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ON THE SIMPLE CUBIC LATTICE GREEN FUNCTION†

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CONTENTS

The analytical properties of the simple cubic lattice Green function

$$G(t) = \frac{1}{\pi^3}\iiint_0^{\pi}[t-(\cos x_1+\cos x_2+\cos x_3)]^{-1}\mathrm{d}x_1\,\mathrm{d}x_2\,\mathrm{d}x_3$$

are investigated. In particular, it is shown that $tG(t)$ can be written in the form

$$tG(t) = [F(9, -\tfrac{3}{4}; \tfrac{1}{4}, \tfrac{3}{4}, 1, \tfrac{1}{2}; 9/t^2)]^2,$$

where $F(a, b; \alpha, \beta, \gamma, \delta; z)$ denotes a Heun function. The standard analytic continuation formulae for Heun functions are then used to derive various expansions for the Green function

$$G^-(s) \equiv G_R(s) + \mathrm{i}G_I(s) = \lim_{\epsilon\to 0+} G(s-\mathrm{i}\epsilon) \quad (0 \leqslant s < \infty)$$

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about the points $s = 0, 1$ and 3. From these expansions accurate numerical values of $G_R(s)$ and $G_I(s)$ are obtained in the range $0 \leqslant s \leqslant 3$, and certain new summation formulae for Heun functions of unit argument are deduced. Quadratic transformation formulae for the Green function $G(t)$ are discussed, and a connexion between $G(t)$ and the Lamé–Wangerin differential equation is established. It is also proved that $G(t)$ can be expressed as a product of two complete elliptic integrals of the first kind. Finally, several applications of the results are made in lattice statistics.

1. Introduction

Recently, there has been considerable interest in the lattice Green function for the simple cubic lattice (Katsura *et al.* 1971 *a*, *b*; Morita & Horiguchi 1971)

$$G(t) = \frac{1}{\pi^3}\iiint_0^{\pi} \frac{dx_1\,dx_2\,dx_3}{t-(\cos x_1+\cos x_2+\cos x_3)}. \tag{1.1}$$

This integral defines a single-valued analytic function $G(t)$ in the complex t-plane cut along the real axis from -3 to $+3$. In most physical applications one usually requires the limiting behaviour of the Green function (1.1) as t approaches the real axis. It is convenient, therefore, to introduce the additional definitions

$$G^{\pm}(s) \equiv \lim_{\epsilon\to 0+} G(s \pm i\epsilon) \equiv G_R(s) \mp iG_I(s), \tag{1.2}$$

where $-\infty < s < \infty$. Since the real part $G_R(s)$ and the imaginary part $G_I(s)$ of $G^-(s)$ satisfy the symmetry relations

$$\left.\begin{aligned} G_R(-s) &= -G_R(s),\\ G_I(-s) &= +G_I(s),\end{aligned}\right\} \tag{1.3}$$

we shall restrict our attention to the Green function $G^-(s)$ with s in the range $0 < s < \infty$. The behaviour of $G^+(s)$ is readily obtained by using the formula

$$G^+(s) = G^-(s)^*. \tag{1.4}$$

It can be shown that the functions $G^{\pm}(s)$ display branch-point singularities at $s = \pm 1$ and $s = \pm 3$.

Katsura *et al.* (1971 *b*) transformed the Green function (1.1) into a Mellin–Barnes type integral, and hence derived Taylor series expansions for $G^+(s)$ about $s = 0$, and $s = \sqrt{5}$ in powers of s^2, and $\frac{1}{4}(s^2-5)$ respectively. In a second paper (Inawashiro, Katsura & Abe 1971) an expansion for $G^-(s)$ was developed about the singular point $s = 1$, in powers of $(s^2-1)^{\frac{1}{2}}$. These authors also showed that the leading-order coefficient in all these expansions could be determined exactly in terms of complete elliptic integrals of the first kind. However, the higher-order coefficients were, in general, expressed as *infinite* series and were *not* evaluated exactly in terms of standard functions. Furthermore, the important expansion about the singular point $s = 3$ was not discussed.

The main aim of this paper is to give a detailed account of the analytic properties of the lattice Green function (1.1). In particular, it will be proved in §3 that $tG(t)$ can be written as the square of a Heun function (Heun 1889). In §§4 and 5 this basic result and the standard transformation formulae for Heun functions will be used to obtain various expansions for $G^-(s)$ about $s = 0$, $s = 1$ *and* $s = 3$. It is shown that the coefficients in these expansions can, in principle, all be generated *exactly* by means of simple recurrence relations.

In §6 a close connexion between the simple cubic lattice Green function and the Lamé–Wangerin differential equation is established. Certain quadratic transformation formulae for

$G(t)$ are also derived. In §7 it is proved that the simple cubic lattice Green function can be evaluated, for *arbitrary* t, as a product of two complete elliptic integrals of the first kind. Some applications of the results are described in §8.

2. Basic results

We begin by considering the closely related lattice Green's function

$$P(z) \equiv \left(\frac{3}{z}\right) G\left(\frac{3}{z}\right) = \frac{1}{\pi^3}\iiint_0^\pi \frac{dx_1\,dx_2\,dx_3}{1-\frac{1}{3}z(\cos x_1+\cos x_2+\cos x_3)}. \tag{2.1}$$

It is interesting to note that this Green function plays an important role in the theory of random walks on a simple cubic lattice (Montroll & Weiss 1965). By inspecting the integrand in equation (2.1) we see that the integral (2.1) represents a single-valued analytic function throughout the z^2-plane cut along the real axis from $+1$ to $+\infty$. (It is convenient to consider the z^2-plane since $P(-z) = P(z)$.)

A power series representation for $P(z)$, valid when $|z| < 1$, may be readily established by expanding the integrand in (2.1) in powers of z and integrating term by term. We find

$$P(z) = \sum_{n=0}^{\infty} a_n z^{2n} \quad (|z| < 1), \tag{2.2}$$

where

$$a_n = \frac{1}{\pi^3}\iiint_0^\pi [\tfrac{1}{3}(\cos x_1+\cos x_2+\cos x_3)]^{2n}\,dx_1\,dx_2\,dx_3. \tag{2.3}$$

An explicit expression for the coefficients a_n can be derived from equation (2.3), in terms of a *terminating* generalized hypergeometric series. The final result is

$$a_n = \frac{1}{3^{2n}}\frac{(\frac{1}{2})_n}{(1)_n}\,{}_3F_2\left[\begin{matrix}\frac{1}{2}, -n, -n; \\ 1, 1;\end{matrix}\ 4\right], \tag{2.4}$$

where $(b)_n = \Gamma(n+b)/\Gamma(b)$. In the theory of random walks the coefficient a_n gives the probability that a random walker will return to his starting-point (not necessarily for the first time) after a walk of $2n$ steps on a simple cubic lattice. The number of random walks r_{2n} which return to the origin after $2n$ steps is

$$r_{2n} = 6^{2n} a_n. \tag{2.5}$$

For large n the behaviour of a_n is described by the asymptotic expansion (Domb 1954)

$$a_n \sim \frac{1}{4}\left(\frac{3}{\pi n}\right)^{\frac{3}{2}}\left[1-\frac{3}{8n}+\frac{13}{128n^2}+\frac{27}{1024n^3}+\frac{723}{32768n^4}+\dots\right], \tag{2.6}$$

as $n \to \infty$. It follows from this asymptotic formula that the range of validity of (2.2) can be extended to include all points on the circle $|z| = 1$. In particular

$$P(1) = \sum_{n=0}^{\infty} a_n. \tag{2.7}$$

The evaluation of $P(1)$ was first carried out by Watson (1939). His result is

$$\begin{aligned} P(1) &= 12\pi^{-2}(18+12\sqrt{2}-10\sqrt{3}-7\sqrt{6})\,K_2^2 \\ &\approx 1.516\,386\,059\,151\,978, \end{aligned} \tag{2.8}$$

where K_2 denotes a complete elliptic integral of the first kind with a modulus

$$k = (2-\sqrt{3})(\sqrt{3}-\sqrt{2}).$$

Unfortunately, Watson's ingenious analysis has not been generalized to the case $z \neq 1$.

In order to obtain a recurrence relation for the coefficient a_n we now introduce the exponential probability generating function

$$E(\theta) = \frac{1}{\pi^3}\iiint_0^{\pi} \exp\left[\tfrac{1}{3}\theta\left(\cos x_1 + \cos x_2 + \cos x_3\right)\right] dx_1\, dx_2\, dx_3 \tag{2.9}$$

$$= \sum_{n=0}^{\infty} a_n \frac{\theta^{2n}}{(2n)!}, \quad |\theta^2| < \infty. \tag{2.10}$$

From equation (2.9) we also have the alternative expression

$$E(\theta) = I_0^3\left(\frac{\theta}{3}\right) = \sum_{n=0}^{\infty} d_n \left(\frac{\theta}{3}\right)^{2n}, \tag{2.11}$$

where

$$d_n = \frac{3^{2n}}{(2n)!} a_n, \tag{2.12}$$

and $I_0(x)$ is a modified Bessel function of the first kind. Watson (1910) has shown that the coefficients d_n satisfy the following three-term recurrence relation

$$16(n+1)^4 d_{n+1} - 4(10n^2+10n+3)\, d_n + 9d_{n-1} = 0 \quad (n \geqslant 0), \tag{2.13}$$

with the initial conditions $d_0 = 1$, and $d_{-1} \equiv 0$. The substitution of (2.12) in (2.13) yields the required recurrence relation

$$36(n+1)^3 a_{n+1} - 2(2n+1)\,(10n^2+10n+3)\, a_n + n(4n^2-1)\, a_{n-1} = 0 \quad (n \geqslant 0) \tag{2.14}$$

with $a_0 = 1$, and $a_{-1} \equiv 0$. We see, therefore, that the number of returns to the origin r_{2n} satisfies the recurrence relation

$$(n+1)^3 r_{2n+2} - 2(2n+1)\,(10n^2+10n+3)\, r_{2n} + 36n(4n^2-1)\, r_{2n-2} = 0 \quad (n \geqslant 0), \tag{2.15}$$

with $r_0 = 1$, and $r_{-2} \equiv 0$. In table 1 is given a list of the numerical values of r_{2n}, which was generated by using the recurrence relation (2.15).

TABLE 1. NUMBER OF RETURNS TO THE ORIGIN r_{2n} FOR THE SIMPLE CUBIC LATTICE

n	r_{2n}	n	r_{2n}
0	1	8	27 770 358 330
1	6	9	842 090 474 940
2	90	10	25 989 269 017 140
3	1 860	11	813 689 707 488 840
4	44 730	12	25 780 447 171 287 900
5	1 172 556	13	825 043 888 527 957 000
6	32 496 156	14	26 630 804 377 937 061 000
7	936 369 720	15	865 978 374 333 905 289 360

The recurrence relation (2.14) is of basic importance since it enables us to establish the following third-order linear homogeneous differential equation for the probability generating function (2.2):

$$4x^2(x-1)\,(x-9)\frac{d^3P}{dx^3} + 12x(2x^2-15x+9)\frac{d^2P}{dx^2} + 3(9x^2-44x+12)\frac{dP}{dx} + 3(x-2)\,P = 0, \tag{2.16}$$

where $x = z^2$. It is readily verified that this differential equation is a Fuchsian equation (Ince

1927; Poole 1936) with four regular singular points at $x = 0, 1, 9$ and ∞. The Riemann P-symbol (see Ince 1927) associated with the differential equation (2.16) is

$$P\begin{bmatrix} 0 & 1 & 9 & \infty & \\ 0 & 0 & 0 & \frac{1}{2} & \\ 0 & 1 & 1 & \frac{3}{2} & x \\ 0 & \frac{1}{2} & \frac{1}{2} & 1 & \end{bmatrix}. \tag{2.17}$$

In this scheme the singular points are placed in the first row with the roots of the corresponding indicial equations beneath them. (The Riemann P-symbol notation should not be confused with the Green function $P(z)$.)

For an *arbitrary* nth order Fuchsian equation with a regular singular point at ∞ and ν regular singular points in the finite x-plane, it can be shown (Ince 1927, p. 371) that the sum of *all* the exponents in the Riemannian scheme is an *invariant* equal to $\frac{1}{2}n(n-1)(\nu-1)$. We see directly from equation (2.17) that the differential equation (2.16) has the correct Fuchsian invariant of 6.

A differential equation for the Green function $G(t)$ may be obtained by applying the transformation (2.1) to equation (2.16). The final result is

$$(t^4-10t^2+9)\frac{d^3G}{dt^3}+6t(t^2-5)\frac{d^2G}{dt^2}+(7t^2-12)\frac{dG}{dt}+tG = 0. \tag{2.18}$$

This Fuchsian differential equation has five regular singular points in the t-plane at $t = \pm 1$, ± 3 and ∞, with a Fuchsian invariant of 9. The Riemann P-symbol associated with equation (2.18) is

$$P\begin{bmatrix} -3 & -1 & 1 & 3 & \infty & \\ 0 & 0 & 0 & 0 & 1 & \\ 1 & 1 & 1 & 1 & 1 & t \\ \frac{1}{2} & \frac{1}{2} & \frac{1}{2} & \frac{1}{2} & 1 & \end{bmatrix}. \tag{2.19}$$

3. Connexion with Heun's differential equation

Appell (1880) has shown that, if y_1 and y_2 are independent solutions of the second-order differential equation

$$\frac{d^2y}{dx^2}+f(x)\frac{dy}{dx}+g(x)\,y = 0, \tag{3.1}$$

then the general solution of the third-order differential equation

$$\frac{d^3y}{dx^3}+3f(x)\frac{d^2y}{dx^2}+\left[2f(x)^2+\frac{df}{dx}+4g(x)\right]\frac{dy}{dx}+\left[4f(x)\,g(x)+2\frac{dg}{dx}\right]y = 0 \tag{3.2}$$

is

$$y = Ay_1^2+By_1y_2+Cy_2^2, \tag{3.3}$$

where A, B and C are arbitrary constants. The application of this result to the differential equation (2.16) enables us to write the lattice Green function $P(x)$ in the product form

$$P(x) = Ay_1^2+By_1y_2+Cy_2^2, \tag{3.4}$$

where y_1 and y_2 are independent solutions of the second-order differential equation

$$\frac{d^2y}{dx^2}+\left[\frac{1}{x}+\frac{1}{2(x-1)}+\frac{1}{2(x-9)}\right]\frac{dy}{dx}+\frac{3(x-4)}{16x(x-1)(x-9)}\,y = 0. \tag{3.5}$$

We now introduce the normal form of Heun's differential equation (Heun 1889; Snow 1952)

$$\frac{\mathrm{d}^2y}{\mathrm{d}x^2}+\left[\frac{\gamma}{x}+\frac{1+\alpha+\beta-\gamma-\delta}{x-1}+\frac{\delta}{x-a}\right]\frac{\mathrm{d}y}{\mathrm{d}x}+\frac{\alpha\beta x+b}{x(x-1)(x-a)}y = 0. \tag{3.6}$$

The Riemannian scheme associated with Heun's equation is

$$P\begin{bmatrix} 0 & 1 & a & \infty & \\ 0 & 0 & 0 & \alpha & x \\ 1-\gamma & \gamma+\delta-\alpha-\beta & 1-\delta & \beta & \end{bmatrix}. \tag{3.7}$$

(In order to provide a *complete* characterization of equation (3.6) one must give the P-symbol, *and* the value of the *accessory parameter* b.) It is evident from equation (3.6) that the differential equation (3.5) is a particular case of Heun's equation with $\alpha = \frac{1}{4}$, $\beta = \frac{3}{4}$, $\gamma = 1$, $\delta = \frac{1}{2}$; $a = 9$, $b = -\frac{3}{4}$. Thus the Riemann P-symbol for equation (3.5) is

$$P\begin{bmatrix} 0 & 1 & 9 & \infty & \\ 0 & 0 & 0 & \frac{1}{4} & x \\ 0 & \frac{1}{2} & \frac{1}{2} & \frac{3}{4} & \end{bmatrix}. \tag{3.8}$$

The solution of equation (3.6) which is regular in the neighbourhood of $x = 0$, with an exponent zero, is Heun's function† defined by the series

$$y_1(x) \equiv F(a, b; \alpha, \beta, \gamma, \delta; x) = \sum_{n=0}^{\infty} c_n x^n, \tag{3.9}$$

where the coefficients c_n satisy the recurrence relation

$$(n+1)(n+\gamma)\,ac_{n+1} = \{(a+1)\,n^2+[\gamma+\delta-1+(\alpha+\beta-\delta)\,a]\,n-b\}\,c_n-(n-1+\alpha)(n-1+\beta)\,c_{n-1} \quad (n \geqslant 0) \tag{3.10}$$

with $c_0 = 1$, and $c_{-1} \equiv 0$. It follows, therefore, that the solution of equation (3.5) which is regular in the neighbourhood of $x = 0$, is given by

$$y_1 = F(9, -\tfrac{3}{4}; \tfrac{1}{4}, \tfrac{3}{4}, 1, \tfrac{1}{2}; x). \tag{3.11}$$

The independent second solution y_2 of equation (3.5) must display a logarithmic singularity at $x = 0$, since the roots of the indicial equation at $x = 0$ are coincident. If these results are applied to equation (3.4) we obtain the basic formula

$$P(z) = [F(9, -\tfrac{3}{4}; \tfrac{1}{4}, \tfrac{3}{4}, 1, \tfrac{1}{2}; x)]^2, \tag{3.12}$$

with $x = z^2$. From equations (2.1) and (3.12) we also have

$$G(t) = \frac{1}{t}\left[F\left(9, -\tfrac{3}{4}; \tfrac{1}{4}, \tfrac{3}{4}, 1, \tfrac{1}{2}; \frac{9}{t^2}\right)\right]^2. \tag{3.13}$$

It is interesting to note that the lattice Green function $P(z)$ for the body-centred cubic lattice can be written as the square of an ${}_2F_1$ hypergeometric function (Joyce 1971*a*)

$$P(z)_{\mathrm{bcc}} = [{}_2F_1(\tfrac{1}{4}, \tfrac{1}{4}; 1; z^2)]^2. \tag{3.14}$$

In the following sections we shall use equations (3.12) and (3.13) to investigate the analytic properties of $P(z)$ and $G(t)$.

† In this paper we shall adopt the Heun function notation used by Snow (1952).

4. Transformation formulae for $P(z)$

We shall discuss in this section the behaviour of $P(z)$ in the neighbourhood of the singular points $x = 1$, 9 and ∞.

(a) *Analytic continuation about* $x = 1$

The application of a standard transformation formula (see Snow (1952) p. 123, equation (20)) to the Heun function in equation (3.12) enables us to write

$$[P(z)]^{\frac{1}{2}} = AF(-8, \tfrac{9}{16}; \tfrac{1}{4}, \tfrac{3}{4}, \tfrac{1}{2}, \tfrac{1}{2}; 1-x) + B(1-x)^{\frac{1}{2}}F(-8, \tfrac{69}{16}; \tfrac{5}{4}, \tfrac{3}{4}, \tfrac{3}{2}, \tfrac{1}{2}; 1-x), \tag{4.1}$$

where A and B are constants. Fortunately, the *joining factors* A and B can be calculated *exactly*. The joining factor A is readily determined by applying Watson's result (2.8) to (4.1). We find

$$A = [P(1)]^{\frac{1}{2}} = (2\sqrt{3}/\pi)\,(18+12\sqrt{2}-10\sqrt{3}-7\sqrt{6})^{\frac{1}{2}}K_2. \tag{4.2}$$

To determine the joining factor B we apply Darboux's theorem (Darboux 1878) to the *singular part* of the square of equation (4.1). This procedure yields the asymptotic formula

$$a_n \sim -B[P(1)/\pi]^{\frac{1}{2}} n^{-\frac{3}{2}}, \quad \text{as} \quad n \to \infty. \tag{4.3}$$

If we compare this result with the asymptotic expansion (2.6) we see that

$$B = -(3/4\pi)\,[3/P(1)]^{\frac{1}{2}}. \tag{4.4}$$

The substitution of (4.2) and (4.4) in equation (4.1) leads to the important analytic continuation formula

$$P(z) = P(1)\,[F(-8, \tfrac{9}{16}; \tfrac{1}{4}, \tfrac{3}{4}, \tfrac{1}{2}, \tfrac{1}{2}; 1-x)]^2 + \frac{27}{16\pi^2 P(1)}(1-x)\,[F(-8, \tfrac{69}{16}; \tfrac{5}{4}, \tfrac{3}{4}, \tfrac{3}{2}, \tfrac{1}{2}; 1-x)]^2$$
$$-\frac{3\sqrt{3}}{2\pi}(1-x)^{\frac{1}{2}}F(-8, \tfrac{9}{16}; \tfrac{1}{4}, \tfrac{3}{4}, \tfrac{1}{2}, \tfrac{1}{2}; 1-x)F(-8, \tfrac{69}{16}; \tfrac{5}{4}, \tfrac{3}{4}, \tfrac{3}{2}, \tfrac{1}{2}; 1-x), \tag{4.5}$$

where $|\arg(1-x)| < \pi$, and $|\arg x| < \pi$.

We can now use the Taylor series (3.9) and the recurrence relation (3.10) to expand the analytic continuation (4.5) in the form

$$P(z) = \sum_{n=0}^{\infty}\left[P(1)\,B_n^{(0)} + \frac{27}{16\pi^2 P(1)}\,B_n^{(1)}\right](1-z^2)^n - \frac{3\sqrt{3}}{2\pi}(1-z^2)^{\frac{1}{2}}\sum_{n=0}^{\infty} C_n(1-z^2)^n, \tag{4.6}$$

where $|1-z^2| < 1$, and $|\arg(1-z^2)| < \pi$. The exact values of the coefficients $B_n^{(0)}$, $B_n^{(1)}$ and C_n are listed in table 2 for $n \leqslant 8$. We give below the numerical values of the leading order terms in the expansion (4.6):

$$P(z) = 1.516\,386\,059\,151\,978 - \frac{3\sqrt{3}}{2\pi}(1-z^2)^{\frac{1}{2}}$$
$$+\,0.539\,238\,175\,081\,581\,(1-z^2) - \frac{3\sqrt{3}}{4\pi}(1-z^2)^{\frac{3}{2}} + \dots. \tag{4.7}$$

The expansions (4.6) and (4.7) are of considerable importance in the theory of random walks (Montroll & Weiss 1965; Domb & Joyce 1972), and in the theories of ferromagnetism such as the spherical model (Berlin & Kac 1952; Joyce 1972*a*). A comparison of equation (4.7) with the earlier calculations of Montroll & Weiss (1965) indicates that the coefficient of $1-z^2$ obtained by these authors is in error.

Next we apply the method of Frobenius (Ince 1927; Poole 1936) to the regular singular point $x = 1$ of the differential equation (2.16), and hence derive a general series solution of (2.16) in

TABLE 2. COEFFICIENTS $B_n^{(0)}$, $B_n^{(1)}$ AND C_n IN THE EXPANSION (4.6)

n	$B_n^{(0)}$	$B_n^{(1)}$	C_n
0	1	0	1
2	$\frac{9}{32}$	1	$\frac{1}{2}$
2	$\frac{175}{1\,024}$	$\frac{23}{32}$	$\frac{7}{20}$
3	$\frac{2\,025}{16\,384}$	$\frac{1\,477}{2\,560}$	$\frac{19}{70}$
4	$\frac{102\,235}{1\,048\,576}$	$\frac{555\,273}{1\,146\,880}$	$\frac{25}{112}$
5	$\frac{1\,356\,047}{16\,777\,216}$	$\frac{38\,466\,649}{91\,750\,400}$	$\frac{67}{352}$
6	$\frac{37\,160\,123}{536\,870\,912}$	$\frac{1\,711\,814\,393}{4\,613\,734\,400}$	$\frac{205}{1\,232}$
7	$\frac{6\,771\,931\,925}{111\,669\,149\,696}$	$\frac{48\,275\,151\,899}{144\,686\,710\,784}$	$\frac{3\,389}{22\,880}$
8	$\frac{772\,428\,184\,055}{14\,293\,651\,161\,088}$	$\frac{28\,127\,429\,172\,349}{92\,599\,494\,901\,760}$	$\frac{24\,469}{183\,040}$

powers of $1-x$. If this series solution is compared with the expansion (4.6) we obtain the following four-term recurrence relations for the coefficients $B_n^{(0)}$, $B_n^{(1)}$ and C_n:

$$16n(n+1)(2n+1)B_{n+1}^{(i)} - n(60n^2+9)B_n^{(i)} + 3(2n-1)^3 B_{n-1}^{(i)} + (n-1)(2n-1)(2n-3)B_{n-2}^{(i)} = 0 \quad (n \geqslant 1) \tag{4.8}$$

and

$$8(n+1)(2n+1)(2n+3)C_{n+1} - 6(2n+1)(5n^2+5n+2)C_n + 24n^3 C_{n-1} + 2n(n-1)(2n-1)C_{n-2} = 0 \quad (n \geqslant 0), \tag{4.9}$$

where $i = 0, 1$. The initial conditions for these recurrence relations are

$$\left.\begin{aligned} B_0^{(0)} &= 1, \quad B_1^{(0)} = \tfrac{9}{32}, \quad i = 0, \\ B_1^{(1)} &= 0, \quad B_1^{(1)} = 1, \quad i = 1, \end{aligned}\right\} \tag{4.10}$$

with $C_0 = 1$. The recurrence relations (4.8) and (4.9) provide us with a simple *independent* method for generating the coefficients in table 2.

Further analytic continuations for $P(z)$ about $x = 1$ can be established using the transformation formulae derived by Snow (1952). For example, it can be shown that (see Snow (1952), p. 121, equation (17))

$$[P(z)]^{\frac{1}{2}} = \frac{[P(1)]^{\frac{1}{2}}(8/9)^{\frac{1}{4}}}{(1-\frac{1}{9}x)^{\frac{1}{4}}} F\left(9, -\tfrac{11}{16}; \tfrac{1}{4}, \tfrac{3}{4}, \tfrac{1}{2}, \tfrac{1}{2}; \frac{1-x}{1-\frac{1}{9}x}\right) - \frac{3\sqrt{3}(8/9)^{\frac{3}{4}}(1-x)^{\frac{1}{2}}}{4\pi[P(1)]^{\frac{1}{2}}(1-\frac{1}{9}x)^{\frac{3}{4}}} F\left(9, -\tfrac{87}{16}; \tfrac{3}{4}, \tfrac{5}{4}, \tfrac{3}{2}, \tfrac{1}{2}; \frac{1-x}{1-\frac{1}{9}x}\right). \tag{4.11}$$

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The application of the Euler-type theorem (Snow 1952)

$$F(a,b;\alpha,\beta,\gamma,\delta;z) = (1-z)^{-\alpha} F\left[\frac{a}{a-1}, -\frac{(b+a\alpha\gamma)}{a-1}; \alpha, \gamma+\delta-\beta, \gamma, \delta; \frac{z}{z-1}\right] \tag{4.12}$$

to the Heun functions in (4.11) yields the additional relation

$$\begin{aligned} P(z) = {} & P(1)\, x^{-\frac{1}{2}} \left[F\left(\tfrac{9}{8}, -\tfrac{7}{128}; \tfrac{1}{4}, \tfrac{1}{4}, \tfrac{1}{2}, \tfrac{1}{2}; \frac{9(x-1)}{8x}\right)\right]^2 \\ & + \frac{27x^{-\frac{3}{2}}}{16\pi^2 P(1)} (1-x) \left[F\left(\tfrac{9}{8}, -\tfrac{75}{128}; \tfrac{3}{4}, \tfrac{3}{4}, \tfrac{3}{2}, \tfrac{1}{2}; \frac{9(x-1)}{8x}\right)\right]^2 \\ & - \frac{3\sqrt{3}}{2\pi} x^{-1}(1-x)^{\frac{1}{2}} F\left(\tfrac{9}{8}, -\tfrac{7}{128}; \tfrac{1}{4}, \tfrac{1}{4}, \tfrac{1}{2}, \tfrac{1}{2}; \frac{9(x-1)}{8x}\right) \\ & \times F\left(\tfrac{9}{8}, -\tfrac{75}{128}; \tfrac{3}{4}, \tfrac{3}{4}, \tfrac{3}{2}, \tfrac{1}{2}; \frac{9(x-1)}{8x}\right). \end{aligned} \tag{4.13}$$

This result is valid throughout the x-plane cut along the real axis from $-\infty$ to 0, and $+1$ to $+\infty$.

(b) *Analytic continuation about* $x = 9$

The behaviour of $P(z)$ in the neighbourhood of $x = 9$ may be established by applying a suitable transformation formula (see Snow (1952), p. 125, equation (24)) to the Heun function in equation (3.12). It is found that

$$\begin{aligned} [P(z)]^{\frac{1}{2}} = {} & A(\tfrac{1}{9}x)^{-\frac{1}{4}} F\left(-8, \tfrac{1}{16}; \tfrac{1}{4}, \tfrac{1}{4}, \tfrac{1}{2}, \tfrac{1}{2}; \frac{x-9}{x}\right) \\ & + B(\tfrac{9}{8})^{\frac{1}{2}} \left(\frac{9-x}{x}\right)^{\frac{1}{2}} (\tfrac{1}{9}x)^{-\frac{1}{4}} F\left(-8, \tfrac{29}{16}; \tfrac{3}{4}, \tfrac{3}{4}, \tfrac{3}{2}, \tfrac{1}{2}; \frac{x-9}{x}\right), \end{aligned} \tag{4.14}$$

where x is either in the upper or lower half of the x-plane cut along the real axis from $-\infty$ to $+\infty$, and A and B are constants which take *different* values in the upper and lower half of the x-plane. For convenience, we shall suppose that x is in the upper half of the cut x-plane.

In order to calculate the joining factors A and B we now use equations (4.14), (2.1) and (1.2) to determine the behaviour of $G^-(s)$ in the neighbourhood of $s = 1$. This procedure gives

$$G^-(s) = A^2 + \tfrac{3}{\sqrt{2}} AB(s^2-1)^{\frac{1}{2}} + O(s^2-1). \tag{4.15}$$

Fortunately, Inawashiro *et al.* (1971) have evaluated the leading-order coefficients in this expansion *exactly*. Their result is

$$G^-(s) = (1+\mathrm{i}\sqrt{2})\, G_{\mathrm{R}}(1) - (3\mathrm{i}/2\pi)\,(s^2-1)^{\frac{1}{2}} + O(s^2-1), \tag{4.16}$$

where

$$G_{\mathrm{R}}(1) = \tfrac{1}{2}\pi[\Gamma(\tfrac{5}{8})\,\Gamma(\tfrac{7}{8})]^{-2} \tag{4.17}$$

$$= (1-2^{-\frac{1}{2}})\,(2/\pi)^2[K((2\sqrt{2}-2)^{\frac{1}{2}})]^2, \tag{4.18}$$

and $K(k)$ denotes a complete elliptic integral of the first kind. The following alternative expression for $G_{\mathrm{R}}(1)$ is also of interest:

$$G_{\mathrm{R}}(1) = 2^{-\frac{1}{2}} P(\pm \mathrm{i})_{\mathrm{bcc}}, \tag{4.19}$$

where $P(z)_{\mathrm{bcc}}$ is the lattice Green function for the body-centred cubic lattice.†

† The relation (4.19) may be derived by comparing equation (4.17) with equation (2.48) in Joyce (1971 *a*).

Exact formulae for the constants A and B are now readily obtained by comparing (4.15) with (4.16). The substitution of these formulae in equation (4.14) finally yields the complete analytic continuation

$$P(z) = (\tfrac{1}{9}x)^{-\frac{1}{2}}\Big\{(1+\mathrm{i}\sqrt{2})\,G_{\mathrm{R}}(1)\left[F\left(-8,\tfrac{1}{16};\tfrac{1}{4},\tfrac{1}{4},\tfrac{1}{2},\tfrac{1}{2};\frac{x-9}{x}\right)\right]^2 + \frac{3(\mathrm{i}\sqrt{2}-1)}{16\pi^2 G_{\mathrm{R}}(1)}\left(\frac{9-x}{x}\right)\left[F\left(-8,\tfrac{29}{16};\tfrac{3}{4},\tfrac{3}{4},\tfrac{3}{2},\tfrac{1}{2};\frac{x-9}{x}\right)\right]^2 - \frac{3\mathrm{i}}{2\pi}\left(\frac{9-x}{x}\right)^{\frac{1}{2}}F\left(-8,\tfrac{1}{16};\tfrac{1}{4},\tfrac{1}{4},\tfrac{1}{2},\tfrac{1}{2};\frac{x-9}{x}\right)F\left(-8,\tfrac{29}{16};\tfrac{3}{4},\tfrac{3}{4},\tfrac{3}{2},\tfrac{1}{2};\frac{x-9}{x}\right)\Big\}, \tag{4.20}$$

where x is in the upper half of the cut x-plane.

Further analytic continuations for $P(z)$ about $x = 9$ can be derived using the appropriate transformation formulae given by Snow (1952). For example, it can be shown that (see Snow (1952), p. 124, equation (22))

$$P(z) = (1+\mathrm{i}\sqrt{2})\,G_{\mathrm{R}}(1)\left[F\left(\tfrac{9}{8},-\tfrac{15}{128};\tfrac{1}{4},\tfrac{3}{4},\tfrac{1}{2},1;\frac{9-x}{8}\right)\right]^2 + \frac{(\mathrm{i}\sqrt{2}-1)}{48\pi^2 G_{\mathrm{R}}(1)}(9-x)\left[F\left(\tfrac{9}{8},-\tfrac{115}{128};\tfrac{3}{4},\tfrac{5}{4},\tfrac{3}{2},1;\frac{9-x}{8}\right)\right]^2 - \frac{\mathrm{i}}{2\pi}(9-x)^{\frac{1}{2}}F\left(\tfrac{9}{8},-\tfrac{15}{128};\tfrac{1}{4},\tfrac{3}{4},\tfrac{1}{2},1;\frac{9-x}{8}\right)F\left(\tfrac{9}{8},-\tfrac{115}{128};\tfrac{3}{4},\tfrac{5}{4},\tfrac{3}{2},1;\frac{9-x}{8}\right), \tag{4.21}$$

where x is in the upper half of the cut x-plane.

(c) *Analytic continuation about $x = \infty$*

The behaviour of $P(z)$ about the point at infinity is readily determined by using the relation (see Snow (1952), p. 123, equation (21*a*))

$$[P(z)]^{\frac{1}{2}} = A(x\mathrm{e}^{-\mathrm{i}\pi})^{-\frac{1}{4}}F(9,-\tfrac{1}{8};\tfrac{1}{4},\tfrac{1}{4},\tfrac{1}{2},\tfrac{1}{2};9/x) + B(x\mathrm{e}^{-\mathrm{i}\pi})^{-\frac{3}{4}}F(9,-\tfrac{21}{8};\tfrac{3}{4},\tfrac{3}{4},\tfrac{3}{2},\tfrac{1}{2};9/x), \tag{4.22}$$

where x is in the x-plane cut along the real axis from 0 to ∞ with $0 < \arg x < 2\pi$, and A and B are constants. From this relation and equations (2.1) and (1.2) we find that

$$G^{-}(s) = \tfrac{1}{3}A^2\mathrm{i} - \tfrac{2}{9}ABs + O(s^2). \tag{4.23}$$

However, from the work of Katsura *et al.* (1971*b*) we have the alternative *exact* expansion

$$G^{-}(s) = G_{\mathrm{I}}(0)\,\mathrm{i} + \frac{2}{\pi\sqrt{3}}s + O(s^2), \tag{4.24}$$

where

$$G_{\mathrm{I}}(0) = 3[\Gamma(\tfrac{1}{3})]^6/2^{\frac{14}{3}}\pi^4, \tag{4.25}$$

$$= \frac{2}{\pi^2}K(\tfrac{1}{2}(2+\sqrt{3})^{\frac{1}{2}})\,K(\tfrac{1}{2}(2-\sqrt{3})^{\frac{1}{2}}), \tag{4.26}$$

$$= \frac{2\sqrt{3}}{\pi^2}\left[K\left(\frac{(\sqrt{3}-1)}{2\sqrt{2}}\right)\right]^2. \tag{4.27}$$

The following additional expression for $G_{\mathrm{I}}(0)$ is also of interest:

$$G_{\mathrm{I}}(0) = \tfrac{2}{3}P(1)_{\mathrm{fcc}}, \tag{4.28}$$

where $P(z)_{\mathrm{fcc}}$ is the lattice Green function for the face-centred cubic lattice (Montroll & Weiss 1965; Joyce 1971*b*).

We can now calculate the joining factors A and B in equation (4.22) by comparing equation (4.23) with equation (4.24). This procedure finally yields the complete analytic continuation

$$
\begin{aligned}
P(z) = {} & 3G_{\mathrm{I}}(0)\,(x\,\mathrm{e}^{-\mathrm{i}\pi})^{-\frac{1}{2}}\,[F(9, -\tfrac{1}{8}; \tfrac{1}{4}, \tfrac{1}{4}, \tfrac{1}{2}, \tfrac{1}{2}; 9/x)]^2 \\
& + \frac{9}{\pi^2 G_{\mathrm{I}}(0)}\,(x\,\mathrm{e}^{-\mathrm{i}\pi})^{-\frac{3}{2}}[F(9, -\tfrac{21}{8}; \tfrac{3}{4}, \tfrac{3}{4}, \tfrac{3}{2}, \tfrac{1}{2}; 9/x)]^2 \\
& - \frac{6\sqrt{3}}{\pi}\,(x\,\mathrm{e}^{-\mathrm{i}\pi})^{-1}F(9, -\tfrac{1}{8}; \tfrac{1}{4}, \tfrac{1}{4}, \tfrac{1}{2}, \tfrac{1}{2}; 9/x)\,F(9, -\tfrac{21}{8}; \tfrac{3}{4}, \tfrac{3}{4}, \tfrac{3}{2}, \tfrac{1}{2}; 9/x),
\end{aligned}
$$

where $0 < \arg x < 2\pi$. We see from (4.29) that $P(z)$ displays a branch-point singularity at $x = \infty$.

5. Expansions for $G_{\mathrm{R}}(s)$ and $G_{\mathrm{I}}(s)$

In this section the general analytic continuation formulae obtained in §4 will be used to derive various expansions for the real and imaginary parts of the Green function $G^{-}(s)$.

(a) *Expansions about* $s = 0$

In order to develop expansions for $G_{\mathrm{R}}(s)$ and $G_{\mathrm{I}}(s)$ about $s = 0$, we substitute $x = 9/t^2$ in equation (4.29) and apply the relations (2.1) and (1.2). This procedure gives

$$G_{\mathrm{R}}(s) = \frac{2s}{\pi\sqrt{3}}F(9, -\tfrac{1}{8}; \tfrac{1}{4}, \tfrac{1}{4}, \tfrac{1}{2}, \tfrac{1}{2}; s^2)F(9, -\tfrac{21}{8}; \tfrac{3}{4}, \tfrac{3}{4}, \tfrac{3}{2}, \tfrac{1}{2}; s^2), \tag{5.1}$$

and

$$G_{\mathrm{I}}(s) = G_{\mathrm{I}}(0)\,[F(9, -\tfrac{1}{8}; \tfrac{1}{4}, \tfrac{1}{4}, \tfrac{1}{2}, \tfrac{1}{2}; s^2)]^2 - \frac{s^2}{3\pi^2 G_{\mathrm{I}}(0)}[F(9, -\tfrac{21}{8}; \tfrac{3}{4}, \tfrac{3}{4}, \tfrac{3}{2}, \tfrac{1}{2}; s^2)]^2, \tag{5.2}$$

Table 3. Coefficients $D_n^{(0)}$, $D_n^{(1)}$ and E_n in the expansion (5.4) and (5.3)

n	$D_n^{(0)}$	$D_n^{(1)}$	E_n
0	1	0	1
1	$\frac{1}{18}$	1	$\frac{2}{9}$
2	$\frac{11}{648}$	$\frac{7}{18}$	$\frac{8}{81}$
3	$\frac{19}{2\,160}$	$\frac{5}{24}$	$\frac{496}{8\,505}$
4	$\frac{7861}{1\,399\,680}$	$\frac{3\,635}{27\,216}$	$\frac{9\,088}{229\,635}$
5	$\frac{301\,259}{75\,582\,720}$	$\frac{557\,485}{5\,878\,656}$	$\frac{12\,032}{413\,343}$
6	$\frac{451\,526\,509}{149\,653\,785\,600}$	$\frac{7\,596\,391}{105\,815\,808}$	$\frac{12\,004\,352}{531\,972\,441}$
7	$\frac{6\,427\,914\,623}{2\,693\,768\,140\,800}$	$\frac{19\,681\,954\,039}{346\,652\,587\,008}$	$\frac{4\,139\,008}{227\,988\,189}$
8	$\frac{16\,794\,274\,237}{8\,620\,058\,050\,560}$	$\frac{32\,139\,541\,115}{693\,305\,174\,016}$	$\frac{51\,347\,456}{3\,419\,822\,835}$

where $-1 \leqslant s \leqslant 1$. We can now use the Heun function series (3.9) and the recurrence relation (3.10) to expand equations (5.1) and (5.2) in the form

$$G_R(s) = \frac{2s}{\pi\sqrt{3}} \sum_{n=0}^{\infty} E_n s^{2n}, \tag{5.3}$$

and

$$G_I(s) = \sum_{n=0}^{\infty} \left[G_I(0)\, D_n^{(0)} - \frac{D_n^{(1)}}{3\pi^2 G_I(0)} \right] s^{2n}, \tag{5.4}$$

where $-1 \leqslant s \leqslant 1$. The coefficients $D_n^{(0)}$, $D_n^{(1)}$ and E_n are listed in table 3 for $n \leqslant 8$.

Recurrence relations for the coefficients $D_n^{(0)}$, $D_n^{(1)}$ and E_n are readily obtained by applying the method of Frobenius to the *ordinary point* $t = 0$ of the differential equation (2.18). The final results are given below:

$$36n(n+1)(2n+1)\, D_{n+1}^{(i)} - 4n(20n^2+1)\, D_n^{(i)} + (2n-1)^3 D_{n-1}^{(i)} = 0 \quad (n \geqslant 1; i = 0, 1) \tag{5.5}$$

and

$$9(n+1)(2n+1)(2n+3)\, E_{n+1} - 2(2n+1)(10n^2+10n+3)\, E_n + 4n^3 E_{n-1} = 0 \quad (n \geqslant 0) \tag{5.6}$$

with the initial conditions

$$\left.\begin{aligned} &D_0^{(0)} = 1, \quad D_1^{(0)} = 1/18 \quad (i=0),\\ &D_0^{(1)} = 0, \quad D_1^{(1)} = 1 \quad\quad (i=1),\end{aligned}\right\} \tag{5.7}$$

and $E_0 = 1$. It is evident that the combination of these recurrence relations with equations (5.3) and (5.4) provides us with a simple accurate procedure for calculating the numerical values of $G_R(s)$ and $G_I(s)$ in the range $0 < s^2 < 1$. (The scheme is rapidly convergent for $s^2 \lesssim \frac{1}{2}$.)

A comparison of the expansions (5.3) and (5.4) with the corresponding *double* series derived by Katsura *et al.* (1971*b*) yields the following apparently new summation formulae:

$$\sum_{m=0}^{\infty} \frac{[\Gamma(m+\frac{1}{2})]^3(\frac{1}{4})^m}{[\Gamma(\frac{1}{2}+m-n)]^2 m!} = \frac{4}{\sqrt{3}}(n!)\,\Gamma(n+\tfrac{3}{2})\, E_n, \tag{5.8}$$

and

$$\frac{1}{2\pi^2} \sum_{m=0}^{\infty} \frac{[\Gamma(m+n+\frac{1}{2})]^3(\frac{1}{4})^m}{(m+n)!(m!)^2} [-3\psi(m+n+\tfrac{1}{2}) + 2\psi(m+1) + \psi(m+n+1) + \ln 4]$$
$$= 4^n n!\,\Gamma(n+\tfrac{1}{2}) \left[G_I(0)\, D_n^{(0)} - \frac{D_n^{(1)}}{3\pi^2 G_I(0)} \right]. \tag{5.9}$$

(*b*) *Expansions about* $s = 1$

The behaviour of $G^-(s)$ in the neighbourhood of $s = 1$ may be determined by substituting $x = 9/t^2$ in the analytic continuation (4.20). It is found that

$$G^-(s) \equiv G_R(s) + iG_I(s) = (1+i\sqrt{2})\, G_R(1)\, [F(-8, \tfrac{1}{16}; \tfrac{1}{4}, \tfrac{1}{4}, \tfrac{1}{2}, \tfrac{1}{2}; 1-s^2)]^2$$
$$+ \frac{3(1-i\sqrt{2})}{16\pi^2 G_R(1)} (1-s^2)\, [F(-8, \tfrac{29}{16}; \tfrac{3}{4}, \tfrac{3}{4}, \tfrac{3}{2}, \tfrac{1}{2}; 1-s^2)]^2$$
$$- \frac{3i}{2\pi}(s^2-1)^{\frac{1}{2}} F(-8, \tfrac{1}{16}; \tfrac{1}{4}, \tfrac{1}{4}, \tfrac{1}{2}, \tfrac{1}{2}; 1-s^2)\, F(-8, \tfrac{29}{16}; \tfrac{3}{4}, \tfrac{3}{4}, \tfrac{3}{2}, \tfrac{1}{2}; 1-s^2), \tag{5.10}$$

where $0 \leqslant s^2 \leqslant 9$, with $s \geqslant 0$, and

$$\left.\begin{aligned} (s^2-1)^{\frac{1}{2}} &= (s^2-1)^{\frac{1}{2}} & (s^2 \geqslant 1)\\ &= -i(1-s^2)^{\frac{1}{2}} & (s^2 \leqslant 1).\end{aligned}\right\} \tag{5.11}$$

We can now use the Heun function series (3.9) and the recurrence relation (3.10) to expand (5.10) in the form

$$G^{-}(s) \equiv G_{\mathrm{R}}(s)+\mathrm{i}G_{\mathrm{I}}(s) = \sum_{n=0}^{\infty}\left[(1+\mathrm{i}\surd 2)\,G_{\mathrm{R}}(1)\,U_n^{(0)}+\frac{3(1-\mathrm{i}\surd 2)}{16\pi^2 G_{\mathrm{R}}(1)}\,U_n^{(1)}\right](1-s^2)^n$$
$$-\frac{3\mathrm{i}}{2\pi}(s^2-1)^{\frac{1}{2}}\sum_{n=0}^{\infty}V_n(1-s^2)^n, \tag{5.12}$$

where $|1-s^2| \leqslant 1$ and $s \geqslant 0$. A list of the coefficients $U_n^{(0)}$, $U_n^{(1)}$ and V_n is given in table 4.

TABLE 4. COEFFICIENTS $U_n^{(0)}$, $U_n^{(1)}$ AND V_n IN THE EXPANSION (5.12)

n	$U_n^{(0)}$	$U_n^{(1)}$	V_n
0	1	0	1
1	$\frac{1}{32}$	1	$\frac{1}{6}$
2	$\frac{15}{1\,024}$	$\frac{29}{96}$	$\frac{1}{12}$
3	$\frac{637}{81\,920}$	$\frac{785}{4\,608}$	$\frac{1}{20}$
4	$\frac{186\,161}{36\,700\,160}$	$\frac{32\,515}{294\,912}$	$\frac{173}{5\,040}$
5	$\frac{2\,129\,373}{587\,202\,560}$	$\frac{372\,295}{4\,718\,592}$	$\frac{563}{22\,176}$
6	$\frac{259\,064\,949}{93\,952\,409\,600}$	$\frac{298\,904\,291}{4\,982\,833\,152}$	$\frac{73}{3\,696}$
7	$\frac{42\,740\,829\,483}{19\,542\,101\,196\,800}$	$\frac{3\,793\,413\,169}{79\,725\,330\,432}$	$\frac{41}{2\,574}$
8	$\frac{6\,266\,337\,923\,043}{3\,501\,944\,534\,466\,560}$	$\frac{132\,419\,161\,225}{3\,401\,614\,098\,432}$	$\frac{369\,581}{28\,005\,120}$

In order to establish recurrence relations for the coefficients in table 4 we transform the independent variable t in the differential equation (2.18) to $\theta = (1-t^2)$ and apply the method of Frobenius about the regular singular point $\theta = 0$. This procedure yields the recurrence relations

$$32n(n+1)(2n+1)\,U_{n+1}^{(i)}-n(56n^2+2)\,U_n^{(i)}-(2n-1)^3\,U_{n-1}^{(i)} = 0 \quad (n \geqslant 1;\, i = 0, 1) \tag{5.13}$$

and
$$4(n+1)(2n+1)(2n+3)\,V_{n+1}-(2n+1)(7n^2+7n+2)\,V_n-2n^3V_{n-1} = 0 \quad (n \geqslant 0), \tag{5.14}$$

with the initial conditions

$$\left.\begin{array}{lll} U_0^{(0)} = 1, & U_1^{(0)} = 1/32 & (i = 0) \\ U_0^{(1)} = 0, & U_1^{(1)} = 1 & (i = 1), \end{array}\right\} \tag{5.15}$$

and $V_0 = 1$. These recurrence relations and expansions (5.12) provide us with a simple *rapidly* convergent scheme for calculating $G_{\mathrm{R}}(s)$ and $G_{\mathrm{I}}(s)$ in the range $\frac{1}{2} \lesssim s^2 \lesssim \frac{3}{2}\,(s > 0)$.

An alternative formula for $G^-(s)$ about $s = 1$ may be derived from the analytic continuation (4.21). We find

$$sG^-(s) = (1+i\sqrt{2})\,G_R(1)\,[F(\tfrac{9}{8}, -\tfrac{15}{128}; \tfrac{1}{4}, \tfrac{3}{4}, \tfrac{1}{2}, 1; \omega)]^2 + \frac{(i\sqrt{2}-1)}{6\pi^2 G_R(1)}\,\omega[F(\tfrac{9}{8}, -\tfrac{115}{128}; \tfrac{3}{4}, \tfrac{5}{4}, \tfrac{3}{2}, 1; \omega)]^2 - \frac{i\sqrt{2}}{\pi}\,\omega^{\frac{1}{2}} F(\tfrac{9}{8}, -\tfrac{15}{128}; \tfrac{1}{4}, \tfrac{3}{4}, \tfrac{1}{2}, 1; \omega) F(\tfrac{9}{8}, -\tfrac{115}{128}; \tfrac{3}{4}, \tfrac{5}{4}, \tfrac{3}{2}, 1; \omega), \tag{5.16}$$

where
$$\omega = 9(s^2-1)/8s^2, \tag{5.17}$$

and $0 < s^2 \leqslant 9$ $(s > 0)$. (When $0 < s < 1$ the square root $\omega^{\frac{1}{2}}$ should be replaced by $-i|\omega|^{\frac{1}{2}}$.) From this basic formula and the series (3.9) we can now obtain the expansion

$$sG^-(s) = \sum_{n=0}^{\infty} \left[(1+i\sqrt{2})\,G_R(1)\,Y_n^{(0)} + \frac{(i\sqrt{2}-1)}{6\pi^2 G_R(1)}\,Y_n^{(1)}\right]\omega^n - \frac{i\sqrt{2}}{\pi}\,\omega^{\frac{1}{2}} \sum_{n=0}^{\infty} Z_n \omega^n, \tag{5.18}$$

provided that $\frac{9}{17} \leqslant s^2 \leqslant 9$ $(s > 0)$. The coefficients $Y_n^{(0)}$, $Y_n^{(1)}$ and Z_n are listed in table 5. From the numerical point of view this alternative expansion about $s = 1$ is particularly important since it converges fairly rapidly in the extended range $\frac{3}{4} \lesssim s^2 \lesssim 3$ $(s > 0)$.

Table 5. Coefficients $Y_n^{(0)}$, $Y_n^{(1)}$ and Z_n in the expansion (5.18)

n	$Y_n^{(0)}$	$Y_n^{(1)}$	Z_n
0	1	0	1
1	$\frac{5}{12}$	1	$\frac{20}{27}$
2	$\frac{13}{48}$	$\frac{115}{108}$	$\frac{16}{27}$
3	$\frac{7\,721}{38\,880}$	$\frac{5\,945}{5\,832}$	$\frac{1\,792}{3\,645}$
4	$\frac{201\,461}{1\,306\,368}$	$\frac{132\,895}{139\,968}$	$\frac{172\,288}{413\,343}$
5	$\frac{539\,561}{4\,354\,560}$	$\frac{6\,619\,375}{7\,558\,272}$	$\frac{4\,891\,648}{13\,640\,319}$
6	$\frac{718\,530\,527}{7\,054\,387\,200}$	$\frac{7\,226\,561\,965}{8\,979\,227\,136}$	$\frac{12\,763\,136}{40\,920\,957}$
7	$\frac{1\,338\,333\,359}{15\,721\,205\,760}$	$\frac{4\,442\,038\,075}{5\,986\,151\,424}$	$\frac{187\,105\,280}{683\,964\,567}$

Finally, we note that the coefficients $Y_n^{(0)}$, $Y_n^{(1)}$ and Z_n satisfy the following recurrence relations:

$$162n(n+1)(2n+1)\,Y_{n+1}^{(i)} - 45n(20n^2+3)\,Y_n^{(i)} + 8(2n-1)(52n^2-52n+21)\,Y_{n-1}^{(i)} - 64(n-1)(2n-1)(2n-3)\,Y_{n-2}^{(i)} = 0 \quad (n \geqslant 1; i = 0, 1) \tag{5.19}$$

and
$$81(n+1)(2n+1)(2n+3)\,Z_{n+1} - 90(2n+1)(5n^2+5n+2)\,Z_n + 64n(13n^2+2)\,Z_{n-1} - 128n(n-1)(2n-1)\,Z_{n-2} = 0 \quad (n \geqslant 0), \tag{5.20}$$

with the initial conditions

$$\left.\begin{aligned} Y_0^{(0)} &= 1, \quad Y_1^{(0)} = \tfrac{5}{12}, \quad (i = 0), \\ Y_0^{(1)} &= 0, \quad Y_1^{(1)} = 1, \quad (i = 1), \end{aligned}\right\} \tag{5.21}$$

and $Z_0 = 1$.

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(c) *Expansions about $s = 3$ and $s = \infty$*

For the case $s = 3$ we use the analytic continuation (4.13) and equations (2.1) and (1.2) to obtain the formula

$$\begin{aligned} G^{-}(s) \equiv G_{\mathrm{R}}(s) + \mathrm{i}G_{\mathrm{I}}(s) = {} & \tfrac{1}{3}P(1)\left[F\left(\tfrac{9}{8}, -\tfrac{7}{128}; \tfrac{1}{4}, \tfrac{1}{4}, \tfrac{1}{2}, \tfrac{1}{2}; \frac{9-s^2}{8}\right)\right]^2 \\ & - \frac{(9-s^2)}{16\pi^2 P(1)}\left[F\left(\tfrac{9}{8}, -\tfrac{75}{128}; \tfrac{3}{4}, \tfrac{3}{4}, \tfrac{3}{2}, \tfrac{1}{2}; \frac{9-s^2}{8}\right)\right]^2 \\ & + \frac{\mathrm{i}}{2\pi\sqrt{3}}(9-s^2)^{\frac{1}{2}} F\left(\tfrac{9}{8}, -\tfrac{7}{128}; \tfrac{1}{4}, \tfrac{1}{4}, \tfrac{1}{2}, \tfrac{1}{2}; \frac{9-s^2}{8}\right) \\ & \times F\left(\tfrac{9}{8}, -\tfrac{75}{128}; \tfrac{3}{4}, \tfrac{3}{4}, \tfrac{3}{2}, \tfrac{1}{2}; \frac{9-s^2}{8}\right), \end{aligned} \tag{5.22}$$

where $1 \leqslant s < \infty$, and

$$\left.\begin{aligned} (9-s^2)^{\frac{1}{2}} &= (9-s^2)^{\frac{1}{2}} & (s^2 \leqslant 9) \\ &= \mathrm{i}(s^2-9)^{\frac{1}{2}} & (s^2 \geqslant 9). \end{aligned}\right\} \tag{5.23}$$

From this result we can now derive the following expansion about $s = 3$:

$$G^{-}(s) = \sum_{n=0}^{\infty}\left[\tfrac{1}{3}P(1)\,W_n^{(0)} - \frac{W_n^{(1)}}{2\pi^2 P(1)}\right]\left(\frac{9-s^2}{8}\right)^n + \frac{\mathrm{i}}{2\pi\sqrt{3}}(9-s^2)^{\frac{1}{2}}\sum_{n=0}^{\infty} X_n\left(\frac{9-s^2}{8}\right)^n, \tag{5.24}$$

where $1 \leqslant s^2 \leqslant 17$ $(s > 0)$. A list of the coefficients $W_n^{(0)}$, $W_n^{(1)}$ and X_n is given in table 6. The expansion (5.24) provides us with a fairly rapidly convergent scheme for calculating $G_{\mathrm{R}}(s)$ and $G_{\mathrm{I}}(s)$ in the range $3 \lesssim s^2 \lesssim 15$ $(s > 0)$. (It should be noted that the imaginary part $G_{\mathrm{I}}(s)$ is equal to zero for *all* $s \geqslant 3$.)

Table 6. Coefficients $W_n^{(0)}$, $W_n^{(1)}$ and X_n in the expansion (5.24)

n	$W_n^{(0)}$	$W_n^{(1)}$	X_n
0	1	0	1
1	$\frac{7}{36}$	1	$\frac{4}{9}$
2	$\frac{127}{1\,296}$	$\frac{25}{36}$	$\frac{112}{405}$
3	$\frac{485}{7\,776}$	$\frac{559}{1\,080}$	$\frac{1\,664}{8\,505}$
4	$\frac{24\,745}{559\,872}$	$\frac{221\,021}{544\,320}$	$\frac{4\,864}{32\,805}$
5	$\frac{1\,007\,881}{30\,233\,088}$	$\frac{48\,460\,849}{146\,966\,400}$	$\frac{533\,504}{4\,546\,773}$
6	$\frac{28\,520\,107}{1\,088\,391\,168}$	$\frac{2\,281\,896\,119}{8\,314\,099\,200}$	$\frac{3\,915\,776}{40\,920\,957}$
7	$\frac{5\,403\,016\,003}{254\,683\,533\,312}$	$\frac{1\,706\,616\,756\,923}{7\,333\,035\,494\,400}$	$\frac{90\,963\,968}{1\,139\,940\,945}$
8	$\frac{71\,572\,670\,015}{4\,074\,936\,532\,992}$	$\frac{134\,250\,885\,145}{670\,448\,959\,488}$	$\frac{231\,538\,688}{3\,419\,822\,835}$

The recurrence relations for the coefficients $W_n^{(0)}$, $W_n^{(1)}$ and X_n are given below:

$$18n(n+1)(2n+1)W_{n+1}^{(i)} - n(68n^2+7)W_n^{(i)} + 4(2n-1)^3 W_{n-1}^{(i)} = 0 \quad (n \geqslant 1; i = 0, 1) \tag{5.25}$$

and

$$9(n+1)(2n+1)(2n+3)X_{n+1} - 2(2n+1)(17n^2+17n+6)X_n + 32n^3 X_{n-1} = 0 \quad (n \geqslant 0), \tag{5.26}$$

with the initial conditions

$$\left.\begin{aligned} W_0^{(0)} &= 1, \quad W_1^{(0)} = \tfrac{7}{36} \quad (i = 0), \\ W_0^{(1)} &= 0, \quad W_1^{(1)} = 1 \quad (i = 1), \end{aligned}\right\} \tag{5.27}$$

and $X_0 = 1$.

An expansion for $G^-(s)$ about $s = \infty$ may be obtained directly from equation (3.13). We find

$$G^-(s) \equiv G_{\mathrm{R}}(s) = s^{-1} \sum_{n=0}^{\infty} a_n (9/s^2)^n, \tag{5.28}$$

where the coefficients a_n satisfy the 3-term recurrence relation (2.14), and $9 \leqslant s^2 < \infty$. This expansion converges fairly rapidly provided that $15 \lesssim s^2 < \infty$.

(d) *Numerical evaluation of $G_{\mathrm{R}}(s)$ and $G_{\mathrm{I}}(s)$*

Expansions (5.3), (5.4), (5.12), (5.18), (5.24) and (5.28) have been used to construct a combined subroutine for the numerical evaluation of $G_{\mathrm{R}}(s)$ and $G_{\mathrm{I}}(s)$ in the range $0 \leqslant s < \infty$. A short tabulation of $G_{\mathrm{R}}(s)$ and $G_{\mathrm{I}}(s)$ for $0 \leqslant s \leqslant 3$ is presented in the appendix.† Since this scheme does not involve *double* series or numerical integration it is considerably simpler than any proposed previously (Katsura *et al.* 1971 *b*; Morita & Horiguchi 1971; Jelitto 1969); (for a review of earlier methods see Katsura *et al.* 1971 *a*).

6. Related results

(a) *Heun function summation formulae*

In the theory of the ${}_2F_1(a, b; c; z)$ hypergeometric function the summation formula

$${}_2F_1(a, b; c; 1) = \frac{\Gamma(c)\,\Gamma(c-a-b)}{\Gamma(c-a)\,\Gamma(c-b)} \tag{6.1}$$

is of considerable importance. Unfortunately, a *general* summation formula does not appear to be known for the Heun function $F(a, b; \alpha, \beta, \gamma, \delta; z)$ with unit argument. However, we shall now show that the analytic continuations given in the previous section can be used to derive $F(1)$ summation formulae for *particular* values of $a, b; \alpha, \beta, \gamma, \delta$.

We first substitute $s = 1$ in equations (5.1) and (5.2), and solve these equations for the two $F(1)$ Heun functions. The application of the relations $G_{\mathrm{I}}(1) = \surd 2 G_{\mathrm{R}}(1)$, (4.18) and (4.27) to the resulting expressions then yields the following summation formulae‡:

$$F(9, -\tfrac{1}{8}; \tfrac{1}{4}, \tfrac{1}{4}, \tfrac{1}{2}, \tfrac{1}{2}; 1) = (2/3)^{\frac{1}{4}} (\surd 3 + \surd 2)^{\frac{1}{2}} (1+\surd 2)^{-\frac{1}{2}} K(\surd 2 - 1) \Big/ K\left(\frac{\surd 3 - 1}{2\surd 2}\right), \tag{6.2}$$

and

$$F(9, -\tfrac{21}{8}; \tfrac{3}{4}, \tfrac{3}{4}, \tfrac{3}{2}, \tfrac{1}{2}; 1) = (6^{\frac{3}{4}}\surd 2/\pi)(\surd 3 - \surd 2)^{\frac{1}{2}} (1+\surd 2)^{-\frac{1}{2}} K(\surd 2 - 1)\, K\left(\frac{\surd 3 - 1}{2\surd 2}\right). \tag{6.3}$$

† A more extensive tabulation of $G_{\mathrm{R}}(s)$ and $G_{\mathrm{I}}(s)$ is currently being prepared in collaboration with J. A. Webb.

‡ In order to simplify the modulus of the elliptic integral in equation (4.18) we have also used the relation $K((2\surd 2 - 2)^{\frac{1}{2}}) = \surd 2 K(\surd 2 - 1)$.

If we set $s = 0$ in equation (5.10) and proceed in a similar manner we find that

$$F(-8, \tfrac{1}{16}; \tfrac{1}{4}, \tfrac{1}{4}, \tfrac{1}{2}, \tfrac{1}{2}; 1) = (6^{\frac{1}{4}}/4)\,(\sqrt{3}+\sqrt{2})^{\frac{1}{2}}\,(1+\sqrt{2})^{\frac{1}{2}}\,K\left(\frac{\sqrt{3}-1}{2\sqrt{2}}\right)\Big/K(\sqrt{2}-1), \tag{6.4}$$

and
$$F(-8, \tfrac{29}{16}; \tfrac{3}{4}, \tfrac{3}{4}, \tfrac{3}{2}, \tfrac{1}{2}; 1) = 6^{-\frac{1}{4}}(8/\pi)\,(\sqrt{3}-\sqrt{2})^{\frac{1}{2}}\,(1+\sqrt{2})^{-\frac{1}{2}}\,K(\sqrt{2}-1)\,K\left(\frac{\sqrt{3}-1}{2\sqrt{2}}\right). \tag{6.5}$$

Further $F(1)$ summation formulae are readily obtained from equations (5.16) and (5.22) with $s = 3$ and $s = 1$ respectively. The final results are given below:

$$\begin{aligned} F(\tfrac{9}{8}, -\tfrac{7}{128}; \tfrac{1}{4}, \tfrac{1}{4}, \tfrac{1}{2}, \tfrac{1}{2}; 1) &= \frac{\sqrt{3}}{2}\,(1+\sqrt{3})\,[F(\tfrac{9}{8}, -\tfrac{15}{128}; \tfrac{1}{4}, \tfrac{3}{4}, \tfrac{1}{2}, 1; 1)]^{-1} \\ &= 2^{-\frac{1}{4}}(1+\sqrt{2})^{-\frac{1}{2}}\,(1+\sqrt{3})^{\frac{1}{2}}\,(18+12\sqrt{2}-10\sqrt{3}-7\sqrt{6})^{-\frac{1}{2}} \\ &\quad\times\frac{K(\sqrt{2}-1)}{K((2-\sqrt{3})\,(\sqrt{3}-\sqrt{2}))}, \end{aligned} \tag{6.6}$$

and
$$\begin{aligned} F(\tfrac{9}{8}, -\tfrac{75}{128}; \tfrac{3}{4}, \tfrac{3}{4}, \tfrac{3}{2}, \tfrac{1}{2}; 1) &= 3^{-\frac{1}{2}}F(\tfrac{9}{8}, -\tfrac{115}{128}; \tfrac{3}{4}, \tfrac{5}{4}, \tfrac{3}{2}, 1; 1) \\ &= (8\sqrt{3}/\pi 2^{\frac{1}{4}})\,(1+\sqrt{2})^{-\frac{1}{2}}(1+\sqrt{3})^{-\frac{1}{2}}(18+12\sqrt{2}-10\sqrt{3}-7\sqrt{6})^{\frac{1}{2}} \\ &\quad\times K(\sqrt{2}-1)\,K((2-\sqrt{3})\,(\sqrt{3}-\sqrt{2})). \end{aligned} \tag{6.7}$$

(*b*) *Quadratic transformations*

Most of the Heun functions which occur in the previous sections satisfy the conditions

$$\gamma = \alpha+\beta \quad \text{and} \quad \delta = \tfrac{1}{2}.$$

Under these circumstances the Heun function $F(a, b; \alpha, \beta, \gamma, \delta; z)$ is known to undergo quadratic transformations (Snow 1952). For example, it can be shown that (see Snow (1952), p. 126, equation (27*a*))

$$\begin{aligned} [P(z)]^{\frac{1}{2}} &= F(9, -\tfrac{3}{4}; \tfrac{1}{4}, \tfrac{3}{4}, 1, \tfrac{1}{2}; x) \\ &= (1-\tfrac{3}{4}x_1)^{\frac{1}{4}}F(\tfrac{4}{3}, -\tfrac{1}{2}; \tfrac{1}{2}, 1, 1, \tfrac{1}{2}; x_1), \end{aligned} \tag{6.8}$$

where
$$x_1 = \tfrac{1}{2}+\tfrac{1}{6}x-\tfrac{1}{2}(1-x)^{\frac{1}{2}}\,(1-\tfrac{1}{9}x)^{\frac{1}{2}}. \tag{6.9}$$

Next we apply the Euler-type transformation (4.12) to the second Heun function in (6.8). This procedure gives

$$[P(z)]^{\frac{1}{2}} = (1-\tfrac{3}{4}x_1)^{\frac{1}{4}}\,(1-x_1)^{-\frac{1}{2}}F(4, -\tfrac{1}{2}; \tfrac{1}{2}, \tfrac{1}{2}, 1, \tfrac{1}{2}; x_2), \tag{6.10}$$

where $x_2 = x_1/(x_1-1)$. After carrying out a further quadratic transformation on the Heun function (6.10), we finally obtain the following *biquadratic* transformation formula:

$$[P(z)]^{\frac{1}{2}} = (1-\tfrac{3}{4}x_1)^{\frac{1}{4}}\,(1-x_1)^{-\frac{1}{2}}\,(1-\tfrac{8}{9}x_3)^{\frac{1}{2}}F(\tfrac{9}{8}, -\tfrac{3}{4}; 1, 1, 1, 1; x_3), \tag{6.11}$$

where
$$x_3 = \tfrac{1}{2}+\tfrac{1}{4}x_2-\tfrac{1}{2}(1-x_2)^{\frac{1}{2}}\,(1-\tfrac{1}{4}x_2)^{\frac{1}{2}}. \tag{6.12}$$

Quadratic transformations may also be derived in a similar manner for the Heun functions $F(a, b; \tfrac{1}{4}, \tfrac{1}{4}, \tfrac{1}{2}, \tfrac{1}{2}; x)$ and $F(a, b'; \tfrac{3}{4}, \tfrac{3}{4}, \tfrac{3}{2}, \tfrac{1}{2}; x)$ which occur in §§4 and 5.

We have so far represented the various solutions of Heun's differential equation (3.6) by means of power series. However, Erdélyi (1942, 1944) has developed an alternative scheme in which the solutions of (3.6) are expanded as a series of hypergeometric functions. The application of Erdélyi's results to the basic Heun function in equation (3.12) yields the expansion

$$[P(z)]^{\frac{1}{2}} = \sum_{n=0}^{\infty} c_n(\tfrac{1}{4}x)^n\, {}_2F_1(n+\tfrac{1}{4}, n+\tfrac{3}{4}; 2n+\tfrac{3}{2}; x), \tag{6.13}$$

where the coefficients c_n satisfy the recurrence relation

$$36(n+1)^2 c_{n+1} + 2(28n^2+14n+3)\, c_n + 9(2n-1)^2 c_{n-1} = 0, \tag{6.14}$$

with $c_0 = 1$, $c_{-1} = 0$ and $n \geqslant 0$. A considerable simplification of this expansion can be achieved by using the standard quadratic transformation formula

$${}_2F_1(a, b; a+b+\tfrac{1}{2}; x) = {}_2F_1[2a, 2b; a+b+\tfrac{1}{2}; \tfrac{1}{2}-\tfrac{1}{2}(1-x)^{\frac{1}{2}}]. \tag{6.15}$$

We find

$$[P(z)]^{\frac{1}{2}} = [\tfrac{1}{2}+\tfrac{1}{2}(1-x)^{\frac{1}{2}}]^{-\frac{1}{2}} \sum_{n=0}^{\infty} c_n \left[\frac{1-(1-x)^{\frac{1}{2}}}{1+(1-x)^{\frac{1}{2}}}\right]^n, \tag{6.16}$$

provided that $|1-(1-x)^{\frac{1}{2}}| \leqslant |1+(1-x)^{\frac{1}{2}}|$.

(c) *Lamé–Wangerin equation*

We shall now discuss the connexion between the simple cubic lattice Green's function and the Lamé–Wangerin differential equation (Snow 1952)

$$L_m(y) \equiv \frac{d^2y}{dx^2} + \frac{1}{2}\left[\frac{1}{x}+\frac{1}{x-1}+\frac{1}{x-a}\right]\frac{dy}{dx} + \frac{[b+\frac{1}{4}(\frac{1}{4}-m^2)\,x]}{x(x-1)\,(x-a)}\,y = 0, \tag{6.17}$$

where m is an integer. This differential equation is a particular case of Heun's equation (3.6) with $\alpha = \frac{1}{4}+\frac{1}{2}m$, $\beta = \frac{1}{4}-\frac{1}{2}m$ and $\gamma = \delta = \frac{1}{2}$, and has a general series solution about $x = 0$ which can be written in the form

$$y(x) = AF(a, b; \tfrac{1}{4}+\tfrac{1}{2}m, \tfrac{1}{4}-\tfrac{1}{2}m, \tfrac{1}{2}, \tfrac{1}{2}; x) + Bx^{\frac{1}{2}}F[a, b-\tfrac{1}{4}(a+1); \tfrac{3}{4}+\tfrac{1}{2}m, \tfrac{3}{4}-\tfrac{1}{2}m, \tfrac{3}{2}, \tfrac{1}{2}; x]. \tag{6.18}$$

We see from equation (6.18) that the Heun functions which occur in the basic formulae (5.1), (5.2), (5.10) and (5.22) are *all* essentially solutions of the Lamé–Wangerin $L_0(y) = 0$. It may also be readily verified, by using equation (4.22), that the transformed function

$$\phi(\theta) \equiv (z^2)^{\frac{1}{4}}[P(z)]^{\frac{1}{2}} \quad (z^2 = 9/\theta) \tag{6.19}$$

satisfies the Lamé–Wangerin equation $L_0(\phi) = 0$, with $a = 9$, $b = -\frac{1}{8}$ and $x \equiv \theta$. Finally, we note that the application of a quadratic transformation to (6.18) enables one to solve the Lamé–Wangerin equation in *finite* form, *providing* $m \neq 0$ (Snow 1952).

7. Evaluation of $P(z)$ and $G(t)$ in terms of elliptic integrals

(a) *General results*

It has been suggested by several authors (Katsura *et al.* 1971*b*; Iwata 1969) that the simple cubic lattice Green function can be expressed as a product of two complete elliptic integrals. The main purpose in this section is to prove that such a product form does in fact exist.

We begin by considering the face-centred cubic lattice Green function (Montroll & Weiss 1965)

$$P(z)_{\text{fcc}} = \frac{1}{\pi^3}\iiint_0^{\pi} \frac{dx_1\, dx_2\, dx_3}{1-\frac{1}{3}z(\cos x_1 \cos x_2 + \cos x_2 \cos x_3 + \cos x_3 \cos x_1)}. \tag{7.1}$$

For this Green function the following product formula has been derived by Iwata (1969), and independently by the present author (Joyce 1971*b*):

$$P(z)_{\text{fcc}} = (12/\pi^2)\,(3+z)^{-1}K(k_+)\,K(k_-), \tag{7.2}$$

where
$$k_\pm^2 = \frac{1}{2} \pm \frac{2\sqrt{3z}}{(3+z)^{\frac{3}{2}}} - \frac{\sqrt{3}}{2}\frac{(3-z)\,(1-z)^{\frac{1}{2}}}{(3+z)^{\frac{3}{2}}}, \tag{7.3}$$

and $K(k)$ is the complete elliptic integral of the first kind with modulus k. More recently, it has also been shown that (G. S. Joyce, unpublished work)

$$P(z)_{\text{fcc}} = [F(-3, 0; \tfrac{1}{2}, 1, 1, 1; z)]^2, \tag{7.4}$$

where $F(a, b; \alpha, \beta, \gamma, \delta; z)$ denotes a Heun function.

The standard linear transformation formulae

$$F(a, b; \alpha, \beta, \gamma, \delta; z) = \left(1-\frac{z}{a}\right)^{-\alpha} F\left[\frac{1}{1-a}, -\left(\frac{b+\alpha\gamma}{1-a}\right); \alpha, 1+\alpha-\delta, \gamma, 1+\alpha+\beta-\gamma-\delta; \frac{z}{z-a}\right], \tag{7.5}$$

and
$$F(a, b; \alpha, \beta, \gamma, \delta; z) = F\left(\frac{1}{a}, \frac{b}{a}; \alpha, \beta, \gamma, 1+\alpha+\beta-\gamma-\delta; \frac{z}{a}\right), \tag{7.6}$$

are next applied successively to the Heun function in equation (7.4). This procedure yields the alternative expression

$$P(z)_{\text{fcc}} = 3(3+z)^{-1}\left[F\left(4, -\tfrac{1}{2}; \tfrac{1}{2}, \tfrac{1}{2}, 1, \tfrac{1}{2}; \frac{4z}{3+z}\right)\right]^2. \tag{7.7}$$

If the substitution $z = 3\eta/(4-\eta)$ is made in equations (7.2) and (7.7), we obtain the important relation

$$[F(4, -\tfrac{1}{2}; \tfrac{1}{2}, \tfrac{1}{2}, 1, \tfrac{1}{2}; \eta)]^2 = 4\pi^{-2}K(k_+)\,K(k_-), \tag{7.8}$$

where
$$k_\pm^2 = \tfrac{1}{2} \pm \tfrac{1}{4}\eta(4-\eta)^{\frac{1}{2}} - \tfrac{1}{4}(2-\eta)\,(1-\eta)^{\frac{1}{2}}. \tag{7.9}$$

(It is interesting to note that the expression (7.8) with $\eta = z^2$ is just the lattice Green function $P(z)$ for the *diamond* lattice.)

The required product form for the simple cubic lattice Green function is now readily established by comparing equation (7.8) with the quadratic transformation formula (6.10). We give the final result below:†

$$P(z)_{\text{sc}} = (1-\tfrac{3}{4}x_1)^{\frac{1}{2}}\,(1-x_1)^{-1}(2/\pi)^2K(k_+)\,K(k_-), \tag{7.10}$$

where
$$k_\pm^2 = \tfrac{1}{2} \pm \tfrac{1}{4}x_2(4-x_2)^{\frac{1}{2}} - \tfrac{1}{4}(2-x_2)\,(1-x_2)^{\frac{1}{2}}, \tag{7.11}$$

$$x_1 = \tfrac{1}{2} + \tfrac{1}{6}z^2 - \tfrac{1}{2}(1-z^2)^{\frac{1}{2}}\,(1-\tfrac{1}{9}z^2)^{\frac{1}{2}}, \tag{7.12}$$

and
$$x_2 = x_1/(x_1-1). \tag{7.13}$$

The corresponding expression for the Green function $G(t)$ may be obtained from this result by using the relation

$$G(t) = t^{-1}P(z)_{\text{sc}} \quad (z = 3/t). \tag{7.14}$$

† The product formula (7.10) was first given without detailed proof in Joyce (1972*b*).

(*b*) *Special cases*

We can check the validity of equation (7.10) by evaluating it for particular values of z^2. When $z^2 = 1$ we find that

$$P(1)_{\text{sc}} = (6\sqrt{2}/\pi^2)\,K(k_+)\,K(k_-), \tag{7.15}$$

where

$$\left.\begin{aligned} k_+^2 &= -\tfrac{1}{2}(2\sqrt{3}-1+\sqrt{6}) \approx -2.4567\,9568,\\ k_-^2 &= -\tfrac{1}{2}(2\sqrt{3}-1-\sqrt{6}) \approx -0.0073\,0594.\end{aligned}\right\} \tag{7.16}$$

Next we apply the standard transformation formula (Erdélyi *et al.* 1953)

$$\begin{aligned}(2/\pi)\,K(k) &= {}_2F_1(\tfrac{1}{2},\tfrac{1}{2};1;k^2)\\ &= (1-k^2)^{-\frac{1}{2}}{}_2F_1(\tfrac{1}{2},\tfrac{1}{2};1;k^2/k^2-1)\end{aligned} \tag{7.17}$$

to the elliptic integrals in (7.15). This procedure yields

$$P(1)_{\text{sc}} = (12\sqrt{2}/\pi^2)\,(2-\sqrt{3})\,K(k_+)\,K(k_-), \tag{7.18}$$

where

$$k_\pm^2 = \frac{2\sqrt{3}-1\pm\sqrt{6}}{2\sqrt{3}+1\pm\sqrt{6}} = (2-\sqrt{3})^2(\sqrt{3}\pm\sqrt{2})^2. \tag{7.19}$$

If the relation

$$K(k_+) = (3/2)^{\frac{1}{2}}(1+k_-)\,K(k_-) \tag{7.20}$$

is substituted in equation (7.18) we finally obtain

$$P(1)_{\text{sc}} = (12/\pi^2)\,(18+12\sqrt{2}-10\sqrt{3}-7\sqrt{6})\,[K(k_-)]^2, \tag{7.21}$$

where $k_- = (2-\sqrt{3})\,(\sqrt{3}-\sqrt{2})$. This result is in complete agreement with that obtained previously by Watson (1939).

The Green function $P(z)_{\text{sc}} \equiv \tilde{P}(z^2)_{\text{sc}}$ is a single-valued analytic function in the z^2-plane cut along the real axis from $+1$ to $+\infty$. In order to evaluate (7.10) along the edges of the branch cut we must replace z^2 by $z^2 \pm \mathrm{i}\epsilon$, and use the formula

$$[1-(\xi\pm\mathrm{i}\epsilon)]^{\frac{1}{2}} = \mp\mathrm{i}(\xi-1\pm\mathrm{i}\epsilon)^{\frac{1}{2}}, \tag{7.22}$$

where $1 < \xi < \infty$, and $\epsilon \gtrsim 0$. For the special case $z^2 = 9\pm\mathrm{i}\epsilon$ a considerable simplification occurs, and (7.10) reduces to

$$\begin{aligned}\lim_{\epsilon\to 0+}\tilde{P}(9\pm\mathrm{i}\epsilon)_{\text{sc}} &= G_{\mathrm{R}}(1)\pm\mathrm{i}G_{\mathrm{I}}(1)\\ &= \pm\mathrm{i}(2\sqrt{2}/\pi^2)\,K(k_-)\lim_{\varDelta\to 0+}K(k_+),\end{aligned} \tag{7.23}$$

where

$$\left.\begin{aligned} k_+^2 &= \tfrac{1}{2}(\sqrt{2}+1)\mp\mathrm{i}\varDelta,\\ k_-^2 &= -\tfrac{1}{2}(\sqrt{2}-1).\end{aligned}\right\} \tag{7.24}$$

The application of standard transformation formulae to the elliptic integrals in equation (7.23) enables one to write

$$\lim_{\varDelta\to 0+}K(k_+) = \sqrt{2}(\sqrt{2}-1)^{\frac{1}{2}}K(\sqrt{2}-1)\,(\sqrt{2}\mp\mathrm{i}), \tag{7.25}$$

$$K(k_-) = \sqrt{2}(\sqrt{2}-1)^{\frac{1}{2}}K(\sqrt{2}-1). \tag{7.26}$$

We now substitute these equations in (7.23), and use the relation

$$\sqrt{2}K(\sqrt{2}-1) = K((2\sqrt{2}-2)^{\frac{1}{2}}). \tag{7.27}$$

In this manner we obtain

$$G_{\mathrm{R}}(1) = \tfrac{1}{2}(2-\sqrt{2})\,(2/\pi)^2[K((2\sqrt{2}-2)^{\frac{1}{2}})]^2, \tag{7.28}$$

$$G_{\mathrm{I}}(1) = \sqrt{2}G_{\mathrm{R}}(1). \tag{7.29}$$

These results for $G_{\mathrm{R}}(1)$ and $G_{\mathrm{I}}(1)$ agree with those derived by Katsura *et al.* (1971*b*).

The evaluation of (7.10) for the special case $z^2 = (\frac{9}{5}) \pm i\epsilon$ is rather more complicated. After some tedious manipulations we find that

$$\lim_{\epsilon\to 0+} \tilde{P}(\tfrac{9}{5} \pm i\epsilon) = \surd 5[G_R(\surd 5) \pm iG_I(\surd 5)]$$
$$= \tfrac{1}{2}\surd 5(1 \pm i)\,(2/\pi^2)K(k_-)\,K(k_+), \tag{7.30}$$

where
$$\left.\begin{aligned} k_+^2 &= \tfrac{1}{2} \mp i(\surd 5+2)^{\frac{1}{2}},\\ k_-^2 &= \tfrac{1}{2} - (\surd 5 - 2)^{\frac{1}{2}}. \end{aligned}\right\} \tag{7.31}$$

It is possible to write the elliptic integral $K(k_+)$ in the alternative form†

$$K(k_+) = \tfrac{1}{2}(\surd 5 - 2)^{\frac{1}{2}}[(1 \mp i)\,K(k'_-) + (1 \pm i)\,K(k_-)], \tag{7.32}$$

where k'_- is the modulus complementary to k_-. If equation (7.32) is substituted in (7.30) we obtain

$$G_R(\surd 5) = \tfrac{1}{2}(\surd 5 - 2)^{\frac{1}{2}}\,(2/\pi)^2 K(k_-)\,K(k'_-), \tag{7.33}$$

$$G_I(\surd 5) = \tfrac{1}{2}(\surd 5 - 2)^{\frac{1}{2}}\,(2/\pi)^2[K(k_-)]^2. \tag{7.34}$$

These expressions are in agreement with those derived by Katsura *et al.* (1971 *b*).

The behaviour of $\tilde{P}(z^2 \pm i\epsilon)$ as $z \to +\infty$ may be readily established from the general formula (7.10). It is found that

$$\lim_{\epsilon\to 0+} \tilde{P}(z^2 \pm i\epsilon) = \pm i(3/z)\,(2/\pi^2)\,K(k_-)\,K(k'_-), \tag{7.35}$$

as $z \to +\infty$, where
$$k_-^2 = \tfrac{1}{4}(2 - \surd 3). \tag{7.36}$$

Hence, we have
$$G_I(0) = (2/\pi^2)\,K(k_-)\,K(k'_-), \tag{7.37}$$

with $G_R(0) = 0$. This result, which was first derived by Katsura *et al.* (1971 *b*), provides us with a further check on equation (7.10).

Finally, we note that equation (7.10) is particularly convenient for investigating the behaviour of $P(z)$ along the imaginary z-axis.

8. Applications

In this section we shall briefly discuss some applications of the above results in lattice statistics.

(*a*) *Spin-wave theory*

According to ideal spin-wave theory (Mattis 1965) the relative magnetization of the general spin S Heisenberg model for the simple cubic lattice is given by

$$[M(T)/M(0)] = 1 - S^{-1}\Phi(\alpha), \tag{8.1}$$

where
$$\Phi(\alpha) \equiv \frac{1}{\pi^3}\int\!\!\int\!\!\int_0^{\pi} \frac{dx_1\,dx_2\,dx_3}{\exp[\alpha\epsilon(\boldsymbol{x})] - 1}, \tag{8.2}$$

$$\epsilon(\boldsymbol{x}) = 1 - \tfrac{1}{3}(\cos x_1 + \cos x_2 + \cos x_3), \tag{8.3}$$

and
$$\alpha = 6JS/k_B\,T. \tag{8.4}$$

† The relation (7.32) may be proved by using various quadratic transformation formulae for hypergeometric functions.

In equation (8.4) the constant J is *twice* the nearest neighbour exchange integral, and k_B is the Boltzmann constant.

The low-temperature behaviour of the relative magnetization may be investigated by first writing the thermal Green function (8.2) in the alternative form†

$$\Phi(\alpha) = \sum_{n=1}^{\infty} e^{-n\alpha}[I_0(\tfrac{1}{3}n\alpha)]^3. \tag{8.5}$$

We can now substitute the *dominant* asymptotic expansion

$$[I_0(\tfrac{1}{3}x)]^3 \sim \left(\frac{3}{2\pi x}\right)^{\frac{3}{2}} e^x \sum_{n=0}^{\infty} g_n x^{-n} \quad \text{as} \quad x \to \infty, \tag{8.6}$$

in equation (8.5), where the coefficients are defined by the formal identity

$$\left[\sum_{n=0}^{\infty} \frac{(\frac{1}{2})_n^2}{n!} (\tfrac{3}{2})^n x^{-n}\right]^3 \equiv \sum_{n=0}^{\infty} g_n x^{-n}. \tag{8.7}$$

This procedure yields the basic low-temperature expansion

$$\Phi(\alpha) \sim \left(\frac{3}{2\pi\alpha}\right)^{\frac{3}{2}} \sum_{n=0}^{\infty} g_n \zeta(n+\tfrac{3}{2})\, \alpha^{-n}, \tag{8.8}$$

where $\zeta(x)$ denotes the Riemann zeta function.

In order to establish a connexion between the above analysis and the lattice Green function $G(t)$ we next introduce the Laplace transform

$$G(t) = \int_0^{\infty} e^{-tz}[I_0(z)]^3 dz, \tag{8.9}$$

where Re $(t) \geqslant 3$. Using this integral and equation (8.6), Maradudin *et al.* (1960) have shown that the behaviour of $G(t)$ in the neighbourhood of the branch-point $t = 3$ is described by an analytic continuation of the form

$$G(t) = \sum_{n=0}^{\infty} e_n(t-3)^n - \frac{1}{\pi\sqrt{2}} \sum_{n=0}^{\infty} f_n(t-3)^{n+\frac{1}{2}} \quad (|t-3| \leqslant 2), \tag{8.10}$$

where
$$f_n = \frac{(-)^n g_n}{3^n(\frac{3}{2})_n}. \tag{8.11}$$

However, we can also derive the analytic continuation (8.10) by applying the method of Frobenius to the regular singular point $t = 3$ of the differential equation (2.18). This alternative procedure leads to the following recurrence relation for the coefficient f_n:

$$\begin{aligned} 96(n+1)(2n+1)(2n+3)f_{n+1} + 8(2n+1)(22n^2+22n+9)f_n \\ + 24n(4n^2+1)f_{n-1} + (2n-1)^3 f_{n-2} = 0 \quad (n \geqslant 0) \end{aligned} \tag{8.12}$$

with the initial conditions $f_0 = 1$, and $f_{-1} = f_{-2} \equiv 0$.

If we substitute equation (8.11) in equation (8.12) we readily find that the coefficients in the ideal spin wave expansion (8.8) satisfy the recurrence relation

$$256(n+1)\, g_{n+1} - 32(22n^2+22n+9)\, g_n + 144n(4n^2+1)\, g_{n-1} - 9(2n-1)^4 g_{n-2} = 0 \quad (n \geqslant 0), \tag{8.13}$$

with the initial conditions $g_0 = 1$ and $g_{-1} = g_{-2} \equiv 0$. A list of the coefficients g_n, which was generated by using (8.13), is given in table 7.

† A detailed derivation of (8.5) is given in Mattis (1965), p. 246.

TABLE 7. COEFFICIENTS g_n IN THE SPIN WAVE EXPANSION (8.8)

n	g_n
0	1
1	$\frac{9}{8}$
2	$\frac{297}{128}$
3	$\frac{7\,587}{1\,024}$
4	$\frac{1\,086\,939}{32\,768}$
5	$\frac{51\,064\,263}{262\,144}$
6	$\frac{5\,995\,159\,677}{4\,194\,304}$
7	$\frac{423\,959\,714\,955}{33\,554\,432}$
8	$\frac{281\,014\,370\,213\,715}{2\,147\,483\,648}$
9	$\frac{26\,702\,465\,299\,878\,195}{17\,179\,869\,184}$
10	$\frac{5\,723\,872\,792\,950\,096\,855}{274\,877\,906\,944}$

It should be stressed that the higher-order coefficients $g_3, g_4, \ldots$ are of little *physical* interest, since the interactions between spin waves (Dyson 1956*a*, *b*) give rise to contributions to equation (8.1) of order α^{-4}. However, the results derived above for the function $\Phi(\alpha)$ are of *mathematical* interest in nonlinear spin wave theory (Mattis 1965), and in the various Green function theories of ferromagnetism (Tahir-Kheli & ter Haar 1962; Callen 1963; Dalton & Wood 1967; Flax & Raich 1969). Finally, we note that the ideal spin-wave coefficients for the body-centred cubic lattice also satisfy a four-term recurrence relation (see Joyce (1971*a*), p. 1397, equation (3.28)) which is very similar to (8.13).

(*b*) *Theory of random walks*

The analytic continuation (4.6) of the probability generating function $P(z)$ has numerous applications in the theory of random walks (Montroll & Weiss 1965; Domb & Joyce 1972). In the present section we shall use (4.6) to derive an asymptotic expansion for the expected number S_n of *distinct* lattice sites visited during an n-step random walk on a simple cubic lattice (Dvoretzky & Erdös 1951; Vineyard 1963; Montroll & Weiss 1965). (Further applications of (4.6) in the theory of random walks will be discussed elsewhere.)

We begin by considering the generating function (Montroll & Weiss 1965)

$$S(z) \equiv \sum_{n=0}^{\infty} S_n z^n = (1-z)^{-2}[P(z)]^{-1} = 1+2z+\frac{17}{6}z^2+\frac{11}{3}z^3+\frac{107}{24}z^4+\frac{21}{4}z^5 + \frac{23\,407}{3\,888}z^6+\frac{13\,201}{1\,944}z^7+\frac{234\,755}{31\,104}z^8+\frac{43\,049}{5\,184}z^9+\ldots. \tag{8.14}$$

This function has two singularities on the circle of convergence $|z| = 1$, at $z = \pm 1$. The behaviour of $S(z)$ in the neighbourhood of the singularity at $z = 1$ may be established by inverting equation (4.6). The final result is

$$S(z) = [P(1)]^{-1}\Big[(1-z)^{-2}+\frac{3\sqrt{6}}{2\Delta}(1-z)^{-\frac{3}{2}}+\frac{9}{16\Delta^2}(18-\Delta^2)(1-z)^{-1}+\frac{9\sqrt{6}}{16\Delta^3}(18-\Delta^2)(1-z)^{-\frac{1}{2}}$$
$$+\frac{1}{128\Delta^4}(7290-243\Delta^2-11\Delta^4)+\frac{\sqrt{6}}{2560\Delta^5}(131\,220-309\Delta^4)(1-z)^{\frac{1}{2}}+\dots\Big], \tag{8.15}$$

where $\Delta = \pi P(1)$. In the neighbourhood of the singularity $z = -1$, we find

$$S(z) = \tfrac{1}{4}[P(1)]^{-1}[1+(3\sqrt{6}/2\Delta)(1+z)^{\frac{1}{2}}+\dots]. \tag{8.16}$$

The application of the method of Darboux (1878) to the *singular* parts of (8.15) *and* (8.16) yields the asymptotic expansion

$$S_n \sim [P(1)]^{-1}n\Big\{1+\frac{3}{\Delta}\Big(\frac{6}{\pi n}\Big)^{\frac{1}{2}}+\frac{1}{16\Delta^2}(162+7\Delta^2)n^{-1}+\frac{9}{16\Delta^3}\Big(\frac{6}{\pi n^3}\Big)^{\frac{1}{2}}(18+\Delta^2)$$
$$-\frac{1}{5120\Delta^5}\Big(\frac{6}{\pi n^5}\Big)^{\frac{1}{2}}[131\,220+6480\Delta^2+171\Delta^4+(-)^n 960\Delta^4]+\dots\Big\}, \tag{8.17}$$

as $n\to\infty$. It is readily seen that, in general, the 'weak' cusp singularity at $z = -1$ gives rise to contributions to the expansion (8.17) of the type $(-)^n/n^{m+\frac{3}{2}}$, with $m = 0, 1, 2, \dots$. Similar asymptotic formulae for S_n have also been derived for the body-centred and face-centred cubic lattices (Joyce 1971*a*, *b*).

(*c*) *Spherical model*

The analytic continuation (4.6) is of basic importance in the spherical model of ferromagnetism (Berlin & Kac 1952) since it enables one to determine the *detailed* critical behaviour of the model (Joyce 1972*a*) as the temperature $T\to T_c\pm$, where T_c is the Curie temperature. In order to illustrate this application we shall now investigate the critical behaviour of the zero-field isothermal susceptibility χ of the spherical model on a simple cubic lattice.

It can be shown (Berlin & Kac 1952) that the susceptibility χ for the simple cubic lattice is given by

$$(k_B T/m^2)\chi = K^{-1}(\xi_s-1)^{-1} \quad (T > T_c), \tag{8.18}$$

where $K \equiv 6J/k_B T$, and m is the magnetic moment of each 'spin' in the system. The 'saddle-point' parameter ξ_s is determined as a function of K from the implicit saddle-point equation

$$K = \xi_s^{-1}P(\xi_s^{-1}) = \frac{1}{\pi^3}\iiint_0^\pi \frac{dx_1\,dx_2\,dx_3}{\xi_s-\frac{1}{3}(\cos x_1+\cos x_2+\cos x_3)}$$
$$= \xi_s^{-1}\sum_{n=0}^{\infty} a_n\xi_s^{-2n} \quad (|\xi_s| \geqslant 1), \tag{8.19}$$

where the coefficients a_n satisfy the recurrence relation (2.14). We see from (8.19) that at very high temperatures the parameter ξ_s is positive with $\xi_s \simeq K^{-1}$, and that as the temperature is lowered ξ_s decreases monotonically. When the saddle-point parameter ξ_s coincides with the branch point $\xi_s = 1$ a phase transition occurs at a Curie temperature given by

$$K_c \equiv 6J/k_B T = P(1). \tag{8.20}$$

An analysis of the saddle-point equation in the critical region $\xi_s \gtrsim 1$ can be carried out using the expansion (4.6). After some manipulation we find

$$(K_c - K) = \frac{3\sqrt{6}}{2\pi}(\xi_s - 1)^{\frac{1}{2}} + \left(\frac{7K_c}{16} - \frac{27}{8\pi^2 K_c}\right)(\xi_s - 1) + O[(\xi_s - 1)^{\frac{3}{2}}]. \tag{8.21}$$

We next revert this expansion and substitute the resulting formula for $\xi_s - 1$ in equation (8.18). This procedure yields

$$(k_B T/m^2)\,\chi = C^+(t^*)^{-2}(1+\lambda t^*) + O(1), \tag{8.22}$$

as $t^* \to 0+$, where

$$t^* = 1 - (K/K_c), \tag{8.23}$$

$$C^+ = (27/2\pi^2)\,K_c^{-3}, \tag{8.24}$$

and

$$\lambda = (1/108)\,(54 + 7\pi^2 K_c^2). \tag{8.25}$$

If the reversion of the series in (8.19) is used to eliminate ξ_s from the expression (8.18) we obtain the following high-temperature series for the susceptibility (Dalton & Wood 1968; Stanley 1969; Joyce 1972*a*):

$$\begin{aligned}(k_B T/m^2)\,\chi = \sum_{n=0}^{\infty} c_n K^n = {} & 1 + 6(\tfrac{1}{6}K) + 30(\tfrac{1}{6}K)^2 + 144(\tfrac{1}{6}K)^3 + 666(\tfrac{1}{6}K)^4 \\ & + 3024(\tfrac{1}{6}K)^5 + 13\,476(\tfrac{1}{6}K)^6 + 59\,328(\tfrac{1}{6}K)^7 \\ & + 258\,354(\tfrac{1}{6}K)^8 + 1\,115\,856(\tfrac{1}{6}K)^9 + 4784\,508(\tfrac{1}{6}K)^{10} \\ & + 20\,393\,856(\tfrac{1}{6}K)^{11} + 86\,473\,548(\tfrac{1}{6}K)^{12} + \dots .\end{aligned} \tag{8.26}$$

This series expansion displays just *one* singularity on its circle of convergence at $K = K_c$, and does *not* have an antiferromagnetic singularity at $K = -K_c$. Outside the circle of convergence $|K| = K_c$, the analytic continuation of the series (8.26) also exhibits *non-physical* branch-point singularities† at $K = \pm K_u$, where $K_u \approx 1.9398\,1075$.

It is clear, therefore, that the *dominant* asymptotic behaviour of the coefficients c_n can be determined by applying Darboux's theorem (1878) to equation (8.22). We find

$$c_n \sim C^+(n+\lambda+1)\,K_c^{-n} \quad \text{as} \quad n \to \infty. \tag{8.27}$$

The non-physical singularities at $K = \pm K_u$ contribute an additional *factor* to (8.27) of the form $1 + O\{(K_c/K_u)^n\}$. Since this factor approaches 1 exponentially fast as $n \to \infty$, we see that the effect of the singularities at $\pm K_u$ will become negligible, providing n is sufficiently large. It follows from (8.27) that the asymptotic behaviour of the ratio of terms c_n/c_{n-1} is described by the simple representation

$$c_n/c_{n-1} \sim K_c^{-1}[1 + (n+\lambda)^{-1}], \tag{8.28}$$

as $n \to \infty$. The asymptotic formula (8.27) is also *formally* valid for most other three-dimensional lattices with isotropic ferromagnetic interactions. (In general we define $K \equiv qJ/k_B T$ where q is the coordination number of the lattice.) However, the susceptibility series for the diamond lattice (Joyce 1972*a*) with nearest neighbour interactions has two 'weak' non-physical branch-point singularities on the circle of convergence at $K = \pm iK_\omega$, where K_ω is *less than* K_c. Under these circumstances it is evident that an asymptotic formula of the type (8.27) no longer holds.

† A more detailed discussion of these non-physical singularities is given in Joyce (1972*a*).

(d) *Lattice dynamics*

The lattice dynamics of a set of N^3 identical particles which interact with nearest neighbour interactions on an $N \times N \times N$ simple cubic lattice has been investigated in considerable detail by Montroll (1956). In particular, he showed that for large N the frequency spectrum $g(\nu)$ of the model can be written in the form

$$g(\nu) = 4\pi\omega N^3 \hat{G}(\gamma_1, \gamma_2, \gamma_3; \omega^2), \tag{8.29}$$

where

$$\hat{G}(\gamma_1, \gamma_2, \gamma_3; \omega^2) = \frac{1}{\pi}\int_0^\infty \cos\left[(\omega^2 - 2\gamma_1 - 2\gamma_2 - 2\gamma_3)\,\alpha\right] J_0(2\gamma_1\alpha)\, J_0(2\gamma_2\alpha)\, J_0(2\gamma_3\alpha)\,\mathrm{d}\alpha, \tag{8.30}$$

$\omega = 2\pi\nu$, and the parameter γ_1 denotes the central force constant while γ_2, γ_3 represent the non-central force constants. The maximum 'cut-off' frequency for the model is given by

$$\omega_L^2 = 4(\gamma_1 + \gamma_2 + \gamma_3). \tag{8.31}$$

If we restrict our attention to the special case $\gamma_1 = \gamma_2 = \gamma_3 = \gamma$ and compare (8.30) with the standard integral representation (Koster & Slater 1954; Wolfram & Callaway 1963)

$$G_{\mathrm{I}}(s) = \int_0^\infty \cos(sx)\,[J_0(x)]^3\,\mathrm{d}x, \tag{8.32}$$

we obtain the basic relation

$$\omega_L^2\, \hat{G}(\gamma, \gamma, \gamma; \omega^2) = (6/\pi)\, G_{\mathrm{I}}(s), \tag{8.33}$$

where

$$s = 3[1 - 2(\omega/\omega_L)^2], \tag{8.34}$$

and $\omega_L^2 = 12\gamma$. We see therefore that the transformation formulae given in §5 enable one to carry out a complete analysis of the spectral density function $\hat{G}(\gamma, \gamma, \gamma; \omega^2)$. The low-frequency expansion for $\hat{G}(\gamma, \gamma, \gamma; \omega^2)$ may be readily derived by applying (8.10) to (8.33). It is found that

$$\omega_L^2\, \hat{G}(\gamma, \gamma, \gamma; \omega^2) = \frac{6\sqrt{3}}{\pi^2}\left(\frac{\omega}{\omega_L}\right) \sum_{n=0}^{\infty} \frac{g_n 2^n}{(\frac{3}{2})_n}\left(\frac{\omega}{\omega_L}\right)^{2n} \quad (\omega^2 \leqslant \tfrac{1}{3}\omega_L^2), \tag{8.35}$$

where the 'spin-wave' coefficients g_n satisfy the four-term recurrence relation (8.13).

Finally, we note that the Green function $G_{\mathrm{I}}(s)$ is also directly related to the density of states in spin-wave theory and in the tight-binding approximation for electrons.

9. Concluding remarks

The results derived in the previous sections provide us with a fairly complete picture of the analytical properties of the Green's function $G(t)$. However, there are still many associated mathematical problems which remain unresolved. For example, it may be possible to express $G_{\mathrm{R}}(s)$ and $G_{\mathrm{I}}(s)$ in terms of complete elliptic integrals for s in the ranges $0 < s < 1$ and $1 < s < 3$. More generally, one might now optimistically expect that the complete Green's function

$$G(\mathbf{l}; t, \alpha) = \frac{1}{\pi^3}\iiint_0^\pi \frac{\cos l_1x_1 \cos l_2x_2 \cos l_3x_3}{t - (\cos x_1 + \cos x_2 + \alpha\cos x_3)}\,\mathrm{d}x_1\,\mathrm{d}x_2\,\mathrm{d}x_3 \tag{9.1}$$

for the anisotropic simple cubic lattice can be evaluated in terms of complete elliptic integrals.

The special case $G(\mathbf{0}; t, \alpha)$ is particularly intriguing since Montroll (1956) has already shown that

$$G(\mathbf{0}; 2+\alpha, \alpha) = (4/\pi^2\alpha^{\frac{1}{2}})\,[(\gamma+1)^{\frac{1}{2}}-(\gamma-1)^{\frac{1}{2}}]\,K(k_+)\,K(k_-), \tag{9.2}$$

where

$$k_\pm = \tfrac{1}{2}[(\gamma-1)^{\frac{1}{2}}\pm(\gamma-3)^{\frac{1}{2}}]\,[(\gamma+1)^{\frac{1}{2}}-(\gamma-1)^{\frac{1}{2}}],$$

$$\gamma = (4+3\alpha)/\alpha. \tag{9.3}$$

It is hoped to discuss these problems in future publications.

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Appendix

Below is given a short table of values for the real part $G_R(s)$ and the imaginary part $G_I(s)$ of the Green function

$$\lim_{\epsilon\to 0+}\frac{1}{\pi^3}\iiint_0^\pi \frac{dx_1\,dx_2\,dx_3}{s-i\epsilon-(\cos x_1+\cos x_2+\cos x_3)}$$

in the range $0 \leqslant s \leqslant 3$.

s	$G_R(s)$	$G_I(s)$
0	0	0.896 440 788 776 763
0.1	0.036 837 303 222 745	0.896 562 114 473 980
0.2	0.074 175 844 749 651	0.896 926 772 749 037
0.3	0.112 564 301 852 041	0.897 536 820 366 793
0.4	0.152 659 626 011 071	0.898 395 729 875 683
0.5	0.195 322 880 928 494	0.899 508 458 513 518
0.6	0.241 797 659 193 004	0.900 881 548 820 933
0.7	0.294 101 634 298 992	0.902 523 265 487 469
0.8	0.356 090 544 780 607	0.904 443 774 841 813
0.9	0.437 633 958 796 167	0.906 655 375 828 984
1.0	0.642 882 248 294 458	0.909 172 794 546 930
1.1	0.633 184 743 623 919	0.700 154 316 589 861
1.2	0.623 923 540 314 459	0.617 640 713 783 929
1.3	0.615 064 356 547 705	0.556 473 298 337 678
1.4	0.606 576 783 898 185	0.506 448 945 066 514
1.5	0.598 433 718 602 123	0.463 544 765 191 000
1.6	0.590 610 894 805 526	0.425 656 571 021 183
1.7	0.583 086 498 372 508	0.391 505 200 745 014
1.8	0.575 840 844 951 127	0.360 232 899 869 855
1.9	0.568 856 109 750 251	0.331 220 782 139 748
2.0	0.562 116 099 272 940	0.303 993 825 678 427
2.1	0.555 606 057 350 799	0.278 165 263 291 800
2.2	0.549 312 499 418 529	0.253 399 689 591 420
2.3	0.543 223 070 191 414	0.229 384 167 638 284
2.4	0.537 326 420 855 799	0.205 799 773 412 628
2.5	0.531 612 102 622 276	0.182 284 855 335 886
2.6	0.526 070 474 073 471	0.158 373 626 234 242
2.7	0.520 692 620 199 918	0.133 367 106 772 626
2.8	0.515 470 281 386 060	0.105 986 195 066 048
2.9	0.510 395 790 904 645	0.073 006 133 685 561
3.0	0.505 462 019 717 326	0

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