n \geq 2)} < 0.54 < 2\, e^{-2\gamma}$, the right-hand side being $\inf_n C_n$.   **QED**

Theorem 3 suggests that D_n, E_n may both follow a truly exponential-decay asymptotic, and numerical work suggests further a universal decay constant, whence we posit:

Conjecture 2 D_n, E_n *both decay exponentially, with the same decay constant. That is, there exist positive constants δ, Δ, ϕ such that*

$$D_n \sim \frac{\delta}{\Delta^n} \ \ and \ E_n \sim \frac{\phi}{\Delta^n},$$

so that ratios behave as

$$\lim_{n\to\infty} \frac{D_n}{D_{n+1}} = \lim_{n\to\infty} \frac{E_n}{E_{n+1}} = \Delta,$$

$$and \ \lim_{n\to\infty} \frac{D_n}{E_n} = \delta/\phi.$$

Remark 3 If this conjecture is true, we expect, based on the quasi-Monte Carlo (qMC) integrations of Section 8, that $\Delta \approx 5$ and $\delta/\phi \approx 0.7$. Moreover, given our rigorous result Theorem 3, is it perhaps reasonable anyway to expect Δ to be of order $b \approx 4.7$.

8 Further dimensional reduction of D_n and E_n

We have seen that D_n, E_n can each be defined by an $(n-1)$-dimensional integral, via relations (3), (5), and that C_n can be reduced to an $(n-2)$-dimensional integral, as in (24) and further to an $(n-3)$-dimensional form (27). However, it turns out that D_n, E_n can *also* be reduced to $(n-2)$-dimensional forms, albeit with considerable combinatorial complications, as we shall now establish.

We begin by considering the integrand factor $\mathcal{A}$ appearing in (3), (5), and noting the combinatorial recursion that results from an attempt to factor out terms involving only t_2:

$$\mathcal{A}_n(t_2,\ldots,t_n) = \left(\frac{1-t_2}{1+t_2}\right)^2 \left(\frac{1-t_2 t_3}{1+t_2 t_3}\right)^2 \cdots \left(\frac{1-t_2\cdots t_n}{1+t_2\cdots t_n}\right)^2 \mathcal{A}_{n-1}(t_3,\ldots,t_n).$$

Observe also that we may write

$$B_n(t_2,\ldots,t_n) = \frac{b^{-1}}{(1+t_2(1+t_3+t_3 t_4 + \cdots + t_3\cdots t_n))\cdot(1+(a/b)\,t_2)}$$

with

$$a \ := \ t_3\cdots t_n, \ b := 1+t_n + t_n t_{n-1} + \cdots + t_n\cdots t_3.$$

Next, we observe a key formal identity

$$\left(\frac{1-z}{1+z}\right)^2 = \frac{\partial}{\partial\lambda}\Big|_{\lambda=1}\left(\lambda + \frac{4}{1+\lambda z}\right)$$

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which will allow us to create terms $(1-z)^2/(1+z)^2$ via partial differentiation. Now for a parameter vector $\vec{\lambda}$ of dimension $(n-1)$, define

$$\mathcal{G}_n(\vec{\lambda}; t_2, \ldots, t_n) \ := \ 2\prod_{k=1}^{n-1}\left(\lambda_k + \frac{4}{1 + \lambda_k \prod_{j=2}^{k+1} t_j}\right).$$

Putting all this together yields

$$D_n \ = \ \int_0^1 \cdots \int_0^1 \mathcal{A}_{n-1}(t_3, \ldots, t_n)\left(\frac{\partial^{n-1}}{\partial\lambda_1 \cdots \partial\lambda_{n-1}}|_{\lambda_k=1}\int_0^1 \mathcal{G}_n\mathcal{B}_n \ dt_2\right) \ dt_3 \cdots dt_n$$

$$E_n \ = \ \int_0^1 \cdots \int_0^1 \mathcal{A}_{n-1}(t_3, \ldots, t_n)\left(\frac{\partial^{n-1}}{\partial\lambda_1 \cdots \partial\lambda_{n-1}}|_{\lambda_k=1}\int_0^1 \mathcal{G}_n \ dt_2\right) \ dt_3 \cdots dt_n.$$

Remarkably, as we shall presently show, $\mathcal{G}_n$ and $\mathcal{G}_n\mathcal{B}_n$—for any n—can each be integrated in closed form with respect to the t_2 coordinate. and furthermore these closed forms may be differentiated with respect to the λ_k and then evaluated at $\lambda_k = 1$ to provide a legitimate, $(n-2)$-dimensional integral over $(t_3, \ldots, t_n)$. Indeed, we have a general reduction theorem:

Theorem 4 *For every integer $n > 2$, each of C_n, D_n, E_n can be written as an $(n-2)$-dimensional integral with elementary integrand consisting of algebraic multivariate functions of logarithms.*

Proof. For a parameter collection $(\sigma_k : k = 1, \ldots, M)$ we know from partial-fraction decomposition that

$$\int_0^1 \prod_{k=1}^M \frac{1}{1+\sigma_k t} \ dt \ = \ \sum_{i=1}^M \frac{\sigma_i^{M-2}\log(1+\sigma_i)}{\prod_{j\neq i}(\sigma_i - \sigma_j)}.$$

Now the t_2-dependent part of the product integrand $\mathcal{G}_n\mathcal{B}_n$ for D_n can be written as a product of the type in the integral here, with $M = n+1$, $t := t_2$, and the σ_k involving subsets of variables taken only from $(t_3, \ldots, t_n)$, so immediately we have an algebraic function of logs for an integral over the one coordinate t_2. Then we differentiate inside with respect to $\lambda_1, \ldots, \lambda_{n-1}$ and arrive at an $(n-2)$-dimensional integral. The same argument goes through for the simpler integrand $\mathcal{G}_n$ of E_n, with $M = n-1$. **QED**

Note that if need be, C_n can be processed as above, with integrand $2\mathcal{B}_n$—see (4)—but the previous result (24) gives equivalent reduction. A specific manifestation of the reduction procedure is detailed in Section 12, where we provide some numerical values for D_5, E_5, D_6, E_6.

We were able to reduce E_4 entirely to one dimensional integrals and ultimately to evaluate it symbolically but for higher dimensions this seems impracticable.

Part II. Various numerical algorithms

9 Algorithm for Bessel-kernel evaluation of C_n

As implied in our Abstract and elsewhere, we first approached the C_n integrals experimentally. Our central strategy for a high-precision numerical evaluation scheme for $F(t) = K_0(t)$ in relation (9) is to utilize a combination of an ascending series $F^{(asc)}(t)$ (which is well-suited for small t) and an asymptotic series $F^{(asy)}(t)$ (which is well-suited for large t), together with a chosen parameter λ that is the boundary between the "small" arguments and the "large" t.

Given the formulae (11), (12) for the modified Bessel function K_0, there are two approaches to computing C_n from (9). The first, suitable for those who have access to symbolic computing software, is simply to write the integral (9) as a sum of two integrals, one from 0 to λ, and the second from λ to ∞, and then to symbolically expand suitably truncated versions of (11) and (12) and evaluate the numerous individual integrals that result. We have obtained reliable results by taking $\lambda = D/2$, where D is the desired precision level in digits, and truncating the two series after $3n\lambda$ and 2λ terms, respectively. This approach suffices to obtain modestly high precision results (at least 30 digits) for n up to eight or so. Beyond this level, the symbolic computing costs become too great to complete in reasonable time.

A second approach is to directly evaluate the integral in (9) using the *tanh-sinh numerical quadrature* scheme [6], [9, pg. 312–313], where the integrand function is evaluated by either the ascending series (11) or the descending series (12), depending on whether the argument t is less than or greater than λ. For these calculations, we found it satisfactory to take $\lambda = D$, and to truncate the series summations when the absolute value of the term being added is less than 10^{-D} times the absolute value of the current sum.

Tanh-sinh quadrature is remarkably effective in evaluating integrals to very high precision, even in cases where the integrand function has an infinite derivative or blow-up singularity at one or both endpoints. It is well-suited for highly parallel evaluation [4], and is also amenable to computation of provable bounds on the error [5]. It is based on the transformation $x = g(t)$, where $g(t) = \tanh[\pi/2 \cdot \sinh(t)]$. In a straightforward implementation of the tanh-sinh scheme, one first calculates a set of *abscissas* x_k and *weights* w_k

$$
\begin{aligned}
x_j &:= \tanh[\pi/2 \cdot \sinh(jh)] \\
w_j &:= \frac{\pi/2 \cdot \cosh(jh)}{\cosh^2[\pi/2 \cdot \sinh(jh)]},
\end{aligned}
$$

where h is the interval of integration. Then the integral of the function $f(t)$ on $[-1, 1]$ is performed as

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

20

where N is chosen so that the terms $w_j f(x_j)$ are sufficiently small that they can be ignored for $j > N$. Full details of a robust implementation are given in [6]. Note that in this particular application, multiple C_n can be efficiently computed for different n, since the abscissas, weights and $K_0(t)$ function values at these abscissas are independent of n.

Using this approach, we have been able to evaluate C_n to very high precision (500-digit accuracy), for n as large as 1024, which is equivalent to performing a 1024-fold iterated integral in (8). Each of these runs (regardless of n) requires only about 100 seconds on a 2006-era single-processor computer. Selected high-precision results are exhibited in Appendix 1.

10   Hypergeometric-kernel representation for D_n

Now to numerical issues for the Ising-susceptibility integrals D_n. It is highly suggestive that we were able to transform the C_n integral into a 1-dimensional form that admits of arbitrary-precision evaluation. For the D_n, a 1-dimensional form is *also* possible, at least formally: We do not yet know the precise convergence rate of the approach; consequently, the 1-dimensional representation we achieve below may well not be practical.

A hyperbolic representation for D_n similar to (8) develops as

$$D_n \quad := \quad \frac{1}{n!} \int \frac{\mathcal{D}\vec{x}}{(\cosh x_1 + \cdots + \cosh x_n)^2} \prod_{i<j} \tanh^2 \left(\frac{x_i - x_j}{2} \right). \quad (33)$$

Knowing the identity

$$\tanh(t - u) \quad = \quad \frac{\tanh t - \tanh u}{1 - \tanh t \tanh u},$$

we fix n and ponder the formal power series

$$\prod_{i<k} \left(\frac{t_i - t_k}{1 - t_i t_k} \right)^2 \quad = \quad \sum_{m_1, \ldots, m_n \geq 0} A(m_1, \ldots, m_n) t_1^{m_1} \cdots t_n^{m_n}.$$

We intend that this *define* the set of A coefficients. So, formally at least, we have

$$D_n \quad = \quad \int_0^\infty d_n(p) \, dp, \quad (34)$$

where the kernel d_n is represented

$$d_n(p) \quad := \quad \frac{2^n p}{n!} \sum_{m_k \geq 0, \text{ even}} A(m_1, \ldots, m_n) \prod_{k=1}^n T_{m_k}(p),$$

where

$$T_m(p) \quad := \quad \int_0^\infty \tanh^m \left(\frac{t}{2} \right) e^{-p \cosh t} \, dt,$$

21

a *confluent hypergeometric function* [1] in disguise. In fact,

$$T_m(p) \;=\; e^{-p}\,\Gamma\left(\frac{m+1}{2}\right)U\left(\frac{m+1}{2},1,2p\right),$$

where U is the standard confluent hypergeometric function [1]. Still formally, without regard to convergence, we claim a 1-dimensional kernel for the D_n as

$$d_n(p) \;:=\; \frac{2^n p e^{-np}}{n!}\sum_{m_k\geq 0,\ \text{even}} A(m_1,\ldots,m_n)\prod_{k=1}^{n}\Gamma\left(\frac{m_k+1}{2}\right)U\left(\frac{m_k+1}{2},1,2p\right).$$

(35)

This kernel d_n is more complicated than the Bessel kernel c_n, which is not unexpected on the basis of the combinatorial product's stultifying appearance in the original D_n integrand. As previously intimated, we do not know the convergence rate for d_n, not to mention the efficiency of the integral (34), say in terms of precision vs. a computational bound on the m_k indices.

It is therefore admitted that this hypergeometric-kernel representation remains of theoretical interest but with as yet untapped numerical power. We do, however, posit the

Conjecture 3 *For fixed n, the 1-dimensional kernel $d_n(p)$ defined by (35) converges to an integrable function on $p \in (0,\infty)$, and therefore gives via (34) the correct Ising integral D_n.*

In future research it may be useful to analyze the character of the A tensor. For $n = 2$, the pattern of the A coefficients is evident in the small collection:

$$\{A(2x,2y)\}_{0\leq x,y\leq 6} \;=\; \begin{pmatrix} 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 1 & -4 & 3 & 0 & 0 & 0 & 0 \\ 0 & 3 & -8 & 5 & 0 & 0 & 0 \\ 0 & 0 & 5 & -12 & 7 & 0 & 0 \\ 0 & 0 & 0 & 7 & -16 & 9 & 0 \\ 0 & 0 & 0 & 0 & 9 & -20 & 11 \\ 0 & 0 & 0 & 0 & 0 & 11 & -24 \end{pmatrix}$$

Useful for calculations on the d_n kernel may be the ascending and asymptotic series, respectively

$$\Gamma(a)\,U(a,1,z) \;=\; \sum_{k\geq 0}\frac{(a)_k z^k}{k!^2}(2\psi(k+1)-\psi(k+a)-\log z), \qquad (36)$$

and

$$\Gamma(a)\,U(a,1,z) \;\sim\; \sum_{m\geq 0}\frac{(a)_m(-1)^m\Gamma(m+a)}{m!z^{m+a}}. \qquad (37)$$

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n	D_n	D_{n-1}/D_n	E_n	E_{n-1}/E_n	D_n/E_n
1*	2.00000000	—	2.00000000	—	1.0000000
2*	0.33333333	6.0000000	0.45482256	4.3973192	0.73288665
3*	0.06430739	5.183437	0.09011020	5.047403	0.7136527
4*	0.01262502	5.093647	0.01774490	5.078089	0.7114729
5	0.00248461	5.08129	0.00349365*	5.079181*	0.7111768
6	4.8914e-04	5.079520	6.8783e-04	5.079219	0.711134
7	9.6301e-05	5.079313	1.3542e-04	5.07925	0.71112
8	1.8960e-05	5.07898	2.666e-05	5.0790	0.7111

Table 2: Results of qMC integration for various D_n, E_n.

11 Heuristic asymptotics via quasi-Monte Carlo (qMC) methods

We have shown (Theorem 3) that D_n, E_n are bounded above and below by exponential decay. We also have the decay Conjecture 2 that D_n, E_n share the same decay constant Δ. Contrast this to our proven result $C_n \to$ constant.

The *quasi-Monte Carlo* (qMC) integrations as shown below in Table 2 suggest that the decay conjecture is true and that $\Delta \approx 5$. Similar theorems and conjectures appear to be reasonable and similar for the related E_n, the ratios E/D, and so on. Yet, there are interesting open questions, such as: Is D_{n-1}/D_n eventually monotonic decreasing in n, as Table 2 suggests? Is the same true for D_n/E_n? The qMC algorithm we employed—a "spacefill-Halton hybrid"—is, for some integrands, suitable for high dimensions lying somewhat beyond the reach of the classical *Halton sequences*, [10, 11]. This qMC approach we employed evidently yields several good decimals even up to dimension $n = 32$. We draw this supposition from the stability of qMC for various n-regions, together with tests on the very much more accurately known C_n. (See also the recent survey on qMC, [12].)

Referring to Table 2: Rows marked '*' (and two items likewise marked) are exactly known (see closed-form evaluations for $n = 1, 2, 3, 4$ and E_5 in Table 1) but all other entities are only numerically understood. Each table entry, for each n, involved $2 \cdot 10^9$ qMC points. Errors are not all rigorously known—entries here are to "believed" precision, based on the qMC trends, and we admit to the usual degradation of precision with increasing dimension. Note that all of the tabulated ratios appear to approach respective constants. Though such limits are only conjectured, we have already proven that D_n, E_n themselves decay at least exponentially rapidly to zero as $n \to \infty$.

There is an additional question which further computation may well address. Namely, J-M. Maillard has suggested that ratios D_n/D_{n+2}, meaning ratios of consecutive even or odd D_n values, might converge more efficiently (or more

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smoothly?) based on general principles of Ising susceptibility expansions [14]. Unfortunately, the qMC values in our Table 2 are evidently too imprecise to decide such an issue. Generally speaking, though, such "parity acceleration" is not uncommon in other fields; for example, the pure-even, pure-odd convergents of continued fractions are examples of split sequences that can each converge efficiently and independently to an actual common limit.

12   Quadrature for higher-dimensional D_n, E_n

Compared with the one-dimensional quadrature calculations we described earlier, multi-dimensional extreme-precision quadrature is very expensive indeed. Thus, to perform numerical quadrature for entities such as D_5, E_5 and beyond requires a representation in the lowest possible dimension. We have seen in Section 8 that D_n, E_n can each be reduced to an $(n-2)$-dimensional form. The details of this extra reduction can be quite intricate, so we shall summarize the explicit algebra for the elusive D_5, E_5, knowing from Theorem 4 that in higher dimensions we can in principle follow the prescription.

For $n = 5$ let us denote variables w, x, y, z and symbolically perform the interior integration over w (which was t_2 in Section 8). We use

$$
\begin{aligned}
\mathcal{A}_4(x,y,z) \;&:=\; \left(\frac{(1-x)(1-xy)(1-xyz)(1-y)(1-yz)(1-z)}{(1+x)(1+xy)(1+xyz)(1+y)(1+yz)(1+z)}\right)^2 \\
\mathcal{G}_5 \;&:=\; 2\left(\lambda_1 + \frac{4}{1+\lambda_1 w}\right)\left(\lambda_2 + \frac{4}{1+\lambda_2 wx}\right)\left(\lambda_3 + \frac{4}{1+\lambda_3 wxy}\right) \\
&\quad\; \cdot\left(\lambda_4 + \frac{4}{1+\lambda_4 wxyz}\right) \\
\mathcal{B}_5^{-1} \;&:=\; (1+z+zy+zyx)\,(1+w(1+x+xy+xyz)) \\
&\quad\; \cdot\left(1 + \frac{zyx}{1+z+zy+zyx}w\right).
\end{aligned}
$$

Then we have, from Section 8,

$$
\begin{aligned}
D_5 \;&=\; \int_0^1 \int_0^1 \int_0^1 \mathcal{A}_4(x,y,z)\left(\frac{\partial^4}{\partial\lambda_1\partial\lambda_2\partial\lambda_3\partial\lambda_4}\Big|_{\lambda_k=1}\int_0^1 \mathcal{G}_5\mathcal{B}_5\,dw\right)\,dx\,dy\,dz \\
E_5 \;&=\; \int_0^1 \int_0^1 \int_0^1 \mathcal{A}_4(x,y,z)\left(\frac{\partial^4}{\partial\lambda_1\partial\lambda_2\partial\lambda_3\partial\lambda_4}\Big|_{\lambda_k=1}\int_0^1 \mathcal{G}_5\,dw\right)\,dx\,dy\,dz.
\end{aligned}
$$

The results for this procedure are two respective integrals for D_5, E_5, over the three variables x, y, z. As we have intimated, the details are overwhelmingly complicated, producing enormous expressions involving multivariate polynomials, rational functions and logarithms. To give but one example, we present here the stultifying triple integral we used to compute D_5:

$$D_5 = \int_0^1 \int_0^1 \int_0^1 \left[2(1-x)^2(1-y)^2(1-xy)^2(1-z)^2(1-yz)^2(1-xyz)^2 \right.$$

$$\left(- \left[4(x+1)(xy+1)\log(2) \left(y^5 z^3 x^7 - y^4 z^2 (4(y+1)z+3)x^6 - y^3 z \left(\left(y^2+1\right)z^2 + 4(y+ \right. \right. \right.$$

$$1)z+5) x^5 + y^2 \left(4y(y+1)z^3 + 3\left(y^2+1\right)z^2 + 4(y+1)z-1 \right) x^4 + y \left(z \left(z^2 + 4z \right. \right.$$

$$+5) y^2 + 4\left(z^2+1\right)y + 5z + 4 \right) x^3 + \left(\left(-3z^2 - 4z+1\right)y^2 - 4zy+1 \right) x^2 - (y(5z+4)$$

$$+4)x-1) / \left[(x-1)^3(xy-1)^3(xyz-1)^3 \right] + \left[3(y-1)^2 y^4 (z-1)^2 z^2 (yz \right.$$

$$-1)^2 x^6 + 2y^3 z \left(3(z-1)^2 z^3 y^5 + z^2 \left(5z^3 + 3z^2 + 3z + 5 \right) y^4 + (z-1)^2 z \right.$$

$$\left(5z^2 + 16z + 5 \right) y^3 + \left(3z^5 + 3z^4 - 22z^3 - 22z^2 + 3z + 3 \right) y^2 + 3 \left(-2z^4 + z^3 + 2 \right.$$

$$z^2 + z - 2) y + 3z^3 + 5z^2 + 5z + 3 \right) x^5 + y^2 \left(7(z-1)^2 z^4 y^6 - 2z^3 \left(z^3 + 15z^2 \right. \right.$$

$$+15z+1) y^5 + 2z^2 \left(-21z^4 + 6z^3 + 14z^2 + 6z - 21 \right) y^4 - 2z \left(z^5 - 6z^4 - 27z^3 \right.$$

$$-27z^2 - 6z + 1) y^3 + \left(7z^6 - 30z^5 + 28z^4 + 54z^3 + 28z^2 - 30z + 7 \right) y^2 - 2 \left(7z^5 \right.$$

$$+15z^4 - 6z^3 - 6z^2 + 15z + 7) y + 7z^4 - 2z^3 - 42z^2 - 2z + 7 \right) x^4 - 2y \left(z^3 \left(z^3 \right. \right.$$

$$-9z^2 - 9z + 1) y^6 + z^2 \left(7z^4 - 14z^3 - 18z^2 - 14z + 7 \right) y^5 + z \left(7z^5 + 14z^4 + 3 \right.$$

$$z^3 + 3z^2 + 14z + 7) y^4 + \left(z^6 - 14z^5 + 3z^4 + 84z^3 + 3z^2 - 14z + 1 \right) y^3 - 3 \left(3z^5 \right.$$

$$+6z^4 - z^3 - z^2 + 6z + 3) y^2 - \left(9z^4 + 14z^3 - 14z^2 + 14z + 9 \right) y + z^3 + 7z^2 + 7z$$

$$+1) x^3 + \left(z^2 \left(11z^4 + 6z^3 - 66z^2 + 6z + 11 \right) y^6 + 2z \left(5z^5 + 13z^4 - 2z^3 - 2z^2 \right. \right.$$

$$+13z+5) y^5 + \left(11z^6 + 26z^5 + 44z^4 - 66z^3 + 44z^2 + 26z + 11 \right) y^4 + \left(6z^5 - 4 \right.$$

$$z^4 - 66z^3 - 66z^2 - 4z + 6) y^3 - 2 \left(33z^4 + 2z^3 - 22z^2 + 2z + 33 \right) y^2 + \left(6z^3 + 2 \right.$$

$$6z^2 + 26z + 6) y + 11z^2 + 10z + 11 \right) x^2 - 2 \left(z^2 \left(5z^3 + 3z^2 + 3z + 5 \right) y^5 + z \left(22z^4 \right. \right.$$

$$+5z^3 - 22z^2 + 5z + 22) y^4 + \left(5z^5 + 5z^4 - 26z^3 - 26z^2 + 5z + 5 \right) y^3 + \left(3z^4 - \right.$$

$$22z^3 - 26z^2 - 22z + 3) y^2 + \left(3z^3 + 5z^2 + 5z + 3 \right) y + 5z^2 + 22z + 5 \right) x + 15z^2 + 2z$$

$$+2y(z-1)^2(z+1) + 2y^3(z-1)^2 z(z+1) + y^4 z^2 \left(15z^2 + 2z + 15 \right) + y^2 \left(15z^4 \right.$$

$$-2z^3 - 90z^2 - 2z + 15) + 15 \right] / \left[(x-1)^2(y-1)^2(xy-1)^2(z-1)^2(yz-1)^2 \right.$$

$$(xyz-1)^2] - \left[4(x+1)(y+1)(yz+1) \left(-z^2 y^4 + 4z(z+1)y^3 + \left(z^2+1\right)y^2 \right. \right.$$

$$-4(z+1)y + 4x \left(y^2 - 1 \right) \left(y^2 z^2 - 1 \right) + x^2 \left(z^2 y^4 - 4z(z+1)y^3 - \left(z^2+1\right)y^2 \right.$$

$$+4(z+1)y+1) - 1) \log(x+1) \right] / \left[(x-1)^3 x(y-1)^3(yz-1)^3 \right] - \left[4(y+1)(xy \right.$$

$$+1)(z+1) \left(x^2 \left(z^2 - 4z - 1 \right) y^4 + 4x(x+1) \left(z^2 - 1 \right) y^3 - \left(x^2+1\right) \left(z^2 - 4z - 1 \right) \right.$$

$$y^2 - 4(x+1) \left(z^2 - 1 \right) y + z^2 - 4z - 1 \right) \log(xy+1) \right] / \left[x(y-1)^3 y(xy-1)^3(z- \right.$$

$$1)^3] - \left[4(z+1)(yz+1) \left(x^3 y^5 z^7 + x^2 y^4 (4x(y+1) + 5)z^6 - xy^3 \left(\left(y^2+ \right. \right. \right.$$

$$1) x^2 - 4(y+1)x - 3) z^5 - y^2 \left(4y(y+1)x^3 + 5\left(y^2+1\right)x^2 + 4(y+1)x + 1 \right) z^4 +$$

$$y \left(y^2 x^3 - 4y(y+1)x^2 - 3\left(y^2+1\right)x - 4(y+1) \right) z^3 + \left(5x^2 y^2 + y^2 + 4x(y+1) \right.$$

$$y+1) z^2 + ((3x+4)y+4)z - 1) \log(xyz+1) \right] / \left[xy(z-1)^3 z(yz-1)^3(xyz-1 \right.$$

$$)^3] \right) \right] / \left[(x+1)^2(y+1)^2(xy+1)^2(z+1)^2(yz+1)^2(xyz+1)^2 \right] \, dx \, dy \, dz$$

There is a similar integrand for E_5. The corresponding expressions for D_6 and E_6 are several times more complicated still—the parse tree for the D_6 integrand has over 27,000 leaves, even after some simplification! In Appendix 2 we display the numerical results for D_5, E_5, D_6, E_6 obtained in this fashion. Note that we expended more machine work for $n = 5$ because that n marks the spot where previous research had reached a kind of blockade.

Based on the numerical value for E_5, we applied a PSLQ integer relation detection program to recognize this constant as exhibited in Table 1, where as one can see the constants π, $\log 2$, $\zeta(3)$ and $\mathrm{Li}_4(1/2)$ are involved. Note the use there of the notation $\overset{?}{=}$, meaning that we have not yet worked out a formal proof. This experimental detection for E_5 is quite strong, though—190 orders of magnitude beyond the level that could reasonably be ascribed to numerical round-off error.

Alas, we still have not been successful in identifying either C_5 or D_5. However, we have established, via a PSLQ computation and based on the 500-digit values given in Appendix 2, that *neither C_5 nor D_5 satisfies a integer linear relation* with the following set of constants, where the vector of integer coefficients in the linear relation has Euclidean norm less than $4 \cdot 10^{12}$:

$$1,\ \pi,\ \log 2,\ \pi^2,\ \pi \log 2,\ \log^2 2,\ \mathrm{L}_{-3}(2),\ \pi^3,\ \pi^2 \log 2,\ \pi \log^2 2,\ \log^3 2,$$
$$\zeta(3),\ \pi\,\mathrm{L}_{-3}(2),\ \log 2 \cdot \mathrm{L}_{-3}(2),\ \pi^4\,\pi^3 \log 2,\ \pi^2 \log^2 2,\ \pi \log^3 2,\ G,\ G\pi^2,$$
$$\mathrm{Li}_4(1/2),\ \sqrt{3}\,\mathrm{L}_{-3}(2),\ \log^4 2,\ \pi\zeta(3),\ \log 2 \cdot \zeta(3),\ \pi^2\mathrm{L}_{-3}(2),\ \pi^2\mathrm{L}_{-3}(2),$$
$$\pi \log 2 \cdot \mathrm{L}_{-3}(2),\ \log^2 2 \cdot \mathrm{L}_{-3}(2),\ \mathrm{L}_{-3}^2(2),\ \mathrm{Im}[\mathrm{Li}_4(e^{2\pi i/5})],\ \mathrm{Im}[\mathrm{Li}_4(e^{4\pi i/5})],$$
$$\mathrm{Im}[\mathrm{Li}_4(i)],\ \mathrm{Im}[\mathrm{Li}_4(e^{2\pi i/3})]$$

Here $G = \sum_{n \geq 0}(-1)^n/(2n + 1)^2$ is the Catalan constant. Some constants that may appear to be "missing" from this list are actually linearly redundant with this set, and thus were not included in the PSLQ search. These include $\mathrm{Re}[\mathrm{Li}_3(i)]$, $\mathrm{Im}[\mathrm{Li}_3(i)]$, $\mathrm{Re}[\mathrm{Li}_3(e^{2\pi i/3})]$, $\mathrm{Im}[\mathrm{Li}_3(e^{2\pi i/3})]$, $\mathrm{Re}[\mathrm{Li}_4(i)]$, $\mathrm{Re}[\mathrm{Li}_4(e^{2\pi i/3})]$, $\mathrm{Re}[\mathrm{Li}_4(e^{2\pi i/5})]$, $\mathrm{Re}[\mathrm{Li}_4(e^{4\pi i/5})]$, $\mathrm{Re}[\mathrm{Li}_4(e^{2\pi i/6})]$ and $\mathrm{Im}[\mathrm{Li}_4(e^{2\pi i/6})]$.

We should note that computing numerical integrals sufficiently high precision to enable serious PSLQ relation searches, which typically require several hundred to several thousand digits, has only recently been achieved for a wide range of integrand functions, even for one-dimensional integrals [8, 9]. Thus our examples here of 3-dimensional and 4-dimensional quadrature, which require thousands of times as much computation as one-dimensional integrals, truly lie on the edge of currently available numerical techniques and computing technology. Indeed, we are not aware of any other instance of a successful three-dimension quadrature of a nontrivial function to an accuracy of 500 or more digits. In any case, our reductions to $(n-2)$ dimensions yield dramatic reductions in computational cost, compared to direct quadrature of the original n-dimensional integral, such as (1).

As we have noted, reasonably extensive—but far from conclusive—PSLQ experiments have failed to identify any evaluations of C_n, D_n, E_n for $n > 4$,

except for the experimental evaluation of E_5 mentioned above. The profusion of potential polylogarithmic constants of order 4 and higher, such as $\mathrm{Li}_4(1/2)$, is one of the problems. While the numerical values for D_6 and E_6 in Appendix 2 may not yet be precise enough for experimental-mathematical closed-form capture, the values of C_n and D_5 given in Appendix 1 likely are sufficiently accurate, if one could only surmise the right set of test constants.

13   The susceptibility amplitudes

It is interesting that, via *Painlevé* differential analysis B. Nickel [15], using the differential theory in [21], has resolved numerical values for two infinite sums relating to the susceptibility amplitudes mentioned in the introduction, namely, recalling $I_n := \pi D_n/(2\pi)^n$,

$$\sum_{n=1,3,5,\dots} I_n = 1.000815260440212647119476363047210236 9375\dots \qquad (38)$$

and

$$\sum_{n=2,4,6,\dots} I_n = 0.0265512973592523253210722731298625636 2526\dots. \qquad (39)$$

Our qMC values from Table 2, optionally augmented by the above higher precision D_5, E_5, D_6, E_6 values, are entirely consistent with these Nickel numbers, in that we get about 20-decimal-place agreement when adding up D_n terms directly. Indeed, it would be wonderful to capture closed forms for these infinite sums.

In the same vein, for comparison we have considered $H_n := \pi C_n/(2\pi)^n$. In this case we may use (9) to write

$$\sum_{n=1,3,5,\dots} H_n \; = \; \pi \int_0^\infty p\,\sinh(K_0(p)/\pi)\;dp \qquad (40)$$

$$= \; 1.01011422864199451701704796866927057660215362408\dots$$

and

$$\sum_{n=2,4,6,\dots} H_n \; = \; \pi \int_0^\infty p\,(\cosh(K_0(p)/\pi) - 1)\;dp \qquad (41)$$

$$= \; 0.81024856380868082565191010347800614283172529480320\dots$$

with the values in Table 1 allowing one to confirm these values to about five places. The use of numerical values from (9) and/or estimates from (22) would allow further confirmation.

One might well ask: If the Painlevé analysis leads to high-precision values for the above sums, why does one need a closed form for say D_5 or its relatives? One answer, as posited by J-M. Maillard, is that new Ising theoretical avenues involving Fuchsian ODEs might require precise knowledge of these higher D_n, starting with $n = 5$ [14].

14 Open problems

- We have in a sense solved what had been an open computational problem, which is to provide a workable quadrature approach for some higher susceptibility integrals $D_{(n>4)}$. But (referring to Appendix 2) what is a closed form for D_5, and how far do we need to take D_6, E_6 quadrature to perform successful detection? (E_6 may well be easier that D_5, D_6 based on our success with E_5.)

- Can the the two-dimensional integral (28) for C_5 be symbolically resolved? The constants obtained would most likely shed light on those involved in D_5.

- Is there a way to calculate the hypergeometric D_n-kernel (35) efficiently, say by adroit grouping of the confluent summands?

- Can the methods of the exponential-decay Theorem 3 be extended to find the universal decay constant Δ in Conjecture 2?

Appendix 1. Numerical values for C_n

Some 500-digit calculated values of C_n are as follows, obtained via the Bessel-kernel method (i.e., quadrature on formula (9), as in Section 9). Note that C_3, C_4 are known in closed form, as in Table 1.

C_3:

```
0.78130241289648629686718742962409235636513433654528542022210006296688698465161
82180928695708322098610210423502565090357688658705524403079992607844199895749
30756967213098085932160953364386339574767285839770325515898564777091242889924100
249818885371308788489523887682281593269542022747136358189370747905938376851614
62178991779208603613530239422760382506422626830545731011203552572648910458111
49527253980249667997964454799602663333658422275946005535371765622825623963016
9896793875768209458304
```

C_4:

```
0.7.011998601764299998165139275483458279462420038652910143788250739494056200420
15969275432592938778900585282842047235419660786997665892748541369564821704608
42751479937338712670558619508572130812164231091228063739358650947253889655021
324661906964500056599300900498070564285656606639594353880299078826360564499250
```

250870873041513555541412129934724348326081023294168461319146078445158603840665
084683055462842935104448102000145675906901520606312335807041636897619159644520
4652919110034651864637 50

C_5:

0.665759800199937428315733808307066598197496382079497659539442703531227043 7672
123478677190150803692930858439949243118560403492593300507536805638668747409055
607471404754882341066312938102997876653928987866647777851800194632991842202782
881930971967588244497326327120253320328103353361480393173992677581082957282289
987428199147001511367793049306753355670504636033628816986290031029311864222938
745624200206539386546929990227698204769881089755395376987248969753929624465607
964265964375050 74037855

C_6:

0.648634209031007075263149843450351690889772509481627995615050887184781781 7880
055792368251624350867887463057785602639802770153606228510777288132190464518642
302249158778483830174783217968153522057328386481386398255864693634234127677654
715476907789871401844503982271880785106722328596251260428231725242036155739839
855032766143883409792517723339172060440519563661300113143929003292790581887272
231047465849738073291087102833123639827238382208616555735577378415362320125128
57683488361001 999048111

C_8:

0.635484026759163226139684899936898393485446063736278309835724508002389169 0329
370273397566840640435235412445863041497295480683521480881673604135213106589949
509550400483852455903797822155130617495416682684784946714237427133251149418721
486065815539916962821415815733807796383198779187152804352512401360865903524067
274041121457033579533593762862388990615273407222566160112092016558205944022503
563800033727339733873276161874833986524785410240352426906097139269551866969548
054684897181037 70282950

C_16:

0.630503946173237263505295657560687419484316217208103047750879119737058711 3428
518776591927635011910666019821885772282625005863790302590212510471642111230055
846525034440766011716943063675091961344295295167762531039303033076338954225849
425176347989010624576159605228245752442523276560004610937432747935264686038248
528719167665214134983765365722519250395916835193811814313121457043515985621220
385335330522425818627568844202427436280607422676722152074638421633970966585698
338058642562858657 88069

C_32:

0.630473504207339806379189843197962510193081141118420178126828333519119779 2172
680052468980756563089169460868733933972620014105552124844464239636721146902818
175987798891827352305809004725922423284700044572641202869901551465064480643904
699788294367863650303756804752685806270481005305890012892529506202937208989842

97836797755839036805489809610349580676450908789472965991228901183202092008278
87406124694849389245932117778177403146723333068650325125909672275939538179275
12282127651621637283187308

C_64:

0.630473503374386796488362088165338625359988808600159169054746716997441328971
54884050888776670638013971973130286525829423166980188271504960922428136760548
13825896829428890200757474414834491919486830723130043582819515980123032348189
04015476905081982491781473477053899423295429758958541155473364936794642857668
87686730631584905481746584288981131703304158096488766771370178615321623342497
47232867090089874823932376334503191432600881162531433337874835400175572553022
1758518690730950772643090414

C_128:

0.630473503374386796122040192710878904393135639979012750412245536553653956121
99745963568405730892166096335045732333272064904008554179739117491488914922380
48110357261778621257307041695580947450808464566684183319055237096966724588862
09964538837590295720117169632429702138426059061323858481321440983541931533314
95702583393518081622908409825299531147659677097465731463175740794225357349429
32683252667726334444652688176921571410757119316024362324215026414600624339353
2596169814986166310642230045

C_256:

0.630473503374386796122040192710878904354587078712732341573817983708970003830
18132633220670569732505003156116078064125733976805180527123982291926485330139
02317816300226839886370730710220773908440994719390995730717338559773855708533
26794060393912060962938279200444746633890279607770845068818243593284360885869
89583087705081607706525967622639501571557249483749667003287329366389623386840
08584950094211059621803322458407345794846673067719636541666816173680885756937
2870696032385323505649883915

C_512:

0.630473503374386796122040192710878904354587078712732341573817983708970003829
95819110189954165781719099450136225650411661308404743188411243430397157807755
85089603235132616205196210238564188359446248757017396988479875856101106619790
75138750251792562100557640869824062649551788317881009825941597948346588141535
42400119458049669018990845728292342952924883567082996313016413961349382235124
95974460405874210134977109407433351684494246332857884173161253528568665810160
192883983234576412903981345

C_1024:

0.630473503374386796122040192710878904354587078712732341573817983708970003829
95819110189954165781719099450136225650411661308404743188411243430397157807755
46845400730961720508654433686665598180980358272744760386111258149048208141490
91790648796301483682260404530555672606139009414570030164542749891640788518827
35623

14645512583127319234933825869992711015296606693152669923037568020986453295018902893350120088207565493545058798221213433349376075739795188427691651570635222481857844009406944470212

Appendix 2. Numerical values for D_n, E_n

The values for D_n, E_n below all started with the respective, dimensionally reduced integrands as described in Section 12. Each integral in this Appendix is thus $(n-2)$-dimensional. As intimated in the main text, we expended less effort on D_6, E_6; their values below were obtained via direct application of the `NIntegrate[]` function in *Mathematica*, with a chosen working precision. Even so, D_6, E_6 each required more than one CPU day on a 1.5 GHz. G5 workstation. This is testimony to the rapidly growing complexity of the integrand with n.

As for D_5, E_5, these were done by converting the relevant integrands to valid Fortran-90 code, by means of a combination of the *Mathematica* `FortranForm` function, together with some offline processing to divide the full expression into "chunks" that could be handled by the IBM XLFortran compiler. We then prepared a special three-dimensional, high-precision Gaussian integration program, implemented using the Message Passing Interface (MPI) parallel programming constructs. The resulting programs was then run on the "Bassi" system at the Lawrence Berkeley National Laboratory, which is a large cluster of IBM Power5 nodes.

Computing E_5 to 240 digits in this manner required 96 minutes on 64 CPUs. In regard to D_5, we were not able to recognize this constant based on a 240-digit value, so we extended the computation to 500 digits (although we were still unsuccessful in recognizing it). The 500-digit run was significantly more expensive, requiring 18.2 hours run time on 256 CPUs.

$D_5 =$

0.0024846057623403154799505091539097496350606776424875161587076921618221378569154357537926899487245120187068721106392520511862069944997542265656264670853828412450011668223000454570326876973848961519824796130355252585151071543863811369617492242985578076280428947770278710921198111606340631254136038598401982807864018693072681098854823037887884875830583512578552364199694869146314091127363094605240934008871628387064364218612045090299733566341137276122024088345463150171135408441978409224566685...

$D_6 =$

0.000489141700188034...

$E_5 =$

0.00349365371172952174068806727918425156963294495514131468369898233699924152717266576695087067520893264332903998566861235384768599443866815487779823641439966119140137365416727476965866845233975094131294703225222116183255112718650890146021418...

$E_6 =$

`0.0006878328718264094437004784...`

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