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Singular behaviour of the lattice Green function for the *d*-dimensional hypercubic lattice

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Abstract

The analytic properties of the d-dimensional hypercubic lattice Green function

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

are investigated, where $w = u + \mathrm{i}v$ is a complex variable in the (u, v) plane. In particular, the detailed behaviour of $G(d, w)$ in the immediate neighbourhood of the branch-point singularities $w = \pm d$ is determined. These results are used to derive an asymptotic expansion in powers of $1/n$ for the number of random walks on the hypercubic lattice which return to their starting point (not necessarily for the first time) after a walk of $2n$ steps. Finally, it is shown that this asymptotic expansion enables one to calculate extremely accurate values for the generalized d-dimensional Watson integral

$$W_d(s) \equiv \frac{1}{\pi^d}\int_0^\pi \cdots \int_0^\pi [d-(\cos\theta_1+\cdots+\cos\theta_d)]^s\,\mathrm{d}\theta_1\cdots\mathrm{d}\theta_d$$

where $s > -d/2$ and $s \neq 1, 2, \ldots$.

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1. Introduction

The Green function

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

where $w = u + \mathrm{i}v$ is a complex variable in the (u, v) plane, plays an important role in many lattice statistical models which involve the d-dimensional hypercubic lattice with nearest-neighbour interactions (Berlin and Kac 1952, Montroll 1956, Montroll and Weiss 1965, Joyce 1972, Gerber and Fisher 1974). We find that the d-fold integral (1.1) defines a single-valued analytic function $G(d, w)$ in the complex (u, v) plane provided that a cut is made along the real axis from $w = -d$ to $w = d$.

In many applications one needs to know the limiting behaviour of $G(d, w)$ as w approaches the real u axis. It is convenient, therefore, to introduce the definitions

$$G^{\pm}(d, u) = \lim_{\epsilon\to 0+} G(u \pm \mathrm{i}\epsilon) \equiv G_{\mathrm{R}}(d, u) \mp \mathrm{i}G_{\mathrm{I}}(d, u) \tag{1.2}$$

where $-\infty < u < \infty$ and ϵ is a positive number. We can use the function $G_{\mathrm{I}}(d, u)$ to express (1.1) in the alternative compact form

$$G(d, w) = \int_{-d}^{d} \frac{\rho(d, u)}{w - u}\,\mathrm{d}u \tag{1.3}$$

where w is any point in the cut (u, v) plane and

$$\rho(d, u) = \frac{1}{\pi} G_{\mathrm{I}}(d, u) \tag{1.4}$$

is a density-of-states function (Wolfram and Callaway 1963, Katsura *et al* 1971).

A series representation for $G(d, w)$ can be established by expanding the integrand in (1.3) in powers of $1/w$. We find that

$$G(d, w) = \frac{1}{w}\sum_{n=0}^{\infty} \mu_{2n}(d)\frac{1}{w^{2n}} \tag{1.5}$$

where $|w| > d$ and

$$\mu_{2n}(d) = 2\int_0^d u^{2n}\rho(d, u)\,\mathrm{d}u. \tag{1.6}$$

It should be noted that the odd moments of the density function $\rho(d, u)$ are zero because $\rho(d, u)$ is an even function of u. An alternative more useful formula for $\mu_{2n}(d)$ can also be obtained by expanding the integrand in (1.1) in powers of $1/w$. This procedure yields

$$\mu_{2n}(d) = \frac{1}{\pi^d}\int_0^{\pi}\cdots\int_0^{\pi} (\cos\theta_1 + \cdots + \cos\theta_d)^{2n}\,\mathrm{d}\theta_1\cdots\mathrm{d}\theta_d. \tag{1.7}$$

In the context of random walk theory (Montroll and Weiss 1965) we can express $\mu_{2n}(d)$ in the further form

$$\mu_{2n}(d) = d^{2n} p_{2n}(d) \tag{1.8}$$

where $p_{2n}(d)$ is the probability that a random walker on the simple hypercubic lattice will return to his starting point (not necessarily for the first time) after a walk of $2n$ nearest-neighbour steps.

From the work of Montroll and Weiss (1965) it is known that $G(d, w)$ exhibits branch-point singularities on the circle of convergence of the moment series (1.5) at the points $w = \pm d$. When d is *odd* the singular behaviour of $G(d, w)$ in the immediate neighbourhood of the points $w = \pm d$ is described by the analytic continuation formula

$$G(d, w) = \pm\left[\sum_{n=0}^{\infty} A_n(d)(\pm w - d)^n + (\pm w - d)^{\frac{1}{2}d-1}\sum_{n=0}^{\infty} B_n(d)(\pm w - d)^n\right] \tag{1.9}$$

while for *d even* we have the alternative formula

$$G(d, w) = \pm\left[\sum_{n=0}^{\infty} C_n(d)(\pm w - d)^n + (\pm w - d)^{\frac{1}{2}d-1}\ln(\pm w - d)\sum_{n=0}^{\infty} D_n(d)(\pm w - d)^n\right] \tag{1.10}$$

where $\{A_n(d), B_n(d), C_n(d), D_n(d) : n = 0, 1, 2, \ldots\}$ are constants which only depend on d. In equations (1.9) and (1.10) the upper signs apply in the neighbourhood of the singular point $w = d$, while the lower signs apply in the neighbourhood of the singular point $w = -d$.

For the case $d = 1$ it readily follows from the simple formula

$$G(1, w) = \frac{1}{w}\left(1 - \frac{1}{w^2}\right)^{-1/2} \tag{1.11}$$

that $\{A_n(1) \equiv 0 : n = 0, 1, 2, \ldots\}$ and

$$B_n(1) = \frac{(-1)^n}{2^n\sqrt{2}} \frac{\left(\frac{1}{2}\right)_n}{n!} \tag{1.12}$$

where $(a)_n$ denotes the Pochhammer symbol and $n = 0, 1, 2, \ldots$. When $d = 2$ we can use the exact result (Katsura and Inawashiro 1971)

$$G(2, w) = \frac{1}{w}{}_2F_1\left(\frac{1}{2}, \frac{1}{2}; 1; \frac{4}{w^2}\right) \tag{1.13}$$

and the second-order differential equation associated with the ${}_2F_1$ hypergeometric function to prove that the coefficients $C_n(2)$, $D_n(2)$ satisfy the recurrence relations:

$$8(n+1)^2 D_{n+1}(2) + 2(3n^2 + 3n + 1)D_n(2) + n^2 D_{n-1}(2) = 0 \tag{1.14}$$

and

$$\begin{aligned}8(n+1)^2 C_{n+1}(2) + 2(3n^2 + 3n + 1)C_n(2) + n^2 C_{n-1}(2) + 16(n+1)D_{n+1}(2)\\ + 6(2n+1)D_n(2) + 2nD_{n-1}(2) = 0\end{aligned} \tag{1.15}$$

where $n = 0, 1, 2, \ldots$. The initial values of $C_0(2)$ and $D_0(2)$ can be determined from the standard analytic properties of the ${}_2F_1$ function in (1.13). It is found that

$$C_0(2) = \frac{2}{\pi}\ln 2 \tag{1.16}$$

$$D_0(2) = -\frac{1}{2\pi}. \tag{1.17}$$

These results and the recurrence relations (1.14) and (1.15) enable one to generate exact values for the coefficients $\{C_n(2), D_n(2) : n = 1, 2, \ldots\}$. Recently, Joyce (2001) has shown that a similar recurrence relation scheme can also be used to generate exact results for the coefficients $\{A_n(3), B_n(3) : n = 0, 1, 2, \ldots\}$.

The main aim in this paper is to derive *general* formulae for $A_n(d), B_n(d)$ and $C_n(d)$, $D_n(d)$ in the expansions (1.9) and (1.10) respectively. The results are used to establish an asymptotic expansion for the random walk probability $p_{2n}(d)$ in powers of $1/n$. Finally, it is shown that this expansion enables one to calculate extremely accurate values for the generalized *d*-dimensional Watson integral.

2. Basic results

We begin by applying the formula

$$\frac{1}{\lambda} = \int_0^\infty \exp(-\lambda t)\,\mathrm{d}t \tag{2.1}$$

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

$$\frac{1}{\pi}\int_0^\pi \exp(t\cos\theta)\,\mathrm{d}\theta = I_0(t) \tag{2.2}$$

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

$$G(d, w) = \int_0^\infty \exp(-wt) I_0^d(t)\,\mathrm{d}t \tag{2.3}$$

where $\mathrm{Re}(w) > d$.

We now follow a procedure which was first developed by Maradudin *et al* (1960) for the case $d = 3$. In particular, we split the range of integration in (2.3) into two intervals $[0, T]$ and $[T, \infty)$ with $T > 0$, and write

$$G(d, w) = J_1(d, T, w) + J_2(d, T, w) \tag{2.4}$$

where

$$J_1(d, T, w) \equiv \int_0^T \exp(-wt) I_0^d(t)\,\mathrm{d}t \tag{2.5}$$

$$J_2(d, T, w) \equiv \int_T^\infty \exp(-wt) I_0^d(t)\,\mathrm{d}t. \tag{2.6}$$

In order to determine the behaviour of $J_1(d, T, w)$ in the immediate neighbourhood of the point $w = d$, we expand the exponential factor in (2.5) as a Taylor series about $w = d$. This procedure yields the required result

$$J_1(d, T, w) = \sum_{n=0}^\infty \frac{(-1)^n}{n!}(w-d)^n \int_0^T t^n \exp(-dt) I_0^d(t)\,\mathrm{d}t. \tag{2.7}$$

It should be noted that $J_1(d, T, w)$ is an *analytic* function at the point $w = d$.

Next we apply the standard asymptotic formula

$$I_0(t) \sim \frac{\exp(t)}{(2\pi t)^{1/2}}\, {}_2F_0\left(\frac{1}{2}, \frac{1}{2}; -; \frac{1}{2t}\right) \tag{2.8}$$

as $t \to \infty$, to the integrand in (2.6), where ${}_2F_0$ is a generalized hypergeometric series. Hence, we obtain the asymptotic representation

$$J_2(d, T, w) \sim \frac{(w-d)^{\frac{1}{2}d-1}}{(2\pi)^{d/2}} \sum_{j=0}^\infty a_j(d)\Gamma\left[-\frac{1}{2}d + 1 - j, T(w-d)\right](w-d)^j \tag{2.9}$$

as $T \to \infty$, where $\Gamma(a, z)$ denotes the incomplete gamma function. The coefficients $\{a_j(d) : j = 0, 1, 2, \ldots\}$ in (2.9) are defined by the formal generating function

$$\left[{}_2F_0\left(\frac{1}{2}, \frac{1}{2}; -; \frac{z}{2}\right)\right]^d = \sum_{j=0}^\infty a_j(d) z^j. \tag{2.10}$$

Explicit formulae for the coefficients $\{a_j(d) : j = 0, 1, 2, \ldots, 5\}$ have been given by Joyce and Zucker (2001). In order to complete the analysis it is necessary to consider the two cases d odd and d even separately.

2.1. Coefficients $A_n(d)$ and $B_n(d)$ for d odd

When $d = 1, 3, 5, \ldots$ we can derive an expansion for $J_2(d, T, w)$ in powers of $w - d$ by applying the formula (Davis 1965)

$$\Gamma(a, z) = \Gamma(a) - z^a \sum_{n=0}^\infty \frac{(-z)^n}{(n+a)n!} \tag{2.11}$$

Table 1. Numerical values of $\{A_n(5) : n = 0, 1, 2, \ldots, 10\}$.

n	$A_n(5)$
0	0.231 261 624 968 046 235 741 427 024 387 713 397 109 085 469 701 028
1	−0.773 976 576 152 940 464 533 831 405 283 196 296 308 355 492 812 747 × 10^{-1}
2	0.959 700 755 773 849 730 065 905 763 800 918 995 361 021 720 304 974 × 10^{-2}
3	−0.124 070 433 372 942 912 213 155 150 795 104 346 543 474 067 393 562 × 10^{-2}
4	0.171 129 040 600 369 909 872 423 604 046 278 565 895 837 639 352 857 × 10^{-3}
5	−0.250 930 253 739 836 185 846 078 704 402 708 507 729 019 230 254 701 × 10^{-4}
6	0.389 001 623 747 206 380 881 268 268 022 686 350 883 098 839 769 690 × 10^{-5}
7	−0.634 079 672 624 924 332 385 394 910 214 928 511 175 547 550 689 334 × 10^{-6}
8	0.108 098 173 407 339 965 561 507 803 434 961 454 875 586 363 794 499 × 10^{-6}
9	−0.191 746 527 196 052 091 260 230 450 074 579 328 601 181 931 621 289 × 10^{-7}
10	0.352 148 803 560 499 158 697 065 730 842 215 470 802 193 438 684 315 × 10^{-8}

to (2.9), where $|z| < \infty$ and $|\arg(z)| < \pi$. We now substitute this expansion for $J_2(d, T, w)$ and the expansion (2.7) for $J_1(d, T, w)$ in (2.4). Finally, we take the limit $T \to \infty$ in the asymptotic formula for $G(d, w)$ and make a comparison with (1.9). In this manner, we find that

$$B_n(d) = \frac{(-1)^{(d-1)/2}\pi}{(2\pi)^{d/2}} \frac{(-1)^n a_n(d)}{\Gamma\left(n + \frac{1}{2}d\right)} \tag{2.12}$$

and

$$A_n(d) = \lim_{T\to\infty} \left[U_n(d, T) + \frac{(-1)^n T^{n+1}}{(2\pi T)^{d/2} n!} \sum_{j=0}^{M} \frac{a_j(d)}{\left(j + \frac{1}{2}d - n - 1\right) T^j} \right] \tag{2.13}$$

where

$$U_n(d, T) \equiv \frac{(-1)^n}{n!} T^{n+1} \int_0^1 u^n \exp(-dTu) I_0^d(Tu)\, \mathrm{d}u \tag{2.14}$$

$M \geqslant \max(0, n + 1 - [d/2])$ and $[a]$ is the largest integer less than or equal to a. Formula (2.12) enables one to derive *exact* values for $\{B_n(d) : n = 0, 1, 2, \ldots\}$ when d is any positive odd integer.

The expression on the right-hand side of (2.13) has been used to determine the numerical values of $\{A_n(d) : n = 0, 1, 2, \ldots\}$ for various odd values of $d \geqslant 1$. In particular, $U_n(d, 8000)$ was first calculated for given values of d and n with an accuracy of 100 digits using *Mathematica* (Wolfram 1991) and the terms in the truncated asymptotic series were then summed until their contribution to the value of $A_n(d)$ was less than 10^{-100}. It should be noted that when $n \geqslant [d/2]$ the leading-order terms in the truncated series in (2.13) will tend to infinity as $T \to \infty$. This property will lead to a large rounding error in the calculated value of $A_n(d)$, especially for $n \gg [d/2]$. In table 1 the final results for $\{A_n(5) : n = 0, 1, 2, \ldots, 10\}$ are listed with an accuracy of 51 digits after the decimal point in unrounded form.

The numerical values of the coefficients $\{A_n(3) : n = 0, 1, 2, \ldots\}$ have also been determined using (2.13) and agreement was found with the exact recurrence relation method developed by Joyce (2001).

2.2. Coefficients $C_n(d)$ and $D_n(d)$ for d even

When $d = 2, 4, 6, \ldots$ we can derive formulae for the coefficients $C_n(d)$ and $D_n(d)$ in (1.10) by following a similar procedure to that described in subsection 2.1. However, for this case (2.11)

Table 2. Numerical values of $\{C_n(4) : n = 0, 1, 2, \ldots, 10\}$.

n	$C_n(4)$
0	0.309 866 780 462 120 428 169 674 416 214 750 177 538 322 267 290 439
1	−0.103 825 397 195 273 302 515 146 683 443 075 515 078 940 615 274 711
2	0.178 180 138 599 791 569 202 095 513 776 168 246 898 750 588 143 251 × 10^{-1}
3	−0.338 599 199 333 426 839 146 857 947 507 583 324 476 386 945 045 057 × 10^{-2}
4	0.731 937 444 756 344 362 648 753 634 053 480 233 880 101 878 457 170 × 10^{-3}
5	−0.180 319 928 883 781 312 026 766 508 830 400 413 073 923 341 895 442 × 10^{-3}
6	0.502 062 536 829 980 618 696 028 272 994 053 079 392 491 636 529 977 × 10^{-4}
7	−0.155 339 074 181 472 711 051 831 696 600 319 403 714 756 109 971 929 × 10^{-4}
8	0.523 093 428 400 629 800 316 463 244 957 894 225 116 714 126 562 147 × 10^{-5}
9	−0.187 960 612 217 849 410 775 478 204 467 817 002 690 300 544 005 016 × 10^{-5}
10	0.709 183 103 240 333 399 997 297 572 287 634 244 320 460 039 324 084 × 10^{-6}

is no longer valid because the parameter $a = -N$, where $N = 0, 1, 2, \ldots$ and it is necessary to use the alternative formula

$$\Gamma(-N, x) = \frac{(-1)^N}{N!}[\psi(N+1) - \ln x] - x^{-N} {\sum_{m=0}^{\infty}}' \frac{(-x)^m}{(m-N)m!} \tag{2.15}$$

where $\psi(z)$ is the digamma function and the prime on the summation sign indicates that the term $m = N$ must be excluded. The final result for the coefficient $D_n(d)$ is

$$D_n(d) = \left(-\frac{1}{2\pi}\right)^{d/2} \frac{(-1)^n a_n(d)}{\Gamma\left(n + \frac{1}{2}d\right)}. \tag{2.16}$$

For the coefficient $C_n(d)$ we find that

$$C_n(d) = \lim_{T\to\infty}\left\{U_n(d, T) + \frac{(-1)^n T^{n+1}}{(2\pi T)^{d/2} n!} {\sum_{j=0}^{M}}' \frac{a_j(d)}{\left(j + \frac{1}{2}d - n - 1\right) T^j} \right.$$
$$\left. + \frac{(-1)^n}{(2\pi)^{d/2} n!} a_{n-\frac{1}{2}d+1}(d)[\psi(n+1) - \ln T]\right\} \tag{2.17}$$

where $M \geqslant \max\left(0, n + 2 - \frac{1}{2}d\right)$ and the prime on the summation sign indicates that when $n \geqslant \frac{1}{2}d - 1$ we must exclude the term $j = n - \frac{1}{2}d + 1$. In formula (2.17) we have also defined $\{a_{-k}(d) \equiv 0 : k = 1, 2, \ldots\}$.

The expression on the right-hand side of (2.17) has been used to determine the numerical values of $\{C_n(d) : n = 0, 1, 2, \ldots\}$ for various even values of $d \geqslant 2$ by following the procedure described in subsection 2.1. In table 2 the final results for $\{C_n(4) : n = 0, 1, 2, \ldots, 10\}$ are listed with an accuracy of 51 digits after the decimal point in unrounded form.

The numerical values of the coefficients $\{C_n(2) : n = 0, 1, 2, \ldots\}$ have also been determined using (2.17). It was found that the results were consistent with the exact recurrence relations (1.14) and (1.15).

3. Asymptotic expansion for $p_{2n}(d)$ as $n \to \infty$

The analytic continuation formulae (1.9) and (1.10) enable one to analyse the critical behaviour of many lattice statistical models of phase transitions such as the Gaussian and spherical models of ferromagnetism (Berlin and Kac 1952, Joyce 1972). They also have important applications in the theory of random walks on the d-dimensional hypercubic lattice (Montroll and Weiss 1965).

In this section we shall demonstrate how (1.9) and (1.10) can be used to investigate the asymptotic behaviour of the return probability $p_{2n}(d)$ as $n \to \infty$. We begin the analysis by considering the probability generating function (Montroll and Weiss 1965)

$$P(d, z) = \sum_{n=0}^{\infty} p_{2n}(d) z^{2n} \qquad |z| < 1. \tag{3.1}$$

It follows from (1.5) and (1.8) that

$$P(d, z) = \left(\frac{d}{z}\right) G\left(d, \frac{d}{z}\right). \tag{3.2}$$

Next we determine the singular behaviour of $P(d, z)$ in the neighbourhood of $z = \pm 1$ by applying the relation (3.2) to the expansions (1.9) and (1.10). When d is odd we find that

$$P(d, z) = \sum_{n=0}^{\infty} \widetilde{A}_n(d)(1 \pm z)^n + (1 \pm z)^{\frac{1}{2}d-1} \sum_{n=0}^{\infty} \widetilde{B}_n(d)(1 \pm z)^n \tag{3.3}$$

where

$$\widetilde{A}_n(d) = d \sum_{m=0}^{n} \frac{d^m (m+1)_{n-m}}{(n-m)!} A_m(d) \tag{3.4}$$

and

$$\widetilde{B}_n(d) = d^{d/2} \sum_{m=0}^{n} \frac{d^m \left(m + \frac{1}{2}d\right)_{n-m}}{(n-m)!} B_m(d). \tag{3.5}$$

For the case d even we have the alternative form

$$P(d, z) = \sum_{n=0}^{\infty} \widetilde{C}_n(d)(1 \pm z)^n + (1 \pm z)^{\frac{1}{2}d-1} \ln(1 \pm z) \sum_{n=0}^{\infty} \widetilde{D}_n(d)(1 \pm z)^n \tag{3.6}$$

where

$$\begin{aligned} \widetilde{C}_n(d) = {} & d \sum_{m=0}^{n} \frac{d^m (m+1)_{n-m}}{(n-m)!} C_m(d) + d^{d/2} \ln(d) \sum_{m=0}^{n-\frac{1}{2}d+1} \frac{d^m \left(m + \frac{1}{2}d\right)_{n-\frac{1}{2}d+1-m}}{\left(n - \frac{1}{2}d + 1 - m\right)!} D_m(d) \\ & + d^{d/2} \sum_{k=0}^{n-\frac{1}{2}d} \sum_{m=0}^{n-\frac{1}{2}d-k} \frac{d^m \left(m + \frac{1}{2}d\right)_{n-\frac{1}{2}d-m-k}}{(k+1)\left(n - \frac{1}{2}d - m - k\right)!} D_m(d). \end{aligned} \tag{3.7}$$

and

$$\widetilde{D}_n(d) = d^{d/2} \sum_{m=0}^{n} \frac{d^m \left(m + \frac{1}{2}d\right)_{n-m}}{(n-m)!} D_m(d). \tag{3.8}$$

In equations (3.3) and (3.6) the upper signs apply in the neighbourhood of the singular point $z = -1$, while the lower signs apply in the neighbourhood of the singular point $z = 1$. It should also be noted that if a summation in (3.7) has an upper limit which is equal to a negative integer then its value is taken to be zero.

We now restrict our attention to the case d odd and apply the method of Darboux (see Dingle 1973) to the analytic continuation formula (3.3). In this manner we obtain the asymptotic representation

$$p_{2n}(d) \sim 2 \sum_{m=0}^{\infty} \binom{m + \frac{1}{2}d - 1}{2n} \widetilde{B}_m(d) \tag{3.9}$$

as $n \to \infty$ and $d = 1, 3, 5, \ldots$. Next the standard result (Luke 1969)

$$\binom{x}{n} \sim (-1)^n \frac{n^{-(x+1)}}{\Gamma(-x)} \sum_{k=0}^{\infty} \frac{(x+1)_k}{n^k k!} B_k^{(-x)} \tag{3.10}$$

as $n \to \infty$, is substituted in (3.9), where $B_k^{(a)}$ is a generalized Bernoulli number. This procedure yields the required asymptotic expansion

$$p_{2n}(d) \sim 2\left(\frac{d}{4\pi n}\right)^{d/2} \sum_{t=0}^{\infty} \frac{Q_t(d)}{(2n)^t} \tag{3.11}$$

as $n \to \infty$, where

$$Q_t(d) = \sum_{m=0}^{t} \frac{(-1)^m B_{t-m}^{(-m-\frac{1}{2}d+1)}}{(t-m)!} \sum_{j=0}^{m} \frac{(-d)^j \left(j+\frac{1}{2}d\right)_{m-j} \left(j+\frac{1}{2}d\right)_{t-j} a_j(d)}{(m-j)!} \tag{3.12}$$

and $d = 1, 3, 5, \ldots$. In the appendix we list formulae for $\{Q_t(d) : t = 0, 1, 2, \ldots, 10\}$. We can carry out a similar analysis for the case d even by applying the method of Darboux to (3.6). It is found that the basic formulae (3.11) and (3.12) *also remain valid* when $d = 2, 4, 6, \ldots$.

A check on the asymptotic expansion (3.11) can be carried out by considering the special case $d = 2$. In particular, we can use (1.13) and (3.2) to show that

$$p_{2n}(2) = \binom{-\frac{1}{2}}{n}^2. \tag{3.13}$$

The application of (3.10) to (3.13) then yields the alternative formula

$$Q_t(2) = \frac{2^t \left(\frac{1}{2}\right)_t}{t!} \sum_{m=0}^{t} \frac{(-t)_m \left(\frac{1}{2}\right)_m}{m! \left(\frac{1}{2}-t\right)_m} B_m^{(\frac{1}{2})} B_{t-m}^{(\frac{1}{2})}. \tag{3.14}$$

We have used (3.14) to calculate the values of $\{Q_t(2) : t = 0, 1, 2, \ldots\}$ and the results were found to be in agreement with those derived from (3.12) with $d = 2$.

When $d = 1$ it is possible to evaluate the second summation in (3.12) in closed form. In this manner we obtain the simplified result

$$Q_t(1) = \frac{\left(\frac{1}{2}\right)_t}{t!} \sum_{m=0}^{t} \frac{(-t)_m \left(\frac{1}{2}\right)_m}{2^m m!} B_{t-m}^{(-m+\frac{1}{2})}. \tag{3.15}$$

However, we can also determine $Q_t(1)$ by applying (3.10) to the well-known formula

$$p_{2n}(1) = (-1)^n \binom{-\frac{1}{2}}{n}. \tag{3.16}$$

Hence we find that

$$Q_t(1) = \frac{2^t \left(\frac{1}{2}\right)_t}{t!} B_t^{(\frac{1}{2})}. \tag{3.17}$$

If formulae (3.15) and (3.17) are compared we obtain the unusual mathematical identity

$$B_t^{(\frac{1}{2})} = \frac{1}{2^t} \sum_{m=0}^{t} \frac{(-t)_m \left(\frac{1}{2}\right)_m}{2^m m!} B_{t-m}^{(-m+\frac{1}{2})}. \tag{3.18}$$

Finally, we note that Domb (1954) has investigated the asymptotic behaviour of $p_{2n}(d)$ as $n \to \infty$ by applying the method of Laplace to the multiple integral in (1.8). The disadvantage of this approach is that it involves a large amount of complicated multivariable algebra and it does not lead to a closed-form expression for the coefficient $Q_t(d)$ in the expansion (3.11).

4. Generalized *d*-dimensional Watson integrals

It will now be shown how the asymptotic expansion (3.11) can be used to determine extremely accurate values for the generalized *d*-dimensional Watson integral

$$W_d(s) \equiv \frac{1}{\pi^d}\int_0^\pi \cdots \int_0^\pi [d - (\cos\theta_1 + \cdots + \cos\theta_d)]^s \, \mathrm{d}\theta_1 \cdots \mathrm{d}\theta_d \tag{4.1}$$

where $s > -d/2$ and $s \neq 1, 2, \ldots$. We begin by applying the binomial expansion theorem to the integrand in (4.1). This procedure yields

$$W_d(s) = d^s \sum_{n=0}^{\infty} \binom{s}{2n} p_{2n}(d). \tag{4.2}$$

Next we write (4.2) in the form

$$W_d(s) = d^s \left[\sum_{n=0}^{J-1} \binom{s}{2n} p_{2n}(d) + \sum_{n=J}^{\infty} \binom{s}{2n} p_{2n}(d) \right] \tag{4.3}$$

where J is taken to be a *large* positive integer.

The binomial coefficient and $p_{2n}(d)$ in the second sum in (4.3) are now replaced by the asymptotic expansions (3.10) and (3.11) respectively. After some rearrangement of the series we obtain the required result

$$W_d(s) = \lim_{J\to\infty} \left[d^s \sum_{n=0}^{J-1} \binom{s}{2n} p_{2n}(d) + \frac{1}{2^s \Gamma(-s)} \left(\frac{d}{4\pi}\right)^{d/2} \times \sum_{m=0}^{L} \zeta\left(m + 1 + s + \frac{d}{2}, J\right) H_m(d, s) \right] \tag{4.4}$$

where $\zeta(u, v)$ denotes the generalized zeta function,

$$H_m(d, s) = \frac{d^s}{2^m} \sum_{t=0}^{m} \frac{(s+1)_{m-t}}{(m-t)!} B_{m-t}^{(-s)} Q_t(d) \tag{4.5}$$

and L is any fixed non-negative integer.

We have used the expression on the right-hand side of (4.4) with $J = 1200$ and $L = 50$ to determine the numerical value of the $W_3(1/2)$. The final result, in unrounded form, is

$$\begin{aligned} W_3(1/2) = 1.&688\,289\,736\,702\,226\,504\,976\,422\,397\,009\,472\,719\,095\,560\,398\,997\,965 \\ &169\,226\,641\,383\,944\,938\,324\,486\,268\,240\,541\,119\,113\,654\,611\,721\,128 \\ &215\,360\,609\,043\,835\,54\ldots . \end{aligned} \tag{4.6}$$

The integral $W_d(1/2)$ is of some importance in a lattice dynamical model which was solved exactly by Montroll (1956). In this idealized model N identical particles of mass M interact with only nearest-neighbour harmonic forces on a *d*-dimensional hypercubic lattice. It was shown by Montroll that the quantum mechanical zero-point energy E_0 for this model is expressible in the reduced form

$$\left(\frac{2M}{\gamma}\right)^{1/2} \frac{E_0}{\hbar N} = W_d(1/2) \tag{4.7}$$

where γ is the nearest-neighbour force constant.

It has also been checked that formula (4.4) gives the correct numerical value for the well-known integral (Watson 1939)

$$W_3(-1) = \left(18 + 12\sqrt{2} - 10\sqrt{3} - 7\sqrt{6}\right) \left[\frac{2}{\pi} K\left(\left(2 - \sqrt{3}\right)\left(\sqrt{3} - \sqrt{2}\right)\right)\right]^2 \tag{4.8}$$

where $K(k)$ denotes the complete elliptic integral of the first kind with a modulus k.

Appendix. Formulae for the coefficients $\{Q_t(d) : t = 0, 1, 2, \ldots, 10\}$

$$Q_0(d) = 1$$

$$Q_1(d) = -\frac{d}{4}$$

$$Q_2(d) = \frac{d}{96}(4 - 3d + 2d^2)$$

$$Q_3(d) = \frac{d^2}{128}(12 - 9d + 2d^2)$$

$$Q_4(d) = -\frac{d}{92\,160}(384 + 11\,440d - 21\,480d^2 + 13\,105d^3 - 2484d^4 - 20d^5)$$

$$Q_5(d) = \frac{d^2}{73\,728}(9600 - 48\,080d + 57\,336d^2 - 26\,783d^3 + 4308d^4 + 28d^5)$$

$$\begin{aligned} Q_6(d) = \frac{d}{185\,794\,560}&(368\,640 - 23\,256\,576d + 294\,330\,176d^2 - 638\,044\,848d^3 \\ &+ 548\,326\,380d^4 - 208\,375\,839d^5 + 28\,969\,494d^6 + 145\,908d^7 + 280d^8) \end{aligned}$$

$$\begin{aligned} Q_7(d) = \frac{d^2}{106\,168\,320}&(12\,902\,400 - 374\,376\,960d + 1\,418\,461\,120d^2 - 2\,004\,204\,816d^3 \\ &+ 1\,338\,160\,740d^4 - 427\,532\,445d^5 + 52\,318\,470d^6 + 197\,676d^7 + 440d^8) \end{aligned}$$

$$\begin{aligned} Q_8(d) = -\frac{d}{356\,725\,555\,200}&(743\,178\,240 + 44\,558\,106\,624d - 2\,664\,102\,481\,920d^2 \\ &+ 17\,068\,299\,864\,320d^3 - 37\,450\,664\,240\,640d^4 + 39\,108\,629\,715\,232d^5 \\ &- 21\,319\,970\,933\,520d^6 + 5\,869\,656\,474\,105d^7 - 641\,112\,913\,800d^8 \\ &- 1\,809\,398\,456d^9 - 3\,732\,960d^{10} - 2800d^{11}) \end{aligned}$$

$$\begin{aligned} Q_9(d) = \frac{d^2}{475\,634\,073\,600}&(61\,683\,793\,920 - 7\,325\,487\,710\,208d + 77\,090\,128\,957\,440d^2 \\ &- 253\,582\,218\,056\,960d^3 + 389\,354\,678\,182\,400d^4 - 321\,897\,397\,752\,224d^5 \\ &+ 148\,178\,495\,110\,800d^6 - 35\,826\,809\,146\,965d^7 + 3\,532\,333\,021\,080d^8 \\ &+ 7\,511\,314\,232d^9 + 13\,084\,960d^{10} + 14\,000d^{11}) \end{aligned}$$

$$\begin{aligned} Q_{10}(d) = \frac{d}{376\,702\,186\,291\,200}&(1\,426\,902\,220\,800 - 47\,123\,587\,399\,680d \\ &+ 11\,802\,678\,455\,107\,584d^2 - 199\,162\,900\,657\,864\,704d^3 \\ &+ 958\,124\,727\,510\,725\,632d^4 - 2\,082\,070\,618\,279\,238\,400d^5 \\ &+ 2\,450\,443\,462\,388\,808\,832d^6 - 1\,675\,452\,415\,814\,936\,352d^7 \\ &+ 667\,321\,990\,357\,286\,836d^8 - 143\,817\,610\,864\,969\,635d^9 \\ &+ 12\,919\,114\,945\,471\,514d^{10} + 21\,013\,640\,968\,056d^{11} \\ &+ 29\,519\,821\,232d^{12} + 33\,319\,440d^{13} + 12\,320d^{14}). \end{aligned}$$

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