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Singular behaviour of the cubic lattice Green functions and associated integrals

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Abstract

The behaviour of the three cubic lattice Green functions

$$G_j(w) = \frac{1}{\pi^3}\int_0^\pi\int_0^\pi\int_0^\pi \frac{d\theta_1\, d\theta_2\, d\theta_3}{w-\lambda_j(\theta_1,\theta_2,\theta_3)} \qquad (j=1,2,3)$$

where

$$\lambda_1(\theta_1,\theta_2,\theta_3) = \tfrac{1}{3}(\cos\theta_1+\cos\theta_2+\cos\theta_3)$$
$$\lambda_2(\theta_1,\theta_2,\theta_3) = \cos\theta_1\cos\theta_2\cos\theta_3$$
$$\lambda_3(\theta_1,\theta_2,\theta_3) = \tfrac{1}{3}(\cos\theta_1\cos\theta_2+\cos\theta_2\cos\theta_3+\cos\theta_3\cos\theta_1)$$

is determined in the neighbourhood of the singular point $w = 1$. The results are used to investigate the singular behaviour of the associated integrals

$$L_j(w) = \frac{1}{\pi^3}\int_0^\pi\int_0^\pi\int_0^\pi \ln\left[w-\lambda_j(\theta_1,\theta_2,\theta_3)\right] d\theta_1\, d\theta_2\, d\theta_3 \qquad (j=1,2,3).$$

Finally, a new method is developed which enables one to calculate the numerical values of the constants $\{L_j(1) : j = 1, 2, 3\}$ with extremely high precision.

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1. Introduction

We define the lattice Green functions at the origin for the simple cubic (sc), body-centred cubic (bcc) and face-centred cubic (fcc) lattices as

$$\text{sc}: \quad G_1(w) = \frac{1}{\pi^3}\int_0^\pi\int_0^\pi\int_0^\pi \frac{d\theta_1\, d\theta_2\, d\theta_3}{w-\frac{1}{3}(\cos\theta_1+\cos\theta_2+\cos\theta_3)} \tag{1.1}$$

$$\text{bcc}: \quad G_2(w) = \frac{1}{\pi^3}\int_0^\pi\int_0^\pi\int_0^\pi \frac{d\theta_1\, d\theta_2\, d\theta_3}{w-\cos\theta_1\cos\theta_2\cos\theta_3} \tag{1.2}$$

$$\text{fcc}: \quad G_3(w) = \frac{1}{\pi^3}\int_0^\pi\int_0^\pi\int_0^\pi \frac{d\theta_1\, d\theta_2\, d\theta_3}{w-\frac{1}{3}(\cos\theta_1\cos\theta_2+\cos\theta_2\cos\theta_3+\cos\theta_3\cos\theta_1)} \tag{1.3}$$

where w is a complex variable in a suitably cut w plane. For $G_1(w)$ and $G_2(w)$ the cut is made along the real axis from $w = -1$ to $w = 1$, while the cut for $G_3(w)$ is made from $w = -1/3$ to $w = 1$. The functions (1.1)–(1.3) appear in the theory of lattice vibrations (Montroll 1956) and in many lattice statistical models of phase transitions such as the Gaussian and spherical models of ferromagnetism (Berlin and Kac 1952, Joyce 1972), while in the theory of random walks on cubic lattices they play a fundamental role as probability generating functions (Montroll and Weiss 1965).

Series representations for $\{G_j(w) : j = 1, 2, 3\}$ can be obtained by expanding the integrands in (1.1)–(1.3) in inverse powers of w and then integrating term-by-term. It is found that

$$G_j(w) = \frac{1}{w}\sum_{n=0}^{\infty}\frac{p_n^{(j)}}{w^n} \qquad (j = 1, 2, 3) \tag{1.4}$$

where $1 \leqslant |w| < \infty$,

$$p_n^{(j)} = \frac{1}{\pi^3}\int_0^{\pi}\int_0^{\pi}\int_0^{\pi}\left[\lambda_j\,(\theta_1, \theta_2, \theta_3)\right]^n \mathrm{d}\theta_1\,\mathrm{d}\theta_2\,\mathrm{d}\theta_3 \qquad (j = 1, 2, 3) \tag{1.5}$$

and

$$\lambda_1\,(\theta_1, \theta_2, \theta_3) = \tfrac{1}{3}\,(\cos\theta_1 + \cos\theta_2 + \cos\theta_3) \tag{1.6}$$

$$\lambda_2\,(\theta_1, \theta_2, \theta_3) = \cos\theta_1\cos\theta_2\cos\theta_3 \tag{1.7}$$

$$\lambda_3\,(\theta_1, \theta_2, \theta_3) = \tfrac{1}{3}\,(\cos\theta_1\cos\theta_2 + \cos\theta_2\cos\theta_3 + \cos\theta_3\cos\theta_1)\,. \tag{1.8}$$

We also note that $p_n^{(1)}$ and $p_n^{(2)}$ are both equal to zero when n is an odd integer and $\{p_1^{(j)} = 0 : j = 1, 2, 3\}$. In random walk theory the quantity $p_n^{(j)}$ gives the probability that a random walker on the jth cubic lattice will return to his starting point (not necessarily for the first time) after a walk of n nearest-neighbour steps.

If one wishes to analyse the asymptotic properties of random walks on cubic lattices or the critical behaviour of the Gaussian and spherical models then it is necessary to determine the singular behaviour of $\{G_j(w) : j = 1, 2, 3\}$ as $w \to 1+$. In this limit the expansions (1.4) become slowly convergent and they do not exhibit the singularity structure of $\{G_j(w) : j = 1, 2, 3\}$ at $w = 1$. Montroll and Weiss (1965) overcame these difficulties by constructing analytic continuation formulae of the type

$$G_j(w) = \sum_{n=0}^{\infty} A_n^{(j)}\,(w-1)^n - \sum_{n=0}^{\infty} B_n^{(j)}\,(w-1)^{n+1/2} \qquad (j = 1, 2, 3) \tag{1.9}$$

where the variable w lies in a sufficiently small neighbourhood of the singularity $w = 1$ and $\{A_n^{(j)}, B_n^{(j)} : n = 0, 1, 2, \ldots\}$ are constants. There are also similar series expansions for $G_1(w)$ and $G_2(w)$ in powers of $-(w + 1)$ which are valid in the neighbourhood of the singularity at $w = -1$.

The main aim in this paper is to derive recurrence relations for the series coefficients $\{p_n^{(j)} : j = 1, 2, 3\}$ and $\{A_n^{(j)}, B_n^{(j)} : j = 1, 2, 3\}$ which occur in (1.4) and (1.9) respectively. These results are then used to investigate the singular behaviour of the three associated integrals

$$L_j(w) = \frac{1}{\pi^3}\int_0^{\pi}\int_0^{\pi}\int_0^{\pi}\ln\left[w - \lambda_j\,(\theta_1, \theta_2, \theta_3)\right]\mathrm{d}\theta_1\,\mathrm{d}\theta_2\,\mathrm{d}\theta_3 \qquad (j = 1, 2, 3) \tag{1.10}$$

in the neighbourhood of $w = 1$. In particular, a new method is developed which can be used to calculate the numerical values of $\{L_j(1) : j = 1, 2, 3\}$ with extremely high accuracy. The functions $\{L_j(w) : j = 1, 2, 3\}$ with $1 \leqslant w < \infty$ occur in the formulae for the free energy of the Gaussian and spherical models (Berlin and Kac 1952, Joyce 1972), while the constant $L_1(1)$ is involved in the calculation of the number of spanning trees on the sc lattice (Rosengren 1987) and in the theory of collapsing branched polymers (Madras *et al* 1990).

2. Recurrence relations for the sc coefficients $p_{2n}^{(1)}$, $A_n^{(1)}$ and $B_n^{(1)}$

From the work of Joyce (1973) it is known that the probabilities $\{p_{2n}^{(1)} : n = 0, 1, 2, \ldots, \}$ for the sc lattice satisfy the recurrence relation

$$36(n+1)^3 p_{2n+2}^{(1)} - 2(2n+1)\left(10n^2+10n+3\right) p_{2n}^{(1)} + n\left(4n^2-1\right) p_{2n-2}^{(1)} = 0 \tag{2.1}$$

where $n = 0, 1, 2, \ldots,$ with the initial conditions $p_0^{(1)} = 1$ and $p_{-2}^{(1)} = 0$. It follows from this result and (1.4) that the sc Green function $G_1(w)$ is a solution of the linear third-order differential equation

$$\left(w^2-1\right)\left(9w^2-1\right)\frac{\mathrm{d}^3G_1}{\mathrm{d}w^3} + 6w\left(9w^2-5\right)\frac{\mathrm{d}^2G_1}{\mathrm{d}w^2} + 3\left(21w^2-4\right)\frac{\mathrm{d}G_1}{\mathrm{d}w} + 9wG_1 = 0. \tag{2.2}$$

Next we determine the general series solution of (2.2) which is valid in the neighbourhood of the regular singular point $w = 1$. In this manner, we find that $\{A_n^{(1)} : n = 0, 1, 2, \ldots\}$ satisfy the recurrence relation

$$8n(n+1)(2n+1)A_{n+1}^{(1)} + n\left(44n^2+7\right)A_n^{(1)} + 9(2n-1)\left(2n^2-2n+1\right)A_{n-1}^{(1)} + 9(n-1)^3A_{n-2}^{(1)} = 0 \tag{2.3}$$

where $n = 1, 2, 3, \ldots,$ with $A_{-1}^{(1)} = 0$, while the recurrence relation for the coefficients $\{B_n^{(1)} : n = 0, 1, 2, \ldots\}$ is given by

$$32(n+1)(2n+1)(2n+3)B_{n+1}^{(1)} + 8(2n+1)\left(22n^2+22n+9\right)B_n^{(1)} + 72n\left(4n^2+1\right)B_{n-1}^{(1)} + 9(2n-1)^3B_{n-2}^{(1)} = 0 \tag{2.4}$$

where $n = 0, 1, 2, \ldots,$ with $B_{-1}^{(1)} = 0$ and $B_{-2}^{(1)} = 0$. It is clear that we can use the relations (2.3) and (2.4) to generate the values of the coefficients $\{A_n^{(1)} : n = 2, 3, \ldots\}$ and $\{B_n^{(1)} : n = 1, 2, \ldots\}$, provided that the values of $A_0^{(1)}$, $A_1^{(1)}$ and $B_0^{(1)}$ are known.

These initial values can be determined by expanding the formula (Joyce 1998, p 5113)

$$G_1(w) = \frac{\left(1-9\xi^4\right)}{w(1-\xi)^3(1+3\xi)}\left[\frac{2}{\pi}K(k_1)\right]^2 \tag{2.5}$$

in powers of $w - 1$, where

$$k_1^2 = k_1^2(\xi) = \frac{16\xi^3}{(1-\xi)^3(1+3\xi)} \tag{2.6}$$

$$\xi = \xi(w) = \left(1+\sqrt{1-\frac{1}{w^2}}\right)^{-1/2}\left(1-\sqrt{1-\frac{1}{9w^2}}\right)^{1/2} \tag{2.7}$$

and $K(k)$ is the complete elliptic integral of the first kind with a modulus k. This procedure eventually yields the following results:

$$A_0^{(1)} = G_1(1) \tag{2.8}$$

$$A_1^{(1)} = -\frac{1}{16}\left[7G_1(1) - \frac{54}{\pi^2 G_1(1)}\right] \tag{2.9}$$

$$B_0^{(1)} = \frac{3\sqrt{3}}{\pi\sqrt{2}}. \tag{2.10}$$

Watson (1939) has proved that $G_1(1)$ can be expressed in the form

$$G_1(1) = 3\left(18+12\sqrt{2}-10\sqrt{3}-7\sqrt{6}\right)\left[\frac{2}{\pi}K\left(\left(2-\sqrt{3}\right)\left(\sqrt{3}-\sqrt{2}\right)\right)\right]^2. \tag{2.11}$$

3. Recurrence relations for the bcc coefficients $p_{2n}^{(2)}$, $A_n^{(2)}$ and $B_n^{(2)}$

For the bcc lattice we have the simple formula

$$p_{2n}^{(2)} = \left[\left(\tfrac{1}{2}\right)_n / n!\right]^3 \tag{3.1}$$

where $n = 0, 1, 2, \ldots$, and $(a)_n$ is the Pochhammer symbol. From this result we readily obtain the recurrence relation

$$8(n+1)^3 p_{2n+2}^{(2)} = (2n+1)^3 p_{2n}^{(2)} \tag{3.2}$$

where $n = 0, 1, 2, \ldots$, with the initial condition $p_0^{(2)} = 1$. If the formula (3.1) is substituted in (1.4) it is seen that (Katsura and Horiguchi 1971, Joyce 1971)

$$G_2(w) = \frac{1}{w}\, {}_3F_2\left(\frac{1}{2}, \frac{1}{2}, \frac{1}{2}; 1, 1; \frac{1}{w^2}\right) \tag{3.3}$$

where ${}_3F_2$ denotes a generalized hypergeometric function. It follows from this result that $G_2(w)$ is a solution of the linear third-order differential equation

$$w^2\left(w^2-1\right)\frac{\mathrm{d}^3G_2}{\mathrm{d}w^3} + 3w\left(2w^2-1\right)\frac{\mathrm{d}^2G_2}{\mathrm{d}w^2} + \left(7w^2-1\right)\frac{\mathrm{d}G_2}{\mathrm{d}w} + wG_2 = 0. \tag{3.4}$$

We now derive the general series solution of (3.4) which is valid in the neighbourhood of the regular singular point $w = 1$. In this manner, we find that $\{A_n^{(2)} : n = 0, 1, 2, \ldots\}$ satisfy the recurrence relation

$$n(n+1)(2n+1)A_{n+1}^{(2)} + n\left(5n^2+1\right)A_n^{(2)} + (2n-1)\left(2n^2-2n+1\right)A_{n-1}^{(2)} + (n-1)^3 A_{n-2}^{(2)} = 0 \tag{3.5}$$

where $n = 1, 2, 3, \ldots$, with $A_{-1}^{(2)} = 0$, while the recurrence relation for the coefficients $\{B_n^{(2)} : n = 0, 1, 2, \ldots\}$ is given by

$$4(n+1)(2n+1)(2n+3)B_{n+1}^{(2)} + (2n+1)\left(20n^2+20n+9\right)B_n^{(2)} + 8n\left(4n^2+1\right)B_{n-1}^{(2)} + (2n-1)^3 B_{n-2}^{(2)} = 0 \tag{3.6}$$

where $n = 0, 1, 2, \ldots$, with $B_{-1}^{(2)} = 0$ and $B_{-2}^{(2)} = 0$. The relations (3.5) and (3.6) can be used to generate the values of $\{A_n^{(2)} : n = 2, 3, \ldots\}$ and $\{B_n^{(2)} : n = 1, 2, \ldots\}$, provided that the values of $A_0^{(2)}$, $A_1^{(2)}$ and $B_0^{(2)}$ are known.

We can determine these initial values by expanding the formula (Maradudin *et al* 1960)

$$G_2(w) = \frac{1}{w}\left[\frac{2}{\pi}K(k_2)\right]^2 \tag{3.7}$$

in powers of $w - 1$, where

$$k_2^2 = k_2^2(w) = \frac{1}{2} - \frac{1}{2}\sqrt{1 - \frac{1}{w^2}}. \tag{3.8}$$

The final results are

$$A_0^{(2)} = G_2(1) \tag{3.9}$$

$$A_1^{(2)} = -\frac{1}{2}\left[G_2(1) - \frac{4}{\pi^2 G_2(1)}\right] \tag{3.10}$$

$$B_0^{(2)} = \frac{2\sqrt{2}}{\pi} \tag{3.11}$$

with

$$G_2(1) = \left[\frac{2}{\pi}K\left(\frac{1}{\sqrt{2}}\right)\right]^2. \tag{3.12}$$

4. Recurrence relations for the fcc coefficients $p_n^{(3)}$, $A_n^{(3)}$ and $B_n^{(3)}$

The derivation of the recurrence relations for the fcc lattice Green function $G_3(w)$ is rather more complicated. We begin the analysis by considering the exact formula (Joyce 1994, p 472)

$$[wG_3(w)]^{1/2} = \frac{(1-3\rho)}{\left(1-6\rho-3\rho^2\right)^{1/2}}\ {}_2F_1\left[\frac{1}{4},\frac{3}{4};1;\frac{64\rho^3}{\left(1-6\rho-3\rho^2\right)^2}\right] \tag{4.1}$$

where

$$\rho = \rho(w) = -\frac{w}{3}\left(1-\sqrt{1-\frac{1}{w}}\right)^2. \tag{4.2}$$

It can be shown from (4.1) by applying various algebraic transformations to the ${}_2F_1$ hypergeometric differential equation (Erdélyi *et al* 1953, p 56) that the function

$$Y_3(w) \equiv [G_3(w)]^{1/2} \tag{4.3}$$

is a solution of the Heun differential equation (see Snow 1952, Ronveaux 1995)

$$\frac{d^2Y_3}{dw^2} + \left[\frac{\gamma}{w} + \frac{(1+\alpha+\beta-\gamma-\delta)}{w-1} + \frac{\delta}{w-a}\right]\frac{dY_3}{dw} + \frac{(\alpha\beta w+b)}{w(w-1)(w-a)}Y_3 = 0 \tag{4.4}$$

with $a=-\frac{1}{3}$, $b=-\frac{1}{12}$, $\alpha=\beta=\gamma=\frac{1}{2}$ and $\delta=1$. This differential equation can be written in the alternative form

$$\frac{d^2Y_3}{dw^2} + f(w)\frac{dY_3}{dw} + g(w)Y_3 = 0 \tag{4.5}$$

where

$$f(w) = \frac{12w^2-7w-1}{2w(w-1)(3w+1)} \tag{4.6}$$

$$g(w) = \frac{3w-1}{4w(w-1)(3w+1)}. \tag{4.7}$$

We can now derive a differential equation for $G_3(w)$ by applying a theorem of Appell (1880) to (4.5). Hence, we find that

$$\frac{d^3G_3}{dw^3} + 3f(w)\frac{d^2G_3}{dw^2} + \left[2f(w)^2 + \frac{df}{dw} + 4g(w)\right]\frac{dG_3}{dw} + \left[4f(w)g(w) + 2\frac{dg}{dw}\right]G_3 = 0. \tag{4.8}$$

From equations (4.6)–(4.8) we obtain the required result

$$2w(w-1)(3w+1)^2\frac{d^3G_3}{dw^3} + 3(3w+1)\left(12w^2-7w-1\right)\frac{d^2G_3}{dw^2} + 6\left(21w^2-3w-2\right)\frac{dG_3}{dw} + 18wG_3 = 0. \tag{4.9}$$

If the expansion (1.4) is substituted in (4.9) we obtain the recurrence relation

$$18(n+1)^3p_{n+1}^{(3)} - 3n(n+1)(2n+1)p_n^{(3)} - 2n\left(5n^2+1\right)p_{n-1}^{(3)} - n(n-1)(2n-1)p_{n-2}^{(3)} = 0 \tag{4.10}$$

where $n=0,1,2,\ldots$, with the initial conditions $p_0^{(3)}=1$, $p_{-1}^{(3)}=0$ and $p_{-2}^{(3)}=0$.

Next we derive the general series solution of (4.9) which is valid in the neighbourhood of the regular singular point $w = 1$. In this manner, we find that the series coefficients $\{A_n^{(3)} : n = 0, 1, 2, \ldots\}$ satisfy the recurrence relation

$$16n(n+1)(2n+1)A_{n+1}^{(3)} + 16n\left(5n^2+1\right)A_n^{(3)} + 3(2n-1)\left(11n^2-11n+6\right)A_{n-1}^{(3)} + 18(n-1)^3 A_{n-2}^{(3)} = 0 \tag{4.11}$$

where $n = 1, 2, 3, \ldots,$ with $A_{-1}^{(3)} = 0$, while the recurrence relation for the coefficients $\{B_n^{(3)} : n = 0, 1, 2, \ldots\}$ is

$$32(n+1)(2n+1)(2n+3)B_{n+1}^{(3)} + 8(2n+1)\left(20n^2+20n+9\right)B_n^{(3)} + 6n\left(44n^2+13\right)B_{n-1}^{(3)} + 9(2n-1)^3 B_{n-2}^{(3)} = 0 \tag{4.12}$$

where $n = 0, 1, 2, \ldots,$ with $B_{-1}^{(3)} = 0$ and $B_{-2}^{(3)} = 0$. It is evident that the relations (4.11) and (4.12) can be used to generate the values of the coefficients $\{A_n^{(3)} : n = 2, 3, \ldots\}$ and $\{B_n^{(3)} : n = 1, 2, \ldots\}$, provided that we know the values of $A_0^{(3)}$, $A_1^{(3)}$ and $B_0^{(3)}$.

These initial values can be obtained by expanding the elliptic integral formula (Joyce 1998, p 5113)

$$G_3(w) = \frac{\left(1+3\xi^2\right)^2}{w(1-\xi)^3(1+3\xi)}\left[\frac{2}{\pi}K(k_3)\right]^2 \tag{4.13}$$

in powers of $w - 1$, where

$$k_3^2 = k_3^2(\xi) = \frac{16\xi^3}{(1-\xi)^3(1+3\xi)} \tag{4.14}$$

$$\xi = \xi(w) = \left(1+\sqrt{1-\frac{1}{w}}\right)^{-1}\left(-1+\sqrt{1+\frac{1}{3w}}\right). \tag{4.15}$$

The final results are

$$A_0^{(3)} = G_3(1) \tag{4.16}$$

$$A_1^{(3)} = -\frac{1}{16}\left[8G_3(1) - \frac{27}{\pi^2 G_3(1)}\right] \tag{4.17}$$

$$B_0^{(3)} = \frac{3\sqrt{3}}{2\pi}. \tag{4.18}$$

It has been shown by Watson (1939) that

$$G_3(1) = \frac{3\sqrt{3}}{4}\left[\frac{2}{\pi}K\left(\frac{\sqrt{3}-1}{2\sqrt{2}}\right)\right]^2. \tag{4.19}$$

5. Singular behaviour of $\{L_j(w) : j = 1, 2, 3\}$ as $w \to 1+$

In order to analyse the associated integrals $\{L_j(w) : j = 1, 2, 3\}$ we first expand the integrand in (1.10) in inverse powers of w and then integrate term-by-term. This procedure leads to the series representations

$$L_j(w) = \ln(w) - \sum_{n=2}^{\infty}\frac{p_n^{(j)}}{nw^n} \qquad (j = 1, 2, 3) \tag{5.1}$$

where $1 \leqslant |w| < \infty$. These expansions converge more slowly as $w \to 1+$ and they do not give an explicit specification of the singular behaviour of the associated integrals $\{L_j(w) : j = 1, 2, 3\}$ in the immediate neighbourhood of $w = 1$.

These problems can be resolved by applying (1.9) to the relation

$$L_j(w) = L_j(1) + \int_1^w G_j(w)\,\mathrm{d}w. \tag{5.2}$$

In this manner, we obtain the analytic continuation formula

$$L_j(w) = L_j(1) + \sum_{n=0}^{\infty} C_n^{(j)}\,(w-1)^{n+1} - \sum_{n=0}^{\infty} D_n^{(j)}\,(w-1)^{n+3/2} \qquad (j = 1, 2, 3) \tag{5.3}$$

where

$$C_n^{(j)} = A_n^{(j)}/(n+1) \tag{5.4}$$

$$D_n^{(j)} = B_n^{(j)}/\left(n + \tfrac{3}{2}\right). \tag{5.5}$$

The series expansion (5.3) provides a convergent representation for $L_j(w)$, provided that $|w-1| < R_j$, where $j = 1, 2, 3$ and $R_1 = 2/3$, $R_2 = R_3 = 1$.

The remaining task of calculating the critical constants $\{L_j(1) : j = 1, 2, 3\}$ can be carried out by first substituting (5.1) in equation (5.3). Hence, we find that

$$L_j(1) = \ln(w) - \sum_{n=1}^{\infty} \frac{p_{2n}^{(j)}}{2nw^{2n}} - \sum_{n=0}^{\infty} C_n^{(j)}\,(w-1)^{n+1} + \sum_{n=0}^{\infty} D_n^{(j)}\,(w-1)^{n+3/2} \tag{5.6}$$

where $|w-1| < R_j$, $j = 1, 2$, and

$$L_3(1) = \ln(w) - \sum_{n=2}^{\infty} \frac{p_n^{(3)}}{nw^n} - \sum_{n=0}^{\infty} C_n^{(3)}\,(w-1)^{n+1} + \sum_{n=0}^{\infty} D_n^{(3)}\,(w-1)^{n+3/2} \tag{5.7}$$

where $|w-1| < R_3$. It is clear that the right-hand sides of (5.6) and (5.7) must have values which are *independent* of the value of w, provided that $|w-1| < R_j$, $j = 1, 2$ and $|w-1| < R_3$, respectively.

Next we use the various recurrence relations derived in sections 2–4 to calculate the numerical values of the partial sums of all the series in (5.6) and (5.7) when the variable w has the mid-point value

$$w = w_j \equiv 1 + \tfrac{1}{2}R_j \tag{5.8}$$

where $j = 1, 2, 3$. The number of terms included in each partial summation is increased until the absolute value of the truncation error is less than 10^{-202}. For the sc case $j = 1$ it is found that the required accuracy is achieved when one uses 777, 325 and 645 terms in the partial summations for the first, second and third series in (5.6) respectively. In this manner, we obtain the numerical value

$$\begin{aligned} L_1(1) = -0.118\,370\,166\,257\,858\,268\,529\,046\,736\,725\,104\,197\,465\,283\,570\,836\,908 \\ 603\,380\,226\,486\,573\,773\,929\,605\,054\,188\,435\,199\,608\,053\,509\,939\,877 \\ 452\,869\,481\,052\,658\,403\,157\,124\,389\,478\,346\,211\,128\,969\,993\,803\,369 \\ 107\,777\,943\,621\,869\,598\,071\,128\,280\,811\,276\,019\,590\,455\,955\,389\ldots. \end{aligned} \tag{5.9}$$

We can understand why this procedure leads to an extremely accurate value for $L_1(1)$ by analysing the asymptotic behaviour of the coefficients $p_{2n}^{(1)}$, $C_n^{(1)}$ and $D_n^{(1)}$ as $n \to \infty$. In particular, we find that

$$p_{2n}^{(1)} \sim \frac{3^{3/2}}{4\pi^{3/2}n^{3/2}} \tag{5.10}$$

$$C_n^{(1)} \sim \frac{9}{\sqrt{2}\,\pi^{3/2}\,n^{5/2}}\left(-\frac{3}{4}\right)^n \tag{5.11}$$

$$D_n^{(1)} \sim \frac{3^{5/2}}{2^{3/2}\,\pi^{3/2}\,n^{5/2}}\left(-\frac{3}{2}\right)^n \tag{5.12}$$

as $n \to \infty$. If these formulae are applied to (5.6) with $j = 1$ and $w = 1 + \frac{1}{2}R_1$, it is seen that the nth terms in the first, second and third series have an asymptotic behaviour which involves an exponential decay factor of the type $\exp(-cn)$, where $c = 2\ln(4/3)$, $2\ln 2$ and $\ln 2$ respectively. These decay factors would have been expected on general grounds because all the series in (5.6) with $j = 1$ have been evaluated at a point $w = w_1$ which lies *inside* the regions of convergence for the series. Similar calculations for the bcc and fcc lattices yield the following results:

$$\begin{aligned} L_2(1) = -0.&089\,250\,123\,407\,895\,156\,541\,177\,278\,941\,164\,711\,281\,140\,399\,609\,931\\ &562\,459\,992\,456\,917\,036\,027\,084\,318\,302\,074\,258\,149\,361\,771\,544\,247\\ &593\,661\,296\,756\,518\,249\,697\,319\,729\,183\,176\,297\,649\,787\,645\,656\,156\\ &709\,641\,813\,477\,295\,606\,926\,191\,334\,751\,219\,935\,584\,655\,740\,278\ldots \end{aligned} \tag{5.13}$$

$$\begin{aligned} L_3(1) = -0.&071\,986\,750\,484\,474\,338\,477\,286\,030\,656\,731\,641\,715\,455\,097\,848\,611\\ &019\,588\,955\,104\,682\,108\,473\,365\,270\,800\,446\,883\,235\,638\,644\,845\,833\\ &284\,144\,091\,332\,507\,794\,845\,752\,516\,605\,119\,614\,803\,518\,173\,805\,198\\ &223\,991\,406\,022\,712\,822\,369\,964\,078\,096\,859\,172\,405\,698\,270\,748\ldots. \end{aligned} \tag{5.14}$$

The values (5.9), (5.13) and (5.14) have been checked by evaluating the series in (5.6) and (5.7) for various other values of w which satisfy the inequality $|w-1| < R_j$, with $j = 1, 2, 3$. Rosengren (1987) obtained the value $L_1(1) = -0.118\,370\,16\ldots$ by using the formula (5.1) with $w = 1$ and $j = 1$. The disadvantage of this method is that it involves the calculation of a rather *slowly* convergent series with terms which have the asymptotic behaviour $dn^{-5/2}$ as $n \to \infty$, where d is a constant.

There is some evidence that the associated integrals $\{L_j(1) : j = 1, 2, 3\}$ may be expressible in terms of familiar mathematical constants. For example, it is known that

$$\frac{1}{\pi^2}\int_0^\pi\int_0^\pi \ln\left[1 - \frac{1}{2}(\cos\theta_1 + \cos\theta_2)\right] d\theta_1\, d\theta_2 = \frac{4G}{\pi} - 2\ln 2 \tag{5.15}$$

where G is the Catalan constant, while Glasser (private communication) has proved the formula

$$\begin{aligned} \frac{1}{\pi^3}\int_0^\pi\int_0^\pi\int_0^\pi \ln\left[1 - \frac{1}{2}(\cos\theta_1 + \cos\theta_2 + \cos\theta_3 - \cos\theta_1\cos\theta_2\cos\theta_3)\right] d\theta_1\, d\theta_2\, d\theta_3 \\ = \frac{8G}{\pi} - 4\ln 2. \end{aligned} \tag{5.16}$$

It is hoped that the highly accurate values (5.9), (5.13) and (5.14) will provide a useful basis for further mathematical investigations of the integrals $\{L_j(1) : j = 1, 2, 3\}$.

Finally, we note that the associated integral $L_2(w)$ can also be written in the generalized hypergeometric form

$$L_2(w) = \ln(w) - \frac{1}{16w^2}\, {}_5F_4\left[\begin{matrix} \frac{3}{2}, & \frac{3}{2}, & \frac{3}{2}, & 1, & 1; \\ 2, & 2, & 2, & 2; & \end{matrix}\; 1/w^2\right] \tag{5.17}$$

where $1 \leqslant |w| < \infty$.

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