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Evaluation of the Watson integral and associated logarithmic integral for the d-dimensional hypercubic lattice

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Abstract

The Watson integral for the d-dimensional hypercubic lattice

$$W_d = \frac{1}{\pi^d}\int_0^\pi \cdots \int_0^\pi \frac{\mathrm{d}\theta_1 \cdots \mathrm{d}\theta_d}{d - (\cos\theta_1 + \cdots + \cos\theta_d)}$$

and the associated logarithmic integral

$$L_d = \frac{1}{\pi^d}\int_0^\pi \cdots \int_0^\pi \ln\left[d - (\cos\theta_1 + \cdots + \cos\theta_d)\right] \mathrm{d}\theta_1 \cdots \mathrm{d}\theta_d$$

are investigated. In particular, a new method is developed which enables one to calculate the numerical values of $\{L_d : d = 1, 2, \ldots\}$ and $\{W_d : d = 3, 4, \ldots\}$ with extremely high precision. The asymptotic behaviour of L_d and W_d as $d \to \infty$ is also determined. Finally, some generalizations of the results are briefly discussed.

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1. Introduction

The d-fold Watson integral

$$W_d = \frac{1}{\pi^d}\int_0^\pi \cdots \int_0^\pi \frac{\mathrm{d}\theta_1 \cdots \mathrm{d}\theta_d}{d - (\cos\theta_1 + \cdots + \cos\theta_d)} \tag{1.1}$$

and the associated logarithmic integral

$$L_d = \frac{1}{\pi^d}\int_0^\pi \cdots \int_0^\pi \ln\left[d - (\cos\theta_1 + \cdots + \cos\theta_d)\right] \mathrm{d}\theta_1 \cdots \mathrm{d}\theta_d \tag{1.2}$$

appear in the theory of the Gaussian and spherical models of ferromagnetism for the d-dimensional hypercubic lattice with nearest-neighbour interactions (Berlin and Kac 1952, Joyce 1972, Gerber and Fisher 1974). The integral W_d also plays an important role in the theory of random walks on the d-dimensional hypercubic lattice (Montroll and Weiss 1965), while the integral L_d is involved in the calculation of the total number of spanning trees on a hypercubic lattice (Rosengren 1987) and in the theory of collapsing branched polymers (Madras *et al* 1990).

Watson (1939) has proved that W_3 can be expressed in the form

$$W_3 = \left(18 + 12\sqrt{2} - 10\sqrt{3} - 7\sqrt{6}\right)\left[\frac{2}{\pi}K\left(\left(2-\sqrt{3}\right)\left(\sqrt{3}-\sqrt{2}\right)\right)\right]^2 \tag{1.3}$$

where $K(k)$ denotes the complete elliptic integral of the first kind with a modulus k. It is also possible to write W_3 in terms of the gamma function using the work of Borwein and Zucker (1992). We find that

$$W_3 = \frac{1}{96\pi^3}\left(\sqrt{3}-1\right)\left[\Gamma\left(\frac{1}{24}\right)\Gamma\left(\frac{11}{24}\right)\right]^2. \tag{1.4}$$

(It should be noted that the improper integral W_d does not exist when $d = 1$ and $d = 2$.) Unfortunately, it does not appear to be possible to generalize Watson's ingenious method for evaluating W_3 to higher dimensions $d \geqslant 4$. However, Maradudin *et al* (1960) have shown that a major simplification can be achieved by applying the formula

$$\frac{1}{\lambda} = \int_0^\infty \exp(-\lambda t)\,\mathrm{d}t \tag{1.5}$$

where $\Re(\lambda) > 0$, to the integrand in (1.1). The resulting multiple integral can then be reduced to a *single* integral using the standard result

$$\frac{1}{\pi}\int_0^\pi \exp(t\cos\theta)\,\mathrm{d}\theta = I_0(t) \tag{1.6}$$

where $I_0(t)$ is a modified Bessel function of the first kind. In this manner, we find that

$$W_d = \int_0^\infty \exp(-dt)\, I_0^d(t)\,\mathrm{d}t \tag{1.7}$$

where $d \geqslant 3$.

For the logarithmic integral L_d with $d = 1$ and $d = 2$ we have the well known results

$$L_1 = -\ln 2 \tag{1.8}$$

$$L_2 = \frac{4G}{\pi} - \ln 2 \tag{1.9}$$

where G is the Catalan constant. When $d \geqslant 3$ there are no further exact formulae available in the literature for L_d and the reduction of (1.2) to a single integral of the type (1.7) has not previously been carried out. Recently, Joyce (2001) has calculated an extremely accurate value for L_3 by applying the method of analytic continuation to the exact elliptic integral formula for the simple cubic lattice Green function.

The main aim in this paper is to derive a *single* integral representation for L_d, which is valid for all $d \geqslant 1$. This new formula will be used to determine accurate numerical values for $\{L_d : d = 2, 3, \ldots\}$ and to establish the asymptotic behaviour of L_d as $d \to \infty$. Finally, various generalizations of the results will be briefly discussed.

2. Evaluation of the integrals L_d and W_d

We begin the analysis by noting the following identity:

$$\int_0^\infty \left[\exp(-t) - \exp(-zt)\right]\frac{\mathrm{d}t}{t} = \ln z \tag{2.1}$$

where $\Re(z) > 0$. A rigorous proof of this result has been given by Whittaker and Watson (1927, p 116). If the formula (2.1) is applied to the integrand in (1.2) then we can use (1.6) to reduce the resulting multiple integral to the single quadrature

$$L_d = \int_0^\infty \left[\exp(-t) - \exp(-dt)\, I_0^d(t)\right] \frac{\mathrm{d}t}{t} \tag{2.2}$$

where $d \geqslant 1$. It is interesting to note that the structure of this new formula for L_d is very similar to that of the integral representation (1.7) for W_d.

In order to calculate the numerical values of L_d we first split the range of integration in (2.2) into two intervals $(0, T]$ and $[T, \infty)$ where $T > 0$. In this manner, we find that

$$L_d = J_d(T) - \int_T^\infty \exp(-dt)\, I_0^d(t) \frac{\mathrm{d}t}{t} + \Gamma(0, T) \tag{2.3}$$

where

$$J_d(T) = \int_0^1 \left[\exp(-Tu) - \exp(-dTu)\, I_0^d(Tu)\right] \frac{\mathrm{d}u}{u} \tag{2.4}$$

and $\Gamma(0, T)$ is an incomplete gamma function. Next we make use of the asymptotic representation

$$\exp(-dt)\, I_0^d(t) \sim \frac{1}{(2\pi t)^{d/2}} \sum_{j=0}^{M} \frac{c_j(d)}{t^j} \tag{2.5}$$

as $t \to \infty$, where $M = 0, 1, 2, \ldots$ and the coefficients $\{c_j(d) : j = 0, 1, 2, \ldots\}$ are defined by the formal generating function

$$\left[{}_2F_0\left(\frac{1}{2}, \frac{1}{2}; -; \frac{z}{2}\right)\right]^d = \sum_{j=0}^{\infty} c_j(d)\, z^j \tag{2.6}$$

where ${}_2F_0$ denotes a generalized hypergeometric function. By expanding the left-hand side of (2.6) in powers of z it is found that $c_0(d) = 1$, $c_1(d) = d/8$, and

$$c_2(d) = \frac{d}{128}(8 + d) \tag{2.7}$$

$$c_3(d) = \frac{d}{3\,072}\left(200 + 24d + d^2\right) \tag{2.8}$$

$$c_4(d) = \frac{d}{98\,304}(24 + d)\left(416 + 24d + d^2\right) \tag{2.9}$$

$$c_5(d) = \frac{d}{3\,932\,160}\left(824\,064 + 65\,920d + 2\,960d^2 + 80d^3 + d^4\right). \tag{2.10}$$

The application of (2.5) to the integrand in (2.3) yields the basic formula

$$L_d = \lim_{T\to\infty}\left[J_d(T) - \frac{1}{(2\pi T)^{d/2}} \sum_{j=0}^{M} \frac{c_j(d)}{\left(j + \frac{d}{2}\right) T^j} + \Gamma(0, T)\right] \tag{2.11}$$

where $\Gamma(0, T)$ is an incomplete gamma function, M is any fixed non-negative integer and $d \geqslant 1$.

We have used the expression on the right-hand side of (2.11) to determine the numerical values of $\{L_d : d = 1, 2, \ldots, 10\}$. In particular, the integral $J_d(300)$ was first calculated with an accuracy of 55 digits using *Mathematica* (Wolfram 1991) and the terms in the truncated asymptotic series were then summed until their contribution to the value of L_d was less than 10^{-55}. (The term $\Gamma(0, T)$ was ignored because $\Gamma(0, 300) \ll 10^{-55}$.) We list the final results for $\{L_d : d = 2, 3, \ldots, 10\}$ in table 1 with an accuracy of 51 digits after the decimal point in

Table 1. Numerical values of $\{L_d : d = 2, 3, \ldots, 10\}$.

d	L_d
2	0.473 096 435 563 329 811 136 305 704 415 403 107 380 764 481 583 093
3	0.980 242 122 410 251 422 866 198 500 197 421 507 182 206 986 985 840
4	1.306 560 463 957 367 250 270 667 182 565 231 588 846 918 868 575 098
5	1.549 340 879 251 435 882 378 312 274 593 388 834 648 927 343 704 651
6	1.743 479 781 440 769 948 878 599 900 066 223 636 015 820 177 721 418
7	1.905 529 123 705 665 419 926 484 935 928 775 748 971 064 554 983 529
8	2.044 720 483 299 361 405 776 140 751 891 651 643 492 629 583 188 815
9	2.166 762 961 780 149 411 740 801 667 304 037 400 446 135 028 813 299
10	2.275 447 303 883 345 867 491 603 112 119 194 500 287 465 549 477 663

Table 2. Numerical values of $\{W_d : d = 3, 4, \ldots, 10\}$.

d	W_d
3	0.505 462 019 717 326 006 052 004 053 227 140 259 985 129 014 817 420
4	0.309 866 780 462 120 428 169 674 416 214 750 177 538 322 267 290 439
5	0.231 261 624 968 046 235 741 427 024 387 713 397 109 085 469 701 028
6	0.186 160 562 204 445 307 280 940 721 994 768 875 442 698 770 398 838
7	0.156 272 330 798 263 999 526 181 689 079 859 980 530 184 282 452 137
8	0.134 830 876 502 115 694 830 335 560 003 426 882 643 791 499 840 442
9	0.118 638 454 042 378 212 553 986 551 283 686 584 460 096 734 255 570
10	0.105 954 374 788 826 107 131 697 595 717 985 275 483 701 891 544 129

unrounded form. The numerical value given for L_2 is consistent with the exact formula (1.9) and the value for L_3 is in agreement with the work of Rosengren (1987) and Joyce (2001).

Similar methods can also been applied to the Watson integral (1.1). In particular, we find that the analogue of formula (2.11) is

$$W_d = \lim_{T\to\infty}\left[W_d(T) + \frac{T}{(2\pi T)^{d/2}}\sum_{j=0}^{M}\frac{c_j(d)}{\left(j+\frac{d}{2}-1\right)T^j}\right] \tag{2.12}$$

where M is any fixed non-negative integer,

$$W_d(T) = T\int_0^1 \exp(-dTu)I_0^d(Tu)\,\mathrm{d}u \tag{2.13}$$

and $d \geqslant 3$. We have used (2.12) to calculate the values of $\{W_d : d = 3, 4, \ldots, 10\}$. The final results are listed in table 2 with an accuracy of 51 digits after the decimal point in unrounded form.

3. Asymptotic behaviour of L_d and W_d as $d \to \infty$

The behaviour of L_d as $d \to \infty$ can be established by considering the series expansion

$$I_0^d(t) = \sum_{j=0}^{\infty} f_j(d)t^{2j} \tag{3.1}$$

where the coefficients $\{f_j(d) : j = 0, 1, 2, \ldots\}$ are defined by the generating function

$$\left[\sum_{j=0}^{\infty}\frac{z^j}{(j!)^2\,4^j}\right]^d = \sum_{j=0}^{\infty} f_j(d)\,z^j \tag{3.2}$$

and $|t| < \infty$. If the left-hand side of (3.2) is expanded in powers of z we find that $f_0(d) = 1$, $f_1(d) = d/4$, and

$$f_2(d) = -\frac{d}{64}(1 - 2d) \tag{3.3}$$

$$f_3(d) = \frac{d}{2\,304}\left(4 - 9d + 6d^2\right) \tag{3.4}$$

$$f_4(d) = -\frac{d}{147\,456}\left(33 - 82d + 72d^2 - 24d^3\right) \tag{3.5}$$

$$f_5(d) = \frac{d}{14\,745\,600}\left(456 - 1\,225d + 1\,250d^2 - 600d^3 + 120d^4\right). \tag{3.6}$$

Next the series (3.1) is applied to the integrand in (2.2). This procedure gives

$$L_d = \ln d - \sum_{j=1}^{\infty} f_j(d)\,\frac{(2j-1)!}{d^{2j}}. \tag{3.7}$$

We can now determine the asymptotic behaviour of L_d for large d by expanding the series in (3.7) in powers of $1/d$. The final result is

$$\begin{aligned} L_d \sim \ln d - \frac{1}{4\,d} - \frac{3}{16\,d^2} - \frac{7}{32\,d^3} - \frac{45}{128\,d^4} - \frac{269}{384\,d^5} - \frac{805}{512\,d^6} - \frac{3\,615}{1\,024\,d^7} \\ - \frac{23\,205}{4\,096\,d^8} + \frac{144\,963}{10\,240\,d^9} + \frac{2\,187\,031}{8\,192\,d^{10}} + \frac{40\,225\,409}{16\,384\,d^{11}} + \frac{1\,277\,353\,077}{65\,536\,d^{12}} \\ + \frac{66\,817\,216\,455}{458\,752\,d^{13}} + \frac{271\,891\,453\,119}{262\,144\,d^{14}} + \frac{10\,764\,825\,180\,395}{1\,572\,864\,d^{15}} + \ldots \end{aligned} \tag{3.8}$$

as $d \to \infty$.

In a similar manner we can derive the asymptotic behaviour of W_d as $d \to \infty$ by substituting the series (3.1) in (1.7). Hence, we obtain

$$W_d = \sum_{j=0}^{\infty} f_j(d)\,\frac{(2j)!}{d^{2j+1}}. \tag{3.9}$$

If the terms in this series are expanded in powers of $1/d$ it is found that

$$\begin{aligned} W_d \sim \frac{1}{d} + \frac{1}{2\,d^2} + \frac{3}{4\,d^3} + \frac{3}{2\,d^4} + \frac{15}{4\,d^5} + \frac{355}{32\,d^6} + \frac{595}{16\,d^7} + \frac{8\,715}{64\,d^8} \\ + \frac{67\,095}{128\,d^9} + \frac{128\,457}{64\,d^{10}} + \frac{3\,461\,073}{512\,d^{11}} + \frac{21\,248\,073}{2\,048\,d^{12}} \\ - \frac{601\,744\,143}{4\,096\,d^{13}} - \frac{5\,200\,528\,905}{2\,048\,d^{14}} - \frac{120\,052\,936\,575}{4\,096\,d^{15}} - \ldots \end{aligned} \tag{3.10}$$

as $d \to \infty$. Gerber and Fisher (1974) have also derived the expansion (3.10) by applying a series reversion procedure to the integrand in (1.7).

4. Generalizations

In this concluding section we shall derive single integral representations for the generalized lattice Green function

$$G_d(\mathbf{n}; s, w) = \frac{1}{\pi^d}\int_0^{\pi}\cdots\int_0^{\pi} \frac{\cos n_1\theta_1 \cdots \cos n_d\theta_d}{[w - (\cos\theta_1 + \cdots + \cos\theta_d)]^s}\,\mathrm{d}\theta_1\cdots\mathrm{d}\theta_d \tag{4.1}$$

and the associated logarithmic integral

$$L_d\,(\mathbf{n}; s, w) = \frac{1}{\pi^d}\int_0^\pi \cdots \int_0^\pi \frac{\cos n_1\theta_1 \cdots \cos n_d\theta_d}{[w - (\cos\theta_1 + \cdots + \cos\theta_d)]^s} \times \ln\,[w - (\cos\theta_1 + \cdots + \cos\theta_d)\,]\ \mathrm{d}\theta_1 \cdots \mathrm{d}\theta_d \qquad (4.2)$$

where $\mathbf{n} = \{n_1, \ldots, n_d\}$ is a set of non-negative integers, $s \geqslant 0$ and $w \geqslant d$.

We begin by applying the formula

$$\frac{1}{\lambda^s} = \frac{1}{\Gamma(s)}\int_0^\infty t^{s-1}\,\exp\,(-\lambda t)\ \mathrm{d}t \qquad (4.3)$$

where $\Re(\lambda) > 0$ and $s > 0$, to the integrand in (4.1). This procedure yields the single integral

$$G_d\,(\mathbf{n}; s, w) = \frac{1}{\Gamma(s)}\int_0^\infty t^{s-1}\,\exp(-wt)\,I_{n_1}(t)\cdots I_{n_d}(t)\,\mathrm{d}t \qquad (4.4)$$

where $w \geqslant d$ and $s > 0$. If equation (4.4) is differentiated with respect to the parameter s we obtain the further result

$$L_d\,(\mathbf{n}; s, w) = \psi(s)\,G_d\,(\mathbf{n}; s, w) - \frac{1}{\Gamma(s)}\int_0^\infty t^{s-1}\,(\ln t)\ \exp(-wt)\,I_{n_1}(t)\cdots I_{n_d}(t)\,\mathrm{d}t \quad (4.5)$$

where $\psi(s)$ is the logarithmic derivative of the gamma function $\Gamma(s)$, $w \geqslant d$ and $s > 0$. It is clear that the formula (4.5) cannot be used to determine $L_d(\mathbf{n}; s, w)$ when $s = 0$. However, for this special case we can apply the identity (2.1) to the integrand in (4.2). In this manner, we find that

$$L_d\,(\mathbf{n}; 0, w) = \int_0^\infty \left[\exp(-t)\,\delta_{\mathbf{n},\mathbf{0}} - \exp(-wt)\,I_{n_1}(t)\cdots I_{n_d}(t)\right]\frac{\mathrm{d}t}{t} \qquad (4.6)$$

where δ denotes the Kronecker symbol. Finally, we note that if $\mathbf{n} \neq \mathbf{0}$ with $n_1 = 1, 2, \ldots$ then we can use the standard recurrence relation

$$\frac{2n_1}{t}\,I_{n_1}(t) = I_{n_1-1}(t) - I_{n_1+1}(t) \qquad (4.7)$$

to express (4.6) in the alternative form

$$L_d\,(\mathbf{n}; 0, w) = \frac{1}{2n_1}\left[G_d\,(n_1+1, n_2, \ldots, n_d; 1, w) - G_d\,(n_1-1, n_2, \ldots, n_d; 1, w)\right] \qquad (4.8)$$

where $n_1 \neq 0$. This result was first derived by Rosengren (1987) for the case $d = 3$.

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