Integrals of the Ising class

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Abstract: From an experimental-mathematical perspective we analyze "Ising-class" integrals. These are structurally related n-dimensional integrals we call C_n, D_n, E_n, where D_n is a magnetic susceptibility integral central to the Ising theory of solid-state physics. We first analyze

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

We had 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 then show that integrals D_n and E_n both decay exponentially with n, in a certain rigorous sense. While C_n, D_n remain unresolved for $n \geq 5$, we were able to conjecture a closed form for E_5. Our experimental results involved extreme-precision, multidimensional quadrature on intricate integrands; thus, highly parallel computation was required.

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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 including works on field-theoretic and form-factor approaches [20, 21, 25, 27, 28, 29, 26, 4]. Very briefly, the importance of D_n in Ising physics runs as follows [23]. 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 [25], 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 [23] and emphasized by J-M. Maillard [17] 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 [10]. 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 our initial motive for defining the entities

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

(not to be confused with the $\mathcal{C}$ amplitudes of Ising theory), and later $C_{n,k}$ as discussed in Part II of this paper.

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 [12, pg. 312–313] and [9, 8, 7]. 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.

Even though our introduction of the C_n, E_n integrals is thus "symbolically motivated," it turns out in retrospect that the C_n do have relevance in Ising physics. Namely, these integrals appear naturally in the analysis of bounds on certain amplitude transforms [23], [21, Lemma 5.1, and p. 384].

We have found the following symbolic machinations particularly useful. For either integral (1) or (2), consider the simplex with constraint $u_1 > u_2 > \cdots > u_n$. 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

[1] By "extreme precision" we mean, loosely, "precision sufficient for reasonable confidence in experimental detection," which in our experience means 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

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

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. The constants $I_3 = D_3/(8\pi^2) \approx 0.00081446$ and $I_4 = D_4/(16\pi^3) \approx 0.000025448$ were resolved in closed form c. 1977 [22][25], while D_5, though still algebraically elusive, was resolved to 30 decimal places by B. Nickel in 1999 [18]—these respective symbolic and numerical achievements being remarkable for their eras. Though I_3 is sometimes known in the literature as the *ferromagnetic constant*, it looms appropriate to honor the pioneering work of [25], by referring to the collections (I_n) and $(I_1, \ldots, I_4)$ as the *McCoy–Tracy–Wu (MTW) integrals and constants*, respectively. Indeed, our Section 9 provides a synopsis of their historical analysis, while Section 14 and Appendix 2 contain our recent extreme-precision rendition of $D_5 = 32\pi^4 I_5$ and also $D_6 = 64\pi^5 I_6$.

In the construction of Table 1, we have invoked a *Dirichlet L-function* that occurs frequently in mathematical physics (see [11, §2.6], [12, Chapter

3]) namely[2]

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

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, which is 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 14). 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 some D_n, E_n, to extreme precision (see Section 14 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

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

[2]Note that some literature treatments (e.g. [22]) use the Clausen function [16] which is algebraically related to the stated L-function.

[3]It is a both a convenience and a pleasure to invoke thus the "curly-$\mathcal{D}$" 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.

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	$=7\zeta(3)/12$	$=4\pi^2/9-1/6-7\zeta(3)/2$	$=22-82\zeta(3)-24\log 2$ $+176\log^2 2-256(\log^3 2)/3$ $+16\pi^2\log 2-22\pi^2/3$
5	$0.6657598001\ldots$	$0.0024846057\ldots$	$\stackrel{?}{=} 42-1984\,\mathrm{Li}_4(1/2)+189\pi^4/10$ $-74\zeta(3)-1272\zeta(3)\log 2$ $+40\pi^2\log^2 2-62\pi^2/3$ $+40(\pi^2\log 2)/3+88\log^4 2$ $+464\log^2 2-40\log 2$
6	$0.6486342090\ldots$	$0.0004891417\ldots$	$0.00068783287\ldots$
$\ldots$			
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: The symbols '$=$' and '$\stackrel{?}{=}$' connote, respectively, 'proven' and 'detected experimentally.' The asymptote $C_\infty = 2e^{-2\gamma}$ is also proven.

which leads to an attractive, 1-dimensional integral

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

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

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

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

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

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

where γ denotes the *Euler constant* and the $H_k := \sum_{m\le k} 1/m$ 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

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

valid for real $x > 0$ and $\mathrm{Re}(\nu) > -1/2$ [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 $|f/g| \le 1$, 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 $\nu \ge 0$ and real $x > 0$, with pivot point p_0, we have*

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

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

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

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

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 11 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

$$C_\infty \quad = \quad 0.630473503374386796122040192710878904354587078712732 34\ldots$$

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:

```
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* $(C_n : n = 1, 2, 3, \ldots)$ *is strictly decreasing. Moreover, we have the finite limit*

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

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

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

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

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

We may therefore express a difference

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

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

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

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: 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* $(C_n : n = 1, 2, 3 \ldots)$ *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

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

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

$$C_n \quad = \quad \frac{2^n}{n!}\left(\int_0^{p_0} + \int_{p_0}^\infty\right) pK_0^n(p)\,dp$$

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

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

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

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

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

$$C_n \quad \sim \quad 2\,e^{-2\gamma} + \frac{n+4}{2^n}e^{-4\gamma} + \frac{2n^2+23n+57}{3^n\cdot 6}e^{-6\gamma} + \ldots \tag{22}$$

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

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

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 $x_1, \ldots$):

$$P := 1 + x_1 + \cdots + x_{n-2}, \tag{25}$$

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

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

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

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

For $n = 4$ we had conjectured, on the basis of numerical values, such as those in Appendix 1, and PSLQ integer relation finding facilities [11], 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

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

by transforming $x \to 1/x$. Here $\mathrm{Li}_2\left(x\right) := \sum x^n/n^2$, is the *dilogarithm*, [11], analytically continued. Now, integrating by parts leads to

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

where each integral is an integral multiple of $\zeta(3)$, as can be obtained from the analysis of the *trilogarithm* $\mathrm{Li}_3\left(x\right) := \sum x^n/n^3$, in [16, §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

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

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

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

where the last equality follows from [16, 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 $C_4 = -(56/3)\,\mathrm{Re}\,\mathrm{Li}_3((-1)^{1/2})/3$.

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 fourth powers of the Bessel terms [3]. Thus C_4 can be derived via the Adamchik method, but evidently C_5 cannot.

To summarize so far: 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

$$\mathcal{A}_3\mathcal{B}_3 = \frac{(t_2-1)^2(t_2t_3-1)^2(t_3-1)^2}{(t_2+1)^2(t_2t_3+1)^2(t_3+1)^2(t_2+t_2t_3+1)(t_2t_3+t_3+1)}$$

Hence, $D_1 = 2$ while

$$\begin{aligned} D_2 &= 2\int_0^1 \frac{(x-1)^2}{(x+1)^4}\,dx = \frac{1}{3} \\ D_3 &= \frac{1}{3}\int_0^1\int_0^1 \mathcal{A}_3\mathcal{B}_3(x,y)\,dx\,dy \\ &= \frac{2}{3}\int_0^1\int_0^x \mathcal{A}_3\mathcal{B}_3(x,y)\,dx\,dy, \end{aligned}$$

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 our Section 9), 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.

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

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

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

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

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

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

[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));
```

Notice the direct involvement of the C_2 value as a 1st-order perturbation 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) [19]:

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

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 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 13).

For convenience in the theorem to follow, we define

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

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 $n > 1$,

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

Observe also that the reduced D_n integrand is the same R-product multiplied by the extra factor $\mathcal{B}_n(x_1, \ldots, x_m) := (1 + x_1 S)^{-1}(T + Ux_1)^{-1}$, where

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

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 $\{A, B\} = \{12, 4\}$.

Remark: 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.

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

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

This establishes strict monotonicity for the sequence (E_n); below we shall tighten this approach to yield a tighter 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

$$R(x_1)R(x_1x_2)\cdots R(x_1\cdots x_m) \quad \leq \quad e^{-2x_1S},$$

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

$$\int_0^1 \frac{e^{-2x_1S}}{(1+x_1S)(T+Ux_1)}\, dx_1 \quad < \quad \frac{0.37}{ST},$$

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 $D_n < 0.37D_{n-1}$.

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 $R(x_i)\,R(x_ix_j)\,R(x_j)$, 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

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

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 $[0,\alpha]^m$. So, 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

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

where $\theta_4(q) := \sum_{n\in Z}(-q)^{n^2}$ is a *Jacobi theta function*, see [12]. 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**

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*

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

so that ratios behave as

$$\begin{aligned} \lim_{n\to\infty}\frac{D_n}{D_{n+1}} &= \lim_{n\to\infty}\frac{E_n}{E_{n+1}} = \Delta, \\ \text{and} \;\; \lim_{n\to\infty}\frac{D_n}{E_n} &= \delta/\phi. \end{aligned}$$

Remark 1 If this conjecture is true, we expect, based on the quasi-Monte Carlo (qMC) integrations of Section 13, 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:

$$\mathcal{A}_n(t_2,\ldots,t_n) \quad = \quad \left(\frac{1-t_2}{1+t_2}\right)^2 \left(\frac{1-t_2t_3}{1+t_2t_3}\right)^2 \cdots \left(\frac{1-t_2\cdots t_n}{1+t_2\cdots t_n}\right)^2 \, \mathcal{A}_{n-1}(t_3,\ldots,t_n).$$

Observe also that we may write

$$B_n(t_2,\ldots,t_n) \quad = \quad \frac{b^{-1}}{(1+t_2(1+t_3+t_3t_4+\cdots+t_3\cdots t_n))\cdot(1+(a/b)\,t_2)}$$

with

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

Next, we observe a key formal identity

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

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

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

Putting all this together yields

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

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

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. Moreover, 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

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

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 14, 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 (as in Table 1) but for higher dimensions this procedure becomes problematic and has not yet been rigorously pursued. The experimentally-detected form for E_5, described in Section 14, appears not to have obvious higher-order analogues and perhaps represents the end of a polylogarithmic ladder.

9 Historical resolution of the MTW constants

In Section 2 we describe the MTW constants as the currently known closed-form cases I_1-through-I_4 (in our present normalization, D_1-through-D_4). It is remarkable that McCoy, Tracy, and Wu were able to resolve these constants in closed form some 30 years ago; moreover, it is likewise remarkable that no further closed forms for the D_n have evolved in all that time.

We now summarize the historical MTW methods, based on some handwritten notes kindly provided to us for the purpose of finally casting those monumental results in a modern symbolic light [24]. The overall technique relies on three clever transforms; we believe it optimally instructive to describe these transforms first for the more tractable integrals C_n, then indicate how the previous researchers handled the D_n. Starting with (2) we write

$$C_n \quad := \quad \frac{4}{n!}\int_{[0,\infty)^n} \frac{\mathcal{D}\vec{u}}{\prod u_k} \int_0^\infty p e^{-p(\sum u_i + \sum 1/u_i)}\, dp. \tag{33}$$

1st MTW transformation: $u_k \to v_k/p$. This leads to the representation

$$C_n \quad := \quad \frac{2}{n!}\int_{[0,\infty)^n} \frac{\mathcal{D}\vec{v}}{\prod v_k} \frac{e^{-\sum v_k}}{\sum \frac{1}{v_k}}. \tag{34}$$

2nd MTW transformation: $v_k \to \alpha_k \sum v_j$. This yields a finite domain of integration :

$$C_n \quad := \quad \frac{2}{n!} \int_{[0,1)^n} \frac{\mathcal{D}\vec{\alpha}}{\prod \alpha_k} \frac{\delta(1 - \sum \alpha_k)}{\sum \frac{1}{\alpha_k}}, \tag{35}$$

where δ is the *Dirac delta-function*.

3rd MTW transformation: Now the key is to find a coordinate system of $(n-1)$ dimensions such that the α_k sum to unity automatically. For example, take $n = 3$ and write (here and beyond, we employ bar-notation, $\bar{x} := 1 - x$ for any variable x):

$$\begin{aligned} \alpha_1 &= x, \\ \alpha_2 &= \bar{x} y, \\ \alpha_3 &= \bar{x} \bar{y}. \end{aligned}$$

The beauty of such a transformation is that the three right-hand sides add up to 1, being as $\bar{z} + z = 1$ always. For $n = 4$ one may take

$$\begin{aligned} \alpha_1 &= xy, \\ \alpha_2 &= x\bar{y}, \\ \alpha_3 &= \bar{x} z. \\ \alpha_4 &= \bar{x} \bar{z}. \end{aligned}$$

These two transforms are what McCoy, Tracy, and Wu actually employed to resolve D_3, D_4, as we shall soon see. Generalization of these $n = 3, 4$ cases is ambiguous, but an example of a universal simplectic scheme having the property $\sum \alpha_k = 1$ is

$$\begin{aligned} \alpha_1 &= x_1, \\ \alpha_2 &= \bar{x}_1 x_2, \\ \alpha_3 &= \bar{x}_1 \bar{x}_2 x_3. \\ &\cdots \\ \alpha_{n-1} &= \bar{x}_1 \bar{x}_2 \cdots \bar{x}_{n-1} x_n, \\ \alpha_n &= \bar{x}_1 \bar{x}_2 \cdots \bar{x}_{n-1} \bar{x}_n, \end{aligned}$$

so that the α_k is a product of k terms, except the last, α_n, is to have $(n-1)$ terms. It is easy to see by adding from the bottom that the sum of the α_k here is unity. Note two things: First, that the historical MTW for $n = 4$ above is *not* this generalization, so that there are other ways to proceed for general n; and second, when doing the above integral with the Dirac delta-function, the rules are a) drop the δ term altogether, and b) introduce the Jacobian from the matrix of $(n-1)^2$ derivatives $(\partial \alpha_k / \partial x_j : j, k \in [1, n-1])$.

Now, a striking feature of the triple-MTW transformation scheme is that *the Ising permutation products are invariant under the MTW transformations.* That is to say, when confronting an Ising susceptibility integral D_n, we may casually insert any permutation product such as

$$\prod_{j<k}\left(\frac{\alpha_j-\alpha_k}{\alpha_j+\alpha_k}\right)^2$$

into (35) and continue on with the 3rd transformation.

Let us work some small-n examples, then. For $n = 2$ we have, from the casual-insertion rule into (35),

$$D_2 \quad = \quad \frac{2}{2!}\int_{[0,1]^2}\frac{d\alpha_1\ d\alpha_2}{\alpha_1+\alpha_2}\ \delta(1-\alpha_1-\alpha_2)\left(\frac{\alpha_1-\alpha_2}{\alpha_1+\alpha_2}\right)^2.$$

In this case we do not even need a 3rd transformation, just the constraint $\alpha_1 + \alpha_2 = 1$, to obtain

$$D_2 \quad = \quad \int_0^1 d\alpha_2(1-2\alpha_2)^2 \ = \ 1/3,$$

consistent with Table 1.

As for C_3, we use (35) with the above simplectic transform for $n = 3$ to get

$$\begin{aligned}
C_3 \quad &= \quad \frac{2}{3!}\int_{[0,1]^3}\frac{d\alpha_1\ d\alpha_2\ d\alpha_3}{\alpha_2\alpha_3+\alpha_1\alpha_3+\alpha_1\alpha_2}\ \delta(1-\alpha_1-\alpha_2-\alpha_3)\\
&= \quad \frac{1}{3}\int_{[0,1]^2}\frac{dx\ dy}{x(1-y+y^2)+y-y^2)}\\
&= \quad -\frac{1}{3}\int_0^1\frac{\log(y^2-y)\ dy}{y^2-y+1}\\
&= \quad \mathrm{L}_{-3}(2),
\end{aligned}$$

using at the end here the same kind of algebra as in Section 5 for C_3.

D_3, in turn, takes the form (recall the rule that the permutation product may simply be inserted, with impunity, into a C_n form to render a D_n):

$$D_3 \quad = \quad \frac{2}{3!}\int_{[0,1]^3}\frac{d\alpha_1\ d\alpha_2\ d\alpha_3\prod_{j<k}\left(\frac{\alpha_j-\alpha_k}{\alpha_j+\alpha_k}\right)^2}{\alpha_2\alpha_3+\alpha_1\alpha_3+\alpha_1\alpha_2}\ \delta(1-\alpha_1-\alpha_2-\alpha_3).$$

Under the same simplectic transformation as for C_3 above, we obtain

$$D_3 \quad = \quad \frac{1}{3}\int_{[0,1]^2}\frac{(1-2y)^2(x(y-2)-y+1)^2(yx+x-y)^2}{((y-1)yx^2+(-2y^2+2y-1)\,x+(y-1)y)^2}\frac{dx\ dy}{x(1-y+y^2)+y-y^2)}.$$

This integral, recondite as it may be, can indeed be resolved and the closed form is given for D_3 in Table 1. Explicitly, integrating the rational function in

Maple with respect to x under the 'assumption' that $x > 0, y > 0, x < 1, y < 1$ and then integrating with respect to y produces the evaluation in the form

$$6\,i\,\mathrm{Li}_2\left(\frac{1}{2} - \frac{1}{2}\,i\sqrt{3}\right)\sqrt{3} - 6\,i\,\mathrm{Li}_2\left(\frac{1}{2} + \frac{1}{2}\,i\,\sqrt{3}\right)\sqrt{3} + \frac{4}{3}\,\pi^2 + 8.$$

At this juncture it is important to point out a refinement due to McCoy, Tracy, Wu that actually simplifies the symbolic analysis for D_3, D_4. This is to observe a connection between permutation products in the deeper perturbation theory of the Ising model [21][25]. For example, in the D_3 case above, one may replace the permutation product $\prod$ of the integrand with

$$\prod \quad \to \quad 6\frac{\alpha_1 - \alpha_2}{\alpha_1 + \alpha_2}\frac{\alpha_2 - \alpha_3}{\alpha_2 + \alpha_3} + 3\left(\frac{\alpha_2 - \alpha_3}{\alpha_2 + \alpha_3}\right)^2.$$

We are not saying this permutation form on the right is algebraically equivalent; we are saying that the integral for D_3 is invariant under this modification. At any rate, the D_3 integral with this modified permutation form is somewhat easier to handle, giving, of course, the correct closed form in Table 1.

Along such lines, the culmination of the MTW historical effort is that D_4 may be written

$$D_4 \quad = \quad \frac{2}{4!}\int_{[0,1]^4} d\alpha_1\; d\alpha_2\; d\alpha_3\; d\alpha_4\; \frac{\delta(1 - \alpha_1 - \alpha_2 - \alpha_3 - \alpha_4)\prod}{\alpha_2\alpha_3\alpha_4 + \alpha_1\alpha_3\alpha_4 + \alpha_1\alpha_2\alpha_4 + \alpha_1\alpha_2\alpha_3},$$

where again the profound knowledge of the underlying perturbation theory allowed those pioneering researchers to use

$$\prod \quad \to \quad \left(\frac{\alpha_1 - \alpha_2}{\alpha_1 + \alpha_2}\frac{\alpha_3 - \alpha_4}{\alpha_3 + \alpha_4} + \frac{\alpha_1 - \alpha_4}{\alpha_1 + \alpha_4}\frac{\alpha_2 - \alpha_3}{\alpha_2 + \alpha_3} - \frac{\alpha_1 - \alpha_3}{\alpha_1 + \alpha_3}\frac{\alpha_2 - \alpha_4}{\alpha_2 + \alpha_4}\right)^2$$

in place of $\prod := \prod_{1\le j<k\le 4}(\alpha_j - \alpha_k)^2/(\alpha_j + \alpha_k)^2$ (although we presume that the latter transformation should go through, perhaps with more difficulty along the way). In this fashion the MTW constant D_4 in Table 1 was established, via the the 3rd MTW transformation above for $n = 4$, those decades ago.

10 Hypergeometric connections

It turns out that Ising-class integrals have a certain connection with hypergeometric functions and their powerful generalization, the *Meijer G-functions*. Such analysis gives rise to fascinating series representations, new closed forms, and rational relations between certain pairs of integrals. We sketch such ideas here, with details to be found in our separate work [5].

This idea is to generalize Ising integrals by modifying intrinsic powers within integrands. Define for integers $k \ge 0$

$$C_{n,k} \quad := \quad \frac{1}{n!}\int \frac{\mathcal{D}\vec{x}}{(\cosh x_1 + \cdots + \cosh x_n)^{k+1}}, \qquad (36)$$

whence, per (8), the original C_n integrals are $C_n := C_{n,1}$. Not surprisingly, the collection $(C_{n,k} : n, k \geq 0)$ provides yet more fertile ground for experimental-mathematical discovery, not to mention clues as to what symbolic behavior might be expected of Ising integrals in general. In addition, one can derive [5] some evidently new exact evaluations of Meijer G-functions themselves.

Now the Bessel-kernel representation (9) likewise generalizes to

$$C_{n,k} \quad := \quad \frac{2^n}{n!}\frac{1}{k!}\int_0^\infty t^k K_0^n(t)\; dt. \tag{37}$$

It is clear from the definition (36) that (i) for fixed n, $C_{n,k}$ is monotonic decreasing in k. The arguments behind Theorems 1 and 2 can be adapted to show first, that (ii) for fixed $k \geq 1$ the set $(C_{n,k})$ is monotonic decreasing in n, and that (iii) for any fixed k we have the large-n asymptote

$$C_{n,k} \quad \sim \quad \frac{1}{k!}\frac{2^{k+1+n}}{(k+1)^{n+1}}e^{-(k+1)\gamma},$$

for which our original, canonical case reads $C_n = C_{n,1} \sim 2e^{-2\gamma}$. This can be verified experimentally.

We next proceed to summarize some closed forms for various $C_{n,k}$, as proven in [5]. One has

$$C_{1,k} \quad = \quad \frac{2^k\,\Gamma\left(\frac{k+1}{2}\right)^2}{k!}.$$

from which it is immediate that

$$C_{1,k} \quad = \quad p_{1,k} + q_{1,k}\;\pi,$$

where the p, q coefficients are always rational, with q vanishing for odd k and p vanishing for even k. Similarly, for $n = 2$, from relation (37) and some manipulations relevant to Meijer G-functions we obtained (see [5])

$$C_{2,k} \quad = \quad \frac{\sqrt{\pi}\,\Gamma\left(\frac{k+1}{2}\right)^3}{2\Gamma\left(\frac{k}{2}+1\right)\Gamma(k+1)},$$

and so

$$C_{2,k} \quad = \quad p_{2,k} + q_{2,k}\;\pi^2,$$

with the same vanishing rule on the rational p, q multipliers as for $n = 1$.

The case $n \geq 3$ on $C_{n,k}$ are problematic. We discovered experimentally the conjectures

$$C_{3,3} \quad \stackrel{?}{=} \quad -\frac{4}{27} + \frac{2}{9}\mathrm{L}_{-3}(2),$$
$$C_{3,5} \quad \stackrel{?}{=} \quad -\frac{92}{1215} + \frac{8}{81}\mathrm{L}_{-3}(2),$$

and several more. We should mention that we found no rational relations whatever between pairs of $C_{3,\text{even}}$ (however, we did find 3-term recurrence relations, as discussed below). Once again on the basis of what to expect, were able to prove the suggested rational-relation conjecture in the form

Theorem 5 (See [5]) *For odd $k \geq 1$, we have*

$$C_{3,k} = p_{3,k} + q_{3,k}\mathrm{L}_{-3}(2),$$

with the p, q coefficients always being rational.

Moreover, a finite form for the rationals q_k can be written down. The method of proof also provides an algorithm for evaluating any $C_{3,\text{odd}}$ rather efficiently. One may arrive quickly at such instances as

$$\begin{aligned} C_{3,15} \quad &:= \quad \frac{1}{3!}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\frac{dx\ dy\ dz}{(\cosh x + \cosh y + \cosh z)^{16}} \\ &= \quad -\frac{11884272896}{837856594575} + \frac{4139008}{227988189}\mathrm{L}_{-3}(2). \end{aligned}$$

See [5] for details.

Continuing our summary, we conjectured pairwise rational relations also for the $C_{4,\text{odd}}$, and carried out an analysis in terms of Meijer G-functions, leading to (again, proof is in [5])

Theorem 6 (See [5]) *For odd $k \geq 1$, we have*

$$C_{4,k} = p_{4,k} + q_{4,k}\ \zeta(3),$$

with the p, q coefficients always being rational.

In these $C_{4,,\text{odd}}$ cases, polynomial-remaindering and rational-arithmetic algorithms [5] quickly yield instances such as

$$\begin{aligned} C_{4,15} \quad &:= \quad \frac{1}{4!}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\frac{dw\ dx\ dy\ dz}{(\cosh w + \cosh x + \cosh y + \cosh z)^{16}} \\ &= \quad -\frac{1744313209}{578605547520000} + \frac{67697}{26990346240}\zeta(3). \end{aligned}$$

One important aspect of this separate work is the following. Beyond the above rational relations, we were not able to find any other relations whatsoever between any pair of $C_{n,k}$, regardless of the parity of k, for $n \geq 4$. However, we did find experimentally m-term relations, where $m = \lfloor (n+3)/2 \rfloor$, involving $(C_{n,k},\, C_{n,k+2}, \cdots, C_{n,k+2m-2})$. Subsequently, and again because we knew on the basis of experiment what to expect, we were able to prove that these universal recurrences do hold for all parameter pairs (n, k) with $n = 1, 2, 3, 4$ and any complex k—these machinations amounting to an interesting application of Wilf–Zeilberger methods [5].

Part II. Various numerical algorithms

11 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 [9], [12, 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 [7], and is also amenable to computation of provable bounds on the error [8]. 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

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

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 [9]. 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 one processor of an Apple G5 computer. Selected high-precision results are exhibited in Appendix 1.

12 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

$$D_n \quad := \quad \frac{1}{n!} \int \frac{\mathcal{D}\vec{x}}{(\cosh x_1 + \cdots + \cosh x_n)^2} \prod_{i<j} \tanh^2 \left(\frac{x_i - x_j}{2} \right). \qquad (38)$$

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

$$D_n \quad = \quad \int_0^\infty d_n(p)\ dp, \qquad (39)$$

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

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

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

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

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

$$d_n(p) \quad := \quad \frac{2^n p e^{-np}}{n!} \sum_{m_k \geq 0,\ \mathrm{even}} A(m_1, \ldots, m_n) \prod_{k=1}^{n} \Gamma\left(\frac{m_k+1}{2}\right) U\left(\frac{m_k+1}{2}, 1, 2p\right). \tag{40}$$

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 (39), 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 (40) converges to an integrable function on $p \in (0, \infty)$, and therefore gives via (39) 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:

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

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

$$\Gamma(a)\, U(a, 1, z) \quad = \quad \sum_{k \geq 0} \frac{(a)_k z^k}{k!^2} (2\psi(k+1) - \psi(k+a) - \log z), \tag{41}$$

and

$$\Gamma(a)\, U(a, 1, z) \quad \sim \quad \sum_{m \geq 0} \frac{(a)_m (-1)^m \Gamma(m+a)}{m! z^{m+a}}. \tag{42}$$

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. Items flagged with * are actually known (or suspected) in closed form; many of the entries are known to much higher precision than is accessible via qMC.

13 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*, [13, 14]. 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, [15].)

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 smoothly?) based on general principles of Ising susceptibility expansions [17]. 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.

14 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,

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

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 on the next page the stultifying triple integral we used to compute E_5.

$$
\begin{aligned}
E_5 \quad = \quad & \int_0^1 \int_0^1 \int_0^1 \, [2(1-x)^2(1-y)^2(1-xy)^2(1-z)^2(1-yz)^2(1-xyz)^2 \\
& (-[4(x+1)(xy+1)\log(2)(y^5z^3x^7 - y^4z^2(4(y+1)z+3)x^6 - y^3z((y^2+1)z^2+4(y+ \\
& 1)z+5)x^5 + y^2(4y(y+1)z^3+3(y^2+1)z^2+4(y+1)z-1)x^4 + y(z(z^2+4z \\
& +5)y^2+4(z^2+1)y+5z+4)x^3+((-3z^2-4z+1)y^2-4zy+1)x^2-(y(5z+4) \\
& +4)x-1)] / [(x-1)^3(xy-1)^3(xyz-1)^3]+[3(y-1)^2y^4(z-1)^2z^2(yz \\
& -1)^2x^6+2y^3z(3(z-1)^2z^3y^5+z^2(5z^3+3z^2+3z+5)y^4+(z-1)^2z \\
& (5z^2+16z+5)y^3+(3z^5+3z^4-22z^3-22z^2+3z+3)y^2+3(-2z^4+z^3+2 \\
& z^2+z-2)y+3z^3+5z^2+5z+3)x^5+y^2(7(z-1)^2z^4y^6-2z^3(z^3+15z^2 \\
& +15z+1)y^5+2z^2(-21z^4+6z^3+14z^2+6z-21)y^4-2z(z^5-6z^4-27z^3 \\
& -27z^2-6z+1)y^3+(7z^6-30z^5+28z^4+54z^3+28z^2-30z+7)y^2-2(7z^5 \\
& +15z^4-6z^3-6z^2+15z+7)y+7z^4-2z^3-42z^2-2z+7)x^4-2y(z^3(z^3 \\
& -9z^2-9z+1)y^6+z^2(7z^4-14z^3-18z^2-14z+7)y^5+z(7z^5+14z^4+3 \\
& z^3+3z^2+14z+7)y^4+(z^6-14z^5+3z^4+84z^3+3z^2-14z+1)y^3-3(3z^5 \\
& +6z^4-z^3-z^2+6z+3)y^2-(9z^4+14z^3-14z^2+14z+9)y+z^3+7z^2+7z \\
& +1)x^3+(z^2(11z^4+6z^3-66z^2+6z+11)y^6+2z(5z^5+13z^4-2z^3-2z^2 \\
& +13z+5)y^5+(11z^6+26z^5+44z^4-66z^3+44z^2+26z+11)y^4+(6z^5-4 \\
& z^4-66z^3-66z^2-4z+6)y^3-2(33z^4+2z^3-22z^2+2z+33)y^2+(6z^3+26 \\
& z^2+26z+6)y+11z^2+10z+11)x^2-2(z^2(5z^3+3z^2+3z+5)y^5+z(22z^4 \\
& +5z^3-22z^2+5z+22)y^4+(5z^5+5z^4-26z^3-26z^2+5z+5)y^3+(3z^4- \\
& 22z^3-26z^2-22z+3)y^2+(3z^3+5z^2+5z+3)y+5z^2+22z+5)x+15z^2+2z \\
& +2y(z-1)^2(z+1)+2y^3(z-1)^2z(z+1)+y^4z^2(15z^2+2z+15)+y^2(15z^4 \\
& -2z^3-90z^2-2z+15)+15] / [(x-1)^2(y-1)^2(xy-1)^2(z-1)^2(yz-1)^2 \\
& (xyz-1)^2]-[4(x+1)(y+1)(yz+1)(-z^2y^4+4z(z+1)y^3+(z^2+1)y^2 \\
& -4(z+1)y+4x(y^2-1)(y^2z^2-1)+x^2(z^2y^4-4z(z+1)y^3-(z^2+1)y^2 \\
& +4(z+1)y+1)-1)\log(x+1)] / [(x-1)^3x(y-1)^3(yz-1)^3]-[4(y+1)(xy \\
& +1)(z+1)(x^2(z^2-4z-1)y^4+4x(x+1)(z^2-1)y^3-(x^2+1)(z^2-4z-1) \\
& y^2-4(x+1)(z^2-1)y+z^2-4z-1)\log(xy+1)] / [x(y-1)^3y(xy-1)^3(z- \\
& 1)^3]-[4(z+1)(yz+1)(x^3y^5z^7+x^2y^4(4x(y+1)+5)z^6-xy^3((y^2+ \\
& 1)x^2-4(y+1)x-3)z^5-y^2(4y(y+1)x^3+5(y^2+1)x^2+4(y+1)x+1)z^4+ \\
& y(y^2x^3-4y(y+1)x^2-3(y^2+1)x-4(y+1))z^3+(5x^2y^2+y^2+4x(y+1) \\
& y+1)z^2+((3x+4)y+4)z-1)\log(xyz+1)] / [xy(z-1)^3z(yz-1)^3(xyz-1 \\
&)^3])] / [(x+1)^2(y+1)^2(xy+1)^2(z+1)^2(yz+1)^2(xyz+1)^2] \; dx\,dy\,dz
\end{aligned}
$$

There is a similar, yet more complicated integrand for D_5. The corresponding expressions for D_6 and E_6 are several times more complicated still—the computer code defining the D_6 integrand extends for over 700 lines of 60 or more characters each, 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.

Based on the numerical value for E_5, we applied a PSLQ integer relation detection program to recognize this constant. We succeeded in finding the experimental result

$$\begin{aligned} E_5 &\stackrel{?}{=} 42 - 1984\,\mathrm{Li}_4(1/2) + \frac{189\pi^4}{10} - 74\zeta(3) - 1272\zeta(3)\log 2 + 40\pi^2\log^2 2 \\ &\quad -\frac{62\pi^2}{3} + \frac{40\pi^2\log 2}{3} + 88\log^4 2 + 464\log^2 2 - 40\log 2. \end{aligned}$$

As before, the notation $\stackrel{?}{=}$ is employed to emphasize that we do not yet have a formal proof for this evaluation. However, this experimental detection is quite strong—190 orders of magnitude beyond the level that could reasonably be ascribed to numerical round-off error or any other artifact.

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 an 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, π, $\log 2$, π^2, $\pi\log 2$, $\log^2 2$, $\mathrm{L}_{-3}(2)$, π^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 $\mathrm{Im}[\mathrm{Li}_4(e^{2\pi i/6})]$.

In a final set of computations, we computed D_6 to 105-digit accuracy, and E_6 to 250-digit accuracy, as shown in Appendix 2. Unfortunately, however, we have not been able to analytically evaluate either of these constants, either experimentally or formally.

Needless to say, these computations were very demanding, both of hardware and software. Just converting the huge expressions for the integrands into working Fortran-90 code proved surprisingly tricky. For these runs, since the integrands are well-behaved at boundaries, we were able to use multi-dimensional

Gaussian quadrature. We could have used tanh-sinh quadrature here, but the run times would have been somewhat longer. The computer runs themselves were performed on the Bassi system, an IBM Power5-based parallel computer system at Lawrence Berkeley Laboratory, and the Terascale Computing Facility, an Apple G5-based parallel computer system at the Virginia Institute of Technology. The computation of D_5 to 500 digits required 18 hours on 256 CPUs; the computation of E_6 to 250 digits required 28 hours on 256 CPUs.

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 [11, 12]. Thus our examples here of 3-dimensional and 4-dimensional high-precision quadrature, which require thousands of times as much computation as one-dimensional integrals, truly lie at the edge of presently available numerical techniques and computing technology. Indeed, we are not aware of any other instance of a successful three-dimensional quadrature of a nontrivial function to several-hundred-digit accuracy, much less a successful four-dimensional quadrature. 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. Perhaps further study will identify the correct terms to use in these evaluations, including perhaps multi-zeta values.

15 Sum rules for susceptibility amplitudes

It is interesting that, via *Painlevé* differential analysis B. Nickel [18], using the differential theory in [25], has resolved numerical values for two infinite sums relating to the susceptibility amplitudes mentioned in the introduction, namely, recalling $I_n := \pi D_n/(2\pi)^n$,

$$\sum_{n=1,3,5,\ldots} I_n = 1.000815260440212647119476363047210236937 5\ldots \tag{43}$$

and

$$\sum_{n=2,4,6,\ldots} I_n = 0.0265512973592523253210722731298625636252 6\ldots. \tag{44}$$

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

$$\sum_{n=1,3,5,\ldots} H_n = \pi \int_0^\infty p \sinh(K_0(p)/\pi)\ dp \tag{45}$$
$$= 1.0101142286419945170170479686692705766021536240 8\ldots$$

and

$$\sum_{n=2,4,6,\ldots} H_n = \pi \int_0^\infty p\,(\cosh(K_0(p)/\pi) - 1)\ dp \tag{46}$$
$$= 0.8102485638086808256519101034780061428317252948032 0\ldots$$

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 $n = 5$ [17].

16 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? A closed form for E_6 may well be more accessible than for D_5, D_6 based on our (conjectured) success with E_5.

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

- Is there a way to calculate the hypergeometric D_n-kernel (40) efficiently, say by adroit grouping of the confluent summands? This would go a long way toward extreme-precision results for the higher D_n.

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

- We discovered that there is a linear, rational relation $aC + bC' = c \neq 0$ between pairs $(C_{n,k}, C' := C_{n,k'})$ with a pair being any of

  $$(C_{1,2r}, C_{1,2r'}), (C_{1,2r+1}, C_{1,2r'+1}), (C_{2,2r}, C_{2,2r'}), (C_{2,2r+1}, C_{2,2r'+1})$$

or any of

$$(C_{3,2r+1}, C_{3,2r'+1}), (C_{4,2r+1}, C_{4,2r'+1}),$$

but could find no others whatsoever. What is a conceivable, abstract-algebraic explanation for the nonexistence of such relations for certain parameter pairs? (Reference [5] has some answers.)

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Appendix 1. Numerical values for C_n

Some 500-digit values of C_n are as follows, obtained via the Bessel-kernel method (i.e., quadrature on formula (9), as in Section 11). Note that C_3, C_4 are known in closed form, as shown in Table 1. Additional data is available online [6].

```
C_3:

0.7813024128964862968671874296240923563651343365452854202221000629668869846516
182180928695708322098610210423502565090357688658705524403079992607844199895749
307569672130980859321609533643863395747672858397703255158985647770912428899241
002498188853713087884895238876822815932695420227471363581893707479059383768516
146217899177920860361353023942276038250642262683054573101120355257264891045811
149527253980249667997964454799602663333658422275946005535371765622825623963016
98967938757682094583043

C_4:

0.7.01199860176429999816513927548345827946242003865291014378825073949405620042
015969275432592938778900585282842047235419660786997665892748541369564821704608
427514799373387126705586195085721308121642310912280637393586509472538896550213
246619069645000565993009004980705642856566060663959435388029907882636056449925
250870873041513555541412129934724348326081023294168461319146078445158603840665
084683055462842935104448102000145675906901520606312335807041636897619159644520
465291911003465186463750

C_5:

0.6657598001999374283157338083070665981974963820794976595394427035312270437672
123478677190150803692930858439949243118560403492593300507536805638668747409055
607471404754882341066312938102997876653928987866647777851800194632991842202782
881930971967588244497326327120253320328103353361480393173992677581082957282289
987428199147001511367793049306753355670504636033628816986290031029311864222938
745624200206539386546929990227698204769881089755395376987248969753929624465607
96426596437505074037855

C_6:

0.6486342090310070752631498434503516908897725094816279956150508871847817817880
055792368251624350867887463057785602639802770153606228510777288132190464518642
302249158778483830174783217968153522057328386481386398255864693634234127677654
715476907789871401844503982271880785106722328596251260428231725242036155739839
855032766143883409792517723339172060440519563661300113143929003292790581887272
231047465849738073291087102833123639827238382208616555735577378415362320125128
57683488361001999048111
```

```
C_8:

0.635484026759163226139684899936898393485446063736278309835724508002389169032937027339756684064043523541244586304149729548068352148088167360413521310658994950955040048385245590379782215513061749541668268478494671423742713325114941872148606581553991696282141581573380779638319877918715280435251240136086590352406727404112145703357953359376286238899061527340722256616011209201655820594402250356380003372733973387327616187483398652478541024035242690609713926955186696954805468489718103770282950

C_16:

0.630503946173237263505295657560687419484316217208103047750879119737058711342851877659192763501191066601982188577228262500586379030259021251047164211123005584652503444076601171694306367509196134429529516776253103930303307633895422584942517634798901062457615960522824575244252327656000461093743274793526468603824852871916766521413498376536572251925039591683519381181431312145704351598562122038533533052242581862756884420242743628060742267672215207463842163397096658569833805864256285865788069

C_64:

0.630473503374386796488362088165338625359988808600159169054746716997441328971548840508887766706380139719731302865258294231669801882715049609224281367605481382589682942889020075747441483449191948683072313004358281951598012303234818904015476905081982491781473477053899423295429758958541155473364936794642857668876867306315849054817465842889811317033041580964887667713701786153216233424974723286709008987482393237633450319143260088116253143333787483540017557255302217585186907309507726430904149

C_256:

0.630473503374386796122040192710878904354587078712732341573817983708970003830181326332206705697325050031561160780641257339768051805271239822919264853301390231781630022683988637073071022077390844099471939099573071733855977385570853326794060393912060962938279200444746633890279607770845068818243593284360885869895830877050816077065259676226395015715572494837496670032873293663896233868400858495009421105962180332245840734579484667306771963654166681617368088575693728706960323853235056498839156

C_1024:

0.630473503374386796122040192710878904354587078712732341573817983708970003829958191101899541657817190994501362256504116613084047431884112434303971578077554684540073096172050865443368665598180980358272744760386111258149048208141490917906487963014836822604045305556726061390094145700301645427498916407885188273562314645512583127319234933825869992711015296606693152669923037568020986453295018902893350120088207565493545058798221213433349376075739795188427691651570635222481857844009406944470212
```

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 14. Each integral in this Appendix is thus $(n-2)$-dimensional. These integrand expressions were then converted to valid Fortran-90 code, via the *Mathematica* `FortranForm[ ]` function, together with some offline processing to divide the full expression into "chunks" of modest enough size that they could be handled by the IBM XLFortran compiler. We then prepared special three-dimensional and four-dimensional, high-precision Gaussian integration programs, which invoked parallel execution using Message Passing Interface (MPI) parallel programming constructs. The resulting programs were then run on the "Bassi" system at the Lawrence Berkeley National Laboratory, which is a large cluster of IBM Power5 nodes, or the Terascale Computing Facility, which is a large cluster of Apple G5 nodes. The computation of D_5 to 500 digits required 18 hours on 256 CPUs; the computation of E_6 to 250 digits required 28 hours on 256 CPUs. As additional data becomes available, it will be made available online [6].

```
D_5:

0.0024846057623403154799505091539097496350606776424875161587076921618221378569
1543575379268994872451201870687211063925205118620699449975422656562646708538828
412450011668223000454570326876973848961519824796130355252585151071543863811369
617492242985578076280428947770278710921198111606340631254136038598401982807864
018693072681098854823037887884875830583512578552364199694869146314091127363094
605240934008871628387064364218612045090299733566341137276122024088345463150171
13540844197840922456685

E_5:

0.0034936537117295217406880672791842515696329449551413146836989823369992415271
726657669508706752089326433290399856686123538476859944386681548777982364143996
611914013736541672747696586684523397509413129470322522211618325511271865089014
6021418

D_6:

0.0004891417001880347751006623153504560332205526275305998837876046083224491394
73517501307771338022995604 44551

E_6:

0.0006878328718264094370047842736902107038148033103222727175338965396792103931
668620590718645325543697533105467758387352231831720375645991880602098222503718
205681784822803225117868730347366955186275157082427875765461445655735856457109
45124403316209068143651100514786250195 9090
```

References

[1] Milton Abramowitz and Irene A. Stegun, *Handbook of Mathematical Functions,* Dover, NY, 1970.

[2] V. Adamchik, "The evaluation of integrals of Bessel functions via G-function identities." *Journal of Computational and Applied Mathematics*, **64**, (1995), 283–290.

[3] V. Adamchik, private communication, Mar 2006.

[4] O. Babelon and D. Bernard, "From form-factors to correlation func- tions: The Ising model," *Phys. Lett.* B 288 (1992) 113 [arXiv:hep- th/9206003].

[5] David H. Bailey, David Borwein, Jonathan M. Borwein and Richard E. Crandall, "Hypergeometric forms for Ising-class integrals," *Experimental Mathematics*, to appear (2007). Also available at `http://crd.lbl.gov/~dhbailey/dhbpapers/meijer.pdf`.

[6] David H. Bailey, Jonathan M. Borwein and Richard E. Crandall, "Ising data," available at `http://crd.lbl.gov/~dhbailey/dhbpapers/ising-data.pdf`

[7] David H. Bailey and Jonathan M. Borwein, "Highly parallel, high-precision numerical integration," D-drive preprint #294, 2005. Also available at `http://crd.lbl.gov/~dhbailey/dhbpapers/quadparallel.pdf`.

[8] David H. Bailey and Jonathan M. Borwein, "Effective error bounds for Euler-Maclaurin-based quadrature schemes," D-drive preprint #297, 2005. Also available at `http://crd.lbl.gov/~dhbailey/dhbpapers/em-error.pdf`.

[9] David H. Bailey, Xiaoye S. Li and Karthik Jeyabalan, "A comparison of three high-precision quadrature schemes," *Experimental Mathematics,* **14** (2005), 317–329. Also available at `http://crd.lbl.gov/~dhbailey/dhbpapers/quadrature.pdf`.

[10] H. E. Boos and V. E. Korepin, "Quantum spin chains and Riemann zeta function with odd argument," preprint hep-th/0104008, 2001.

[11] Jonathan M. Borwein and David H. Bailey, *Mathematics by Experiment,* AK Peters, 2003.

[12] gathan M. Borwein, David H. Bailey and Roland Girgensohn, *Experimentation in Mathematics,* AK Peters, 2004.

[13] Richard E. Crandall, "Theory and applications of space-filling curves," manuscript, 2005.

[14] Richard Crandall and Carl Pomerance, *Prime numbers: A Computational Perspective*, 2nd Ed, Springer-Verlag, New York, 2005.

[15] Frances Y. Kuo and Ian H. Sloan, "Lifting the curse of dimensionality," *Notices of the AMS,* **52**, no. 11, (2005), 1320–1329.

[16] L. Lewin *Polylogarithms and Associated Functions,* North Holland, 1981.

[17] J-M. Maillard, Private communication, Jan 2005.

[18] B. Nickel, "On the singularity structure of the 2D Ising model susceptibility," *Journal of Physics A: Mathematical and General*, **32** (1999), 3889–3906.

[19] F. Oberhettinger, *Tables of Fourier Transforms and Fourier Transforms of Distributions*, Springer-Verlag, 1990.

[20] W. Orrick, B. Nickel, A. Guttmann, and J. Perk, "The susceptibility of the square lattice Ising model: New developments," manuscript, 3 Mar 2001.

[21] J. Palmer and C. Tracy, "Two-dimensional Ising correlations: Convergence of the scaling limit," *Advances in Applied Mathematics,* **2** (1981), 329-388.

[22] C. A. Tracy, "Painlevé transcendents and scaling functions of the two-dimensional Ising model," in *Nonlinear Equations in Physics and Mathematics*, ed. A. O. Barut, D. Reidel Publ. Co., Dordrecht, Holland, (1978), 378–380.

[23] C. Tracy, Private communication, Oct-Jan 2005.

[24] C. Tracy, unpublished notes, 1976.

[25] T. T. Wu, B. M. McCoy, C. A. Tracy and E. Barouch, "Spin-spin correlation functions for the two-dimensional Ising model: Exact theory in the scaling region," *Physical Review* **B13** (1976), 316-374.

[26] V. P. Yurov and A. B. Zamolodchikov, "Correlation Functions Of Integrable 2-D Models Of Relativistic Field Theory. Ising Model, *Int. J. Mod. Phys.* A 6 (1991) 3419.

[27] N. Zenine, S. Boukraa, S. Hassani and J-M Maillard, "Square lattice Ising susceptibility: Connection matrices and singular behaviour of $\chi^{(3)}$ and $\chi^{(4)}$," *Journal of Physics A: Mathematical and General* **38** (2005), 9439-9474.

[28] N. Zenine, S. Boukraa, S. Hassani and J-M Maillard, "Beyond series expansions: Mathematical structures for the susceptibility of the square lattice Ising model," *Journal of Physics Conference* (electronic review of *Journal of Physics*), June 2006.

[29] N. Zenine, S. Boukraa, S. Hassani and J-M Maillard, "Differential Galois groups of high order Fuchsian ODEs," preprint, 2005.