New representations for spin integrals

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Abstract: The correlation integrals for a spin-1/2 antiferromagnet have received much attention in recent years. In 2001, Boos and Korepin conjectured that these spin integrals can always be represented as superpositions of products of odd-Riemann-η values (η(s) = (1 − 21−s)ζ(s)). Though this hypothesis has been settled to the positive, there is still no constructive proof that yields convenient superposition weights. Herein we develop a general series, intended for possible theoretical bounds on spin integrals, together with a finite-domain integral formulation that leads to multiple L-functions as alternative expansion entities. We also provide numerical techniques that were useful in the course of our investigation.

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1 Motivation

The object of our present attention will be the correlation integrals for the Heisenberg spin-1/2 antiferromagnet. This integral given by Boos and Korepin, for a length-$n$ spin chain, as [5, eqn. 2.2]

\[ P(n) := \frac{1}{(2\pi i)^n} \int_{C_n} U_n T_n \, d\vec{\lambda}, \]

(1)

where

\[ U_n := \pi^{n(n+1)/2} \prod_{j<k} \sinh \pi (\lambda_k - \lambda_j) \left( \frac{\pi}{\sinh \pi \lambda_j} \right)^n, \]

(2)

\[ T_n := \prod_{j} \frac{\lambda_j^{j-1} (\lambda_j + i)^{n-j}}{\prod_{j<k} (\lambda_k - \lambda_j - i)}. \]

(3)

The nomenclature is explained as follows. Here and beyond, lone indices such as $j$ run over $[1,n]$. The indicial constraint $j < k$ means $1 \leq j < k \leq n$. The “curly-D” notation—essentially the Feynman path differential—is simply, for arbitrary vector $r$, $D\vec{r} := dr_1 \cdots dr_n$. The integration domain $C^n$ denotes that each $\lambda_j$ runs eastward along the horizontal contour $C := \{ x - i/2 : x \in (-\infty, \infty) \}$.

Much attention has been given to exact resolution of the $P(n)$. Currently, all $P(n)$ for $n \leq 6$ have been given closed forms [3] [4] [5] [6] [7]. In particular, each such exact evaluation involves rational-weighted sums of products of odd-argument $\eta$ functions, where

\[ \eta(s) := (1 - 2^{1-s}) \zeta(s), \]

with $\zeta$ denoting the celebrated Riemann zeta function. Note that $\eta(-1) = 1/4, \eta(1) = \log 2$, and so for example it is known that

\[ P(3) = \eta(-1) - \eta(1) + \frac{1}{2} \eta(3) = \frac{1}{4} - \log 2 + \frac{3}{8} \zeta(3), \]

while the most advanced known case as of this writing is [7, eqn 4.3]

\[ P(6) = \sum_{a,b,c} q_{a,b,c} \eta(a) \eta(b) \eta(c), \]

where the $q_{a,b,c}$ are all rational.\(^1\) Note that we are exploiting the fact of $\eta(-1)$ being rational to effect an $\eta$-sum that is perhaps more symmetrical than those in the literature. Indeed, the rational leading term here for $P(6)$ is \( q_{-1,-1,-1} \eta(-1)^3 \).

\(^1\)And yet, as one of the many open mysteries in regard to the $P(n)$, the coefficients $q_{1,5,7}$ and $q_{1,3,3}$ vanish in the $P(6)$ evaluation, while $q_{3,3,3}$, historically expected to vanish, does not; such observations appear in [7].
The original Boos–Korepin conjecture [3] states that $P(n)$ is always a combination of $\eta$ evaluations as exemplified above. This conjecture has since been interpreted in a “strong” form, in the sense of an explicit postulate on the algebraic character of the $\eta$ combinations entering into $P(n)$ [7, eqns. 4.5, 4.6].

The strong Boos–Korepin conjecture is settled in [2]. However, that resolution can be considered nonconstructive: There is still no effective form for the general coefficients, and certain asymptotic properties of $P(n)$ remain elusive. For example, it is suggested in [4] that

$$P(n) \sim a^{-n^2},$$

with $a$ estimated from what are known as DMRG computations as $a \approx 1.6719 \pm 0.0005$. Incidentally, the present authors concur with $a \approx 1.67$ using quasi-Monte Carlo (qMC) methods, on the relatively stable integrands of our numerical section below.

For these reasons we provide, first, new representations of the spin integrals $P(n)$ in the hope of alternative derivations of the precise coefficients of the Boos–Korepin representation. Second, another natural research avenue is to effect extreme-precision quadrature for the $P(n)$; we address such numerical issues in a later section.

2 New representations via dimensional inflation

The approach we shall take is to attempt formal removal of the denominator terms in (1). Previous treatments have made extensive use of pole calculus—some would call it “poleology,” whereas our own methods focus instead upon certain transformations of the integral to yield infinite-sum representations, especially multiple $L$-functions.

2.1 General real series

We start by assigning $\lambda_j \rightarrow x_j/\pi - i/2$, so that, after some manipulation including the use of sinh, cosh identities we arrive at

$$P(n) = \frac{1}{(2\pi)^n} \int_{\mathbb{R}^n} \mathcal{D}x \prod_j \frac{(x_j - i\pi/2)^{j-1}(x_j + i\pi/2)^{n-j}}{\cosh^n x_j} \prod_{j<k} \frac{\sinh(x_k - x_j - i\pi)}{x_k - x_j - i\pi}, \quad (4)$$

where the $n = 1$ case is interpreted: $P(1) = 1/(2\pi) \int_{-\infty}^{\infty} dx/\cosh x = 1/2$. An initial observation is that the representation (4) can immediately be written as an $M$-fold infinite sum, where $M := n(n-1)/2$, by expanding the sinh terms in classical fashion, to yield a sum over exactly

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2As in the paper [1] of Bailey, Borwein, and Crandall, “extreme precision” in such cases is taken to mean at least 100 decimal digits (or thereabouts). More precisely, we wish the precision to be enough so that integer-detection algorithms, e.g. PSLQ, will succeed in discovering closed forms.
There are $M$ integer indices—called say $m_{k,j}$ with $k > j$ understood—each index being in the positive odd integers $D^+$:

$$
P(n) = \frac{1}{(2\pi)^n} \sum_{m_{k,j} \in D^+} \frac{1}{m_{k,j}!} \int_{\mathbb{R}^n} \frac{D\bar{x}}{\prod_j \cosh^n x_j} \prod_j X_j^{n-j}(X_j^*)^{j-1} \prod_{k>j} (X_k^*-X_j)^{m_{k,j}-1},
$$

where we have denoted $X_j := x_j + i\pi/2$ and its complex conjugate $X_j^*$.

Remarkable, all the integrals implied can be given a closed form, as we shall see. For the moment, we define (setting $X := x + i\pi/2$, with conjugate $X^* = x - i\pi/2$)

$$
G_n(\mu, \nu) := \int_{-\infty}^{\infty} \frac{X(\mu)(X^*)^\nu}{\cosh^n x} \, dx,
$$

and contemplate coefficients $C_n(\vec{m}, \vec{\mu}, \vec{\nu})$, depending on an $M$-vector $\vec{m} := \{m_{k,j} : k > j\}$ having positive odd components and two $n$-vectors $\vec{\mu}, \vec{\nu}$ having nonnegative integer components, said coefficients defined implicitly by

$$
\prod_j X_j^{n-j}(X_j^*)^{j-1} \prod_{k>j} (X_k^*-X_j)^{m_{k,j}-1} =: \sum_{\vec{m},\vec{\mu},\vec{\nu}} C_n(\vec{m}, \vec{\mu}, \vec{\nu}) X_1^{\mu_1}(X_1^*)^{\nu_1} \cdots X_n^{\mu_n}(X_n^*)^{\nu_n}.
$$

Now we can write a general series for spin integrals

$$
P(n) = \frac{1}{(2\pi)^n} \sum_{m_{k,j}} \frac{1}{m_{k,j}!} T_n(\vec{m}),
$$

where

$$
T_n(\vec{m}) := \sum_{\vec{m},\vec{\mu},\vec{\nu}} C_n(\vec{m}, \vec{\mu}, \vec{\nu}) G_n(\mu_1, \nu_1) \cdots G_n(\mu_n, \nu_n)
$$

is a finite superposition of products of doable integrals.

Note that each term $T_n(\vec{m})$ is real, which follows from the fact that the conjugate of integrand in (4) is obtained by the swap-substitution $x_j \rightarrow x_{n+1-j}$. We have thus established a real series for spin integrals.

Stultifying as the expansion (6) and its attendant definitions may seem, it is nevertheless possible at least for smaller $n$ to perform some practical numerics, leading to interesting conjectures, as exhibited in a later section. For the moment, we observe that the leading term of the general series is

$$
T_n(\{1,1,\ldots,1\}) = \prod_{j=0}^{n-1} G_n(j, n-1-j).
$$

This term is easily seen to be real, as $G_n(\mu, \nu) = G_n^*(\mu, \nu)$ and the $G$-product here can be pairwise evaluated except for a possible (real) middle term.

We are aware that the original dimension, $n$, of the spin integral has blown up to a sum of dimension $n(n-1)/2$; we are saying there are nevertheless some advantages to such dimensional inflation.
2.2 Finite-domain integrals

Another representation, this time leading to a certain class of multiple \( L \)-function evaluations, starts also with the form (4) but now uses

\[
\frac{\sinh z}{z} = \frac{1}{2} \int_{-1}^{1} e^{\omega z} d\omega,
\]

and some elementary operator calculus, exemplified by

\[
(x \pm i\pi/2) e^{i\omega x} = \frac{\partial}{\partial \omega} e^{\omega x} \pm i\pi \omega/2.
\]

We anticipate a finite-domain integral, so we denote an origin-centered \( M \)-dimensional cube \([-1,1]^M\) and contemplate \( M \)-dimensional vectors \( \vec{\omega} = \{\omega_{k,j} : k > j\} \) lying in this cube. As before, we have an inflationary dimension \( M := n(n-1)/2 \), and we shall adopt the important symbolic convention that \( \omega_{k,j} := 0 \) when \( k \leq j \):

\[
P(n) = \frac{(-1)^{[n/2]}\pi^n 2^{n(n+1)/2}}{n!} \int_{[-1,1]^M} D\vec{\omega} \prod_{g=1}^{n} \prod_{h<g} \frac{\partial}{\partial \omega_{h,g}} \prod_{h>g} \frac{\partial}{\partial \omega_{g,h}} e^{-\frac{i\pi}{2} \sum_{e}(\omega_{e,g} + \omega_{g,e})} F_n \left( \sum_{d}(\omega_{g,d} - \omega_{d,g}) \right), \quad (7)
\]

where we hereby define

\[
F_n(\omega) = \int_{-\infty}^{\infty} \frac{e^{\omega x}}{\cosh^n x} dx.
\]

This rather abstruse representation (7) is motivated by the fact that the \( F \)-integral can be given closed, elementary form, and thus (7) has the important feature of being a finite-domain integral of rational-elementary functions.

Before we analyze the \( G \) and \( F \) functions that appear from this dimensional-inflation procedure, we clarify the notation of (7) with two examples. First,

\[
P(2) = -\frac{1}{8\pi^2} \int_{-1}^{1} d\omega \left\{ \frac{\partial}{\partial \omega} e^{-i\omega/2} F_2(-\omega) \right\} \left\{ \frac{\partial}{\partial \omega} e^{-i\omega/2} F_2(\omega) \right\}, \quad (8)
\]

which is especially simple because \( M = 1 \) and the only relevant \( \omega_{k,j} \) term is \( \omega := \omega_{2,1} \) in the integral. For \( P(3) \), we begin to see the combinatorial complications. Indeed, when \( n = 3 \) we have \( M = 3 \), and let us simplify by renumbering: \( u_1 := \omega_{2,1}, \ u_2 := \omega_{3,1}, \ u_3 := \omega_{3,2} \). Then

\[
P(3) = -\frac{1}{64\pi^3} \int_{[-1,1]^3} du_1 \, du_2 \, du_3 \right. \left\{ \frac{\partial^2}{\partial u_1 \partial u_2} e^{-i\frac{\pi}{2}(u_1+u_2)} F_3(-u_1 - u_2) \right\} \left\{ \frac{\partial^2}{\partial u_1 \partial u_3} e^{-i\frac{\pi}{2}(u_1+u_3)} F_3(+u_1 - u_3) \right\} \left\{ \frac{\partial^2}{\partial u_2 \partial u_3} e^{-i\frac{\pi}{2}(u_2+u_3)} F_3(+u_2 + u_3) \right\}, \quad (9)
\]
Note the important facts that 1) the factors $\exp(-i\pi/2 \sum)$ always have positive signs for the summed variables, while 2) the number of minus signs in the argument to $F_n$ decrements term-by-term.

An alternative finite-domain integral equivalent to (7) is in some ways easier to analyze. We introduce $2n$ auxiliary parameters $\{\alpha_j, \beta_j : j = 1 \ldots n\}$ (actually, $\beta_1$ and $\alpha_n$ can be taken to vanish a priori):

$$P(n) = \frac{1}{\pi^n 2^{n(n+1)/2}} \prod_{j=1}^{n} \partial_{\alpha_j} \partial_{\beta_j}^{j-1} |_{\alpha_j=\beta_j=0} e^{i\pi/2 \sum_j^{(\alpha_j-\beta_j)}} \int_{[-1,1]^M} D\vec{\omega} \ e^{-i\pi \sum_{k>j} \omega_{k,j}}$$

$$\times \prod_{g=1}^{n} F_n \left( \alpha_g + \beta_g + \sum_d (\omega_{g,d} - \omega_{d,g}) \right).$$

For clarity, we give the $n = 2$ case, simplifying notation via $\alpha = \alpha_1, \beta = \beta_2, \omega = \omega_{2,1}$:

$$P(2) = \frac{1}{8\pi^2} \partial_\alpha \partial_\beta |_{\alpha,\beta=0} e^{i\pi/2 (\alpha-\beta)} \int_{-1}^{1} d\omega \ e^{-i\pi \omega} F_2(\alpha - \omega) F_2(\beta + \omega).$$

Comparing this with the alternative (8), we can see a simpler integrand at the cost of external derivatives.

Before we derive closed forms for the $G, F$ kernels, thereby establishing finite-domain representations in terms of explicit elementary functions, we should remark on the value of numerical support for this theory. Faced with the representation (9), which is already complicated at $n = 3$, we elected to test the integral numerically, using techniques described in a later section. The result of quadrature on (9)—using the closed form we establish below for $F_3$—was

$$P(3) \approx 0.00762415812490254760766968910861717846136972526743182,$$

which agrees with the theoretical result to the implied precision.

[DBAI: You might want to move the above numerical snippet to a better place; no matter what, it is absolutely true what I say above—that this was used as a sanity check on the already tough $P(3)$ integral—Yet another reason to have extreme-numerics tools!]

### 3 Cosh-kernel theory

What we shall call cosh kernels are the functions that lie at the core of our series and integral representations, namely, we recall our two previous definitions (we assume $|\Re(\omega)| < n$ and nonnegative integers $\mu, \nu$):

$$F_n(\omega) := \int_{-\infty}^{\infty} \frac{e^{\omega x}}{\cosh^n x} \ dx,$$
and
\[ G_n(\mu, \nu) := \int_{-\infty}^{\infty} \frac{(x + i\pi/2)^\mu(x - i\pi/2)^\nu}{\cosh^n x} \, dx \] 
\[ = \left. \frac{\partial^{\mu+\nu}}{\partial\alpha^\mu \partial\beta^\nu} e^{i\pi(\alpha-\beta)/2} F_n(\alpha + \beta) \right|_{\alpha,\beta=0}. \] (13)

It is evident that all of the \( \cosh \) kernels here can be derived from \( F_n \) itself.

### 3.1 Analysis of the \( F_n \) kernels

It will be important to our multiple-\( L \)-function theory that \( F_n \) is an even function. It is elementary (and can be found in tables) that
\[ F_1(\omega) = \frac{\pi}{\cos(\pi\omega/2)}, \]
\[ F_2(\omega) = \frac{\pi\omega}{\sin(\pi\omega/2)}. \]

It is likewise easy to establish, via integration by parts, the recurrences
\[ F_n(\omega) = \frac{n + \omega - 2}{n - 1} F_{n-1}(\omega - 1), \]
valid for \( n > 1 \), and
\[ F_{n+2}(\omega) = \frac{n^2 - \omega^2}{n(n + 1)} F_n(\omega), \]
valid for \( n \geq 1 \). These facts give rise to closed forms for all the \( F_n \):

**Theorem 1** The \( \cosh \) kernel \( F_n(\omega) \) is given explicitly for integer \( n \geq 1 \) by

\[ F_{\text{even}} n(\omega) = \frac{\pi}{(n - 1)! \sin(\pi\omega/2)} Q_n(\omega), \]
\[ F_{\text{odd}} n(\omega) = \frac{\pi}{(n - 1)! \cos(\pi\omega/2)} Q_n(\omega), \]

where \( Q_n \) is an integer polynomial of degree \( n - 1 \):

\[ Q_{\text{even}} n(\omega) := \omega \left( 2^2 - \omega^2 \right) \left( 4^2 - \omega^2 \right) \cdots \left( (n - 2)^2 - \omega^2 \right), \]
\[ Q_{\text{odd}} n(\omega) := \left( 1^2 - \omega^2 \right) \left( 3^2 - \omega^2 \right) \cdots \left( (n - 2)^2 - \omega^2 \right). \]
**Proof:** Direct application of the recurrence relations. QED

Now, there are various ways to expand trigonometric reciprocals. One way yields the following Fourier-sum representations

\[
\frac{1}{\sin(\pi \omega/2)} = \mp 2i \sum_{m \geq 0} e^{\pm i \pi (m+1/2)\omega},
\]
\[
\frac{1}{\cos(\pi \omega/2)} = 2 \sum_{m \geq 0} (-1)^m e^{\pm i \pi (m+1/2)\omega},
\]

where here and elsewhere such sums can be interpreted as having a \( z^m \) in each summand, whence the sum is the \( z \to 1^- \) limit. We also exploit the ability to switch signs as indicated, as this will bring some convenience in our multiple-\( L \)-function development. On this understanding we can write

\[
F_2(\omega) := \mp 2\pi i \omega \sum_{m \geq 0} e^{\pm i \pi (m+1/2)\omega}, \tag{14}
\]
\[
F_3(\omega) := \pi (1 - \omega^2) \sum_{m \geq 0} (-1)^m e^{\pm i \pi (m+1/2)\omega}, \tag{15}
\]

and in general \( F_n(\omega) \) can be written as a relevant Fourier sum times \( Q_n(\omega) \).

Alternative reciprocal expansions are based on Bernoulli–Euler series:

\[
F_1(\omega) := \frac{\pi}{\cos(\pi \omega/2)} = \pi \sum_{m \geq 0} (-1)^m \frac{E_{2m}}{(2m)!} (\pi/2)^{2m} \omega^{2m}, \tag{16}
\]
\[
F_2(\omega) := \frac{\pi \omega}{\sin(\pi \omega/2)} = 4 \sum_{m \geq 0} (-1)^{m-1} \left( 2^{2m-1} - 1 \right) \frac{B_{2m}}{(2m)!} (\pi/2)^{2m} \omega^{2m}, \tag{17}
\]

and the phase-shifted forms

\[
e^{\pm i \pi \omega/2} F_1(\omega) = \frac{\pi e^{\pm i \pi \omega/2}}{\cos(\pi \omega/2)} = \pi \sum_{m \geq 0} \frac{E_m(0)}{m!} (\mp i\pi)^m \omega^m. \tag{18}
\]
\[
e^{\pm i \pi \omega/2} F_2(\omega) = \frac{\pi \omega e^{\pm i \pi \omega/2}}{\sin(\pi \omega/2)} = 2 \sum_{m \geq 0} \frac{B_m}{m!} (\mp i\pi)^m \omega^m, \tag{19}
\]
3.2 Analysis of the $G_n$ kernels

The above Bernoulli–Euler expansions allow closed-form evaluation of any cosh kernel $G_n$, in the following way.

**Theorem 2** The cosh kernel is always of the finite form

$$G_n(\mu, \nu) = i^{\mu+\nu} R_{\mu,\nu}(\pi),$$

where $R_{\mu,\nu}$ is a polynomial with rational real coefficients, enjoying the symmetry $R_{\mu,\nu} = (-1)^{\mu+\nu} R_{\nu,\mu}$.

**Proof:** Performing the indicated differentiation in (13), on various of the formulae (16, 17, 18, 19) yields the finite form indicated. The symmetry relations follows from the conjugacy relation $G_n(\mu, \nu) = G^*_n(\nu, \mu)$.

QED

So for example, one has

$$G_4(3,3) = \int_\infty^\infty \frac{(x + i\pi/2)^3(x - i\pi/2)^3}{\cosh^4 x} \, dx = \frac{-2\pi^4}{3} + \frac{32\pi^6}{315},$$

while

$$G_4(2,1) = \int_\infty^\infty \frac{(x + i\pi/2)^2(x - i\pi/2)}{\cosh^3 x} \, dx = i \left( \frac{\pi^4}{8} - \frac{\pi^2}{2} \right).$$

Particular closed forms for $n = 2$ will be useful in the next section:

$$G_2(\mu,0) = G_2(0,\mu)^* = 2(-i\pi)^\mu B_\mu.$$

4 $P(2), P(3)$ series lead to a strong conjecture

Even though it may seem computationally inefficient, let us write the series (6) explicitly for $n = 2$. After binomial expansion of $X_1X_2^*(X_2^* - X_1)^{m-1}$ and application of the evaluation method inherent to Theorem 2, one arrives at a 1-dimensional sum over odd indices

$$P(2) = \sum_{m \in D^+} \binom{(m-1)/2}{m!} \sum_{j=0}^{m-1} \binom{m-1}{j} \cdot \left( \frac{\pi^{m-1}}{m!} \right) B_{j+1} B_{m-j}.$$

It is interesting that this sum must equal the known literature value $P(2) = (1 - \log 2)/3$. One can achieve 100 decimal digits of accuracy using odd $m < 360$, say. Yet more interesting is the numerical suggestion that except for the first term, all summands appear to be negative. The significance of this is that pushing the sum further would yield monotonically decreasing results, and thus possible rigorous bounds on such a spin integral.
For $n = 3$, the series is of the form

$$P(3) = \sum_{m_{2,1}, m_{3,1}, m_{3,2} \in D^+} \frac{1}{m_{2,1}! m_{3,1}! m_{3,2}!} T_3(\vec{m}),$$

where $T$ is of course fairly complicated. But once again, numerical experiments give

$$\sum_{m_{k,j} \leq 19} T_3(\vec{m}) = 0.007626\ldots,$$

which is accurate to 3 significant digits, and more importantly the numerical sum appears to be monotonic decreasing as the limit on the $\vec{m}$ components is increased: The terms beyond the $(1,1,1)$ term appear to be all negative.

These observations lead us to

**Conjecture 1** *In the general series (6) the only positive term is the first, $T_n(\{1,1,\ldots,1\})$, all other terms being $T_n(\vec{m})$ being negative.*

On this conjecture, it is clear that any finite calculation would provide a rigorous upper bound on a spin integral.

## 5 Multiple-$L$-function approach

Let us begin a multiple-$L$-function investigation by working out the exact evaluation of $P(2)$. The idea is to insert the conditionally convergent trigonometric series (14) into the integral (8)—or, alternatively, into (11)—to yield a representation such as

$$P(2) = \frac{1}{2} \sum_{m_1, m_2 \geq 0} \int_{-1}^{1} d\omega \ (1 + i\pi m_1\omega)(1 + i\pi m_2\omega)e^{i\pi(m_1+m_2)\omega}. $$

There is a caution here, however: The precise variant of the integral depends on whether or not one exploits the symmetry, i.e. the evenness, of the $F_k$ kernels. That is, one may choose the signs in (14) arbitrarily, and this changes the form of $L$-series. At any rate, the above integral can be expanded in terms of

$$W(k,p) := \int_{-1}^{1} \omega^k e^{i\pi p\omega} \ d\omega. $$

which we consider for nonnegative integers $k$. It is elementary that

$$W(k,0) = \frac{2}{k+1} \delta_k \text{ even},$$
and that for \( p \neq 0 \)

\[
W(k, p) = \frac{2k!(−1)^{k+p+1}}{π^{k}} \sum_{j \text{ odd}}^{k} (-1)^{(j−1)/2} \frac{\pi^jp^{j−1}}{j!}.
\]

Using the instances \( W(k, m_1 + m_2) \) for \( k = 0, 1, 2 \) we achieve a certain kind of \( L \)-function evaluation

\[
P(2) = 1 + \sum_{m_1, m_2 \geq 0} (-1)^{m_1+m_2} - 2 \sum_{m_1, m_2 \geq 0} \frac{m_1m_2}{(m_1 + m_2)^2} (-1)^{m_1+m_2}.
\]

Here—and importantly—our \( \sum' \) notation means “avoid \( m_1 + m + 2 = 0 \).” This is not always the same as avoiding singular terms—we actually mean that

\[
\sum' (-1)^{m_1+m_2} = \sum_{m_1+m_2 \neq 0} (-1)^{m_1+m_2} = \frac{\lim_{x \to 1^-} \left( \frac{1}{(1 + x)^2} - 1 \right)}{2} = -\frac{3}{4}.
\]

The harder sum is

\[
\sum_{m_1, m_2 \geq 0} \frac{m_1m_2}{(m_1 + m_2)^2} (-1)^{m_1+m_2} = \sum_{d=1}^{\infty} \frac{(-1)^d (d-1)d(d+1)}{6} = \frac{1}{6} \log 2 - \frac{1}{24}.
\]

The known result \( P(2) = (1 - \log 2)/3 \) follows.

The example of \( P(3) \) is not only more complicated, but also indicates the direction in which we may generalize the multiple-\( L \)-function approach. Using the relation (9), or (10) for \( n = 3 \), together with Fourier expansion (15) and adroit choice of signs, we find that \( P(3) \) can be expressed as a superposition of multiple \( L \)-functions, but with form no deeper than

\[
\sum_{m_1, m_2, m_3 \geq 0} \frac{p(m_1, m_2, m_3)(-1)^{m_1+m_2+m_3}}{(m_1 + m_2)^{a_1}(m_1 + m_3)^{a_2}(m_3 - m_2 - 1)^{a_3}},
\]

where \( p \) is polynomial and the \( a_j \leq 4 \) are nonnegative integers. One can find, for example, that

\[
\sum_{m_1, m_2, m_3 \geq 0} \frac{(-1)^{m_1+m_2+m_3}}{(m_1 + m_2)(m_1 + m_3)(m_3 - m_2 - 1)} = -2 + \frac{\pi^2}{8} + 3 \log 2 - 3 \log^2 2,
\]

using the tools of the next section. Even though some of the fundamental constants here must necessarily cancel out to render the final, known form for \( P(3) \) (which for example does not involve \( \pi^2 \)), such sums are interesting in their own right.
6 Recurrence theory for multiple $L$-functions

[JBor: Here I assume goes your theory, which led to the previous section’s 3-dim sum.]

**Theorem 3** The general spin integral $P(n)$ can be written as a superposition of multiple $L$-functions of form involving $n$-dimensional summation over lattice vectors $\vec{m} = (m_1, \ldots, m_n)$, and a collection of $M = n(n-1)/2$ nonnegative integer powers $\{a_{k,j} : k > j\}$:

$$
\sum_{m_j \geq 0}^\prime p(\vec{m}) (-1)^{\sum m_j} \prod_{k>j} (m_k - m_j - 1)^{a_{k,j}},
$$

where the summation $'$ means any term with $m_k = m_j + 1$ is avoided (even if its associated power $a_{k,j}$ be zero). Alternatively, we may also adopt a superposition of functions:

[JBor, DBai: Right here goes same kind of sum, except like our worked case for $P(2)$ previous, some of the denominator terms are $m_j + m_k$ with no minus-one’s, and that allows some conveniences...I have no idea which form is best for finally getting closed forms for all $P(n)$.]

**Proof:** A proof uses (15), multiplied by the appropriate polynomial in $\omega$—with careful choice of signs—in either (7) or (10). For one choice of signs, one gets the first $L$-function display of Theorem 3, while for another, one effectively minimizes the number of denominator terms $m_k - m_j - 1$ in favor of $m_k + m_j$ for many of them.

[JBor, DBai: OBVIOUSLY incomplete...]

QED

It is interesting that our dimensional inflation that started the analysis has brought the benefit that, even though there are $M = n(n-1)/2$ denominator terms in the multiple $L$-functions, the lattice space is back to being $n$-dimensional.

7 Resolution of the Boos–Korepin conjecture

Finally we are able to provide explicit coefficients for $P(n)$, and thus a constructive resolution of the Boos–Korepin (strong) conjecture.

[JBor, DBai: This will be tough, or impossible...the key would appear to be Theorem 3.]

8 Numerical considerations

An immediate difficulty for the numerical quadrature of (1) is the complex character of the variables; another is the infinite domain of integration. We can handle both difficulties with
the multiple substitution

\[ \lambda_j = x_j - i/2, \]
\[ x_j = \frac{1}{\pi} a_j, \]
\[ a_j =: \frac{1}{2} \log \frac{1 + v_j}{1 - v_j}. \]

The result after all of this substitution is an integral over vectors \( \vec{v} \) in the origin-centered cube \([-1, 1]^n\):

\[
P(n) = \left( -1 \right)^{\left\lfloor \frac{n}{2} \right\rfloor} \frac{1}{(2\pi)^n} \int_{[-1,1]^n} D\vec{v} \prod_j \left( 1 - v_j^2 \right)^{n/2-1} \left( a_j - \frac{i\pi}{2} \right)^{j-1} \left( a_j + \frac{i\pi}{2} \right)^{n-j} \prod_{1 \leq k < h \leq n} \sinh(a_h - a_k) a_h - a_k - i\pi.
\]

The natural quadrature setup, then, is to assume each variable \( v_j \) of integration will lie in \((-1, 1)\), and when evaluating the integrand, to create the \( a_j \) from the \( v_j \) via the logarithmic formula above. Note: If \( \vec{v} \) is on any face of the cube—i.e. some \( v_j = \pm 1 \), the logarithm is singular but happily, one may simply take the integrand to be 0 at such points. Thus, an integrand function can return-with-zero if any \( v_j^2 = 1 \). Note that the integral \( P(n) \) is always real—as can be gleaned from symmetry arguments, so one may either use complex arithmetic for the integrand and keep only the real part, or pre-reduce this integrand symbolically so to effect pure-real algebra.

Incidentally, there are various speedups for the integral (21), such as table lookup for pairs \((k, h > k)\) and some reductions, such as

\[
\sinh(a_h - a_k) = \frac{v_h - v_k}{\sqrt{1 - v_h^2} \sqrt{1 - v_k^2}},
\]

which avoids some of the transcendental arithmetic. Indeed, the square root terms here mostly cancel the ones in the numerator, leaving us with

\[
P(n) = \left( -1 \right)^{\left\lfloor \frac{n}{2} \right\rfloor} \frac{1}{(2\pi)^n} \int_{[-1,1]^n} D\vec{v} \prod_j \left( 1 - v_j^2 \right)^{-1/2} \left( a_j - \frac{i\pi}{2} \right)^{j-1} \left( a_j + \frac{i\pi}{2} \right)^{n-j} \prod_{1 \leq k < h \leq n} \frac{v_h - v_k}{a_h - a_k - i\pi}.
\]

If one desires some singularity removal for reasons of numerical stability, the substitutions \( v_j := \sin \phi_j \) yield

\[
P(n) = \left( -1 \right)^{\left\lfloor \frac{n}{2} \right\rfloor} \frac{1}{(2\pi)^n} \int_{-\pi/2}^{\pi/2} \cdots \int_{-\pi/2}^{\pi/2} D\vec{\phi} \prod_j \left( a_j - \frac{i\pi}{2} \right)^{j-1} \left( a_j + \frac{i\pi}{2} \right)^{n-j} \prod_{1 \leq k < h \leq n} \sin \phi_h - \sin \phi_k \frac{a_h - a_k - i\pi}{a_h - a_k - i\pi},
\]
where, now,
\[
a_j = \frac{1}{2} \log \frac{1 + \sin \phi_j}{1 - \sin \phi_j}.
\]

These finite-domain integral formulations are suitable for quasi-Monte Carlo (qMC) (results pending), and hopefully for extreme-precision, modern quadrature (results pending).

9 Computations

The formulation (23) is well-suited for high-precision quadrature, in that it is free from singularities (provided one stays away from certain rational values that possess removable singularities), and is defined on a finite multi-dimensional cube.

Since the integrand function is regular (free from singularities and vertical derivatives), we found that for ordinary multi-dimensional Gaussian quadrature is the best quadrature scheme to use. However, run time very rapidly increases with increasing dimension, due to the need for roughly \(N^m\) evaluations of the integrand function, where \(N\) is the number of evaluations needed in one dimension, and \(m\) is the number of dimensions.

In order to reduce the number of calculations to a minimum, we employed a number of techniques. One that was particularly helpful is to pre-compute each part of the expression in (23), including the \((a_j - \frac{i\pi}{2})^{j-1}\) terms, the \(\sin\) terms and even the denominator of the right-most term (which denominator we pre-computed and stored as a two-dimensional array). We also employed a binary search technique to quickly retrieve the requisite value from our tables.

Even with these changes, these computations are extremely expensive. We were able to compute \(P(n)\) to at least modest precision for \(n\) up to 6; beyond this level seems impractical using our current methods. The run times and processors used shown in the table below underscore the rapidly escalating difficulty of these computations:

<table>
<thead>
<tr>
<th>(n)</th>
<th>Digits</th>
<th>Processors</th>
<th>Run Time</th>
</tr>
</thead>
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<tr>
<td>2</td>
<td>120</td>
<td>1</td>
<td>10 sec.</td>
</tr>
<tr>
<td>3</td>
<td>120</td>
<td>8</td>
<td>55 min.</td>
</tr>
<tr>
<td>4</td>
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<td>64</td>
<td>27 min.</td>
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<td>30</td>
<td>256</td>
<td>39 min.</td>
</tr>
<tr>
<td>6</td>
<td>6</td>
<td>256</td>
<td>59 hrs.</td>
</tr>
</tbody>
</table>

10 Acknowledgements

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References


