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

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

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

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

then the general solution of the third-order differential equation

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

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

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

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

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

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

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

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

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

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

and

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

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

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

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 $G_{\mathrm{R}}(s)$ and $G_{\mathrm{I}}(s)$ 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

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

(*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

$$\begin{aligned} G^-(s) \equiv G_{\mathrm{R}}(s) + \mathrm{i}G_{\mathrm{I}}(s) = {} & (1+\mathrm{i}\sqrt{2})\, G_{\mathrm{R}}(1)\, [F(-8, \tfrac{1}{16}; \tfrac{1}{4}, \tfrac{1}{4}, \tfrac{1}{2}, \tfrac{1}{2}; 1-s^2)]^2 \\ & + \frac{3(1-\mathrm{i}\sqrt{2})}{16\pi^2 G_{\mathrm{R}}(1)} (1-s^2)\, [F(-8, \tfrac{29}{16}; \tfrac{3}{4}, \tfrac{3}{4}, \tfrac{3}{2}, \tfrac{1}{2}; 1-s^2)]^2 \\ & - \frac{3\mathrm{i}}{2\pi} (s^2-1)^{\frac{1}{2}} F(-8, \tfrac{1}{16}; \tfrac{1}{4}, \tfrac{1}{4}, \tfrac{1}{2}, \tfrac{1}{2}; 1-s^2)\, F(-8, \tfrac{29}{16}; \tfrac{3}{4}, \tfrac{3}{4}, \tfrac{3}{2}, \tfrac{1}{2}; 1-s^2), \end{aligned} \tag{5.10}$$

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

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

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

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

$$-\frac{3\mathrm{i}}{2\pi}(s^2-1)^{\frac{1}{2}}\sum_{n=0}^{\infty}V_n(1-s^2)^n, \tag{5.12}$$

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

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

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 $\frac{1}{2} \lesssim s^2 \lesssim \frac{3}{2}$ $(s > 0)$.

(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

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

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:

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

and

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

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 $15\lessapprox s^2<\infty$.

(*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 $G_{\mathrm{I}}(1)=\sqrt{2}G_{\mathrm{R}}(1)$, (4.18) and (4.27) to the resulting expressions then yields the following summation formulae‡:

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

and

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

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

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

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

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)

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

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)

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

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

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

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)

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

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

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

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:†

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

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

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

† 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

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

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

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

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

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

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 $P(z)_{\mathrm{sc}} \equiv \tilde{P}(z^2)_{\mathrm{sc}}$ 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

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

where

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

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

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

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

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*).

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 $\mathrm{Re}\,(t) \geqslant 3$. 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.

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*).

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.

I am extremely grateful to Dr A. J. Guttmann for several stimulating discussions and for assistance in the initial stages of this work, particularly in the derivation of the basic recurrence relation (2.15). I also thank Professor C. Domb and Dr D. S. Gaunt for their interest and encouragement. Finally, I am indebted to J. A. Webb for expert programming assistance.

Appendix

Below is given a short table of values for the real part $G_{\mathrm{R}}(s)$ and the imaginary part $G_{\mathrm{I}}(s)$ of the Green function

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

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

s	$G_{\mathrm{R}}(s)$	$G_{\mathrm{I}}(s)$
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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