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Experimental Mathematics and Mathematical Physics

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Abstract

One of the most effective techniques of experimental mathematics is to compute mathematical entities such as integrals, series or limits to high precision, then attempt to recognize the resulting numerical values. Recently these techniques have been applied with great success to problems in mathematical physics. Notable among these applications are the identification of some key multi-dimensional integrals that arise in Ising theory, quantum field theory and in magnetic spin theory.

1   Introduction

One of the most effective techniques of experimental mathematics is to compute mathematical entities to high precision, then attempt to recognize the resulting numerical values. Techniques for efficiently performing basic arithmetic operations and transcendental functions to high precision have been known for several decades, and within the past few years these have been extended to definite integrals, sums of infinite series and limits of sequences. Recognition of the resulting numerical values is typically done by calculating a list of n possible terms on the right-hand side of an identity, also to high precision, then applying the PSLQ algorithm [19, 11] to see if there is a linear relation in this set of $n + 1$ values. If PSLQ does find a

credible relation, then by solving this relation for the value in question, one obtains a formula. These techniques have been described in detail in [14], [15], and [9].

In almost applications of this methodology, both in sophistication and in computation time, the most demanding step is the computation of the key value to sufficient precision to permit PSLQ detection. As we will show below, computation of some high-dimensional integrals, for instance, often requires several hours on a highly parallel computer system. In contrast, applying PSLQ to find a relation among, say, 20 candidate terms, each computed to 500-digit precision, usually can be done on a single-CPU system in less than a minute.

In our studies of definite integrals, we have used either Gaussian quadrature (in cases where the function is well behaved on a closed interval) or the "tanh-sinh" quadrature scheme due to Takahasi and Mori [24] (in cases where the function has an infinite derivative or blow-up singularity at one or both endpoints). For many integrand functions, these schemes exhibit "quadratic" or "exponential" convergence – dividing the integration interval in half (or, equivalently, doubling the number of evaluation points) approximately doubles the number of correct digits in the result.

The tanh-sinh scheme is based on the observation, rooted in the *Euler-Maclaurin summation* formula, that for certain bell-shaped integrands (namely those where the function and all higher derivatives rapidly approach zero at the endpoints of the interval), a simple block-function or trapezoidal approximation to the integral is remarkably accurate [3, pg. 180]. This principle is exploited in the tanh-sinh scheme by transforming the integral of a given function $f(x)$ on a finite interval such as $[-1, 1]$ to an integral on $(-\infty, \infty)$, by using the change of variable $x = g(t)$, where $g(t) = \tanh(\pi/2 \cdot \sinh t)$. The function $g(t)$ has the property that $g(x) \to 1$ as $x \to \infty$ and $g(x) \to -1$ as $x \to -\infty$, and also that $g'(x)$ and all higher derivatives rapidly approach zero for large positive and negative arguments. Thus one can write, for $h > 0$,

$$\int_{-1}^{1} f(x)\, \mathrm{d}x \;=\; \int_{-\infty}^{\infty} f(g(t)) g'(t)\, \mathrm{d}t \;\approx\; h \sum_{j=-N}^{N} w_j f(x_j), \tag{1}$$

where the abscissas $x_j = g(hj)$, the weights $w_j = g'(hj)$, and N is chosen large enough that terms beyond N (positive or negative) are smaller than the "epsilon" of the numeric precision being used. In many cases, even where $f(x)$ has an infinite derivative or an integrable singularity at one or both endpoints, the transformed integrand $f(g(t)) g'(t)$ is a smooth bell-shaped function for which the Euler-Maclaurin argument applies. In these cases, the error in this approximation (1) decreases more rapidly than any fixed power of h. Full details are given in [12].

Both Gaussian quadrature and the tanh-sinh scheme are appropriate for analytic functions on a finite interval. Functions on a semi-infinite intervals can be handled by a simple transformation such as:

$$\int_{0}^{\infty} f(t)\, \mathrm{d}t \;=\; \int_{0}^{1} f(t)\, \mathrm{d}t + \int_{0}^{1} \frac{f(1/t)\, \mathrm{d}t}{t^2} \tag{2}$$

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Oscillatory integrands such as $\int_0^\infty (1/x \sin x)^p \, \mathrm{d}x$ can be efficiently computed by applying a clever technique recently introduced by Ooura and Mori [22]. Let $x = g(t) = Mt/(1 - \exp(-2\pi \sinh t))$. Then in the case of $p = 2$, for instance,

$$
\begin{aligned}
\int_0^\infty \left(\frac{\sin x}{x} \right)^2 \mathrm{d}x &= \int_{-\infty}^\infty \left(\frac{\sin g(t)}{g(t)} \right)^2 \cdot g'(t) \, \mathrm{d}t \\
&\approx h \sum_{k=-N}^N \left(\frac{\sin g(hk)}{g(hk)} \right)^2 \cdot g'(hk)
\end{aligned}
\tag{3}
$$

Now note that if one chooses $M = \pi/h$, then for large k, the $g(hk)$ values are all very close to $k\pi$, so the $\sin(g(hk))$ values are all very close to zero. Thus the sum can be truncated after a modest number of terms, as in tanh-sinh quadrature. In practice, this scheme is very effective for oscillatory integrands such as this.

In the next four sections we consider Ising integrals, Bessel moment integrals, 'box' integrals, and hyperbolic volumes arising from quantum field theory respectively.

2 Ising integrals

In a recent study, Bailey, Borwein and Richard Crandall applied tanh-sinh quadrature, implemented using the ARPREC package, to study the following classes of integrals [8]. The D_n integrals arise in the Ising theory of mathematical physics, and the C_n have tight connections to quantum field theory.

$$
\begin{aligned}
C_n &= \frac{4}{n!} \int_0^\infty \cdots \int_0^\infty \frac{1}{\left(\sum_{j=1}^n (u_j + 1/u_j) \right)^2} \frac{\mathrm{d}u_1}{u_1} \cdots \frac{\mathrm{d}u_n}{u_n} \\
D_n &= \frac{4}{n!} \int_0^\infty \cdots \int_0^\infty \frac{\prod_{i<j} \left(\frac{u_i - u_j}{u_i + u_j} \right)^2}{\left(\sum_{j=1}^n (u_j + 1/u_j) \right)^2} \frac{\mathrm{d}u_1}{u_1} \cdots \frac{\mathrm{d}u_n}{u_n} \\
E_n &= 2 \int_0^1 \cdots \int_0^1 \left(\prod_{1 \le j < k \le n} \frac{u_k - u_j}{u_k + u_j} \right)^2 \mathrm{d}t_2 \, \mathrm{d}t_3 \cdots dt_n,
\end{aligned}
\tag{4}
$$

where (in the last line) $u_k = \prod_{i=1}^k t_i$.

Needless to say, evaluating these n-dimensional integrals to high precision presents a daunting computational challenge. Fortunately, in the first case, we were able to show that the C_n integrals can be written as one-dimensional integrals:

$$
C_n = \frac{2^n}{n!} \int_0^\infty p K_0^n(p) \, \mathrm{d}p,
\tag{5}
$$

where K_0 is the *modified Bessel function* [1]. After computing C_n to 1000-digit accuracy for various n, we were able to identify the first few instances of C_n in

terms of well-known constants, e.g.,

$$C_3 = \text{L}_{-3}(2) = \sum_{n \geq 0} \left(\frac{1}{(3n+1)^2} - \frac{1}{(3n+2)^2} \right)$$

$$C_4 = \frac{7}{12}\zeta(3), \tag{6}$$

where ζ denotes the Riemann zeta function. When we computed C_n for fairly large n, for instance

$$C_{1024} = 0.63047350337438679612204019271087890435458707871273234\ldots,$$

we found that these values rather quickly approached a limit. By using the new edition of the *Inverse Symbolic Calculator*, available at `http://ddrive.cs.dal.ca/~isc`, this numerical value can be identified as

$$\lim_{n \to \infty} C_n = 2e^{-2\gamma}, \tag{7}$$

where γ is Euler's constant. We later were able to prove this fact—this is merely the first term of an asymptotic expansion—and thus showed that the C_n integrals are fundamental in this context [8].

The integrals D_n and E_n are much more difficult to evaluate, since they are not reducible to one-dimensional integrals (as far as we can tell), but with certain symmetry transformations and symbolic integration we were able to reduce the dimension in each case by one or two. In the case of D_5 and E_5, the resulting 3-D integrals are extremely complicated, but we were nonetheless able to numerically evaluate these to at least 240-digit precision on a highly parallel computer system. In this way, we produced the following evaluations, all of which except the last we subsequently were able to prove:

$$
\begin{aligned}
D_2 &= 1/3 \\
D_3 &= 8 + 4\pi^2/3 - 27\,\text{L}_{-3}(2) \\
D_4 &= 4\pi^2/9 - 1/6 - 7\zeta(3)/2 \\
E_2 &= 6 - 8\log 2 \\
E_3 &= 10 - 2\pi^2 - 8\log 2 + 32\log^2 2 \\
E_4 &= 22 - 82\zeta(3) - 24\log 2 + 176\log^2 2 - 256(\log^3 2)/3 + 16\pi^2 \log 2 - 22\pi^2/3 \\
E_5 &\overset{?}{=} 42 - 1984\,\text{Li}_4(1/2) + 189\pi^4/10 - 74\zeta(3) - 1272\zeta(3)\log 2 + 40\pi^2 \log^2 2 \\
&\quad -62\pi^2/3 + 40(\pi^2 \log 2)/3 + 88\log^4 2 + 464\log^2 2 - 40\log 2, \tag{8}
\end{aligned}
$$

where Li denotes the polylogarithm function. In the case of D_2, D_3 and D_4, these are confirmations of known results. We tried but failed to recognize D_5 in terms of similar constants (the 500-digit numerical value is available if anyone wishes to try). The conjectured identity shown here for E_5 was confirmed to 240-digit accuracy, which is 180 digits beyond the level that could reasonably be ascribed to numerical

round-off error; thus we are quite confident in this result even though we do not have a formal proof.

In a follow-on study [6], we examined the following generalization of the C_n integrals:

$$C_{n,k} = \frac{4}{n!} \int_0^\infty \cdots \int_0^\infty \frac{1}{\left(\sum_{j=1}^n (u_j + 1/u_j)\right)^{k+1}} \frac{\mathrm{d}u_1}{u_1} \cdots \frac{\mathrm{d}u_n}{u_n}. \tag{9}$$

Here we made the initially surprising discovery—now proven in [17] and in outline much earlier [13]—that there are linear relations in each of the rows of this array (considered as a doubly-infinite rectangular matrix), e.g.,

$$
\begin{aligned}
0 &= C_{3,0} - 84C_{3,2} + 216C_{3,4} \\
0 &= 2C_{3,1} - 69C_{3,3} + 135C_{3,5} \\
0 &= C_{3,2} - 24C_{3,4} + 40C_{3,6} \\
0 &= 32C_{3,3} - 630C_{3,5} + 945C_{3,7} \\
0 &= 125C_{3,4} - 2172C_{3,6} + 3024C_{3,8}.
\end{aligned} \tag{10}
$$

3 Bessel moment integrals

In a more recent study of Bessel moment integrals, co-authored with Larry Glasser [7], the first three authors were able to analytically recognize many of the $C_{n,k}$ constants in the earlier study—because, remarkably, these same integrals appear naturally in quantum field theory (for odd k). We also discovered, and then proved with considerable effort, that with $c_{n,k}$ normalized by $C_{n,k} = 2^n c_{n,k}/(n!\,k!)$, we have

$$c_{3,0} = \frac{3\Gamma^6(1/3)}{32\pi 2^{2/3}} = \frac{\sqrt{3}\pi^3}{8} {}_3F_2\left(\begin{matrix} 1/2, 1/2, 1/2 \\ 1, 1 \end{matrix} \,\middle|\, \frac{1}{4} \right)$$

$$c_{3,2} = \frac{\sqrt{3}\pi^3}{288} {}_3F_2\left(\begin{matrix} 1/2, 1/2, 1/2 \\ 2, 2 \end{matrix} \,\middle|\, \frac{1}{4} \right)$$

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

$$
\begin{aligned}
c_{4,2} = \frac{\pi^4}{64} \Bigg[4\, {}_4F_3&\left(\begin{matrix} 1/2, 1/2, 1/2, 1/2 \\ 1, 1, 1 \end{matrix} \,\middle|\, 1 \right) \\
&- 3\, {}_4F_3\left(\begin{matrix} 1/2, 1/2, 1/2, 1/2 \\ 2, 1, 1 \end{matrix} \,\middle|\, 1 \right) \Bigg] - \frac{3\pi^2}{16},
\end{aligned} \tag{11}
$$

where ${}_pF_q$ denotes the *generalized hypergeometric* function [1]. The corresponding values for small odd second indices are $c_{3,1} = 3L_{-3}(2)/4$, $c_{3,3} = L_{-3}(2) - 2/3$, $c_{4,1} = 7\zeta(3)/8$ and $c_{4,3} = 7\zeta(3)/32 - 3/16$.
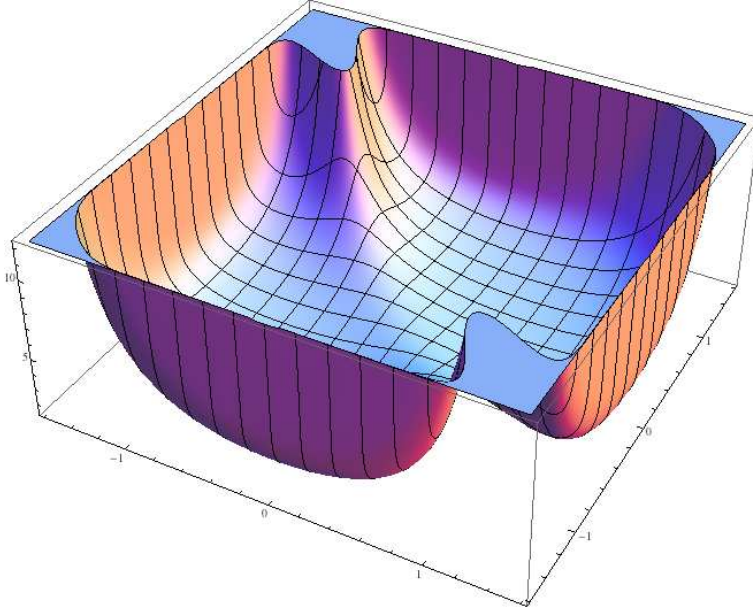
5

Figure 1: Plot of $c_{5,0}$ integrand function.

Integrals in the Bessel moment study were quite challenging to evaluate numerically. As one example, we sought to numerically verify the following identity that we had derived analytically:

$$c_{5,0} \;=\; \frac{\pi}{2} \int_{-\pi/2}^{\pi/2} \int_{-\pi/2}^{\pi/2} \frac{\mathbf{K}(\sin\theta)\,\mathbf{K}(\sin\phi)}{\sqrt{\cos^2\theta\cos^2\phi + 4\sin^2(\theta+\phi)}} \, \mathrm{d}\theta \, \mathrm{d}\phi \,, \tag{12}$$

where $\mathbf{K}$ denotes the elliptic integral of the first kind [1]. Note that this function has blow-up singularities on all four sides of the region of integration, with particularly troublesome singularities at $(\pi/2, -\pi/2)$ and $(-\pi/2, \pi/2)$ (see Figure 1). Nonetheless, after making some minor substitutions, we were able to evaluate (and confirm) this integral to 120-digit accuracy (using 240-digit working precision) in a run of 43 minutes on 1024 cores of the "Franklin" system at LBNL.

In a separate study, the first two authors studied correlation integrals for the Heisenberg spin-1/2 antiferromagnet, as given by Boos and Korepin, for a length-n spin chain [21, eqn. 2.2]:

$$
\begin{aligned}
P(n) \;:=\; & \frac{\pi^{n(n+1)/2}}{(2\pi i)^n} \cdot \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \cdots \int_{-\infty}^{\infty} U(x_1 - i/2, x_2 - i/2, \cdots, x_n - i/2) \\
& \times \, T(x_1 - i/2, x_2 - i/2, \cdots, x_n - i/2) \, \mathrm{d}x_1 \, \mathrm{d}x_2 \cdots \mathrm{d}x_n
\end{aligned}
\tag{13}
$$

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n	Digits	Processors	Run Time
2	120	1	10 sec.
3	120	8	55 min.
4	60	64	27 min.
5	30	256	39 min.
6	6	256	59 hrs.

Table 1: Run times and precision levels for spin integral calculations

where

$$U(x_1 - i/2, x_2 - i/2, \cdots, x_n - i/2) = \frac{\prod_{1 \le k < j \le n} \sinh[\pi(x_j - x_k)]}{\prod_{1 \le j \le n} i^n \cosh^n(\pi x_j)}$$

$$T(x_1 - i/2, x_2 - i/2, \cdots, x_n - i/2) = \frac{\prod_{1 \le j \le n}(x_j - i/2)^{j-1}(x_j + i/2)^{n-j}}{\prod_{1 \le k < j \le n}(x_j - x_k - i)}. \quad (14)$$

They computed numerical values for these n-fold integrals to as great a precision as we could, then attempted to recognize them using PSLQ. They found the following, which confirm some earlier results obtained by others using physical symmetry methods.

$$P(1) = \frac{1}{2}$$

$$P(2) = \frac{1}{3} - \frac{1}{3}\log 2$$

$$P(3) = \frac{1}{4} - \log 2 + \frac{3}{8}\zeta(3)$$

$$P(4) = \frac{1}{5} - 2\log 2 + \frac{173}{60}\zeta(3) - \frac{11}{6}\zeta(3)\log 2 - \frac{51}{80}\zeta^2(3) - \frac{55}{24}\zeta(5) + \frac{85}{24}\zeta(5)\log 2$$

$$P(5) = \frac{1}{6} - \frac{10}{3}\log 2 + \frac{281}{24}\zeta(3) - \frac{45}{2}\zeta(3)\log 2 - \frac{489}{16}\zeta^2(3) - \frac{6775}{192}\zeta(5)$$

$$+ \frac{1225}{6}\zeta(5)\log 2 - \frac{425}{64}\zeta(3)\zeta(5) - \frac{12125}{256}\zeta^2(5) + \frac{6223}{256}\zeta(7)$$

$$- \frac{11515}{64}\zeta(7)\log 2 + \frac{42777}{512}\zeta(3)\zeta(7) \quad (15)$$

These computations underscore the rapidly increasing cost of computing integrals in higher dimensions. Precision levels, processor counts and run times are shown in Table 1.

4   Box integrals

Let us define *box integrals* for dimension n as

$$B_n(s) \; := \; \int_0^1 \cdots \int_0^1 \left(r_1^2 + \cdots + r_n^2 \right)^{s/2} \, \mathrm{d}r_1 \cdots \mathrm{d}r_n \tag{16}$$

$$\Delta_n(s) \; := \; \int_0^1 \cdots \int_0^1 \left((r_1 - q_1)^2 + \cdots + (r_n - q_n)^2 \right)^{s/2} \, \mathrm{d}r_1 \cdots \mathrm{d}r_n \, \mathrm{d}q_1 \cdots \mathrm{d}q_n.$$

As explained in previous treatments [4, 5], these integrals have several physical interpretations:

1. $B_n(1)$ is the expected distance of a random point from the origin (or from any fixed vertex) of the n-cube.

2. $\Delta_n(1)$ is the expected distance *between* two random points of the n-cube.

3. $B_n(-n + 2)$ is the expected electrostatic potential in an n-cube whose origin has a unit charge. Such statements presume that electrostatic potential in n dimensions is $V(r) = 1/r^{n-2}$, and say $\log r$ for $n = 2$; in other words, the negative powers of r can also have physical meaning.

4. $\Delta_n(-n+2)$ is the expected electrostatic energy between two points in a uniform cube of charged "jellium."

5. Recently integrals of this type have arisen in neuroscience e.g., the average distance between synapses in a mouse brain.

Note that the definitions show immediately that both $\Delta_n(2m)$ and $B_n(2m)$ are rational when m, n are natural numbers. A pivotal, original treatment on box integrals is the 1976 work of Anderssen et al [2]. There have been interesting modern treatments of the B_n and related integrals, as in [10], [14, pg. 208], [27], and [25]. Related material may also be found in [20, 26].

Like the Ising integrals, some of these n-dimensional integrals are reducible to 1-dimension integrals. For instance, we found that

$$\Delta_3(-1) \;\; = \;\; \frac{2}{\sqrt{\pi}} \int_0^\infty \frac{\left(-1 + e^{-u^2} + \sqrt{\pi}\, u \operatorname{erf}(u) \right)^3}{u^6} \, \mathrm{d}u. \tag{17}$$

After calculating a 400-digit numerical value for this constant, we were able to recognize it as

$$\Delta_3(-1) = \frac{1}{15} \left(6 + 6\sqrt{2} - 12\sqrt{3} - 10\pi + 30 \log(1 + \sqrt{2}) + 30 \log(2 + \sqrt{3}) \right). \tag{18}$$

A selection of results that we have found are shown in Tables 2, 3, 4 and 5. Here G denotes Catalan's constant, namely, $G := \sum_{n \geq 0} 1/(2n + 1)^2$, $\theta = \arctan((16 - 3\sqrt{15})/11$, Cl denotes *Clausen's function*,

$$\operatorname{Cl}_2(\theta) = \sum_{n \geq 1} \frac{\sin(n\theta)}{n^2},$$

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and Ti denotes Lewin's *inverse-tan function*,

$$\mathrm{Ti}_2(x) = \sum_{n \geq 0} (-1)^n \frac{x^{2n+1}}{(2n+1)^2}.$$

5   Clausen functions and hyperbolic volumes

In an unpublished 1998 study [16] two of the present authors (Borwein and Broadhurst) identified 998 closed hyperbolic 3-manifolds whose volumes are rationally related to Dedekind zeta values, with coprime integers a and b giving

$$\frac{a}{b}\,\mathrm{vol}(\mathcal{M}) \;=\; \frac{(-D)^{3/2}}{(2\pi)^{2n-4}} \frac{\zeta_K(2)}{2\zeta(2)} \tag{19}$$

for a manifold $\mathcal{M}$ whose invariant trace field K has a single complex place, discriminant D, degree n, and Dedekind zeta value $\zeta_K(2)$. While the existence of integers a, b can be established, via algebraic K-theory as in [30], for the most part it was and is not possible to specify the rational a/b other than empirically [30].

The simplest identity implicit in (19) devolves to

$$3\,\mathrm{Cl}_2(\alpha) - 3\mathrm{Cl}_2(2\alpha) + \mathrm{Cl}_2(3\alpha) \;=\; \frac{7\sqrt{7}}{4}\,\mathrm{L}_{-7}(2), \tag{20}$$

with $\alpha = 2\arctan(\sqrt{7})$, as is recorded in [14, p. 91]. Here $L_{-7}(2) := \sum_{n>0} \left(\frac{n}{7}\right)/n^2$ is the primitive Dirichlet L-series modulo 7 evaluated at 2 where $\left(\frac{n}{7}\right)$ is the Legendre symbol. This was rewritten in equivalent and more self-contained form as

$$\frac{24}{7\sqrt{7}} \int_{\pi/3}^{\pi/2} \log\left|\frac{\tan t + \sqrt{7}}{\tan t - \sqrt{7}}\right| \, \mathrm{d}t \;=\; \mathrm{L}_{-7}(2) \tag{21}$$

in [9, p. 61]—and elsewhere.

Note that the integrand function of (21) has a nasty singularity at $\tan^{-1}\sqrt{7}$ (see Figure 2). However, we were able to numerically evaluate this integral to 20,000-digit accuracy, by splitting the integral into two parts, namely on the intervals $[\pi/3, \tan^{-1}\sqrt{7}]$ and $[\tan^{-1}\sqrt{7}, \pi/2]$. Note that tanh-sinh quadrature can be used on each part, since it can readily handle blow-up singularities at one or both endpoints of the interval of integration. This run required 46 minutes on 1024 CPUs of the Virginia Tech Apple cluster. The right-hand side was also evaluated, using *Mathematica*, to 20,000-digit precision. The two values agreed to $19,995$ digits [9, pg. 61]. Alternative representations of the integral in (21) are given in [18].

We shall now provide a proof of Eqn. (20) and hence of Eqn. (21). Actually, an equivalent (if not obviously so) form of identity (20), namely

$$\begin{aligned}
\zeta_{\mathbb{Q}(\sqrt{-7})}(2) &= \frac{\pi^2}{3\sqrt{7}}\left(A\left(\cot\frac{\pi}{7}\right) + A\left(\cot\frac{2\pi}{7}\right) + A\left(\cot\frac{4\pi}{7}\right)\right) \\
&= \frac{2\pi^2}{7\sqrt{7}}\left\{2A(\sqrt{7}) + A(\sqrt{7}+2\sqrt{3}) + A(\sqrt{7}-2\sqrt{3})\right\}
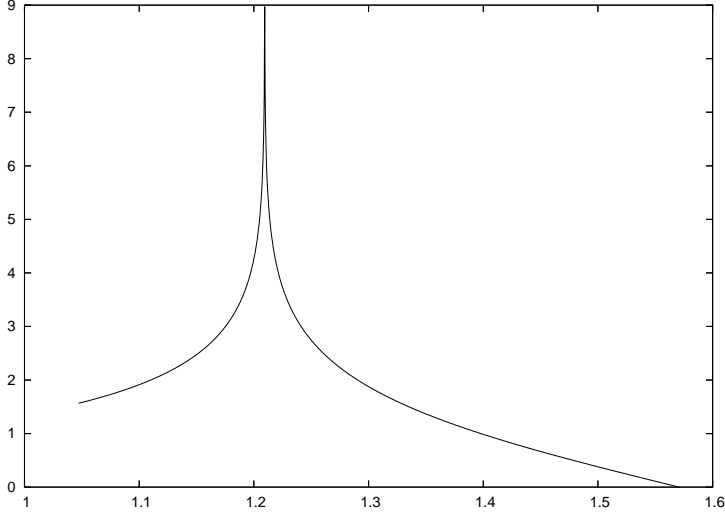\end{aligned} \tag{22}$$

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Figure 2: Plot of integrand function in (21).

with the notation

$$A(x) \quad := \int_0^x \frac{1}{1+t^2} \, \log \frac{4}{1+t^2} \, \mathrm{d}t = \mathrm{Cl}_2(2 \operatorname{arccot} x), \qquad (23)$$

is already established in [28]. The first equality in (22) can be written as

$$\zeta_{\mathbb{Q}(\sqrt{-7})}(2) \quad = \quad \frac{\pi^2}{6} \, \mathrm{L}_{-7}(2) \quad = \quad \zeta(2) \, \mathrm{L}_{-7}(2). \qquad (24)$$

On noting that

$$\cot \arg \frac{\sqrt{7}+i}{2\sqrt{2}} = \sqrt{7}, \quad \cot \arg \frac{(1+i\sqrt{7})(1 \mp i\sqrt{3})}{4\sqrt{2}} = \sqrt{7} \pm 2\sqrt{3}$$

and

$$\mathrm{Cl}_2(\theta) = \mathrm{Im} \sum_{n \geq 1} \frac{e^{in\theta}}{n^2},$$

we can translate the remaining, highly non-trivial, part of (22) to

$$2A(\sqrt{7}) + A(\sqrt{7} + 2\sqrt{3}) + A(\sqrt{7} - 2\sqrt{3}) = 2 \, \mathrm{Im} \sum_{n \geq 1} \frac{1}{n^2} \left(\frac{\sqrt{7}+i}{2\sqrt{2}} \right)^{2n}$$

$$+ \mathrm{Im} \sum_{n \geq 1} \frac{1}{n^2} \left(\frac{(1+i\sqrt{7})(1 - i\sqrt{3})}{4\sqrt{2}} \right)^{2n} + \mathrm{Im} \sum_{n \geq 1} \frac{1}{n^2} \left(\frac{(1+i\sqrt{7})(1 + i\sqrt{3})}{4\sqrt{2}} \right)^{2n}.$$

Now we use

$$\left(\frac{(1+i\sqrt{7})(1 + i\sqrt{3})}{4\sqrt{2}} \right)^2 = \mu e^{2\pi i/3}, \quad \left(\frac{(1+i\sqrt{7})(1 - i\sqrt{3})}{4\sqrt{2}} \right)^2 = \mu e^{-2\pi i/3},$$

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and

$$\mathrm{Im}\left(\frac{\sqrt{7}+i}{2\sqrt{2}}\right)^{2n} = \mathrm{Im}\left(\frac{3+i\sqrt{7}}{4}\right)^{n} = -\mathrm{Im}(-\mu)^{n} \qquad \text{for} \quad n = 0, 1, 2, \dots,$$

where $\mu := (-3 + i\sqrt{7})/4$ has absolute value 1 and $\arg\mu = \alpha = 2\arctan(\sqrt{7})$, to write the latter equality as

$$
\begin{aligned}
2A(\sqrt{7}) + A(\sqrt{7} + 2\sqrt{3}) + A(\sqrt{7} - 2\sqrt{3}) &= \mathrm{Im}\sum_{n \geq 1} \frac{\mu^{n}(e^{2\pi i n/3} + e^{-2\pi i n/3} - 2(-1)^{n})}{n^{2}} \\
&= \mathrm{Im}\left(\sum_{n \geq 1} \frac{\mu^{n}}{n^{2}} - \sum_{n \geq 1} \frac{\mu^{2n}}{n^{2}} + \frac{1}{3}\sum_{n \geq 1} \frac{\mu^{3n}}{n^{2}}\right) \\
&= \mathrm{Cl}_{2}(\alpha) - \mathrm{Cl}_{2}(2\alpha) + \frac{1}{3}\mathrm{Cl}_{2}(3\alpha), \qquad (25)
\end{aligned}
$$

where we have applied the following two standard identities

$$\frac{1}{2}\sum_{n \geq 1} \frac{x^{2n}}{n^{2}} = \sum_{n \geq 1} \frac{x^{n}}{n^{2}} + \sum_{n \geq 1} \frac{(-1)^{n}x^{n}}{n^{2}} \quad \text{and}$$

$$\frac{1}{3}\sum_{n \geq 1} \frac{x^{3n}}{n^{2}} = \sum_{n \geq 1} \frac{x^{n}}{n^{2}} + \sum_{n \geq 1} \frac{e^{2\pi i n/3}x^{n}}{n^{2}} + \sum_{n \geq 1} \frac{e^{-2\pi i n/3}x^{n}}{n^{2}}$$

for the dilogarithm function. It remains to substitute our finding (25) into (22) and (24) to finish a proof of identity (20).

The equivalent identity (21) can be obtained by some reasonably straightforward but tedious manipulation of the Clausen integral representation

$$\mathrm{Cl}_{2}(\theta) = -\int_{0}^{\theta} \log|2\sin\sigma|\, d\sigma \qquad (26)$$

for $0 \leq \theta < 2\pi$, and an appropriate change of variables.

Remark As Don Zagier points out in [28]

> *"we observe that the values of $A(x)$ at algebraic arguments satisfy many non-trivial linear relations over the rational numbers; I know of no direct proof, for instance, of the equality of the right-hand sides of Eqns. (5) and (6)."*

Zagier's Eqns. (5) and (6) are our identity (22).

Let us clarify the current status and somewhat-complicated history of various of the discoveries in [16]. Until recently the authors of [16] after discussion with Zagier believed (22) to be unproven. It was only when Zudilin spent time with Don Zagier in 2008 that he remembered his equivalent pre-dilogarithm (see [29, 30]) result in [28]. Two of the present authors (Borwein and Broadhurst) [16] wrote

> "*While the existence of such relations is understood [28, 29, 30], their precise forms appear to be unpredictable, thus far, by deductive mathematics. They are therefore ripe for the application of experimental mathematics.*"

The great bulk of the results recorded in [16] remain unproven. They were discovered by intensive physically and mathematically motivated computation, using *SnapPea*, *Pari/GP*, *Maple*, and other tools.　　　　　□

Indeed, the cases

$$D = -8, -11, -15, -20, -24$$

are challenging enough! These five respectively yield the following conjectured identities—each of which. First

$$27\mathrm{Cl}_2(\theta_2) - 9\mathrm{Cl}_2(2\theta_2) + \mathrm{Cl}_2(3\theta_2) \ \overset{?}{=} \ 8\mathrm{Cl}_2\left(\frac{2\pi}{8}\right) + 8\mathrm{Cl}_2\left(\frac{6\pi}{8}\right) \qquad (27)$$

with $\theta_2 := 2\arctan\sqrt{2}$. Second

$$15\mathrm{Cl}_2(\theta_{11}) - 10\mathrm{Cl}_2(2\theta_{11}) + \mathrm{Cl}_2(5\theta_{11}) \ \overset{?}{=} \ 11\sum_{k=1}^{5}\left(\frac{k}{11}\right)\mathrm{Cl}_2\left(\frac{2\pi k}{11}\right) \qquad (28)$$

where $\theta_{11} := 2\arctan\sqrt{11}$ and $\left(\frac{k}{11}\right)$ is the Jacobi (or Legendre) symbol for the Dirichlet character. Third

$$24\mathrm{Cl}_2(\theta_{5,3}) - 12\mathrm{Cl}_2(2\theta_{5,3}) - 8\mathrm{Cl}_2(3\theta_{5,3}) + 6\mathrm{Cl}_2(4\theta_{5,3}) \ \overset{?}{=} \ 15\sum_{k=1}^{7}\left(\frac{k}{15}\right)\mathrm{Cl}_2\left(\frac{2\pi k}{15}\right)$$
$$(29)$$

with $\theta_{5,3} := 2\arctan\sqrt{5/3}$. Fourth

$$36\mathrm{Cl}_2(\theta_5) - 30\mathrm{Cl}_2(2\theta_5) + 4\mathrm{Cl}_2(3\theta_5) + 3\mathrm{Cl}_2(4\theta_5) \ \overset{?}{=} \ 20\sum_{k\in\{1,3,7,9\}}\mathrm{Cl}_2\left(\frac{2\pi k}{20}\right)$$
$$(30)$$

with $\theta_5 := 2\arctan\sqrt{5}$. Finally,

$$60\mathrm{Cl}_2(\theta_{3,2}) - 18\mathrm{Cl}_2(2\theta_{3,2}) - 4\mathrm{Cl}_2(3\theta_{3,2}) + 3\mathrm{Cl}_2(4\theta_{3,2}) \ \overset{?}{=} \ 24\sum_{k\in\{1,5,7,11\}}\mathrm{Cl}_2\left(\frac{2\pi k}{24}\right)$$
$$(31)$$

with $\theta_{3,2} := 2\arctan\sqrt{3/2}$. So, for the 5th time, we have a relation that is as easy to check numerically as it appears hard to derive. Needless to say, it it would be interesting to check whether Zagier's 1986 method [28] works for all such small values of D.

As another example of the ubiquity of Clausen values, we complete this section with the most difficult integral evaluation required in [5]:

$$\mathcal{K}_1 \;\; := \;\; \int_3^4 \frac{\arcsec{(x)}}{\sqrt{x^2 - 4\,x + 3}}\, dx \tag{32}$$

$$= \;\; \mathrm{Cl}_2\left(\frac{\theta}{3}\right) - \mathrm{Cl}_2\left(\frac{\theta}{3} + \frac{\pi}{3}\right) - \mathrm{Cl}_2\left(\frac{\theta}{3} - \frac{\pi}{2}\right) + \mathrm{Cl}_2\left(\frac{\theta}{3} - \frac{\pi}{6}\right)$$

$$\mathrm{Cl}_2\left(\theta + \frac{2\pi}{3}\right) - \mathrm{Cl}_2\left(\theta + \frac{\pi}{3}\right) - \mathrm{Cl}_2\left(\theta - \frac{5\pi}{6}\right) + \mathrm{Cl}_2\left(\theta + \frac{5\pi}{6}\right)$$

$$+ \left(2\,\theta - \frac{5\,\pi}{2}\right)\log\left(2 - \sqrt{3}\right).$$

Here

$$\theta := \arctan\left(\frac{16 - 3\sqrt{15}}{11}\right) + \pi.$$

It may well be that this closed form for $\mathcal{K}_1$ can be further simplified.

6   Conclusion

We have presented here a brief survey of the rapidly expanding applications of experimental mathematics (in particular, the application of high-precision arithmetic) in mathematical physics. It is worth noting that all but the last of these examples have arisen in the past five to ten years. Efforts to analyze integrals that arise in mathematical physics have underscored the need for significantly faster schemes to produce high-precision values of 2-D, 3-D and higher-dimensional integrals. Along this line, the "sparse grid" methodology has some promise [23, 31]. Current research is aimed at evaluating such techniques for high-precision applications.

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n	s	$B_n(s)$
any	even $s \geq 0$	rational, e.g., : $B_2(2) = 2/3$
1	$s \neq -1$	$\frac{1}{s+1}$
2	-4	$-\frac{1}{4} - \frac{\pi}{8}$
2	-3	$-\sqrt{2}$
2	-1	$2\log(1+\sqrt{2})$
2	1	$\frac{1}{3}\sqrt{2} + \frac{1}{3}\log(1+\sqrt{2})$
2	3	$\frac{7}{5}\sqrt{2} + \frac{3}{20}\log(1+\sqrt{2})$
2	$s \neq -2$	$\frac{2}{2+s}{}_2F_1\left(\frac{1}{2}, -\frac{s}{2}; \frac{3}{2}; -1\right)$
3	-5	$-\frac{1}{6}\sqrt{3} - \frac{1}{12}\pi$
3	-4	$-\frac{3}{2}\sqrt{2}\arctan\frac{1}{\sqrt{2}}$
3	-2	$-3G + \frac{3}{2}\pi\log(1+\sqrt{2}) + 3\,\mathrm{Ti}_2(3-2\sqrt{2})$
3	-1	$-\frac{1}{4}\pi + \frac{3}{2}\log\left(2+\sqrt{3}\right)$
3	1	$\frac{1}{4}\sqrt{3} - \frac{1}{24}\pi + \frac{1}{2}\log\left(2+\sqrt{3}\right)$
3	3	$\frac{2}{5}\sqrt{3} - \frac{1}{60}\pi - \frac{7}{20}\log\left(2+\sqrt{3}\right)$

Table 2: Recent evaluations of Box integrals

n	s	$B_n(s)$
4	-5	$-\sqrt{8}\arctan\left(\frac{1}{\sqrt{8}}\right)$
4	-3	$4\,G - 12\,\mathrm{Ti}_2(3-2\sqrt{2})$
4	-2	$\pi\log\left(2+\sqrt{3}\right) - 2\,G - \frac{\pi^2}{8}$
4	-1	$2\log 3 - \frac{2}{3}G + 2\,\mathrm{Ti}_2\left(3-2\sqrt{2}\right) - \sqrt{8}\arctan\left(\frac{1}{\sqrt{8}}\right)$
4	1	$\frac{2}{5} - \frac{G}{10} + \frac{3}{10}\mathrm{Ti}_2\left(3-2\sqrt{2}\right) + \log 3 - \frac{7\sqrt{2}}{10}\arctan\left(\frac{1}{\sqrt{8}}\right)$
5	-3	$-\frac{110}{9}G - 10\log\left(2-\sqrt{3}\right)\theta - \frac{1}{8}\pi^2 + 5\log\left(\frac{1+\sqrt{5}}{2}\right) - \frac{5}{2}\sqrt{3}\arctan\left(\frac{1}{\sqrt{15}}\right)$ $-10\,\mathrm{Cl}_2\left(\frac{1}{3}\theta + \frac{1}{3}\pi\right) + 10\,\mathrm{Cl}_2\left(\frac{1}{3}\theta - \frac{1}{6}\pi\right)$ $+\frac{10}{3}\mathrm{Cl}_2\left(\theta + \frac{1}{6}\pi\right) + \frac{20}{3}\mathrm{Cl}_2\left(\theta + \frac{4}{3}\pi\right) - \frac{10}{3}\mathrm{Cl}_2\left(\theta + \frac{5}{3}\pi\right) - \frac{20}{3}\mathrm{Cl}_2\left(\theta + \frac{11}{6}\pi\right)$
5	-2	$\frac{8}{3}B_5(-6) - \frac{1}{3}B_5(-4) + \frac{5}{2}\pi\log(3) + 10\,\mathrm{Ti}_2\left(\frac{1}{3}\right) - 10\,G$
5	-1	$-\frac{110}{27}G + \frac{10}{3}\log\left(2-\sqrt{3}\right)\theta + \frac{1}{48}\pi^2 + 5\log\left(\frac{1+\sqrt{5}}{2}\right) - \frac{5}{2}\sqrt{3}\arctan\left(\frac{1}{\sqrt{15}}\right)$ $+\frac{10}{3}\mathrm{Cl}_2\left(\frac{1}{3}\theta + \frac{1}{3}\pi\right) - \frac{10}{3}\mathrm{Cl}_2\left(\frac{1}{3}\theta - \frac{1}{6}\pi\right)$ $-\frac{10}{9}\mathrm{Cl}_2\left(\theta + \frac{1}{6}\pi\right) + \frac{20}{3}\mathrm{Cl}_2\left(\theta + \frac{4}{3}\pi\right) - \frac{10}{3}\mathrm{Cl}_2\left(\theta + \frac{5}{3}\pi\right) + \frac{20}{9}\mathrm{Cl}_2\left(\theta + \frac{11}{6}\pi\right)$
5	1	$-\frac{77}{81}G + \frac{7}{9}\log\left(2-\sqrt{3}\right)\theta + \frac{1}{360}\pi^2 + \frac{1}{6}\sqrt{5} + \frac{10}{9}\log\left(\frac{1+\sqrt{5}}{2}\right) - \frac{4}{3}\sqrt{3}\arctan\left(\frac{1}{\sqrt{15}}\right) +$ $\frac{7}{9}\mathrm{Cl}_2\left(\frac{1}{3}\theta + \frac{1}{3}\pi\right) - \frac{7}{9}\mathrm{Cl}_2\left(\frac{1}{3}\theta - \frac{1}{6}\pi\right)$ $-\frac{7}{27}\mathrm{Cl}_2\left(\theta + \frac{1}{6}\pi\right) - \frac{14}{27}\mathrm{Cl}_2\left(\theta + \frac{4}{3}\pi\right) + \frac{7}{27}\mathrm{Cl}_2\left(\theta + \frac{5}{3}\pi\right) + \frac{14}{27}\mathrm{Cl}_2\left(\theta + \frac{11}{6}\pi\right)$

Table 3: Recent evaluations of Box integrals, continued

n	s	$\Delta_n(s)$
2	-5	$\frac{4}{3} + \frac{8}{9}\sqrt{2}$
2	-1	$\frac{4}{3} - \frac{4}{3}\sqrt{2} + 4\log(1+\sqrt{2})$
2	1	$\frac{2}{15} + \frac{1}{15}\sqrt{2} + \frac{1}{3}\log(1+\sqrt{2})$
3	-7	$\frac{4}{5} - \frac{16\sqrt{2}}{15} + \frac{2\sqrt{3}}{5} + \frac{\pi}{15}$
3	−2	$2\pi - 12\,G + 12\,\mathrm{Ti}_2\left(3 - 2\sqrt{2}\right) + 6\pi\log\left(1+\sqrt{2}\right) + 2\log 2 - \frac{5}{2}\log 3 - 8\sqrt{2}\arctan\left(\frac{1}{\sqrt{2}}\right)$
3	-1	$\frac{2}{5} - \frac{2}{3}\pi + \frac{2}{5}\sqrt{2} - \frac{4}{5}\sqrt{3} + 2\log\left(1+\sqrt{2}\right) + 12\log\left(\frac{1+\sqrt{3}}{\sqrt{2}}\right) - 4\log\left(2+\sqrt{3}\right)$
3	1	$-\frac{118}{21} - \frac{2}{3}\,\pi + \frac{34}{21}\,\sqrt{2} - \frac{4}{7}\,\sqrt{3} + 2\,\log\left(1+\sqrt{2}\right) + 8\,\log\left(\frac{1+\sqrt{3}}{\sqrt{2}}\right)$
3	3	$-\frac{1}{105} - \frac{2}{105}\,\pi + \frac{73}{840}\,\sqrt{2} + \frac{1}{35}\,\sqrt{3} + \frac{3}{56}\,\log\left(1+\sqrt{2}\right) + \frac{13}{35}\,\log\left(\frac{1+\sqrt{3}}{\sqrt{2}}\right)$

Table 4: Recent evaluations of Box integrals, continued

n	s	$\Delta_n(s)$
4	-10	$-\frac{8}{45}\pi\sqrt{3}-\frac{20}{9}\pi\log(2)+\frac{4}{9}\pi^2+\frac{4}{3}\log(2)+\frac{1}{15}\log(3)+\frac{8}{3}\operatorname{Ti}_2\left(3-2\sqrt{2}\right)$
4	-9	$\frac{16}{5}\pi\sqrt{3}-\frac{32}{3}\pi\log(2)-\frac{2}{3}\pi^2+\frac{16}{5}\pi+8\sqrt{2}\arctan\left(2\sqrt{2}\right)-24\log(2)+\frac{2}{5}\log(3)$ $+12\pi\log\left(\sqrt{2}-1\right)-64\operatorname{Ti}_2\left(3-2\sqrt{2}\right)+\frac{160}{3}G$
4	-3	$-\frac{128}{15}+\frac{1}{63}\pi-8\log\left(1+\sqrt{2}\right)-32\log\left(1+\sqrt{3}\right)+16\log(2)+20\log(3)$ $-\frac{8}{5}\sqrt{2}+\frac{32}{5}\sqrt{3}-32\sqrt{2}\arctan\left(\frac{1}{\sqrt{8}}\right)-96\operatorname{Ti}_2\left(3-2\sqrt{2}\right)+32G$
4	-2	$-\frac{16}{15}\pi\sqrt{3}+\frac{16}{3}\pi\log\left(1+\sqrt{3}\right)-\frac{8}{3}\pi\log(2)+4\pi\log\left(\sqrt{2}+1\right)-\frac{2}{3}\pi^2+\frac{4}{5}\pi$ $+\frac{8}{5}\sqrt{2}\arctan\left(2\sqrt{2}\right)+\frac{2}{5}\log(3)+8\operatorname{Ti}_2\left(3-2\sqrt{2}\right)-\frac{40}{3}G$
4	-1	$\frac{704}{195}-\frac{8}{39}\pi-\frac{100}{13}\log(3)+\frac{120}{13}\log(2)-\frac{8}{65}\sqrt{2}+\frac{128}{65}\sqrt{3}$ $-\frac{140}{13}\log\left(1+\sqrt{2}\right)-\frac{32}{13}\log\left(1+\sqrt{3}\right)+\frac{160}{13}\sqrt{2}\arctan\left(\frac{1}{\sqrt{8}}\right)+\frac{48}{13}G$
4	1	$-\frac{23}{135}-\frac{16}{315}\pi-\frac{52}{105}\log(2)+\frac{197}{420}\log(3)+\frac{73}{630}\sqrt{2}+\frac{8}{105}\sqrt{3}$ $+\frac{1}{14}\log\left(1+\sqrt{2}\right)+\frac{104}{105}\log\left(1+\sqrt{3}\right)-\frac{68}{105}\sqrt{2}\arctan\left(\frac{1}{\sqrt{8}}\right)-\frac{4}{15}G+\frac{4}{5}\operatorname{Ti}_2\left(3-2\sqrt{2}\right)$
5	-3	$-\frac{12304}{63}-\frac{512}{21}\sqrt{2}+\frac{576}{7}\sqrt{3}+\frac{800}{21}\sqrt{5}-\frac{320}{3}B_2(3)+\frac{448}{3}B_2(5)$ $-320B_3(1)+960B_3(3)-\frac{1792}{3}B_3(5)-160B_4(-1)+\frac{4400}{3}B_4(1)-\frac{20720}{9}B_4(3)$ $+896B_4(5)+32B_5(-3)+\frac{800}{3}B_5(-1)-1488B_5(1)+\frac{14336}{9}B_5(3)-448B_5(5)$
5	-1	$\frac{16388}{189}+\frac{1024}{189}\sqrt{2}-\frac{192}{7}\sqrt{3}-\frac{4000}{189}\sqrt{5}+\frac{64}{3}B_2(5)-\frac{192}{7}B_2(7)+\frac{320}{3}B_3(3)$ $-256B_3(5)+\frac{960}{7}B_3(7)+160B_4(1)-\frac{6160}{9}B_4(3)+784B_4(5)-\frac{1760}{7}B_4(7)$ $+32B_5(-1)-400B_5(1)+\frac{8192}{9}B_5(3)-672B_5(5)+\frac{1056}{7}B_5(7)$
5	1	$-\frac{1279}{567}G-\frac{4}{189}\pi+\frac{4}{315}\pi^2-\frac{449}{3465}+\frac{3239}{62370}\sqrt{2}+\frac{568}{3465}\sqrt{3}-\frac{380}{6237}\sqrt{5}$ $+\frac{295}{252}\log(3)+\frac{1}{54}\log\left(1+\sqrt{2}\right)+\frac{20}{63}\log\left(2+\sqrt{3}\right)+\frac{64}{189}\log\left(\frac{1+\sqrt{5}}{2}\right)$ $-\frac{73}{63}\sqrt{2}\arctan\left(\frac{1}{\sqrt{8}}\right)-\frac{8}{21}\sqrt{3}\arctan\left(\frac{1}{\sqrt{15}}\right)+\frac{104}{63}\log\left(2-\sqrt{3}\right)\theta$ $+\frac{5}{7}\operatorname{Ti}_2\left(3-2\sqrt{2}\right)+\frac{104}{63}\operatorname{Cl}_2\left(\frac{1}{3}\theta+\frac{1}{3}\pi\right)-\frac{104}{63}\operatorname{Cl}_2\left(\frac{1}{3}\theta-\frac{1}{6}\pi\right)$ $-\frac{104}{189}\operatorname{Cl}_2\left(\theta+\frac{1}{6}\pi\right)-\frac{208}{189}\operatorname{Cl}_2\left(\theta+\frac{4}{3}\pi\right)+\frac{104}{189}\operatorname{Cl}_2\left(\theta+\frac{5}{3}\pi\right)+\frac{208}{189}\operatorname{Cl}_2\left(\theta+\frac{11}{6}\pi\right)$

Table 5: Recent evaluations of Box integrals, continued

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